

Editors

Timothy J. Barth
Michael Griebel
David E. Keyes
Risto M. Nieminen
Dirk Roose
Tamar Schlick

Habib Ammari (Ed.)

Modeling and Computations in Electromagnetics

A Volume Dedicated to Jean-Claude Nédélec

With 74 Figures and 5 Tables

 Springer

Editor

Habib Ammari

École Polytechnique
CNRS UMR 7641
Centre de Mathématiques Appliquées
91128 Palaiseau Cedex
France
email: ammari@cmapx.polytechnique.fr

Library of Congress Control Number: 2007933491

Mathematics Subject Classification (2000): 78M05, 78M15, 83C50, 35Q60, 35R30, 65R20, 65R32

ISBN 978-3-540-73777-3 Springer Berlin Heidelberg New York

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilm or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer. Violations are liable for prosecution under the German Copyright Law.

Springer is a part of Springer Science+Business Media
springer.com

© Springer-Verlag Berlin Heidelberg 2008

The use of general descriptive names, registered names, trademarks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

Typesetting by the editors and SPi using a Springer L^AT_EX macro package
Cover design: WMX Design GmbH, Heidelberg

Printed on acid-free paper SPIN: 10885101 46/SPi 5 4 3 2 1 0

To Jean-Claude Nédélec

Preface

Modeling and computations in electromagnetics is quite novel and growing discipline, expanding as a result of the steadily increasing demand for designing electrical devices, modeling electromagnetic materials, and simulating electromagnetic fields in nanoscale structures.

The aim of this volume is to bring together prominent worldwide experts to review state-of-the-art developments and future trends of modeling and computations in electromagnetics. This volume is devoted to merging the expertise of scientists working on this active discipline, and to raise interest for challenging issues. The most significant advances in computational techniques developed in the very last years and several challenging technological applications such as those related to communications, to biomedical devices, and to magnetic storage design are presented in this volume. It covers the following topics: fast algorithms for time-dependent electromagnetic waves, high-order methods for high-frequency electromagnetic scattering, non-reflecting boundary conditions for time-dependent electromagnetic waves, multi-scale analysis for Maxwell's equations, time-reversal for electromagnetic waves, and inverse electromagnetic scattering.

This volume is dedicated to Jean-Claude Nédélec in celebration of his 65th birthday and retirement from Ecole Polytechnique in January 2008. Jean-Claude has been one of the most distinguished scientist in the area of computational electromagnetics. His outstanding contributions on finite-elements and fast algorithms for Maxwell's equations have significantly advanced the field.

Paris,

Habib Ammari
May 2007

Contents

1 Stabilized FEM–BEM Coupling for Maxwell Transmission Problems	
<i>R. Hiptmair and P. Meury</i>	1
2 A Posteriori Error Analysis and Adaptive Finite Element Methods for Electromagnetic and Acoustic Problems	
<i>Z. Chen</i>	39
3 Time Domain Adaptive Integral Method for Surface Integral Equations	
<i>H. Bağcı, A.E. Yılmaz, J.-M. Jin, and E. Michielssen</i>	65
4 Local and Nonlocal Nonreflecting Boundary Conditions for Electromagnetic Scattering	
<i>M.J. Grote</i>	105
5 High-Order Methods for High-Frequency Scattering Applications	
<i>O.P. Bruno and F. Reitich</i>	129
6 Recent Studies on Inverse Medium Scattering Problems	
<i>G. Bao, S. Hou, and P. Li</i>	165
7 Time Reversal of Electromagnetic Waves	
<i>J. de Rosny, G. Lerosey, A. Tourin, and M. Fink</i>	187
8 Addition Theorem	
<i>B. He and W.C. Chew</i>	203
Index	227

Stabilized FEM–BEM Coupling for Maxwell Transmission Problems

R. Hiptmair and P. Meury

1.1 Introduction

We consider the electromagnetic scattering of monochromatic incident waves from a penetrable, three-dimensional bounded object $\Omega \subset \mathbb{R}^3$, the scatterer. In applications one usually encounters scatterers with piecewise smooth, Lipschitz continuous boundaries. Thus it is natural to assume the scatterer to be a curvilinear Lipschitz-polyhedron in the parlance of [28, Sect. 1]. For the sake of simplicity, we assume that its surface $\Gamma := \partial\Omega$ is connected. However, with slight changes all theorems can be extended to more general situations. The material parameters ε_r and μ_r may display some spatial variation inside Ω but assume the constant values $\varepsilon_0 > 0$ and $\mu_0 > 0$ in the air region $\Omega^+ := \mathbb{R}^3 \setminus \Omega$.

Let $\mathbf{E}^s$ denote the complex amplitude of the scattered electric field in the air region and $\mathbf{E}$ the total electric field inside the scatterer Ω , which emerge as solutions to the Maxwell transmission problem (cf. [49, Sect. 5.6.3])

$$\begin{aligned} \operatorname{curl} \mu_r(\mathbf{x})^{-1} \operatorname{curl} \mathbf{E} - \kappa^2 \varepsilon_r(\mathbf{x}) \mathbf{E} &= \mathbf{F}(\mathbf{x}) && \text{in } \Omega, \\ \operatorname{curl} \operatorname{curl} \mathbf{E}^s - \kappa^2 \mathbf{E}^s &= \mathbf{0} && \text{in } \Omega^+, \\ \gamma_t^+ \mathbf{E}^s - \gamma_t^- \mathbf{E} &= \mathbf{g}_D \quad \text{on } \Gamma, & \gamma_N^+ \mathbf{E}^s - \mu_r^{-1} \gamma_N^- \mathbf{E} &= \mathbf{g}_N \quad \text{on } \Gamma, \\ \lim_{|\mathbf{x}| \rightarrow \infty} \operatorname{curl} \mathbf{E} \times \mathbf{x} - i\kappa |\mathbf{x}| \mathbf{E} &= \mathbf{0}. \end{aligned} \tag{1.1}$$

Here, $\kappa := \omega \sqrt{\mu_0 \varepsilon_0} L$ (with $\omega > 0$ the fixed angular frequency of the excitation, L the characteristic length of the scatterer) denotes the normalized wave number and should be considered as a real positive parameter. Furthermore, we write $\gamma_t \mathbf{E}$ for the tangential components of $\mathbf{E}$ on Γ and $\gamma_N \mathbf{E}$ for the “magnetic components” $\operatorname{curl} \mathbf{E} \times \mathbf{n}$ on Γ . The exterior unit normal vector field $\mathbf{n}$ on Γ belongs to $\mathbf{L}^\infty(\Gamma)$ and is directed from Ω into Ω^+ . In the

case of excitation by plane electric waves, whose complex amplitude will be denoted by $\mathbf{E}^{\text{inc}}$, the generic jump data $\mathbf{g}_D$ and $\mathbf{g}_N$ evaluate to the following traces

$$\mathbf{g}_D := -\gamma_t \mathbf{E}^{\text{inc}}, \quad \mathbf{g}_N := -\gamma_N \mathbf{E}^{\text{inc}}.$$

Finally, we designate by

$$[\gamma \mathbf{U}]_\Gamma := \mathbf{U}|_{\Omega^+} - \mathbf{U}|_\Omega \quad \text{and} \quad \{\gamma \mathbf{U}\}_\Gamma := \frac{1}{2} (\mathbf{U}|_{\Omega^+} + \mathbf{U}|_\Omega)$$

the jump, respectively the average, of some generic trace γ of a function $\mathbf{U}$ across the boundary Γ .

Using Rellich's lemma and unique continuation techniques, the following result can be established (cf. [36, Theorem 3.1]).

Theorem 1.1. *Provided that the relative material parameters μ_r and $\varepsilon_r > 0$ are piecewise smooth and bounded away from zero everywhere in Ω , the problem (1.1) has a unique solution.*

Boundary element methods (BEM) offer the most flexible way to deal with the homogeneous problem in the unbounded exterior domain Ω^+ . They are based on boundary integral operators on the interface Γ . Due to potentially nonconstant material parameters, the field problem inside Ω may not be amenable to a treatment by means of boundary element methods. Hence, finite element schemes (FEM) have to be used here. Thus the topic of this chapter comes into focus, namely how to derive and discretize stable coupled variational formulations, and how to analyze the resulting FEM-BEM formulation.

The coupling entails expressing the Dirichlet-to-Neumann (DtN) map of the exterior problem by means of boundary integral operators linking the Cauchy data $\gamma_t \mathbf{E}$ and $\gamma_N \mathbf{E}$ for the electric field. There exists a huge variety of integral formulations for the exterior electromagnetic boundary value problem. A comprehensive survey is given in Nédélec's monograph [49]. In principle all these methods furnish Dirichlet-to-Neumann maps. However, in many cases, in particular with so-called indirect formulations, the resulting operator lacks structural properties of the Dirichlet-to-Neumann map, for instance symmetry. This is obviously the case for second-order elliptic problems. If the structure of the DtN map is not preserved, then the linear systems of equations obtained by a Ritz-Galerkin boundary element discretization are adversely affected.

For second-order elliptic problems Costabel [27] discovered that the so-called direct boundary integral equation methods provide a remedy. The main idea is to employ the Calderón projector, which acts on the Cauchy data of the problem. For details and theoretical considerations we refer to [21, Sect. 4.5] and [30]. In short, the Calderón projector yields two sets of boundary integral equations. Judiciously combining them yields a version of the Dirichlet-to-Neumann map, which is perfectly suited for a Ritz-Galerkin discretization.

Costabel’s idea of coupling finite elements with boundary elements is usually referred to as “the symmetric coupling approach.” It has been applied to a wide range of strongly elliptic problems; see, among others [19, 38, 44]. For references to the engineering literature see [53, 55] and the references therein.

Unsurprisingly, the Calderón projector for the Maxwell system has been thoroughly studied, cf. [20, Sect. 1.3.2], [32], [49, Sect. 5.5], and [43, Sect. 3]. The idea of symmetric coupling for the transmission problem was theoretically probed in [1, 2, 4], and in [7] for a related problem involving impedance boundary conditions. All these results employ compactness arguments and the Fredholm alternative. To this end, most authors have studied the integral operators intrinsically on Γ . They have been successful on smooth interface boundaries, but all efforts to adjust the approach to nonsmooth boundaries have been in vain.

The fundamental new insights about the traces of electromagnetic fields, presented in [9, 12, 13, 15], paved the way to further progress. That progress could finally be achieved by remembering a highly effective policy in the modern treatment of boundary integral equations: The guideline is to stay off the boundary as far as possible by studying variational problems instead of the boundary integral operators directly. This policy has demonstrated its efficacy in the work of Costabel [27]. The recent textbook [46] discusses all nuances of this approach for strongly elliptic systems. Moving off the boundary helps steer clear of its awkward geometric features. Thus, the foundation for a theory of electromagnetic boundary integral operators could be laid in [16, 18].

In addition, in order to harness compactness arguments, we have to employ decompositions of the surface vector fields on Γ . The classical composition is the so-called Hodge decomposition [32], which remains a very effective tool on piecewise smooth boundaries, cf. [14], [18], and, in particular [41]. Its counterpart on domains is the Helmholtz decomposition. It is important to realize that there is some leeway in choosing the decomposition, because the exact orthogonality featured by Hodge or Helmholtz decompositions is of minor importance. Instead, we prefer to use related, but simpler, splittings.

Almost all boundary integral equations for the exterior Dirichlet problem in electromagnetic and acoustic scattering are haunted by the presence of “spurious frequencies” [15, 18, 22], for which the equations fail to have unique solutions. Those agree with interior Dirichlet eigenvalues. The symmetrically coupled variational formulation presented in [39] exhibits the same drawback.

In this chapter, we propose a stabilized method for FEM–BEM coupling based on (mixed) Robin-type boundary conditions to ensure unique solvability of the corresponding interior boundary value problem. The use of complex combinations of boundary integral operators has been an invaluable tool for deriving resonance-free combined field integral equations (CFIE) for electromagnetic scattering from a perfect conductor, cf. [35]. Furthermore, our approach also features regularizing operators, already used to stabilize Maxwell scattering problems in [17], to ensure a Gårding inequality for the sesquilinear

form underlying the variational formulation. In our case, both problems are tackled by introducing modified trace operators.

Based on the generalized traces, stabilized versions of Calderón projectors can be defined for the coupling of domain based variational formulations with boundary integral equations. Thus, we can derive new coupled variational formulations, which feature existence, uniqueness, and stability of solutions for all wave numbers $\kappa > 0$. A similar approach to the one presented here can be found in [54].

To discretize the symmetric and the stabilized coupled variational formulations, we rely on discrete differential forms (edge elements, face elements) on triangulations of both Ω and Γ . The Ritz–Galerkin approach is straightforward, and yet, in the discrete setting another challenge arises. The Helmholtz and Hodge-type decompositions do not directly carry over to the discrete spaces. For pure indirect boundary element formulations (Rumsey’s principle) remedies have been explored in [41] and [22]. Direct boundary integral equations were tackled in [18]. All these approaches exploit the fact that appropriate discrete splittings can approximate their continuous counterparts reasonably well. In this chapter we adapt the ideas in [18] and [39] to the symmetrically coupled FEM–BEM problem. We will use variants of these results that do not require sophisticated elliptic regularity theory.

The outline of this chapter is as follows: In the following section we will review the theory of Sobolev spaces and tangential traces. In Sect. 1.3 we will introduce the potentials, which form the building blocks of the Stratton–Chu representation formula and the boundary integral operators for the electric field equation. In Sect. 1.4 we construct decompositions of the electric field in Ω . The theoretical results for the symmetrically coupled variational formulation are reviewed in Sect. 1.5. In Sect. 1.6 the stabilized coupling strategy is presented. So far, all sections have been merely concerned with the analysis of the continuous variational problems. Then, in Sect. 1.7, we introduce the finite element and boundary element spaces, which are used for a Ritz–Galerkin discretization of the coupled problem. In Sect. 1.8 we derive discrete counterparts to the decompositions on the continuous level and establish discrete inf–sup estimates for the underlying sesquilinear forms. Finally, in Sect. 1.10 we will establish a priori convergence estimates for the stabilized coupling approach.

1.2 Traces and Spaces

The main purpose of this section is to define suitable Sobolev spaces, which can be used to derive weak formulations of (1.1), and review some of their most important properties. The notation and notions we introduce closely follow the ones of [39, Sect. 2].

The natural Hilbert space for an analysis of the Maxwell transmission problem (1.1) is the space

$$\mathbf{H}_{\text{loc}}(\mathbf{curl}, D) := \{ \mathbf{V} \in \mathbf{L}_{\text{loc}}^2(D); \mathbf{curl} \mathbf{V} \in \mathbf{L}_{\text{loc}}^2(D) \} .$$

Here and below D denotes a generic domain, which can be either Ω or Ω^+ . For a thorough examination of these spaces we refer to [33, Chap. 1].

The Sobolev spaces of scalar functions and their dual spaces, $H^s(\Gamma)$ and $H^{-s}(\Gamma)$, can be defined invariantly for $0 \leq s \leq 1$, see [34, Theorem 1.3.3]. Furthermore, we denote by $\gamma : H_{\text{loc}}^s(D) \mapsto H^{s-1/2}(\Gamma)$, $\frac{1}{2} < s < \frac{3}{2}$, the natural trace operator, cf. [46, Theorem 3.38]. Superscripts $+$ and $-$ will be attached to the trace operators, when it is important whether they act from Ω or Ω^+ . Furthermore, we denote by $\langle \cdot, \cdot \rangle_\Gamma : H^{-1/2}(\Gamma) \times H^{1/2}(\Gamma) \mapsto \mathbb{C}$ the duality pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$, when $L^2(\Gamma)$ is taken as pivot space.

If Γ is a curvilinear Lipschitz polyhedron in the parlance of [28] with smooth components Γ_j , $j = 1, \dots, N_\Gamma$, we define

$$\begin{aligned} H^s(\Gamma) &:= \{u \in H^1(\Gamma); u|_{\Gamma_j} \in H^s(\Gamma_j), j = 1, \dots, N_\Gamma\} \quad \text{for } s > 1, \\ \mathbf{H}_t^s(\Gamma) &:= \{\mathbf{u} \in \mathbf{L}_t^2(\Gamma); \mathbf{u}|_{\Gamma_j} \in \mathbf{H}^s(\Gamma_j), j = 1, \dots, N_\Gamma\} \quad \text{for } s \geq 0, \end{aligned}$$

where $\mathbf{L}_t^2(\Gamma) := \{\mathbf{u} \in \mathbf{L}^2(\Gamma); \mathbf{u} \cdot \mathbf{n} = 0\}$. We equip all spaces with their natural graph norms.

For any $\mathbf{U} \in \mathbf{C}^\infty(\bar{D})$ the tangential components trace γ_t and the twisted tangential trace $\gamma_\times$ can be defined a.e. on Γ by

$$\gamma_t \mathbf{U}(\mathbf{x}) := \mathbf{n}(\mathbf{x}) \times (\mathbf{U}(\mathbf{x}) \times \mathbf{n}(\mathbf{x})), \quad \gamma_\times \mathbf{U}(\mathbf{x}) := \mathbf{U}(\mathbf{x}) \times \mathbf{n}(\mathbf{x}).$$

For piecewise smooth boundaries their extension onto $\mathbf{H}_{\text{loc}}(\text{curl}, D)$ has been achieved in [9] and [12, Prop. 1.7], and for Lipschitz boundaries in [15, Sect. 2].

Theorem 1.2. *There exist intrinsically defined spaces $\mathbf{H}_\parallel^{1/2}(\Gamma) \subset \mathbf{L}_t^2(\Gamma)$ and $\mathbf{H}_\perp^{1/2}(\Gamma) \subset \mathbf{L}_t^2(\Gamma)$ such that the tangential components trace and the twisted tangential trace*

$$\gamma_t^\pm : \mathbf{H}_{\text{loc}}^1(D) \mapsto \mathbf{H}_\parallel^{1/2}(\Gamma), \quad \gamma_\times^\pm : \mathbf{H}_{\text{loc}}^1(D) \mapsto \mathbf{H}_\perp^{1/2}(\Gamma),$$

are continuous, surjective and possess continuous right inverses.

Proof. For a proof see [12, Prop. 2.7]. $\square$

Their dual spaces will be denoted by $\mathbf{H}_\parallel^{-1/2}(\Gamma)$ and $\mathbf{H}_\perp^{-1/2}(\Gamma)$ respectively. In what follows

$$\langle \boldsymbol{\lambda}, \boldsymbol{\mu} \rangle_t := \int_\Gamma \boldsymbol{\lambda} \cdot \bar{\boldsymbol{\mu}} \, d\mathbf{S}, \quad \boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathbf{L}_t^2(\Gamma),$$

will stand for the inner product on $\mathbf{L}_t^2(\Gamma)$, which can be extended to a sesquilinear duality pairing

$$\langle \cdot, \cdot \rangle_t : \mathbf{H}_\parallel^{-1/2}(\Gamma) \times \mathbf{H}_\parallel^{1/2}(\Gamma) \mapsto \mathbb{C}, \quad \langle \cdot, \cdot \rangle_t : \mathbf{H}_\perp^{-1/2}(\Gamma) \times \mathbf{H}_\perp^{1/2}(\Gamma) \mapsto \mathbb{C},$$

when $\mathbf{L}_t^2(\Gamma)$ is taken as pivot space.

The classical Rellich embedding theorem can be applied to the tangential trace spaces in the following way.

Lemma 1.1. *The embeddings $\mathbf{H}_{\parallel}^{1/2}(\Gamma) \hookrightarrow \mathbf{L}_{\mathbf{t}}^2(\Gamma)$ and $\mathbf{H}_{\perp}^{1/2}(\Gamma) \hookrightarrow \mathbf{L}_{\mathbf{t}}^2(\Gamma)$ are compact.*

Based on surface differential operators, cf. [12, Sect. 3], we can define

$$\begin{aligned}\mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma) &:= \left\{ \mathbf{v} \in \mathbf{H}_{\perp}^{-1/2}(\Gamma); \operatorname{curl}_{\Gamma} \mathbf{v} \in H^{-1/2}(\Gamma) \right\}, \\ \mathbf{H}^{-1/2}(\operatorname{div}_{\Gamma}, \Gamma) &:= \left\{ \boldsymbol{\zeta} \in \mathbf{H}_{\parallel}^{-1/2}(\Gamma); \operatorname{div}_{\Gamma} \boldsymbol{\zeta} \in H^{-1/2}(\Gamma) \right\}.\end{aligned}$$

These spaces are endowed with the natural graph norms and are of great importance as suitable trace spaces for vector fields in $\mathbf{H}_{\text{loc}}(\mathbf{curl}, D)$ (cf. [12, Theorems 2.7 and 2.8], [13, Theorem 4.5] and [9, Sect. 4]):

Theorem 1.3. *The tangential components trace and the twisted tangential trace*

$$\begin{aligned}\gamma_{\mathbf{t}}^{\pm} : \mathbf{H}_{\text{loc}}(\mathbf{curl}, D) &\mapsto \mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma), \\ \gamma_{\times}^{\pm} : \mathbf{H}_{\text{loc}}(\mathbf{curl}, D) &\mapsto \mathbf{H}^{-1/2}(\operatorname{div}_{\Gamma}, \Gamma),\end{aligned}$$

are continuous, surjective with continuous right inverses.

From this theorem we conclude that $\mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma)$ is exactly the right space for the Dirichlet data $\gamma_{\mathbf{t}}^{-} \mathbf{E}$, $\gamma_{\mathbf{t}}^{+} \mathbf{E}^{\text{s}}$ and $\mathbf{g}_D$ in (1.1). Thus we adopt the alternative notation γ_D for $\gamma_{\mathbf{t}}$ to stress the fact that this is the right “Dirichlet” trace space. As has been demonstrated in [13, Sect. 4], $\mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma)$ and $\mathbf{H}^{-1/2}(\operatorname{div}_{\Gamma}, \Gamma)$ can be put into duality, when $\mathbf{L}_{\mathbf{t}}^2(\Gamma)$ is used as pivot space. More precisely, the usual $\mathbf{L}_{\mathbf{t}}^2(\Gamma)$ -inner product can be extended to a sesquilinear duality pairing

$$\langle \cdot, \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\operatorname{div}_{\Gamma}, \Gamma) \times \mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma) \mapsto \mathbb{C}$$

by means of a Green’s formula, $D \in \{\Omega, \Omega^+\}$,

$$\mp \int_D \mathbf{U} \cdot \operatorname{curl} \bar{\mathbf{V}} - \operatorname{curl} \mathbf{U} \cdot \bar{\mathbf{V}} \, d\mathbf{x} = \langle \gamma_{\times}^{\pm} \mathbf{U}, \gamma_{\mathbf{t}}^{\pm} \mathbf{V} \rangle_{\mathbf{t}}$$

for all $\mathbf{U}, \mathbf{V} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}, D)$, where an overbar denotes complex conjugation.

For continuous tangential vector fields $\mathbf{u}$, we define the surface twist operator by

$$\mathbf{R}(\mathbf{u})(\mathbf{x}) := \mathbf{n}(\mathbf{x}) \times \mathbf{u}(\mathbf{x}),$$

which gives rise to an isometric mapping

$$\mathbf{R} : \mathbf{H}^{-1/2}(\operatorname{curl}_{\Gamma}, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{div}_{\Gamma}, \Gamma).$$

We will also need the normal components trace $\gamma_{\mathbf{n}}$ defined by

$$\gamma_{\mathbf{n}} \mathbf{U}(\mathbf{x}) := \mathbf{n}(\mathbf{x}) \cdot \mathbf{U}(\mathbf{x})$$

for almost all $\mathbf{x} \in \Gamma$ and $\mathbf{U} \in \mathbf{C}^\infty(\bar{\Omega})$. This trace can be extended to a continuous and surjective mapping $\gamma_{\mathbf{n}} : \mathbf{H}_{\text{loc}}(\text{div}, \Omega) \mapsto H^{-1/2}(\Gamma)$ (cf. [33, Theorem 2.5]).

Besides the Dirichlet trace γ_D the transmission conditions of (1.1) also feature a second trace, aptly called the Neumann trace γ_N , which has to be introduced in a weak sense: For

$$\mathbf{U} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}^2, D) := \{ \mathbf{V} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}, D); \mathbf{curl} \mathbf{curl} \mathbf{V} \in \mathbf{L}_{\text{loc}}^2(D) \},$$

we define $\gamma_N^\pm \mathbf{U} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ by

$$\mp \int_D \mathbf{curl} \mathbf{U} \cdot \mathbf{curl} \bar{\mathbf{V}} - \mathbf{curl} \mathbf{curl} \mathbf{U} \cdot \bar{\mathbf{V}} \, d\mathbf{x} = \langle \gamma_N^\pm \mathbf{U}, \gamma_D^\mp \mathbf{V} \rangle_{\mathbf{t}}, \quad (1.2)$$

for all $\mathbf{V} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}, D)$. Obviously for smooth vector fields we recover $\gamma_N \mathbf{U} = \gamma_\times(\mathbf{curl} \mathbf{U}) = \mathbf{curl} \mathbf{U} \times \mathbf{n}$. The following lemma shows that $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ is exactly the right space for the “Neumann” data in (1.1).

Lemma 1.2. *The traces $\gamma_N^\pm : \mathbf{H}_{\text{loc}}(\mathbf{curl}^2, D) \mapsto \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ furnish continuous mappings.*

Proof. For a proof see [38, Lemma 3.3]. $\square$

There is some analogy between the Helmholtz and the Maxwell case, which is already indicated by the notation we have chosen. In the Helmholtz case fields of total, scattered and incident waves belong to $H_{\text{loc}}^1(D)$, whereas in the Maxwell case they belong to $\mathbf{H}_{\text{loc}}(\mathbf{curl}, D)$. For smooth functions U or fields $\mathbf{E}$ and any $\mathbf{x} \in \Gamma$, we can establish the following correspondence between the Dirichlet and Neumann traces:

$$\begin{aligned} \gamma_D \mathbf{E}(\mathbf{x}) &= \mathbf{n}(\mathbf{x}) \times (\mathbf{E}(\mathbf{x}) \times \mathbf{n}(\mathbf{x})) & \leftrightarrow & \gamma_D U(\mathbf{x}) = U(\mathbf{x}), \\ \gamma_N \mathbf{E}(\mathbf{x}) &= \mathbf{curl} \mathbf{E}(\mathbf{x}) \times \mathbf{n}(\mathbf{x}) & \leftrightarrow & \gamma_N U(\mathbf{x}) = \mathbf{grad} U(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}). \end{aligned}$$

Furthermore, in the Helmholtz case, the Dirichlet and Neumann traces are part of the $H^{1/2}(\Gamma)$ and $H^{-1/2}(\Gamma)$, whereas in the Maxwell case they belong to $\mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$ and $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$. Nevertheless, the continuity and surjectivity results for both traces are completely analogous.

1.3 Potentials and Boundary Integral Operators

Any distribution $\mathbf{U} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}^2, \Omega^+)$ which satisfies the electric field equation

$$\mathbf{curl} \mathbf{curl} \mathbf{U} - \kappa^2 \mathbf{U} = 0 \quad \text{in } \Omega^+, \quad (1.3)$$

together with the Silver–Müller radiation condition can be written using the *Stratton–Chu representation formula* (cf. [14, Sect. 3], [20, Chap. 3, Sect. 1.3.2], and [49, Sect. 5.5])

$$\mathbf{U} = \boldsymbol{\Psi}_{\text{DL}}^\kappa(\gamma_{\text{D}}^+ \mathbf{U}) - \boldsymbol{\Psi}_{\text{S}}^\kappa(\gamma_{\text{N}}^+ \mathbf{U}) - \mathbf{grad} \Psi_{\text{S}}^\kappa(\gamma_{\text{N}}^+ \mathbf{U}) \quad \text{in } \Omega^+, \quad (1.4)$$

with the potentials:

$$\text{scalar single-layer potential} \quad \Psi_{\text{S}}^\kappa(\varphi)(\mathbf{x}) := \int_{\Gamma} G_\kappa(|\mathbf{x} - \mathbf{y}|) \varphi(\mathbf{y}) \, \mathrm{d}\mathbf{S}(\mathbf{y}),$$

$$\text{vectorial single-layer potential} \quad \boldsymbol{\Psi}_{\text{S}}^\kappa(\boldsymbol{\mu})(\mathbf{x}) := \int_{\Gamma} G_\kappa(|\mathbf{x} - \mathbf{y}|) \boldsymbol{\mu}(\mathbf{y}) \, \mathrm{d}\mathbf{S}(\mathbf{y}),$$

$$\text{Maxwell double-layer potential} \quad \boldsymbol{\Psi}_{\text{DL}}^\kappa(\mathbf{u})(\mathbf{x}) := (\mathbf{curl} \circ \boldsymbol{\Psi}_{\text{S}}^\kappa \circ \mathbf{R})(\mathbf{u})(\mathbf{x}),$$

based on the Helmholtz kernel

$$G_\kappa(z) := \frac{1}{4\pi} \frac{\exp(i\kappa z)}{z}, \quad z \neq 0,$$

and $\mathbf{x} \notin \Gamma$. However, a simplification of (1.4) is possible by observing that [15, (26)]

$$\operatorname{div}_\Gamma(\gamma_{\text{N}}^+ \mathbf{U}) = \gamma_{\text{N}}^+(\mathbf{curl} \, \mathbf{curl} \, \mathbf{U}) = \kappa^2 \gamma_{\text{N}}^+ \mathbf{U} \quad \text{in } H^{-1/2}(\Gamma)$$

for all $\mathbf{U} \in \mathbf{H}_{\text{loc}}(\mathbf{curl}^2, \Omega^+)$ satisfying (1.3). This makes it possible to get rid of the normal components trace in (1.4) and we obtain a much simpler version of the representation formula

$$\mathbf{U} = \boldsymbol{\Psi}_{\text{DL}}^\kappa(\gamma_{\text{D}}^+ \mathbf{U}) - \boldsymbol{\Psi}_{\text{SL}}^\kappa(\gamma_{\text{N}}^+ \mathbf{U}) \quad \text{in } \Omega^+, \quad (1.5)$$

by introducing the Maxwell single-layer potential

$$\boldsymbol{\Psi}_{\text{SL}}^\kappa(\boldsymbol{\mu})(\mathbf{x}) := \boldsymbol{\Psi}_{\text{S}}^\kappa(\boldsymbol{\mu})(\mathbf{x}) + \frac{1}{\kappa^2} \mathbf{grad} \Psi_{\text{S}}^\kappa(\operatorname{div}_\Gamma \boldsymbol{\mu})(\mathbf{x}), \quad \mathbf{x} \notin \Gamma.$$

Lemma 1.3. *The scalar and vectorial single-layer potentials Ψ_{S}^κ and $\boldsymbol{\Psi}_{\text{S}}^\kappa$ give rise to continuous mappings*

$$\Psi_{\text{S}}^\kappa : H^{-1/2}(\Gamma) \mapsto H_{\text{loc}}^1(\mathbb{R}^3), \quad \boldsymbol{\Psi}_{\text{S}}^\kappa : \mathbf{H}_{\parallel}^{-1/2}(\Gamma) \mapsto \mathbf{H}_{\text{loc}}^1(\mathbb{R}^3).$$

Proof. For a proof see [27] or [38, Theorem 5.1]. $\square$

Lemma 1.4. *For $\mathbf{u} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ we have $\operatorname{div} \boldsymbol{\Psi}_{\text{S}}^\kappa(\mathbf{u}) = \Psi_{\text{S}}^\kappa(\operatorname{div}_\Gamma \mathbf{u})$ in $L_{\text{loc}}^2(\mathbb{R}^3)$.*

Proof. A proof can be found in [45, Lemma 2.3]. $\square$

From this we immediately derive the identities

$$\begin{aligned} (\mathbf{curl} \, \mathbf{curl} - \kappa^2 \operatorname{Id}) \boldsymbol{\Psi}_{\text{S}}^\kappa(\boldsymbol{\mu}) &= \mathbf{grad} \Psi_{\text{S}}^\kappa(\operatorname{div}_\Gamma \boldsymbol{\mu}) & \forall \boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma), \\ (\mathbf{curl} \, \mathbf{curl} - \kappa^2 \operatorname{Id}) \boldsymbol{\Psi}_{\text{DL}}^\kappa(\mathbf{u}) &= 0 & \forall \mathbf{u} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma), \end{aligned}$$

off the boundary in a point wise sense, and, globally in $\mathbf{L}_{\text{loc}}^2(\mathbb{R}^3)$. Thus we conclude that both $\boldsymbol{\Psi}_{\text{SL}}^\kappa$ and $\boldsymbol{\Psi}_{\text{DL}}^\kappa$ are radiating solutions to the electric field equation in $\Omega \cup \Omega^+$.

From these relationships and Lemma 1.3 we immediately derive the following continuity properties.

Lemma 1.5. *The Maxwell single-layer potential Ψ_{SL}^κ and the Maxwell double-layer potential Ψ_{DL}^κ provide continuous mappings*

$$\begin{aligned}\Psi_{\text{SL}}^\kappa &: \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \mapsto \mathbf{H}_{\text{loc}}(\text{curl}^2, \Omega \cup \Omega^+), \\ \Psi_{\text{DL}}^\kappa &: \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbf{H}_{\text{loc}}(\text{curl}^2, \Omega \cup \Omega^+),\end{aligned}$$

are continuous mappings.

The potentials also satisfy fundamental jump relations (cf. [25, Theorem 6.11], [49, Theorem 5.5.1] and [38, Sect. 5]).

Lemma 1.6. *The interior and exterior Dirichlet and Neumann traces of the potentials Ψ_{SL}^κ and Ψ_{DL}^κ are well defined and satisfy*

$$\begin{aligned}[\gamma_{\text{D}}\Psi_{\text{SL}}^\kappa(\mu)]_\Gamma &= 0, & [\gamma_{\text{N}}\Psi_{\text{SL}}^\kappa(\mu)]_\Gamma &= -\mu, & \forall \mu \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma), \\ [\gamma_{\text{D}}\Psi_{\text{DL}}^\kappa(\mathbf{u})]_\Gamma &= \mathbf{u}, & [\gamma_{\text{N}}\Psi_{\text{DL}}^\kappa(\mathbf{u})]_\Gamma &= 0, & \forall \mathbf{u} \in \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma).\end{aligned}$$

This theorem in conjunction with Lemma 1.4 and $\Psi_{\text{S}}^\kappa(\mathbf{R}(\mathbf{u})) \in \mathbf{H}_{\text{loc}}^1(\mathbb{R}^3)$ supplies further jump relations

$$[\gamma_{\text{N}}\Psi_{\text{DL}}^\kappa(\mathbf{u})]_\Gamma = 0, \quad [\gamma \text{div} \Psi_{\text{S}}^\kappa(\mu)]_\Gamma = 0.$$

By applying averages of Dirichlet and Neumann traces to the potentials of the representation formula we obtain the relevant boundary integral operators for the electric field equation (cf. [39, Lemma 5.1, Theorem 5.2]). Their continuity properties are immediate from Theorem 1.2 and Lemmas 1.2, 1.3.

Lemma 1.7. *The integral operators*

$$\begin{aligned}\mathbf{S}_\kappa &:= \{\gamma_{\text{D}}\}_\Gamma \circ \Psi_{\text{S}}^\kappa &: \mathbf{H}_{\parallel}^{-1/2}(\Gamma) \mapsto \mathbf{H}_{\parallel}^{1/2}(\Gamma), \\ \mathbf{S}_\kappa^\times &:= \{\gamma_{\times}\}_\Gamma \circ \Psi_{\text{S}}^\kappa \circ \mathbf{R} &: \mathbf{H}_{\perp}^{-1/2}(\Gamma) \mapsto \mathbf{H}_{\perp}^{1/2}(\Gamma), \\ \mathbf{S}_\kappa &:= \{\gamma\}_\Gamma \circ \Psi_{\text{S}}^\kappa &: \mathbf{H}^{-1/2}(\Gamma) \mapsto \mathbf{H}^{1/2}(\Gamma),\end{aligned}$$

are continuous.

Theorem 1.4. *The following integral operators are continuous:*

$$\begin{aligned}\mathbf{V}_\kappa &:= \{\gamma_{\text{D}}\}_\Gamma \circ \Psi_{\text{SL}}^\kappa &: \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma), \\ \mathbf{K}'_\kappa &:= \{\gamma_{\text{N}}\}_\Gamma \circ \Psi_{\text{SL}}^\kappa &: \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma), \\ \mathbf{K}_\kappa &:= \{\gamma_{\text{D}}\}_\Gamma \circ \Psi_{\text{DL}}^\kappa &: \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma), \\ \mathbf{W}_\kappa &:= \{\gamma_{\text{N}}\}_\Gamma \circ \Psi_{\text{DL}}^\kappa &: \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma).\end{aligned}$$

Beyond continuity, the integral operators possess numerous important properties. In particular, the operators $\mathbf{K}_\kappa$ and $\mathbf{K}'_\kappa$ are closely related as expressed in the following lemma, see [39, Lemma 5.4].

Lemma 1.8. *There exists a compact linear operator*

$$\mathbf{T}_\kappa : \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma),$$

such that for all $\zeta \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ and $\mathbf{q} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ there holds

$$\langle \mathbf{K}'_\kappa(\zeta), \mathbf{q} \rangle_t = \langle \zeta, \mathbf{K}_\kappa(\mathbf{q}) \rangle_t - \langle \mathbf{T}_\kappa(\zeta), \mathbf{q} \rangle_t.$$

Since we aim to apply the powerful Fredholm alternative argument, compactness properties of the boundary integral operators are of great importance. It will be crucial that we can switch to the “Laplace kernel” G_0 by a compact perturbation only (cf. [18, Theorem 3.12] and [41, Lemma 3.2]).

Lemma 1.9. *The following integral operators are compact:*

$$\delta \mathbf{S}_\kappa := \mathbf{S}_\kappa - \mathbf{S}_0 : \mathbf{H}^{-1/2}(\Gamma) \mapsto \mathbf{H}^{1/2}(\Gamma),$$

$$\delta \mathbf{S}_\kappa := \mathbf{S}_\kappa - \mathbf{S}_0 : \mathbf{H}_\parallel^{-1/2}(\Gamma) \mapsto \mathbf{H}_\parallel^{1/2}(\Gamma),$$

$$\delta \mathbf{S}_\kappa^\times := \mathbf{S}_\kappa^\times - \mathbf{S}_0^\times : \mathbf{H}_\perp^{-1/2}(\Gamma) \mapsto \mathbf{H}_\perp^{1/2}(\Gamma),$$

$$\delta \mathbf{W}_\kappa := \mathbf{W}_\kappa - \mathbf{W}_0 : \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma).$$

The significance of the case $\kappa = 0$ is highlighted by the following result (cf. [46, Corollary 8.13], [31, Chap. XI, Sect. 2, Theorem 3] and [14, Prop. 4.1]).

Lemma 1.10. *The operators $\mathbf{S}_0$, $\mathbf{S}_0$ and $\mathbf{S}_0^\times$ are continuous, self-adjoint and fulfill*

$$\langle \mu, \mathbf{S}_0(\mu) \rangle_\Gamma \geq C \|\mu\|_{\mathbf{H}^{-1/2}(\Gamma)}^2 \quad \forall \mu \in \mathbf{H}^{-1/2}(\Gamma),$$

$$\langle \mu, \mathbf{S}_0(\mu) \rangle_t \geq C \|\mu\|_{\mathbf{H}_\parallel^{-1/2}(\Gamma)}^2 \quad \forall \mu \in \mathbf{H}_\parallel^{-1/2}(\Gamma), \operatorname{div}_\Gamma \mu = 0,$$

$$\langle \mathbf{v}, \mathbf{S}_0^\times(\mathbf{v}) \rangle_t \geq C \|\mathbf{v}\|_{\mathbf{H}_\perp^{-1/2}(\Gamma)}^2 \quad \forall \mathbf{v} \in \mathbf{H}_\perp^{-1/2}(\Gamma), \operatorname{curl}_\Gamma \mathbf{v} = 0,$$

with constants $C > 0$ depending only on Γ .

At first glance, the Helmholtz and Maxwell cases seem similar, but there are some apparent differences. The most striking among them is the lack of coercivity of the Maxwell single-layer operator $\mathbf{V}_\kappa$ on $\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$. In the Helmholtz case, we can combine Lemmas 1.9 and 1.10 and conclude that the Helmholtz single-layer operator $\mathbf{S}_\kappa$ satisfies a Gårding inequality on $\mathbf{H}^{-1/2}(\Gamma)$, i.e., there exists a constant $C > 0$ and a compact operator $\mathbf{T}_\mathbf{S} := \mathbf{S}_0 - \mathbf{S}_\kappa : \mathbf{H}^{-1/2}(\Gamma) \mapsto \mathbf{H}^{1/2}(\Gamma)$ such that

$$\operatorname{Re} \{ \langle \vartheta, \mathbf{S}_\kappa(\vartheta) \rangle_\Gamma + \langle \vartheta, \mathbf{T}_\mathbf{S}(\vartheta) \rangle_\Gamma \} \geq C \|\vartheta\|_{\mathbf{H}^{-1/2}(\Gamma)}^2, \quad (1.6)$$

for all $\vartheta \in H^{-1/2}(\Gamma)$. However, for the Maxwell single-layer operator $\mathbf{V}_\kappa$ things are different. Since variational formulations are our primary concern, let us inspect the sesquilinear form associated with $\mathbf{V}_\kappa$, see [16, Sect. 5] for details:

$$\langle \boldsymbol{\mu}, \mathbf{V}_\kappa(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} = \langle \boldsymbol{\mu}, \mathbf{S}_\kappa(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} - \kappa^{-2} \langle \operatorname{div}_\Gamma \boldsymbol{\mu}, \mathbf{S}_\kappa(\operatorname{div}_\Gamma \boldsymbol{\lambda}) \rangle_\Gamma, \quad (1.7)$$

for all $\boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathbf{H}_\parallel^{-1/2}(\Gamma)$. Slightly abusing notation, we define

$$\mathbf{V}_0 := \mathbf{S}_0 + \kappa^{-2} \operatorname{grad}_\Gamma \circ \mathbf{S}_0 \circ \operatorname{div}_\Gamma$$

and by recalling Lemma 1.9 we conclude that $\mathbf{V}_\kappa - \mathbf{V}_0$ is compact as a mapping from $\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ onto $\mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$. Although, this result is sufficient to establish coercivity in the Helmholtz case (see (1.6)), it does not guarantee a Gårding inequality for the Maxwell single-layer operator. According to (1.7)

$$\langle \boldsymbol{\mu}, \mathbf{V}_0(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} = \langle \boldsymbol{\mu}, \mathbf{S}_0(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} - \kappa^{-2} \langle \operatorname{div}_\Gamma \boldsymbol{\mu}, \mathbf{S}_0(\operatorname{div}_\Gamma \boldsymbol{\lambda}) \rangle_\Gamma,$$

can be split into a sum of two operators of order minus one and plus one, respectively. In contrast to the Helmholtz case, the operator of order -1 is not elliptic but has an infinite dimensional kernel, which agrees with the kernel of the surface divergence operator $\operatorname{div}_\Gamma$. This clearly indicates that a Gårding inequality for $\mathbf{V}_\kappa$ on $\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ remains elusive.

1.4 Decompositions

This section provides stable splittings of $\mathbf{H}(\operatorname{curl}, \Omega)$ and $\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$, which are needed to establish Gårding inequalities for the sesquilinear forms underlying the coupled variational formulations. We motivate the splitting idea for two particular cases, namely for an interior source problem and for plane wave scattering from a perfect electric conductor.

Let us first consider the *interior source problem* for the electric wave equation in variational form: For any $\mathbf{F} \in \mathbf{L}^2(\Omega)$, find $\mathbf{E} \in \mathbf{H}(\operatorname{curl}, \Omega)$ such that for all $\mathbf{V} \in \mathbf{H}(\operatorname{curl}, \Omega)$ there holds

$$\mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) := (\mu_r^{-1} \operatorname{curl} \mathbf{E}, \operatorname{curl} \mathbf{V})_0 - \kappa^2 (\varepsilon_r \mathbf{E}, \mathbf{V})_0 = (\mathbf{F}, \mathbf{V})_0.$$

The numerical analysis of the indefinite interior source problem is usually based on the Fredholm alternative, which can only be applied to variational formulations, whose underlying sesquilinear forms are coercive. Thus establishing a generalized Gårding inequality for $\mathbf{q}_\kappa(\cdot, \cdot)$ on $\mathbf{H}(\operatorname{curl}, \Omega)$ is essential. Unfortunately, due to a lack of compact embedding of $\mathbf{H}(\operatorname{curl}, \Omega)$ into $\mathbf{L}^2(\Omega)$, a generalized Gårding inequality remains elusive.

However, the lack of coercivity can be overcome by a splitting of the fields into two components

$$\mathbf{H}(\operatorname{curl}, \Omega) = \mathbf{X}(\Omega) \oplus \mathbf{N}(\Omega).$$

In the context of electromagnetic problems this idea has been pioneered by Nédélec and was first applied to integral operators in [32]. Since then, it has emerged as very powerful theoretical tool, see [3, 14, 22] and, in particular, the monograph [49]. The following features of a splitting prove essential:

1. The subspace $\mathbf{N}(\Omega)$ in the splitting agrees with the kernel of the $\mathbf{curl}$.
2. The compact embedding of the complement subspace $\mathbf{X}(\Omega)$ into $\mathbf{L}^2(\Omega)$.
3. Stability of the splitting.
4. Extra regularity of vector fields in the complement space $\mathbf{X}(\Omega)$.

Thus, any $\mathbf{E} \in \mathbf{H}(\mathbf{curl}, \Omega)$ can be decomposed into two components $\mathbf{E} = \mathbf{E}^0 + \mathbf{E}^\perp$, where $\mathbf{E}^0 \in \mathbf{N}(\Omega)$ and $\mathbf{E}^\perp \in \mathbf{X}(\Omega)$. This naturally leads us to the definition of a bounded, linear isomorphism $\mathbf{X}_\Omega : \mathbf{H}(\mathbf{curl}, \Omega) \mapsto \mathbf{H}(\mathbf{curl}, \Omega)$, given by $\mathbf{X}_\Omega(\mathbf{E}) := \mathbf{E}^\perp - \mathbf{E}^0$, which can be employed to “flip signs” in the decomposition. Due to the compact embedding $\mathbf{X}(\Omega) \hookrightarrow \mathbf{L}^2(\Omega)$, we conclude that the following terms

$$(\varepsilon_r \mathbf{E}^\perp, \mathbf{V}^\perp)_0, \quad (\varepsilon_r \mathbf{E}^\perp, \mathbf{V}^0)_0, \quad (\varepsilon_r \mathbf{E}^0, \mathbf{V}^\perp)_0,$$

are compact for all $\mathbf{E}, \mathbf{V} \in \mathbf{H}(\mathbf{curl}, \Omega)$. Thus, there exists a compact sesquilinear form $c_\kappa : \mathbf{H}(\mathbf{curl}, \Omega) \times \mathbf{H}(\mathbf{curl}, \Omega) \mapsto \mathbb{C}$, such that the following estimate holds

$$\begin{aligned} \operatorname{Re} \{ q_\kappa(\mathbf{E}, \mathbf{X}_\Omega(\mathbf{E})) + c_\kappa(\mathbf{E}, \mathbf{X}_\Omega(\mathbf{E})) \} \\ \geq C \left(\|\mathbf{E}^\perp\|_{\mathbf{H}(\mathbf{curl}, \Omega)}^2 + \|\mathbf{E}^0\|_{\mathbf{H}(\mathbf{curl}, \Omega)}^2 \right), \end{aligned}$$

for all $\mathbf{E} \in \mathbf{H}(\mathbf{curl}, \Omega)$. Hence, we immediately derive a generalized Gårding inequality for the sesquilinear form $q_\kappa(\cdot, \cdot)$ on the product space $\mathbf{X}(\Omega) \times \mathbf{N}(\Omega)$.

This motivates the use of the a Helmholtz-type *regular splitting*, whose construction is based on the existence of vector potentials in $\mathbf{H}^1(\Omega)$ (cf. [5, Lemma 3.5]):

Lemma 1.11. *There exists a continuous mapping*

$$\mathbf{L} : \mathbf{H}(\operatorname{div} 0, \Omega) := \{ \mathbf{V} \in \mathbf{L}^2(\Omega); \operatorname{div} \mathbf{V} = 0 \} \mapsto \mathbf{H}^1(\Omega),$$

such that $(\operatorname{div} \circ \mathbf{L})(\mathbf{U}) = 0$ and $(\mathbf{curl} \circ \mathbf{L})(\mathbf{U}) = \mathbf{U}$ for all $\mathbf{U} \in \mathbf{H}(\operatorname{div} 0, \Omega)$.

Based on this device we introduce the following operator

$$\mathbf{P} : \mathbf{H}(\mathbf{curl}, \Omega) \mapsto \mathbf{H}^1(\Omega), \quad \mathbf{P}(\mathbf{U}) := (\mathbf{L} \circ \mathbf{curl})(\mathbf{U}).$$

From the properties of $\mathbf{L}$ we immediately derive numerous features of $\mathbf{P}$.

Lemma 1.12. *The operator $\mathbf{P}$ is a continuous projection that preserves the $\mathbf{curl}$ and satisfies $\operatorname{Ker}(\mathbf{P}) = \operatorname{Ker}(\mathbf{curl}) \cap \mathbf{H}(\mathbf{curl}, \Omega)$.*

Since $\text{Ker}(\mathbf{P}) = \text{Ker}(\mathbf{curl}) \cap \mathbf{H}(\mathbf{curl}, \Omega)$ it is clear that the following closed subspaces

$$\begin{aligned}\mathbf{X}(\mathbf{curl}, \Omega) &:= \mathbf{P}(\mathbf{H}(\mathbf{curl}, \Omega)), \\ \mathbf{N}(\mathbf{curl}, \Omega) &:= \text{Ker}(\mathbf{curl}) \cap \mathbf{H}(\mathbf{curl}, \Omega),\end{aligned}$$

provide a stable and direct Helmholtz-type splitting

$$\mathbf{H}(\mathbf{curl}, \Omega) = \mathbf{X}(\mathbf{curl}, \Omega) \oplus \mathbf{N}(\mathbf{curl}, \Omega). \quad (1.8)$$

For both components we retain the $\mathbf{H}(\mathbf{curl}, \Omega)$ -norm. The extra regularity of the $\mathbf{X}(\mathbf{curl}, \Omega)$ -component, which is contained in $\mathbf{H}^1(\Omega)$, is essential, since it immediately yields the following compact embedding.

Corollary 1.1. *The embedding $\mathbf{X}(\mathbf{curl}, \Omega) \hookrightarrow \mathbf{L}^2(\Omega)$ is compact.*

Summing up, this provides us with a generalized Gårding inequality for the sesquilinear form $\mathbf{q}_\kappa(\cdot, \cdot)$ on the product space $\mathbf{X}(\mathbf{curl}, \Omega) \times \mathbf{N}(\mathbf{curl}, \Omega)$.

It is hardly surprising that the splitting idea has to be adopted for the treatment of boundary integral operators as well. First, we discuss this for a pure scattering problem and related indirect boundary integral equations. Using a single-layer potential ansatz $\mathbf{E} := \Psi_{\text{SL}}^\kappa(\boldsymbol{\mu})$, $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$, as a trial expression for electromagnetic scattering from a perfect electric conductor, we arrive at the following variational problem: For every $\gamma_{\text{D}} \mathbf{E}^{\text{inc}} \in \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$, find $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ such that for all $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ there holds

$$\langle \boldsymbol{\mu}, \mathbf{V}_\kappa(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} = -\langle \boldsymbol{\mu}, \gamma_{\text{D}}^- \mathbf{E}^{\text{inc}} \rangle_{\mathbf{t}}.$$

Our considerations at the end of Sect. 1.3 clearly show, that a Gårding inequality for $\mathbf{V}_\kappa$ on $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ is not available, and, thus an appropriate splitting has to be employed. This time we opt for a Hodge-type splitting of the Neumann trace space into two components:

$$\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) = \mathbf{X}(\Gamma) \oplus \mathbf{N}(\Gamma).$$

In contrast to the splitting employed in [18, Theorem 3.4], we will waive orthogonality for increased regularity in the complement subspace $\mathbf{X}(\Gamma)$ and compact embeddings. We require:

1. The subspace $\mathbf{N}(\Gamma)$ in the splitting agrees with the kernel of div_Γ .
2. The compact embedding of the complement subspace $\mathbf{X}(\Gamma)$ into $\mathbf{L}_{\mathbf{t}}^2(\Gamma)$.
3. Stability of the splitting.
4. Extra regularity of vector fields in the complement space $\mathbf{X}(\Gamma)$.

Again, any $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ can be decomposed into $\boldsymbol{\lambda} = \boldsymbol{\lambda}^\perp + \boldsymbol{\lambda}^0$, where $\boldsymbol{\lambda}^\perp \in \mathbf{X}(\Gamma)$ and $\boldsymbol{\lambda}^0 \in \mathbf{N}(\Gamma)$. This time, the sign-flip isomorphism $\mathbf{X}_\Gamma : \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ is defined by $\mathbf{X}_\Gamma(\boldsymbol{\lambda}) := \boldsymbol{\lambda}^0 - \boldsymbol{\lambda}^\perp$.

Furthermore, the embedding $\mathbf{X}(\Gamma) \hookrightarrow \mathbf{L}_{\mathbf{t}}^2(\Gamma)$ allows us to identify the following compact sesquilinear pairings

$$\begin{aligned} \langle \boldsymbol{\lambda}^\perp, \boldsymbol{\mu}^\perp \rangle_{\mathbf{t}}, & \quad \langle \boldsymbol{\lambda}^\perp, \mathbf{S}_0(\boldsymbol{\mu}^\perp) \rangle_{\mathbf{t}}, & \forall \boldsymbol{\lambda}, \boldsymbol{\mu} \in \mathbf{H}(\mathbf{curl}, \Omega), \\ \langle \boldsymbol{\lambda}^\perp, \mathbf{S}_0(\boldsymbol{\mu}^0) \rangle_{\mathbf{t}}, & \quad \langle \boldsymbol{\lambda}^0, \mathbf{S}_0(\boldsymbol{\mu}^\perp) \rangle_{\mathbf{t}}, \end{aligned}$$

which imply existence of a compact sesquilinear form $c_\kappa : \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma) \times \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma) \mapsto \mathbb{C}$, such that for all $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma)$ the following estimate holds true

$$\begin{aligned} \operatorname{Re} \{ \langle \mathbf{X}_\Gamma(\boldsymbol{\lambda}), \mathbf{V}_\kappa(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} + c_\kappa(\mathbf{X}_\Gamma(\boldsymbol{\lambda}), \boldsymbol{\lambda}) \} \\ \geq C \left(\|\boldsymbol{\lambda}^\perp\|_{\mathbf{H}_{\parallel}^{-1/2}(\Gamma)}^2 + \|\boldsymbol{\lambda}^0\|_{\mathbf{H}_{\parallel}^{-1/2}(\Gamma)}^2 \right). \end{aligned}$$

Thus, we immediately derive a generalized Gårding inequality for the sesquilinear form corresponding to the Maxwell single-layer operator $\mathbf{V}_\kappa$ on the product space $\mathbf{X}(\Gamma) \times \mathbf{N}(\Gamma)$.

This motivates the construction of the following Hodge-type decomposition of $\mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma)$: Pick an arbitrary $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma)$, set $\omega := \mathbf{div}_\Gamma \boldsymbol{\lambda} \in H^{-1/2}(\Gamma)$ and solve the Neumann problem

$$\Psi \in \mathbf{H}^1(\Omega)/\mathbb{R} : \quad \Delta \Psi = 0 \text{ in } \Omega, \quad \gamma_{\mathbf{n}}^- \mathbf{grad} \Psi = \omega \text{ on } \Gamma.$$

Obviously $\mathbf{W} := \mathbf{grad} \Psi \in \mathbf{H}(\mathbf{div} 0, \Omega)$ belongs to the domain of the lifting operator $\mathbf{L}$. Thus we can introduce the operator $\mathbf{J} : H^{-1/2}(\Gamma) \mapsto \mathbf{H}^1(\Omega)$ by $\mathbf{J}(\omega) := \mathbf{L}(\mathbf{W})$. Its continuity is straightforward and, thanks to Theorem 1.2, inherited by the mapping

$$\mathbf{P}^\Gamma : \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma) \mapsto \mathbf{H}_{\perp}^{1/2}(\Gamma), \quad \mathbf{P}^\Gamma := \gamma_{\times} \circ \mathbf{J} \circ \mathbf{div}_\Gamma.$$

Properties of $\mathbf{P}^\Gamma$ matching those of $\mathbf{P}$ can be easily established, cf. [39, Lemma 7.4].

Lemma 1.13. *The operator $\mathbf{P}^\Gamma : \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma) \mapsto \mathbf{H}_{\perp}^{1/2}(\Gamma)$ is a continuous projection that preserves the $\mathbf{div}_\Gamma$ and satisfies $\operatorname{Ker}(\mathbf{P}^\Gamma) = \operatorname{Ker}(\mathbf{div}_\Gamma) \cap \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma)$.*

By defining the components

$$\mathbf{X}(\mathbf{div}_\Gamma, \Gamma) := \mathbf{P}^\Gamma(\mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma)),$$

$$\mathbf{N}(\mathbf{div}_\Gamma, \Gamma) := \operatorname{Ker}(\mathbf{div}_\Gamma) \cap \mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma),$$

we arrive at a stable direct decomposition of the space of magnetic traces:

$$\mathbf{H}^{-1/2}(\mathbf{div}_\Gamma, \Gamma) = \mathbf{X}(\mathbf{div}_\Gamma, \Gamma) \oplus \mathbf{N}(\mathbf{div}_\Gamma, \Gamma).$$

As before, the extra regularity of $\mathbf{X}(\mathbf{div}_\Gamma, \Gamma)$ rewards us with a valuable compact embedding analogous to [18, Theorem 3.4].

Corollary 1.2. *The embedding $\mathbf{X}(\operatorname{div}_\Gamma, \Gamma) \hookrightarrow \mathbf{L}_t^2(\Gamma)$ is compact.*

In short, this provides us with a generalized Gårding inequality for the sesquilinear form corresponding to the Maxwell single-layer operator $\mathbf{V}_\kappa$ on the product space $\mathbf{X}(\operatorname{div}_\Gamma, \Gamma) \times \mathbf{N}(\operatorname{div}_\Gamma, \Gamma)$.

1.5 Symmetric FEM–BEM Coupling

Applying the Green’s formula to the electric wave equation in Ω results in the following variational formulation: Find $\mathbf{E} \in \mathbf{H}(\operatorname{curl}, \Omega)$ such that

$$(\mu_r^{-1} \operatorname{curl} \mathbf{E}, \operatorname{curl} \mathbf{V})_0 - \kappa^2 (\varepsilon_r \mathbf{E}, \mathbf{V})_0 - \langle \mu_r^{-1} \gamma_N^- \mathbf{E}, \gamma_D^- \mathbf{V} \rangle_t = (\mathbf{F}, \mathbf{V})_0 \quad (1.9)$$

for all $\mathbf{V} \in \mathbf{H}(\operatorname{curl}, \Omega)$. The coupling to the exterior domain is taken into account by the transmission conditions

$$\mu_r^{-1} \gamma_N^- \mathbf{E} = \gamma_N^+ \mathbf{E}^s - \mathbf{g}_N, \quad \gamma_D^+ \mathbf{E}^s = \gamma_D^- \mathbf{E} + \mathbf{g}_D. \quad (1.10)$$

In order to incorporate the exterior field on the unbound domain Ω^+ into the variational formulation some realization of the Dirichlet-to-Neumann map has to be provided. It is furnished by the *exterior Calderón projector*, which arises from applying both exterior Dirichlet and Neumann traces to the representation formula (1.5) (cf. [32, (29)], [49, Sect. 5.5], [18, Sect. 3.3], and [43, (24)]). In variational form the resulting identities read

$$\begin{aligned} \langle \mu, \gamma_D^+ \mathbf{E}^s \rangle_t &= \langle \mu, (\tfrac{1}{2} \operatorname{Id} + \mathbf{K}_\kappa) (\gamma_D^+ \mathbf{E}^s) \rangle_t - \langle \mu, \mathbf{V}_\kappa (\gamma_N^+ \mathbf{E}^s) \rangle_t, \\ \langle \gamma_N^+ \mathbf{E}^s, \mathbf{v} \rangle_t &= \langle \mathbf{W}_\kappa (\gamma_D^+ \mathbf{E}^s), \mathbf{v} \rangle_t + \langle (\tfrac{1}{2} \operatorname{Id} - \mathbf{K}'_\kappa) (\gamma_N^+ \mathbf{E}^s), \mathbf{v} \rangle_t, \end{aligned} \quad (1.11)$$

for all $\mu \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ and $\mathbf{v} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$. Now we can use the transmission conditions (1.10) and the second equation of the Calderón projector to replace the boundary term in (1.9). The trick underlying the symmetric coupling approach according to Costabel [26] is to combine the resulting equation together with the first equation of (1.11) (cf. [32, Sect. 4] for Maxwell equations). Adopting the abbreviation $\boldsymbol{\lambda} := \gamma_N^+ \mathbf{E}^s \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ we arrive at the following variational formulation: Find $\mathbf{E} \in \mathbf{H}(\operatorname{curl}, \Omega)$ and $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ such that for all $\mathbf{V} \in \mathbf{H}(\operatorname{curl}, \Omega)$ and $\mu \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$

$$\begin{aligned} \mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) - \langle \mathbf{W}_\kappa (\gamma_D^- \mathbf{E}), \gamma_D^- \mathbf{V} \rangle_t \\ + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2} \operatorname{Id}) (\boldsymbol{\lambda}), \gamma_D^- \mathbf{V} \rangle_t &= \mathbf{f}_1(\mathbf{V}), \\ \langle \mu, (\tfrac{1}{2} \operatorname{Id} - \mathbf{K}_\kappa) (\gamma_D^- \mathbf{E}) \rangle_t + \langle \mu, \mathbf{V}_\kappa (\boldsymbol{\lambda}) \rangle_t &= \mathbf{g}_1(\mu), \end{aligned} \quad (1.12)$$

with right-hand sides

$$\begin{aligned} \mathbf{f}_1(\mathbf{V}) &:= (\mathbf{F}, \mathbf{V})_0 - \langle \mathbf{g}_N, \gamma_D^- \mathbf{V} \rangle_t + \langle \mathbf{W}_\kappa (\mathbf{g}_D), \gamma_D^- \mathbf{V} \rangle_t, \\ \mathbf{g}_1(\mu) &:= \langle \mu, (\mathbf{K}_\kappa - \tfrac{1}{2} \operatorname{Id}) (\mathbf{g}_D) \rangle_t, \end{aligned}$$

and $\mathbf{q}_\kappa(\cdot, \cdot)$ representing the interior sesquilinear form,

$$\mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) := (\mu_r^{-1} \mathbf{curl} \mathbf{E}, \mathbf{curl} \mathbf{V})_0 - \kappa^2 (\varepsilon_r \mathbf{E}, \mathbf{V})_0.$$

Lemma 1.14. *Provided that $\mathbf{curl} \mathbf{curl} \mathbf{U} - \kappa^2 \mathbf{U} = 0$ in Ω and $\gamma_D^- \mathbf{U} = 0$ on Γ implies $\mathbf{U} = 0$, then any solution of (1.12) provides a solution of (1.1) by retaining $\mathbf{E}$ in Ω and using the representation formula (1.5) for the Cauchy data $(\gamma_D^- \mathbf{E} + \mathbf{g}_D, \boldsymbol{\lambda})$ in Ω^+ .*

Proof. For a proof see [39, Lemma 6.1]. $\square$

If κ^2 coincides with an interior Dirichlet eigenvalue, then the solution (1.12) is only unique up to contributions $(0, \boldsymbol{\eta})$, where $\boldsymbol{\eta}$ is contained in the span of Neumann data belonging to interior Dirichlet eigensolutions. In particular, the interior electric field $\mathbf{E}$ and its Dirichlet data $\gamma_D^- \mathbf{E}$ are unique.

Since the sesquilinear form underlying the variational formulation (1.12) features the domain-based part $\mathbf{q}_\kappa(\cdot, \cdot)$, as well as the Maxwell single-layer operator $\mathbf{V}_\kappa$, our considerations from Sect. 1.4 clearly indicate that coercivity on $\mathbf{H}(\mathbf{curl}, \Omega) \times \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ does not hold. Thus, based on the splittings provided in Sect. 1.4, we can decompose the trial and test functions in the variational problem (1.12) according to:

$$\begin{aligned} \mathbf{E} &= \mathbf{E}^\perp + \mathbf{E}^0, & \mathbf{E}^\perp &\in \mathbf{X}(\mathbf{curl}, \Omega), \mathbf{E}^0 \in \mathbf{N}(\mathbf{curl}, \Omega), \\ \mathbf{V} &= \mathbf{V}^\perp + \mathbf{V}^0, & \mathbf{V}^\perp &\in \mathbf{X}(\mathbf{curl}, \Omega), \mathbf{V}^0 \in \mathbf{N}(\mathbf{curl}, \Omega), \\ \boldsymbol{\lambda} &= \boldsymbol{\lambda}^\perp + \boldsymbol{\lambda}^0, & \boldsymbol{\lambda}^\perp &\in \mathbf{X}(\text{div}_\Gamma, \Gamma), \boldsymbol{\lambda}^0 \in \mathbf{N}(\text{div}_\Gamma, \Gamma), \\ \boldsymbol{\mu} &= \boldsymbol{\mu}^\perp + \boldsymbol{\mu}^0, & \boldsymbol{\mu}^\perp &\in \mathbf{X}(\text{div}_\Gamma, \Gamma), \boldsymbol{\mu}^0 \in \mathbf{N}(\text{div}_\Gamma, \Gamma). \end{aligned}$$

In addition, we sort the unknowns according to their “electric” or “magnetic” nature, grouping them as $(\boldsymbol{\lambda}^\perp, \mathbf{E}^0)$ (electric), $(\boldsymbol{\lambda}^0, \mathbf{E}^\perp)$ (magnetic). Thus we arrive at a variational formulation with a distinct block structure on the Hilbert space

$$\mathcal{V} := \mathbf{X}(\text{div}_\Gamma, \Gamma) \times \mathbf{N}(\mathbf{curl}, \Omega) \times \mathbf{N}(\text{div}_\Gamma, \Gamma) \times \mathbf{X}(\mathbf{curl}, \Omega),$$

that is endowed with the natural graph norm: Find $(\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp) \in \mathcal{V}$ such that

$$\widehat{\mathbf{a}}_\kappa^{\text{sym}}((\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp), (\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp)) = \widehat{\mathbf{f}}_\kappa^{\text{sym}}(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp) \quad (1.13)$$

for all $(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp) \in \mathcal{V}$. The sesquilinear form $\widehat{\mathbf{a}}_\kappa^{\text{sym}} : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{C}$ and the linear form $\widehat{\mathbf{f}}_\kappa^{\text{sym}} : \mathcal{V} \mapsto \mathbb{C}$ are defined by

$$\begin{aligned} \widehat{\mathbf{a}}_\kappa^{\text{sym}}((\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp), (\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp)) \\ := \mathbf{a}_\kappa^{\text{sym}}((\mathbf{E}^\perp + \mathbf{E}^0, \boldsymbol{\lambda}^\perp + \boldsymbol{\lambda}^0), (\mathbf{V}^\perp - \mathbf{V}^0, -\boldsymbol{\mu}^\perp + \boldsymbol{\mu}^0)), \\ \widehat{\mathbf{f}}_\kappa^{\text{sym}}(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp) := \mathbf{f}_\kappa^{\text{sym}}(\mathbf{V}^\perp - \mathbf{V}^0, -\boldsymbol{\mu}^\perp + \boldsymbol{\mu}^0), \end{aligned}$$

where $\mathbf{a}_\kappa^{\text{sym}}$ and $\mathbf{f}_\kappa^{\text{sym}}$ are the sesquilinear and the linear form underlying the variational equation (1.12) (see [39, (8.1)] for a detailed structure of $\mathbf{a}_\kappa^{\text{sym}}$). Evidently, the split variational formulation (1.13) produces exactly the same solutions as (1.12) for $\boldsymbol{\lambda} = \boldsymbol{\lambda}^\perp + \boldsymbol{\lambda}^0$ and $\mathbf{E} = \mathbf{E}^\perp + \mathbf{E}^0$, provided that unique solutions exist. The decomposition of test and trial spaces provides us with the following powerful theorem.

Theorem 1.5. *The sesquilinear form $\widehat{\mathbf{a}}_\kappa^{\text{sym}} : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{C}$ satisfies a generalized Gårding inequality; that is, it can be written as a sum $\widehat{\mathbf{a}}_\kappa^{\text{sym}} = \mathbf{a}_\text{E} + \mathbf{a}_\text{C}$ of a $\mathcal{V}$ -elliptic sesquilinear form $\mathbf{a}_\text{E} : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{C}$ and a compact sesquilinear form $\mathbf{a}_\text{C} : \mathcal{V} \times \mathcal{V} \mapsto \mathbb{C}$.*

Proof. For a proof see [39, Theorem 8.3]. $\square$

1.6 Stable FEM–BEM Coupling

As pointed out in Lemma 1.14, the existence of spurious modes is directly linked to the fact that for certain κ there exist nontrivial interior Maxwell solutions $\mathbf{E}$ satisfying $\gamma_\text{D}^- \mathbf{E} = 0$. On the other hand, there are complex Robin-type boundary conditions which ensure unique solvability of the corresponding boundary value problem, namely,

$$\begin{aligned} \operatorname{curl} \operatorname{curl} \mathbf{E} - \kappa^2 \mathbf{E} &= \mathbf{0} & \text{in } \Omega, \\ \gamma_\text{D}^- \mathbf{E} + i\eta \gamma_\text{N}^- \mathbf{E} &= \mathbf{0} & \text{on } \Gamma, \end{aligned} \quad (1.14)$$

for some $\eta \in \mathbb{R} \setminus \{0\}$. Testing (1.2) with $\mathbf{V} := \mathbf{E}$ yields the identity

$$i\eta \|\gamma_\text{N}^- \mathbf{E}\|_{L_t^2(\Gamma)}^2 = \langle \gamma_\text{N}^- \mathbf{E}, \gamma_\text{D}^- \mathbf{E} \rangle_t = \int_\Omega |\operatorname{curl} \mathbf{E}|^2 - \kappa^2 |\mathbf{E}|^2 \, d\mathbf{x} \in \mathbb{R}.$$

Considering the imaginary part only, we arrive at $\gamma_\text{N}^- \mathbf{E} = 0$ and $\gamma_\text{D}^- \mathbf{E} = 0$ immediately follows from the boundary condition in (1.14). Since both traces are equal to zero we conclude that $\mathbf{E}$ must vanish on Ω , which establishes uniqueness of solutions to the boundary value problem (1.14). Note that we can rely on a Robin-type boundary operator to state the transmission conditions of (1.1), as long as we are able to recover the conventional traces.

In order to obtain a stable coupled variational formulation for the Maxwell transmission problem (1.1), we will make use of the idea of complex linear combinations of traces underlying the boundary value problem (1.14). Recalling the Calderón projector in its operator form, we arrive at the following two equations

$$\gamma_\text{D}^+ \mathbf{E}^\text{s} = \left(\frac{1}{2} \operatorname{Id} + \mathbf{K}_\kappa\right) (\gamma_\text{D}^+ \mathbf{E}^\text{s}) - \mathbf{V}_\kappa (\gamma_\text{N}^+ \mathbf{E}^\text{s}) \quad \text{in } H^{-1/2}(\operatorname{curl}_\Gamma, \Gamma), \quad (1.15)$$

$$\gamma_\text{N}^+ \mathbf{E}^\text{s} = \mathbf{W}_\kappa (\gamma_\text{D}^+ \mathbf{E}^\text{s}) + \left(\frac{1}{2} \operatorname{Id} - \mathbf{K}'_\kappa\right) (\gamma_\text{N}^+ \mathbf{E}^\text{s}) \quad \text{in } H^{-1/2}(\operatorname{div}_\Gamma, \Gamma). \quad (1.16)$$

Unfortunately, the trace spaces $\mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$ and $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ do not match, which means that complex linear combinations of Dirichlet and Neumann traces are not well defined. Thus, we cannot simply work with the natural trace spaces of problem (1.1), but have to do a lifting of both traces onto $\mathbf{L}_t^2(\Gamma)$. Now for $\eta > 0$, the complex linear combination (1.15) + $i\eta$ (1.16) yields the identity

$$\begin{aligned} \mathbf{0} &= (\mathbf{K}_\kappa - \tfrac{1}{2}\text{Id} + i\eta \mathbf{W}_\kappa) (\gamma_D^+ \mathbf{E}^s) \\ &\quad - (\mathbf{V}_\kappa + i\eta (\tfrac{1}{2}\text{Id} + \mathbf{K}'_\kappa)) (\gamma_N^+ \mathbf{E}^s) \in \mathbf{L}_t^2(\Gamma), \end{aligned} \quad (1.17)$$

which can be used to replace either (1.15) or (1.16) in a coupled variational formulation. Moreover, in order to get meaningful tangential trace operators, we have to replace $\mathbf{H}(\mathbf{curl}, \Omega)$ by the Hilbert space

$$\mathbf{X} := \{ \mathbf{U} \in \mathbf{H}(\mathbf{curl}, \Omega); \gamma_D^- \mathbf{U} \in \mathbf{L}_t^2(\Gamma) \},$$

which is Hilbert space with respect to the graph norm on $\mathbf{H}(\mathbf{curl}, \Omega)$, cf. [47, Chap. 4].

Thus, introducing the new variable $\boldsymbol{\lambda} := \gamma_N^+ \mathbf{E}^s \in \mathbf{L}_t^2(\Gamma)$ together with (1.9), (1.10), (1.16), and (1.17), we arrive at the following coupled variational formulation: Find $\mathbf{E} \in \mathbf{X}$ and $\boldsymbol{\lambda} \in \mathbf{L}_t^2(\Gamma)$, such that for all $\mathbf{V} \in \mathbf{X}$ and $\boldsymbol{\mu} \in \mathbf{L}_t^2(\Gamma)$ there holds

$$\begin{aligned} &\mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) - \langle \mathbf{W}_\kappa(\gamma_D^- \mathbf{E}), \gamma_D^- \mathbf{V} \rangle_t \\ &\quad + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2}\text{Id}) (\boldsymbol{\lambda}), \gamma_D^- \mathbf{V} \rangle_t = \mathbf{f}_2(\mathbf{V}), \\ &\langle \boldsymbol{\mu}, (\mathbf{V}_\kappa + i\eta (\tfrac{1}{2}\text{Id} + \mathbf{K}_\kappa)) (\gamma_D^- \mathbf{E}) \rangle_t \\ &\quad + \langle \boldsymbol{\mu}, (\tfrac{1}{2}\text{Id} - \mathbf{K}_\kappa - i\eta \mathbf{W}_\kappa) (\boldsymbol{\lambda}) \rangle_t = \mathbf{g}_2(\boldsymbol{\mu}), \end{aligned} \quad (1.18)$$

where the right-hand sides are given by

$$\begin{aligned} \mathbf{f}_2(\mathbf{V}) &= (\mathbf{F}, \mathbf{V})_0 - \langle \mathbf{g}_N, \gamma_D^- \mathbf{V} \rangle_t + \langle \mathbf{W}_\kappa(\mathbf{g}_D), \gamma_D^- \mathbf{V} \rangle_t, \\ \mathbf{g}_2(\boldsymbol{\mu}) &= \langle \boldsymbol{\mu}, (\mathbf{K}_\kappa - \tfrac{1}{2}\text{Id} + i\eta \mathbf{W}_\kappa) (\mathbf{g}_D) \rangle_t. \end{aligned}$$

At first sight, this variational formulation looks promising, since it shares a similar internal structure as the symmetric formulation and in addition there is hope that the additional terms might suppress internal resonances. However, due to a lack of compactness of the boundary integral operators

$$\tfrac{1}{2}\text{Id} + \mathbf{K}_\kappa : \mathbf{L}_t^2(\Gamma) \mapsto \mathbf{L}_t^2(\Gamma), \quad \mathbf{W}_\kappa : \mathbf{L}_t^2(\Gamma) \mapsto \mathbf{L}_t^2(\Gamma),$$

on nonsmooth domains, the sesquilinear form underlying the variational formulation (1.18) is in general not coercive. Unfortunately, switching to smooth domains (1.18) does not provide us with a stable variational formulation either, since $\mathbf{W}_\kappa$ is not even compact on smooth boundaries. This bars us from

applying the Fredholm alternative on either smooth or nonsmooth domains and prevents us from establishing existence and uniqueness of solutions and asymptotic quasi-optimality error estimates. Hence, a simple complex combination of Dirichlet and Neumann traces is not enough to stabilize coupled variational formulations.

The problem concerning the nonmatching Dirichlet and Neumann trace spaces and the lack of coercivity can be overcome by introducing a special trace transformation operator

$$\mathcal{T} : \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma) \times \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma) \times \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$$

defined by

$$\mathcal{T} \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\mu} \end{bmatrix} := \begin{bmatrix} \mathbf{u} + i\eta \mathbf{M}(\boldsymbol{\mu}) \\ \boldsymbol{\mu} \end{bmatrix}, \quad \eta > 0, \quad (1.19)$$

for all $\mathbf{u} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ and $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$.

The main ingredient here is a *regularizing operator*

$$\mathbf{M} : \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma),$$

which satisfies the following assumption.

Assumption 1. *We suppose that*

1. $\mathbf{M} : \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ is compact, and
2. $\operatorname{Re} \{ \langle \boldsymbol{\mu}, \mathbf{M}(\boldsymbol{\mu}) \rangle_{\mathbf{t}} \} > 0$ for all $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \setminus \{0\}$.

After a straightforward application of the trace transformation operator (1.19) to the exterior Calderón projector (1.11) the first equation changes into

$$\begin{aligned} \langle \boldsymbol{\mu}, \gamma_D^+ \mathbf{E}^s + i\eta \mathbf{M}(\gamma_N^+ \mathbf{E}^s) \rangle_{\mathbf{t}} \\ = \langle \boldsymbol{\mu}, (\tfrac{1}{2} \operatorname{Id} + \mathbf{K}_\kappa + i\eta \mathbf{M} \circ \mathbf{W}_\kappa) (\gamma_D^+ \mathbf{E}^s) \rangle_{\mathbf{t}} \\ + \langle \boldsymbol{\mu}, (i\eta \mathbf{M} \circ (\tfrac{1}{2} \operatorname{Id} - \mathbf{K}'_\kappa) - \mathbf{V}_\kappa) (\gamma_N^+ \mathbf{E}^s) \rangle_{\mathbf{t}}. \end{aligned}$$

A simple algebraic transformation yields the following variational identities for the Dirichlet and Neumann traces $\gamma_D^+ \mathbf{E}^s$ and $\gamma_N^+ \mathbf{E}^s$ (cf. [40, Sect. 6] for the Helmholtz case)

$$\begin{aligned} \langle \boldsymbol{\mu}, \gamma_D^+ \mathbf{E}^s \rangle_{\mathbf{t}} &= \langle \boldsymbol{\mu}, (\tfrac{1}{2} \operatorname{Id} + \mathbf{K}_\kappa + i\eta \mathbf{M} \circ \mathbf{W}_\kappa) (\gamma_D^+ \mathbf{E}^s) \rangle_{\mathbf{t}} \\ &\quad - \langle \boldsymbol{\mu}, (\mathbf{V}_\kappa + i\eta \mathbf{M} \circ (\tfrac{1}{2} \operatorname{Id} + \mathbf{K}'_\kappa)) (\gamma_N^+ \mathbf{E}^s) \rangle_{\mathbf{t}}, \quad (1.20) \\ \langle \gamma_N^+ \mathbf{E}^s, \mathbf{v} \rangle_{\mathbf{t}} &= \langle \mathbf{W}_\kappa (\gamma_D^+ \mathbf{E}^s), \mathbf{v} \rangle_{\mathbf{t}} + \langle (\tfrac{1}{2} \operatorname{Id} - \mathbf{K}'_\kappa) (\gamma_N^+ \mathbf{E}^s), \mathbf{v} \rangle_{\mathbf{t}}, \end{aligned}$$

for all $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ and $\mathbf{v} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$. The identity (1.20) provides an alternative realization of the Dirichlet-to-Neumann map.

For the construction of regularizing operators we strongly rely on the techniques already established for the regularization of Maxwell scattering problems (cf. [17, Sect.4]). A crucial tool in the construction of a suitable regularizing operator will be the following trace space

$$\mathbf{H}(\operatorname{curl}_\Gamma, \Gamma) := \{\boldsymbol{\mu} \in \mathbf{L}_t^2(\Gamma); \operatorname{curl}_\Gamma \boldsymbol{\mu} \in L^2(\Gamma)\} \subset \mathbf{L}_t^2(\Gamma).$$

Lemma 1.15. *The space $\mathbf{H}(\operatorname{curl}_\Gamma, \Gamma) \subset \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ is a dense subspace.*

Proof. We start from the dense inclusions $\mathbf{C}^\infty(\Omega) \subset \mathbf{H}^1(\Omega)$ and $\mathbf{H}^1(\Omega) \subset \mathbf{H}(\operatorname{curl}, \Omega)$. By definition and due to Theorem 1.3 we conclude that $\mathbf{V}_\gamma := \gamma_D(\mathbf{C}^\infty(\Omega)) \subset \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ is dense. Since the following inclusions hold $\mathbf{V}_\gamma \subset \mathbf{H}(\operatorname{curl}_\Gamma, \Gamma) \subset \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$, the statement is proved. $\square$

Lemma 1.16. *The embedding $\mathbf{H}(\operatorname{curl}_\Gamma, \Gamma) \hookrightarrow \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ is compact.*

Proof. Our is similar to the one given in [17, Lemma 2.5]. Let $\{\mathbf{u}_n\}_{n \in \mathbb{N}} \subset \mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)$ such that $\|\mathbf{u}_n\|_{\mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)} \leq 1$, for all $n \in \mathbb{N}$. The compact embedding $\mathbf{L}_t^2(\Gamma) \hookrightarrow \mathbf{H}_\perp^{-1/2}(\Gamma)$ directly implies, that there exists $\mathbf{u} \in \mathbf{H}_\perp^{-1/2}(\Gamma)$ and a subsequence $\mathbf{u}_{n_k}$ of $\mathbf{u}_n$ such that $\mathbf{u}_{n_k} \rightarrow \mathbf{u}$ strongly in $\mathbf{H}_\perp^{-1/2}(\Gamma)$.

Due to the continuity of the operator $\operatorname{curl}_\Gamma : \mathbf{H}_\perp^{-1/2}(\Gamma) \mapsto H^{-3/2}(\Gamma)$ we get $\operatorname{curl}_\Gamma \mathbf{u}_{n_k} \rightarrow \operatorname{curl}_\Gamma \mathbf{u}$ strongly in $H^{-3/2}(\Gamma)$ (see [12] for the proof and a definition of $H^{-3/2}(\Gamma)$).

On the other hand we know that $\|\operatorname{curl}_\Gamma \mathbf{u}_{n_k}\|_{L^2(\Gamma)} \leq 1$, which implies up to extraction of a subsequence $\operatorname{curl}_\Gamma \mathbf{u}_{n_k}$, is strongly converging to an element in $H^{-1/2}(\Gamma)$. By uniqueness of the limit we conclude that $\operatorname{curl}_\Gamma \mathbf{u} \in H^{-1/2}(\Gamma)$, and, up to selecting a proper subsequence $\mathbf{u}_{n_k} \rightarrow \mathbf{u} \in \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$, strongly. $\square$

A simple eligible operator $\mathbf{M}$ can be introduced through a variational definition: For any $\boldsymbol{\zeta} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$ find $\mathbf{M}(\boldsymbol{\zeta}) \in \mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)$ such that

$$\langle \mathbf{M}(\boldsymbol{\zeta}), \mathbf{q} \rangle_t + \langle \operatorname{curl}_\Gamma \mathbf{M}(\boldsymbol{\zeta}), \operatorname{curl}_\Gamma \mathbf{q} \rangle_t = \langle \boldsymbol{\zeta}, \mathbf{q} \rangle_t, \quad (1.21)$$

for all $\mathbf{q} \in \mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)$. In order to simplify notations we introduce the associated sesquilinear form

$$\mathbf{b}(\mathbf{p}, \mathbf{q}) := \langle \mathbf{p}, \mathbf{q} \rangle_t + \langle \operatorname{curl}_\Gamma \mathbf{p}, \operatorname{curl}_\Gamma \mathbf{q} \rangle_t. \quad (1.22)$$

Compactness of $\mathbf{M} : \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}^{-1/2}(\operatorname{curl}_\Gamma, \Gamma)$ immediately follows from Lemma 1.16.

Lemma 1.17. *The regularization operator $\mathbf{M} : \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma) \mapsto \mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)$ defined by (1.21) is injective and thus item (2) of Assumption 1 holds true for all $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)$.*

Proof. The proof closely follows the one given in [17, Sect. 4]. Assume that $\mathbf{M}(\boldsymbol{\zeta}) = 0$ from which we conclude that $\langle \boldsymbol{\zeta}, \mathbf{q} \rangle_{\mathbf{t}} = 0$ for all $\mathbf{q} \in \mathbf{H}(\text{curl}_\Gamma, \Gamma)$. Now choose $\boldsymbol{\eta} \in \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$ such that

$$\langle \boldsymbol{\zeta}, \boldsymbol{\eta} \rangle_{\mathbf{t}} = \|\boldsymbol{\zeta}\|_{\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)}^2$$

and since $\mathbf{H}(\text{curl}_\Gamma, \Gamma) \subset \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$ is dense, there exists a sequence $\{\boldsymbol{\eta}_k\}_{k \in \mathbb{N}} \subset \mathbf{H}(\text{curl}_\Gamma, \Gamma)$ such that $\boldsymbol{\eta}_k \rightarrow \boldsymbol{\eta}$ strongly in $\mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$. From the definition of the regularization operator we infer $0 = \langle \boldsymbol{\zeta}, \boldsymbol{\eta}_k \rangle_{\mathbf{t}}$, for all $k \in \mathbb{N}$. Thus taking the limit yields $\boldsymbol{\zeta} = 0$, which finishes the proof. $\square$

Thus we conclude that both items of Assumption 1 are satisfied and hence $\mathbf{M}$ given by the implicit definition (1.21) qualifies as a regularizing operator.

Using the abbreviation $\boldsymbol{\lambda} := \gamma_{\mathbf{N}}^+ \mathbf{E}^s \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ and the same trick as in Sect. 1.5, to couple the boundary integral equations (1.20) together with the variational problem on Ω , we finally end up with the following formulation: Find $\mathbf{E} \in \mathbf{H}(\text{curl}, \Omega)$ and $\boldsymbol{\vartheta} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ such that for all $\mathbf{V} \in \mathbf{H}(\text{curl}, \Omega)$ and $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$

$$\begin{aligned} \mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) - \langle \mathbf{W}_\kappa(\gamma_{\mathbf{D}}^- \mathbf{E}), \gamma_{\mathbf{D}}^- \mathbf{V} \rangle_{\mathbf{t}} \\ + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2} \text{Id}) (\boldsymbol{\lambda}), \gamma_{\mathbf{D}}^- \mathbf{V} \rangle_{\mathbf{t}} = \mathbf{f}_3(\mathbf{V}), \\ \langle \boldsymbol{\mu}, (\tfrac{1}{2} \text{Id} - \mathbf{K}_\kappa - i\eta \mathbf{M} \circ \mathbf{W}_\kappa) (\gamma_{\mathbf{D}}^- \mathbf{E}) \rangle_{\mathbf{t}} \\ + \langle \boldsymbol{\mu}, (\mathbf{V}_\kappa + i\eta \mathbf{M} \circ (\tfrac{1}{2} \text{Id} + \mathbf{K}'_\kappa)) (\boldsymbol{\lambda}) \rangle_{\mathbf{t}} = \mathbf{g}_3(\boldsymbol{\mu}) \end{aligned} \quad (1.23)$$

with the right-hand sides given by

$$\begin{aligned} \mathbf{f}_3(\mathbf{V}) &:= (\mathbf{F}, \mathbf{V})_0 - \langle \mathbf{g}_{\mathbf{N}}, \gamma_{\mathbf{D}}^- \mathbf{V} \rangle_{\mathbf{t}} + \langle \mathbf{W}_\kappa(\mathbf{g}_{\mathbf{D}}), \gamma_{\mathbf{D}}^- \mathbf{V} \rangle_{\mathbf{t}}, \\ \mathbf{g}_3(\boldsymbol{\mu}) &:= \langle \boldsymbol{\mu}, (\mathbf{K}_\kappa - \tfrac{1}{2} \text{Id} + i\eta \mathbf{M} \circ \mathbf{W}_\kappa) (\mathbf{g}_{\mathbf{D}}) \rangle_{\mathbf{t}}. \end{aligned}$$

Summing up, due to the compactness of the regularization operator $\mathbf{M}$ we conclude that all additional off-diagonal terms in the sesquilinear form underlying the regularized variational formulation, compared to the symmetric formulation, are compact. In combination with Theorem 1.5 this results again in a Gårding inequality on $\mathbf{V}$. It remains to establish uniqueness of solutions, which amounts to confirming that (1.23) is really immune to spurious resonances.

Lemma 1.18. *Any solution of (1.23) provides a solution of (1.1) by retaining $\mathbf{E}$ in Ω and using the representation formula (1.5) for the Cauchy data $(\gamma_{\mathbf{D}}^- \mathbf{E} + \mathbf{g}_{\mathbf{D}}, \boldsymbol{\lambda})$ in Ω^+ .*

Proof. Our approach is based on [52, Sect. 4.3] and [18, Sect. 5]. Testing with $\mathbf{V}$ that is compactly supported in Ω confirms that $\mathbf{E}$ satisfies (1.1) in Ω . We conclude (1.9) for any admissible $\mathbf{V}$. This renders (1.23) equivalent to

$$\begin{aligned}
\langle \boldsymbol{\xi}, \gamma_D^- \mathbf{V} \rangle_{\mathbf{t}} - \langle \mathbf{W}_\kappa(\mathbf{u}), \gamma_D^- \mathbf{V} \rangle_{\mathbf{t}} + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2} \text{Id}) (\boldsymbol{\lambda}), \gamma_D^- \mathbf{V} \rangle_{\mathbf{t}} &= \mathbf{0}, \\
\langle \boldsymbol{\mu}, (\tfrac{1}{2} \text{Id} - \mathbf{K}_\kappa - i\eta \mathbf{M} \circ \mathbf{W}_\kappa)(\mathbf{u}) \rangle_{\mathbf{t}} \\
- \langle \boldsymbol{\mu}, (\mathbf{V}_\kappa + i\eta \mathbf{M} \circ (\tfrac{1}{2} \text{Id} + \mathbf{K}'_\kappa)) (\boldsymbol{\lambda}) \rangle_{\mathbf{t}} &= \mathbf{0},
\end{aligned}$$

with $\boldsymbol{\xi} := \mu_r^{-1} \gamma_N^- \mathbf{E} - \mathbf{g}_N$ and $\mathbf{u} := \gamma_D^- \mathbf{E} - \mathbf{g}_D$. Translated into operator notation this yields

$$\left(\mathcal{T} \circ \begin{bmatrix} \tfrac{1}{2} \text{Id} - \mathbf{K}_\kappa & \mathbf{V}_\kappa \\ -\mathbf{W}_\kappa & \tfrac{1}{2} \text{Id} + \mathbf{K}'_\kappa \end{bmatrix} \right) \begin{bmatrix} \mathbf{u} \\ \boldsymbol{\lambda} \end{bmatrix} = \begin{bmatrix} \mathbf{0} \\ \boldsymbol{\lambda} - \boldsymbol{\xi} \end{bmatrix}, \quad (1.24)$$

where the second operator in the product we recognize as an *interior Calderón projector* [18, Sect. 3.3]. By applying the trace transformation operator (1.19) to the Dirichlet and Neumann traces of the following function

$$\mathbf{U}(\mathbf{x}) := \boldsymbol{\Psi}_{\text{SL}}^\kappa(\boldsymbol{\lambda})(\mathbf{x}) - \boldsymbol{\Psi}_{\text{DL}}^\kappa(\mathbf{u})(\mathbf{x}), \quad \mathbf{x} \in \Omega,$$

we obtain the traces

$$\gamma_D^- \mathbf{U} + i\eta \mathbf{M}(\gamma_N^- \mathbf{U}) = \mathbf{0}, \quad \gamma_N^- \mathbf{U} = \boldsymbol{\lambda} - \boldsymbol{\xi}.$$

Furthermore, since $\mathbf{U}$ is a solution to the boundary value problem

$$\mathbf{curl} \mathbf{curl} \mathbf{U} - \kappa^2 \mathbf{U} = \mathbf{0} \text{ in } \Omega, \quad \gamma_D^- \mathbf{U} + i\eta \mathbf{M}(\gamma_N^- \mathbf{U}) = \mathbf{0} \text{ on } \Gamma,$$

integration by parts together with the “test function” $\mathbf{V} := \overline{\mathbf{U}}$ yields

$$i\eta \langle \gamma_N^- \mathbf{U}, \mathbf{M}(\gamma_N^- \mathbf{U}) \rangle_{\mathbf{t}} = \langle \gamma_N^- \mathbf{U}, \gamma_D^- \mathbf{U} \rangle_{\mathbf{t}} = \int_{\Omega} |\mathbf{curl} \mathbf{U}|^2 - \kappa^2 |\mathbf{U}|^2 \, d\mathbf{x} \in \mathbb{R}.$$

Considering the imaginary part of the previous equation we finally arrive at

$$0 = \eta \operatorname{Re} \{ \langle \gamma_N^- \mathbf{U}, \mathbf{M}(\gamma_N^- \mathbf{U}) \rangle_{\mathbf{t}} \}$$

and item (2) of Assumption 1 immediately implies $\boldsymbol{\lambda} = \boldsymbol{\xi}$. From (1.24) we conclude that $(\mathbf{u}, \boldsymbol{\lambda})$ belong to the kernel of the interior Calderón projector, which implies that they represent Cauchy data of an exterior Maxwell solution. Hence, due to the following definition

$$\mathbf{W}(\mathbf{x}) := \boldsymbol{\Psi}_{\text{DL}}^\kappa(\mathbf{u})(\mathbf{x}) - \boldsymbol{\Psi}_{\text{SL}}^\kappa(\boldsymbol{\lambda})(\mathbf{x}), \quad \mathbf{x} \in \Omega^+.$$

we obtain a pair of solutions $(\mathbf{E}, \mathbf{W})$ to the Maxwell transmission problem (1.1). Finally, uniqueness of solutions to the transmission problem carries over to the variational formulation (1.23). $\square$

Eventually, existence of solutions to the variational problem (1.23) follows from their uniqueness and a Fredholm argument, see [46, Theorem 2.33].

Although (1.23) provides us with a stable variational formulation, it cannot be discretized by means of a straightforward Galerkin scheme, due to the various operator products. This suggests to introduce the auxiliary variable

$$\mathbf{p} := \mathbf{M}\left(\left(\frac{1}{2}\text{Id} + \mathbf{K}'_\kappa\right)(\boldsymbol{\lambda}) - \mathbf{W}_\kappa(\gamma_D^-\mathbf{E} + \mathbf{g}_D)\right) \in \mathbf{H}(\text{curl}_\Gamma, \Gamma), \quad (1.25)$$

which converts (1.23) into the following mixed variational formulation: Find $\mathbf{E} \in \mathbf{H}(\text{curl}, \Omega)$, $\boldsymbol{\lambda} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$, and $\mathbf{p} \in \mathbf{H}(\text{curl}_\Gamma, \Gamma)$ such that for all $\mathbf{V} \in \mathbf{H}(\text{curl}, \Omega)$, $\boldsymbol{\mu} \in \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$, and $\mathbf{q} \in \mathbf{H}(\text{curl}_\Gamma, \Gamma)$

$$\begin{aligned} & \mathbf{q}_\kappa(\mathbf{E}, \mathbf{V}) - \langle \mathbf{W}_\kappa(\gamma_D^-\mathbf{E}), \gamma_D^-\mathbf{V} \rangle_{\mathbf{t}} \\ & + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2}\text{Id})(\boldsymbol{\lambda}), \gamma_D^-\mathbf{V} \rangle_{\mathbf{t}} = \mathbf{f}_4(\mathbf{V}), \\ & \langle \boldsymbol{\mu}, (\tfrac{1}{2}\text{Id} - \mathbf{K}_\kappa)(\gamma_D^-\mathbf{E}) \rangle_{\mathbf{t}} + \langle \boldsymbol{\mu}, \mathbf{V}_\kappa(\boldsymbol{\lambda}) \rangle_{\mathbf{t}} - i\eta \langle \boldsymbol{\mu}, \mathbf{p} \rangle_{\mathbf{t}} = \mathbf{g}_4(\boldsymbol{\mu}), \\ & \langle \mathbf{W}_\kappa(\gamma_D^-\mathbf{E}), \mathbf{q} \rangle_{\mathbf{t}} - \langle (\tfrac{1}{2}\text{Id} + \mathbf{K}'_\kappa)(\boldsymbol{\lambda}), \mathbf{q} \rangle_{\mathbf{t}} + \mathbf{b}(\mathbf{p}, \mathbf{q}) = \mathbf{h}_4(\mathbf{q}), \end{aligned} \quad (1.26)$$

with right-hand sides given by

$$\begin{aligned} \mathbf{f}_4(\mathbf{V}) &:= (\mathbf{F}, \mathbf{V})_0 - \langle \mathbf{g}_N, \gamma_D^-\mathbf{V} \rangle_{\mathbf{t}} + \langle \mathbf{W}_\kappa(\mathbf{g}_D), \gamma_D^-\mathbf{V} \rangle_{\mathbf{t}}, \\ \mathbf{g}_4(\boldsymbol{\mu}) &:= \langle \boldsymbol{\mu}, (\mathbf{K}_\kappa - \tfrac{1}{2}\text{Id})(\mathbf{g}_D) \rangle_{\mathbf{t}}, \\ \mathbf{h}_4(\mathbf{q}) &:= -\langle \mathbf{W}_\kappa(\mathbf{g}_D), \mathbf{q} \rangle_{\mathbf{t}}. \end{aligned}$$

An essential feature of the stabilized variational formulation is that the auxiliary unknown $\mathbf{p}$ obtained from the solutions $(\mathbf{E}, \boldsymbol{\lambda}, \mathbf{p})$ to the mixed variational formulation (1.26) can be recast into the following expression

$$\mathbf{p} = \mathbf{M}\left(\left(\tfrac{1}{2}\text{Id} + \mathbf{K}'_\kappa\right)(\boldsymbol{\lambda}) - \mathbf{W}_\kappa(\gamma_D^-\mathbf{E} + \mathbf{g}_D)\right).$$

At second glance, we realize that $\mathbf{p} = \mathbf{0}$, if $(\mathbf{E}, \boldsymbol{\vartheta})$ solves (1.26). This follows directly from Lemma 1.18 and (1.11). Summing up, $\mathbf{p}$ is a “dummy variable.”

Again using the splittings from Sect. 1.4 and grouping the components into electric $(\boldsymbol{\lambda}^\perp, \mathbf{E}^0)$, magnetic $(\boldsymbol{\lambda}^0, \mathbf{E}^\perp)$, and auxiliary ones $\mathbf{p}$ we arrive at a variational formulation on the Hilbert space

$$\mathcal{W} := \mathcal{V} \times \mathbf{H}(\text{curl}_\Gamma, \Gamma),$$

that is endowed with the natural graph norm: Find $(\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp, \mathbf{p}) \in \mathcal{W}$ such that

$$\begin{aligned} & \widehat{\mathbf{a}}_\kappa^{\text{reg}}\left((\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp, \mathbf{p}), (\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp, \mathbf{q})\right) \\ & = \widehat{\mathbf{f}}_\kappa^{\text{reg}}\left(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp, \mathbf{q}\right), \end{aligned} \quad (1.27)$$

for all $(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp, \mathbf{q}) \in \mathcal{W}$. Again, the sesquilinear form and the linear form of the split variational equation are related to those underlying (1.26), namely $\mathbf{a}_\kappa^{\text{reg}}$ and $\mathbf{f}_\kappa^{\text{reg}}$, through the following equations:

$$\begin{aligned} \widehat{\mathbf{a}}_\kappa^{\text{reg}}\left((\boldsymbol{\lambda}^\perp, \mathbf{E}^0, \boldsymbol{\lambda}^0, \mathbf{E}^\perp, \mathbf{p}), (\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp, \mathbf{q})\right) \\ := \mathbf{a}_\kappa^{\text{reg}}\left((\mathbf{E}^\perp + \mathbf{E}^0, \boldsymbol{\lambda}^\perp + \boldsymbol{\lambda}^0, \mathbf{p}), (\mathbf{V}^\perp - \mathbf{V}^0, -\boldsymbol{\mu}^\perp + \boldsymbol{\mu}^0, \mathbf{q})\right), \\ \widehat{\mathbf{f}}_\kappa^{\text{reg}}\left(\boldsymbol{\mu}^\perp, \mathbf{V}^0, \boldsymbol{\mu}^0, \mathbf{V}^\perp, \mathbf{q}\right) := \mathbf{f}_\kappa^{\text{reg}}\left(\mathbf{V}^\perp - \mathbf{V}^0, -\boldsymbol{\mu}^\perp + \boldsymbol{\mu}^0, \mathbf{q}\right). \end{aligned}$$

In order to settle the issue of existence and uniqueness of solutions of (1.26) we first observe that by the very definition of $\mathbf{M}$ in (1.21) and (1.25) the first two components of $(\mathbf{U}, \boldsymbol{\lambda}, \mathbf{p})$ of (1.26) will also solve (1.23) and thus Lemma 1.18 ensures uniqueness.

The next lemma tells us that we do not need to worry about the new terms introduced into the variational equations.

Lemma 1.19. *The following sesquilinear forms are compact*

$$\begin{aligned} \langle \cdot, \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma) &\mapsto \mathbb{C}, \\ \langle \mathbf{W}_\kappa(\cdot), \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma) &\mapsto \mathbb{C}, \\ \langle (\tfrac{1}{2}\text{Id} + \mathbf{K}'_\kappa)(\cdot), \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma) &\mapsto \mathbb{C}. \end{aligned}$$

Proof. It is sufficient to note that the sesquilinear forms

$$\langle \cdot, \cdot \rangle_{\mathbf{t}}, \langle (\tfrac{1}{2}\text{Id} + \mathbf{K}'_\kappa)(\cdot), \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \times \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbb{C}$$

and

$$\langle \mathbf{W}_\kappa(\cdot), \cdot \rangle_{\mathbf{t}} : \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \times \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbb{C}$$

are continuous and that the injection $\mathbf{H}(\text{curl}_\Gamma, \Gamma) \hookrightarrow \mathbf{H}^{-1/2}(\text{curl}_\Gamma, \Gamma)$ is compact due to Lemma 1.16. $\square$

As an immediate consequence of this result we note that all additional off-diagonal terms of (1.26) are compact. Furthermore, the sesquilinear form

$$\mathbf{b}(\cdot, \cdot) : \mathbf{H}(\text{curl}_\Gamma, \Gamma) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma) \mapsto \mathbb{C}$$

is clearly elliptic, since it gives rise to an inner product on $\mathbf{H}(\text{curl}_\Gamma, \Gamma)$. In combination with Theorem 1.5 we conclude that the sesquilinear form $\widehat{\mathbf{a}}_\kappa^{\text{reg}} : \mathcal{W} \times \mathcal{W} \mapsto \mathbb{C}$ from (1.27) satisfies a Gårding inequality on the Hilbert space $\mathcal{W}$.

Again, a Fredholm argument ensures existence of solutions from the uniqueness result. Thus we have obtained a well-posed variational formulation which yields weak solutions to the transmission problem and is amenable to standard Galerkin discretizations.

1.7 Galerkin Discretization

We equip (the curvilinear polyhedron) Ω with a family of tetrahedral, shape regular triangulations $\{\Omega_h\}_h$. The parameter h designates the mesh width, that is the length of the longest edge. Let $\mathbb{H}$ stand for the collection of mesh widths occurring in $\{\Omega_h\}_h$ and, moreover, assume that $\mathbb{H} \subset \mathbb{R}_+$ forms a decreasing series tending to zero. The set $\mathcal{T}_h$ will include all tetrahedra of Ω_h . Restricting Ω_h , $h \in \mathbb{H}$, to Γ gives a sequence $\{\Gamma_h\}_h$ of surface meshes. They inherit shape regularity from $\{\Omega_h\}_h$. We suppose that all Γ_h are aligned with edges of Γ .

Discrete electric fields should be modeled by discrete 1-forms (edge elements). They can be represented by piecewise polynomial vector fields: For a *fixed* degree ν , $\nu \in \mathbb{N}_0$, and any tetrahedron $T \in \mathcal{T}_h$ the local spaces are given by (cf. [48])

$$\mathcal{E}_{\nu+1}^1(T) := \left\{ \mathbf{V} \in (\mathcal{P}_{\nu+1}(T))^3; \mathbf{V}(\mathbf{x}) \cdot \mathbf{x} = 0 \ \forall \mathbf{x} \in T \right\},$$

where $\mathcal{P}_{\nu+1}(T)$ is the space of multivariate polynomials of total degree ν on T . This gives rise to the global finite element space

$$\mathcal{E}_{\nu+1}^1(\Omega_h) := \left\{ \mathbf{U} \in \mathbf{H}(\mathbf{curl}, \Omega); \mathbf{U}|_T \in \mathcal{E}_{\nu+1}^1(T) \ \forall T \in \Omega_h \right\}.$$

This renders degrees of freedom based on moments (of tangential components) on edges, faces, and the elements themselves well defined. See [37] and [24] for details and proof of unisolvence. The discrete 1-forms on $\{\Omega_h\}_h$ form an affine family of finite elements in the sense of [23] with respect to the pullback of 1-forms. Based on the degrees of freedom, we can introduce nodal interpolation operators $\Pi_{\nu+1}^1$ onto $\mathcal{E}_{\nu+1}^1(\Omega_h)$. To begin with they are defined only for continuous vector fields but can be generalized to less regular settings

Lemma 1.20. *If $s > \frac{1}{2}$, then for all $\mathbf{U} \in \mathbf{H}^s(\Omega)$ such that $\mathbf{curl} \mathbf{U} \in \mathbf{H}^s(\Omega)$*

$$\begin{aligned} \|\mathbf{U} - \Pi_{\nu+1}^1(\mathbf{U})\|_{\mathbf{L}^2(\Omega)} &\leq Ch^{\min\{\nu+1, s\}} \left(\|\mathbf{U}\|_{\mathbf{H}^s(\Omega)} + \|\mathbf{curl} \mathbf{U}\|_{\mathbf{H}^s(\Omega)} \right), \\ \|\mathbf{curl}(\mathbf{U} - \Pi_{\nu+1}^1(\mathbf{U}))\|_{\mathbf{L}^2(\Omega)} &\leq Ch^{\min\{\nu+1, s\}} \|\mathbf{curl} \mathbf{U}\|_{\mathbf{H}^s(\Omega)}, \end{aligned}$$

with constants $C > 0$ depending only on Ω , ν , s and the shape-regularity of the meshes.

Proof. For a proof see [24, Lemmas 3.2 and 3.3]. $\square$

The reason why we want to use the nodal interpolation operator $\Pi_{\nu+1}^1$, although it fails to be defined on the entire space $\mathbf{H}(\mathbf{curl}, \Omega)$, is its exceptional algebraic properties. In order to explain them, we need to introduce the $\mathbf{H}(\mathbf{div}, \Omega)$ -conforming spaces $\mathcal{F}_\nu(\Omega_h)$ of discrete 2-forms, also known as face elements, cf. [8, Chap. 3] and [48]. Suitable degrees of freedom for this space are provided by moments of face fluxes and weighted integrals over

elements. They introduce the nodal interpolation operators Π_ν^2 onto $\mathcal{F}_\nu(\Omega_h)$. A straightforward application of the Stokes theorem, cf. [37], confirms the following *commuting diagram property*

$$\mathbf{curl} \circ \Pi_{\nu+1}^1 = \Pi_\nu^2 \circ \mathbf{curl}, \quad (1.28)$$

which is valid for all vector fields contained in the domain $\text{Dom}(\Pi_{\nu+1}^1)$ of $\Pi_{\nu+1}^1$. From relation (1.28) we conclude that $\Pi_{\nu+1}^1$ leaves the kernel of the $\mathbf{curl}$ invariant.

To pick a suitable discrete trial space for $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ we also adopt the perspective of differential forms. Be aware that $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ is the trace space for magnetic fields, and keep in mind that those can also be described by 1-forms. This suggests that $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ should be approximated by traces of discrete 1-forms on the surface. In other words, as $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ -conforming boundary element space we chose $\gamma_\times \mathcal{E}_{\nu+1}^1(\Omega_h)$. Elementary computations reveal that this generates exactly the two-dimensional face elements $\mathcal{F}_\nu(\Gamma_h)$ on the surface mesh, see [50]. The degrees of freedom are also inherited from $\mathcal{E}_{\nu+1}^1(\Omega_h)$. By construction, the induced nodal interpolation operator Φ_ν^2 satisfies

$$\Phi_\nu^2 \circ \gamma_\times = \gamma_\times \circ \Pi_{\nu+1}^1,$$

which, due to (1.28), implies another commuting diagram property,

$$\text{div}_\Gamma \circ \Phi_\nu^2 = Q_\nu^\Gamma \circ \text{div}_\Gamma,$$

for sufficiently smooth tangential surface vector fields. Here, Q_ν^Γ is the plain $L^2(\Gamma)$ -orthogonal projection onto the space $\mathcal{Q}_\nu(\Gamma_h)$ of discontinuous, piecewise polynomials of degree ν on Γ_h . Invariance of $\text{Ker}(\text{div}_\Gamma) \cap \text{Dom}(\Phi_\nu^2)$ under Φ_ν^2 is immediate.

From the results of [50] and [41, Sect. 5] we obtain the following interpolation error estimates.

Lemma 1.21. *If $\mu \in \mathbf{H}_t^s(\Gamma)$, $\text{div}_\Gamma \mu \in H^s(\Gamma)$ for some $s > 0$, then*

$$\begin{aligned} \|\mu - \Phi_\nu^2(\mu)\|_{L^2(\Gamma)} &\leq Ch^{\min\{s, \nu+1\}} \left(|\mu|_{\mathbf{H}_t^s(\Gamma)} + |\text{div}_\Gamma \mu|_{H^s(\Gamma)} \right), \\ \|\text{div}_\Gamma (\mu - \Phi_\nu^2(\mu))\|_{L^2(\Gamma)} &\leq Ch^{\min\{s, \nu+1\}} |\text{div}_\Gamma \mu|_{H^s(\Gamma)}. \end{aligned}$$

Finally, it remains to choose a suitable conforming discrete trial space for $\mathbf{H}(\text{curl}_\Gamma, \Gamma)$. Picking an arbitrary function $\mathbf{u}_h$ from a such trial space, it must feature $\mathbf{q}_h \in \mathbf{L}_t^2(\Gamma)$, as well as $\text{curl}_\Gamma \mathbf{q}_h \in L^2(\Gamma)$. Thus a suitable choice would be to take $\gamma_t \mathcal{E}_1^1(\Omega_h)$, which creates exactly the space of $\mathbf{H}(\text{curl}_\Gamma, \Gamma)$ -conforming surface edge elements $\mathcal{E}_1^1(\Gamma_h)$. The degrees of freedom are again inherited from $\mathcal{E}_1^1(\Omega_h)$. For sufficiently smooth vector fields, the induced nodal interpolation operator Φ_1^1 satisfies the following commuting diagram property

$$\text{curl}_\Gamma \circ \Phi_1^1 = Q_0^\Gamma \circ \text{curl}_\Gamma.$$

Again, we conclude invariance of $\text{Ker}(\text{curl}_\Gamma) \cap \text{Dom}(\Phi_1^1)$ under Φ_1^1 .

Lemma 1.22. *If $\mathbf{q} \in \mathbf{H}_{\mathbf{t}}^s(\Gamma)$, $\operatorname{curl}_\Gamma \mathbf{q} \in H^s(\Gamma)$ for some $0 < s \leq 1$, then*

$$\begin{aligned} \|\mathbf{q} - \Phi_1^1(\mathbf{q})\|_{L^2(\Gamma)} &\leq Ch^s \left(\|\mathbf{q}\|_{\mathbf{H}_{\mathbf{t}}^s(\Gamma)} + |\operatorname{curl}_\Gamma \mathbf{q}|_{H^s(\Gamma)} \right), \\ \|\operatorname{curl}_\Gamma (\mathbf{q} - \Phi_1^1(\mathbf{q}))\|_{L^2(\Gamma)} &\leq Ch^s |\operatorname{curl}_\Gamma \mathbf{q}|_{H^s(\Gamma)}. \end{aligned}$$

Based on the conforming finite element spaces, the Galerkin discretization of the variational problems (1.26) is straightforward: Find $\mathbf{E}_h \in \mathcal{E}_{\nu+1}^1(\Omega_h)$, $\boldsymbol{\vartheta}_h \in \mathcal{F}_\nu(\Gamma_h)$, and $\mathbf{p}_h \in \mathcal{E}_1^1(\Gamma_h)$ such that for all $\mathbf{V}_h \in \mathcal{E}_{\nu+1}^1(\Omega_h)$, $\boldsymbol{\mu}_h \in \mathcal{F}_\nu(\Gamma_h)$, and $\mathbf{q}_h \in \mathcal{E}_1^1(\Gamma_h)$

$$\begin{aligned} &\mathbf{q}_\kappa(\mathbf{E}_h, \mathbf{V}_h) - \langle \mathbf{W}_\kappa(\gamma_D^- \mathbf{E}_h), \gamma_D^- \mathbf{V}_h \rangle_{\mathbf{t}} \\ &\quad + \langle (\mathbf{K}'_\kappa - \tfrac{1}{2} \operatorname{Id}) (\boldsymbol{\lambda}_h), \gamma_D^- \mathbf{V}_h \rangle_{\mathbf{t}} = \mathbf{f}_4(\mathbf{V}_h), \\ &\langle \boldsymbol{\mu}_h, (\tfrac{1}{2} \operatorname{Id} - \mathbf{K}_\kappa) (\gamma_D^- \mathbf{E}_h) \rangle_{\mathbf{t}} \\ &\quad + \langle \boldsymbol{\mu}_h, \mathbf{V}_\kappa(\boldsymbol{\lambda}_h) \rangle_{\mathbf{t}} + i\eta \langle \boldsymbol{\mu}_h, \mathbf{p}_h \rangle_{\mathbf{t}} = \mathbf{g}_4(\boldsymbol{\mu}_h), \\ &\langle \mathbf{W}_\kappa(\gamma_D^- \mathbf{E}_h), \mathbf{q}_h \rangle_{\mathbf{t}} - \langle (\tfrac{1}{2} \operatorname{Id} + \mathbf{K}'_\kappa) (\boldsymbol{\lambda}_h), \mathbf{q}_h \rangle_{\mathbf{t}} + \mathbf{b}(\mathbf{p}, \mathbf{q}_h) = \mathbf{h}_4(\mathbf{q}_h). \end{aligned} \tag{1.29}$$

Remark 1. Why do we have to worry about approximating the auxiliary variable $\mathbf{p}$ at all, though it vanishes and apparently the choice of boundary elements does not affect the convergence of Galerkin solutions? The reason is that the convergence of discrete solutions hinges on sufficiently good approximation properties of the underlying finite element and boundary element spaces. Hence the use of lowest order boundary elements is sufficient to ensure optimal convergence rates for the discretization error.

1.8 Discrete Decompositions

The splitting idea, which was used to prove coercivity on the continuous level, has to be adopted for an analysis on the discrete level as well. We follow a simple guideline, which boils down to applying nodal interpolation operators to the Helmholtz-type splittings in Sect. 1.4.

First we construct a discrete counterpart of $\mathbf{X}(\operatorname{curl}, \Omega)$. We strongly rely on the projector already introduced in Sect. 1.4. According to the recipe outlined above, it is formally defined as $\mathbf{P}_h := \boldsymbol{\Pi}_{\nu+1}^1 \circ \mathbf{P}$. However, even on $\mathbf{P}(\mathbf{H}(\operatorname{curl}, \Omega))$ the nodal interpolation operator $\boldsymbol{\Pi}_{\nu+1}^1$ fails to be bounded, because the smoothness of the curl is not controlled. Nonetheless, we aim to apply $\mathbf{P}_h$ to finite element functions only, the following lemma saves the idea.

Lemma 1.23. *If $\mathbf{U} \in H^s(\Omega)$ and $\operatorname{curl} \mathbf{U} \in \mathcal{F}_\nu(\Omega_h)$, for some $s \geq 1$, then $\mathbf{U} \in \operatorname{Dom}(\boldsymbol{\Pi}_{\nu+1}^1)$ and*

$$\|\mathbf{U} - \boldsymbol{\Pi}_{\nu+1}^1(\mathbf{U})\|_{L^2(\Omega)} \leq Ch^{\min\{\nu+1, s\}} |\mathbf{U}|_{H^s(\Omega)},$$

with $C > 0$ depending only on Ω , ν , and the shape regularity of Ω_h .

Proof. For a proof see [42, Lemma 2.1]. $\square$

Due to the commuting diagram property (1.28) and Lemma 1.12, we conclude that $\mathbf{curl} \mathbf{P}(\mathbf{U}_h) \in \mathcal{F}_\nu(\Omega_h)$ for $\mathbf{U}_h \in \mathcal{E}_{\nu+1}^1(\Omega_h)$.

Lemma 1.24. *The operator $\mathbf{P}_h : \mathcal{E}_{\nu+1}^1(\Omega_h) \mapsto \mathcal{E}_{\nu+1}^1(\Omega_h)$ is a h -uniformly continuous projection and preserves the $\mathbf{curl}$, and $\text{Ker}(\mathbf{P}_h) = \text{Ker}(\mathbf{curl}) \cap \mathcal{E}_{\nu+1}^1(\Omega_h)$.*

Thus by defining

$$\begin{aligned} \mathbf{X}_h(\mathbf{curl}, \Omega_h) &:= \mathbf{P}_h(\mathcal{E}_{\nu+1}^1(\Omega_h)), \\ \mathbf{N}_h(\mathbf{curl}, \Omega_h) &:= \text{Ker}(\mathbf{curl}) \cap \mathcal{E}_{\nu+1}^1(\Omega_h), \end{aligned}$$

we instantly get a h -uniformly $\mathbf{H}(\mathbf{curl}, \Omega)$ -stable direct splitting

$$\mathcal{E}_{\nu+1}^1(\Omega_h) = \mathbf{X}_h(\mathbf{curl}, \Omega_h) \oplus \mathbf{N}_h(\mathbf{curl}, \Omega_h).$$

The following result makes it possible to pursue the same strategy in the case of the face elements space $\mathcal{F}_\nu(\Gamma_h)$, cf. [41, Lemma 6.2].

Lemma 1.25. *If $\boldsymbol{\mu} \in \mathbf{H}_t^s(\Gamma)$ and $\text{div}_\Gamma \boldsymbol{\mu} \in \mathcal{Q}_\nu(\Gamma_h)$, for some $s \geq \frac{1}{2}$, then $\boldsymbol{\mu} \in \text{Dom}(\boldsymbol{\Phi}_\nu^2)$ and*

$$\|\boldsymbol{\mu} - \boldsymbol{\Phi}_\nu^2(\boldsymbol{\mu})\|_{L^2(\Gamma)} \leq Ch^{\min\{\nu+1, s\}} \|\boldsymbol{\mu}\|_{\mathbf{H}_t^s(\Gamma)},$$

with $C > 0$ only depending on Γ , ν , s , and the shape-regularity of the meshes.

Thus, we can define the operator

$$\mathbf{P}_h^\Gamma : \mathcal{F}_\nu(\Gamma_h) \mapsto \mathcal{F}_\nu(\Gamma_h), \quad \mathbf{P}_h^\Gamma := \boldsymbol{\Phi}_\nu^2 \circ \mathbf{P}^\Gamma,$$

and obtain properties similar to those of $\mathbf{P}_h : \mathcal{E}_{\nu+1}^1(\Omega_h) \mapsto \mathcal{E}_{\nu+1}^1(\Omega_h)$.

Lemma 1.26. *The mapping $\mathbf{P}_h^\Gamma : \mathcal{F}_\nu(\Gamma_h) \mapsto \mathcal{F}_\nu(\Gamma_h)$ is a h -uniformly continuous projector, which preserves div_Γ and fulfills $\text{Ker}(\mathbf{P}_h^\Gamma) = \text{Ker}(\text{div}_\Gamma) \cap \mathcal{F}_\nu(\Gamma_h)$.*

The projector $\mathbf{P}_h^\Gamma$ furnishes the desired h -uniformly $\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)$ -stable splitting of the discrete Neumann trace space

$$\mathcal{F}_\nu(\Gamma_h) = \mathbf{X}_h(\text{div}_\Gamma, \Gamma_h) \oplus \mathbf{N}_h(\text{div}_\Gamma, \Gamma_h),$$

with

$$\mathbf{X}_h(\text{div}_\Gamma, \Gamma_h) := \mathbf{P}_h^\Gamma(\mathcal{F}_\nu(\Gamma_h)), \quad \mathbf{N}_h(\text{div}_\Gamma, \Gamma_h) := \text{Ker}(\text{div}_\Gamma) \cap \mathcal{F}_\nu(\Gamma_h).$$

Notice that vector fields in $\mathcal{E}_{\nu+1}^1(\Omega_h)$ are by no means continuous across inter element faces. On the other hand, any vector field in $\mathbf{H}^1(\Omega)$ must possess

continuous components. Furthermore, there are elements in $\mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h)$ that are not twisted tangential traces of continuous vector fields. In short,

$$\begin{aligned}\mathbf{X}_h(\operatorname{curl}, \Omega_h) &\not\subset \mathbf{X}(\operatorname{curl}, \Omega), \quad \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h) \not\subset \mathbf{X}(\operatorname{div}_\Gamma, \Gamma), \\ \mathbf{N}_h(\operatorname{curl}, \Omega_h) &\subset \mathbf{N}(\operatorname{curl}, \Omega), \quad \mathbf{N}_h(\operatorname{div}_\Gamma, \Gamma_h) \subset \mathbf{N}(\operatorname{div}_\Gamma, \Gamma).\end{aligned}$$

Thus by choosing

$$\begin{aligned}\mathcal{W}_h &:= \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h) \times \mathbf{N}_h(\operatorname{curl}, \Omega_h) \\ &\quad \times \mathbf{N}_h(\operatorname{div}_\Gamma, \Gamma_h) \times \mathbf{X}_h(\operatorname{curl}, \Omega_h) \times \mathcal{E}_1^1(\Gamma_h),\end{aligned}$$

as a discrete approximation space for $\mathcal{W}$, we have made a *nonconforming* choice, since $\mathcal{W}_h \not\subset \mathcal{W}$. Note that this is a special type of nonconformity, since it does not arise from the choice of discrete spaces, but from the way they are split. However, the Gårding inequality for $\widehat{\mathbf{a}}_\kappa^{\operatorname{reg}}$ was only established with respect to the split space $\mathcal{W}$. This prevents us from applying the well-known results about convergence of conforming Galerkin discretizations of coercive variational problems [51].

1.9 Discrete Inf–Sup Estimates

We start by recalling the main results of the abstract convergence theory from [18, Sect. 4.1] (see also [10, 11, 22]).

Let W be a Hilbert space with an W -stable decomposition $W = X \oplus N$, such that for any $w \in W$ we have uniquely determined $u \in X$, $v \in N$ with $w = u + v$ and

$$C^{-1} \|w\|_W \leq \|u\|_W + \|v\|_W \leq C \|w\|_W.$$

Based on the splitting we can define the isomorphism $\mathbf{X} : W \mapsto W$ by $\mathbf{X}(w) := \overline{u - v}$.

Assumption 2. *Consider a sequence of closed subspaces $W_h \subset W$ with decompositions $W_h = X_h \oplus N_h$, satisfying the following assumptions:*

1. *The family W_h is approximating in W , i.e.,*

$$\lim_{h \rightarrow 0} \inf_{w_h \in W_h} \|w - w_h\|_W = 0.$$

2. *W_h satisfies a gap property, i.e., there exist two subsets X_h, N_h of W_h such that*

$$\delta_h := \max \{ \delta(X, X_h), \delta(N, N_h) \} \rightarrow 0, \quad \text{as } h \rightarrow 0,$$

where

$$\delta(X, X_h) := \sup_{u_h \in X_h} \inf_{u \in X} \frac{\|u_h - u\|_W}{\|u_h\|_W},$$

$$\delta(N, N_h) := \sup_{v_h \in N_h} \inf_{v \in N} \frac{\|v_h - v\|_W}{\|v_h\|_W}.$$

Remark 2. In the particular case in which $N_h \subset N$, we have of course $\delta(N_h, N) = 0$. This means that the condition $\delta(W, W_h) \rightarrow 0$ for $h \rightarrow 0$ implies that N_h is approximating in N , i.e.,

$$\lim_{h \rightarrow 0} \inf_{v_h \in N_h} \|v - v_h\|_W = 0.$$

The following theorem provides us with a discrete inf-sup estimate on the conforming, discrete trial space, cf. [18, Theorem 4.1] and [10, Theorem 3.7].

Theorem 1.6. *Assume that $\mathbf{A} : W \mapsto W^*$ is continuous and that there exists a compact operator $\mathbf{T} : W \mapsto W^*$ and a constants $\alpha > 0$ such that for all $w \in W$*

$$\operatorname{Re} \{ \langle (\mathbf{A} + \mathbf{T})(w), \mathbf{X}(w) \rangle \} \geq \alpha \|w\|_W^2,$$

where $\langle \cdot, \cdot \rangle$ denotes the duality pairing between W^* and W . Assume further that $\mathbf{A}$ is one-to-one and let $\{W_h\}_h$ denote a sequence of subspaces of W satisfying Assumption 2.

Then there exists $h_0 > 0$ such that for all $h < h_0$ the following inf-sup estimate holds

$$\sup_{v_h \in W_h} \frac{|\langle A(w_h), v_h \rangle|}{\|v_h\|} \geq \frac{\alpha}{2} \|w_h\|_X \quad \text{for all } w_h \in W_h. \quad (1.30)$$

It is well known that the discrete inf-sup condition implies that the discrete Galerkin equation

$$\langle A(w_h), v_h \rangle = \langle f, v_h \rangle \quad \text{for all } v_h \in W_h,$$

has unique solutions for all right-hand sides $f \in W^*$ and that the discretization error is quasi-optimal, in the sense that there exists a constant $C > 0$ such that

$$\|w - w_h\|_W \leq C \inf_{v_h \in W_h} \|w - v_h\|_W,$$

where $w \in W$ satisfies $A(w) = f$.

Remark 3. The approximation and the gap property of Assumption 2 of the family of subspaces $W_h \subset W$ are equivalent to the existence of two bounded, linear operators, namely an *interpolation operator* $\Pi_h : W \mapsto W_h$, and a *bridge mapping* $B_h : W_h \mapsto W$, which satisfy

$$\forall w \in W : \|w - \Pi_h(w)\|_W \rightarrow 0, \quad \|\text{Id} - \mathbf{B}_h\| \rightarrow 0, \quad (1.31)$$

as $h \rightarrow 0$, see [18, Sect. 4.1] and [39, Sect. 11]. Provided we have two such operators on hand, then the following two estimates are straightforward

$$\begin{aligned} \inf_{w_h \in W_h} \|w - w_h\|_W &\leq C \|w - \Pi_h(w)\|_W \rightarrow 0, \\ \delta(W, W_h) &:= \sup_{w_h \in W_h} \inf_{w \in W} \frac{\|w_h - w\|_W}{\|w_h\|_W} \leq C \sup_{w_h \in W_h} \frac{\|w_h - \mathbf{B}_h(w_h)\|_W}{\|w_h\|_W} \rightarrow 0, \end{aligned}$$

as $h \rightarrow 0$. Thus, item (1) and (2) of Assumption 2 hold. In a finite element/boundary element framework the existence of an interpolation estimate is straightforward, since interpolation error estimates are well established.

We return to particular setting of the coupled variational formulation and start by splitting the continuous trial space $\mathbf{W} = \mathbf{X} \oplus \mathbf{N}$ into the following components

$$\begin{aligned} \mathbf{X} &:= \mathbf{X}(\text{div}_\Gamma, \Gamma) \times \{\mathbf{0}\} \times \{\mathbf{0}\} \times \mathbf{X}(\text{curl}, \Omega) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma), \\ \mathbf{N} &:= \{\mathbf{0}\} \times \mathbf{N}(\text{curl}, \Omega) \times \mathbf{N}(\text{div}_\Gamma, \Gamma) \times \{\mathbf{0}\} \times \{\mathbf{0}\}, \end{aligned}$$

and note that the discrete trial $\mathbf{W}_h$ space is approximating in $\mathbf{W}$ due to Lemmas 1.20, 1.21 and 1.22. Thus item (1) of Assumption 2 holds true.

Furthermore, we split the discrete trial space $\mathbf{W}_h = \mathbf{X}_h \oplus \mathbf{N}_h$ according to

$$\begin{aligned} \mathbf{X}_h &:= \mathbf{X}_h(\text{div}_\Gamma, \Gamma_h) \times \{\mathbf{0}\} \times \{\mathbf{0}\} \times \mathbf{X}_h(\text{curl}, \Omega_h) \times \mathcal{E}_1^1(\Gamma_h), \\ \mathbf{N}_h &:= \{\mathbf{0}\} \times \mathbf{N}_h(\text{curl}, \Omega_h) \times \mathbf{N}_h(\text{div}_\Gamma, \Gamma_h) \times \{\mathbf{0}\} \times \{\mathbf{0}\}, \end{aligned}$$

into a nonconforming component $\mathbf{X}_h \not\subset \mathbf{X}$ and a conforming component $\mathbf{N}_h \subset \mathbf{N}$, for which $\delta(\mathbf{N}, \mathbf{N}_h) = 0$ holds. According to Remark 3, we can rely on a suitable bridge mapping to establish the gap property (2) of Assumption 2. A suitable operator can be constructed in a component-wise fashion on the discrete trial spaces $\mathbf{X}_h(\text{curl}, \Omega_h)$ and $\mathbf{X}_h(\text{div}_\Gamma, \Gamma_h)$, see [39, Sect. 11].

First, we define the bridge mapping $\mathbf{B}_\Omega : \mathbf{X}_h(\text{curl}, \Omega_h) \mapsto \mathbf{X}(\text{curl}, \Omega)$ by $\mathbf{B}_\Omega(\mathbf{U}_h) := \mathbf{P}(\mathbf{U}_h)$, $\mathbf{U}_h \in \mathbf{X}_h(\text{curl}, \Omega_h)$. The projection properties from Lemmas 1.24 and 1.12 yields

$$(\Pi_{\nu+1}^1 \circ \mathbf{B}_\Omega)(\mathbf{U}_h) = \mathbf{U}_h, \quad \text{curl } \mathbf{B}_\Omega(\mathbf{U}_h) = \text{curl } \mathbf{U}_h \in \mathcal{F}_\nu(\Omega_h),$$

for all $\mathbf{U}_h \in \mathbf{X}_h(\text{curl}, \Omega_h)$. Thus, Lemma 1.23 permits us to estimate

$$\begin{aligned} \|\mathbf{U}_h - \mathbf{B}_\Omega(\mathbf{U}_h)\|_{L^2(\Omega)} &= \|(\Pi_{\nu+1}^1 - \text{Id}) \circ \mathbf{B}_\Omega(\mathbf{U}_h)\|_{L^2(\Omega)} \\ &\leq Ch \|\mathbf{B}_\Omega(\mathbf{U}_h)\|_{H^1(\Omega)} \\ &\leq Ch \|\text{curl } \mathbf{U}_h\|_{L^2(\Omega)}, \end{aligned} \quad (1.32)$$

where the constant $C > 0$ only depends on Ω , ν , and the shape regularity of Ω_h .

The same construction can also be used for $\mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h)$. We introduce the bridge mapping $\mathbf{B}_\Gamma : \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h) \mapsto \mathbf{X}(\operatorname{div}_\Gamma, \Gamma)$ by $\mathbf{B}_\Gamma(\boldsymbol{\mu}_h) := \mathbf{P}_h^\Gamma(\boldsymbol{\mu}_h)$, $\boldsymbol{\mu}_h \in \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h)$. As above, using the Lemmas 1.26 and 1.13, we obtain

$$(\boldsymbol{\Phi}_\nu^2 \circ \mathbf{B}_\Gamma)(\boldsymbol{\mu}_h) = \boldsymbol{\mu}_h, \quad \operatorname{div}_\Gamma \mathbf{B}_\Gamma(\boldsymbol{\mu}_h) = \operatorname{div}_\Gamma \boldsymbol{\mu}_h \in \mathcal{Q}_\nu(\Gamma_h),$$

for all $\boldsymbol{\mu}_h \in \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h)$. A straightforward application of Lemma 1.25 yields the following estimate

$$\begin{aligned} \|\boldsymbol{\mu}_h - \mathbf{B}_\Gamma(\boldsymbol{\mu}_h)\|_{L^2(\Gamma)} &= \|((\boldsymbol{\Phi}_\nu^2 - \operatorname{Id}) \circ \mathbf{B}_\Gamma)(\boldsymbol{\mu}_h)\|_{L^2(\Gamma)} \\ &\leq Ch^{1/2} \|\mathbf{B}_\Gamma(\boldsymbol{\mu}_h)\|_{\mathbf{H}_\perp^{1/2}(\Gamma)} \\ &\leq Ch^{1/2} \|\operatorname{div}_\Gamma \boldsymbol{\mu}_h\|_{H^{-1/2}(\Gamma)} \end{aligned} \quad (1.33)$$

with $C > 0$ depending only on Γ , ν and the shape regularity of the meshes. Thus we define the bridge mapping $\mathbf{B} : \mathcal{W}_h \mapsto \mathcal{W}$,

$$\mathbf{B}(\boldsymbol{\mu}_h^\perp, \mathbf{U}_h^0, \boldsymbol{\mu}_h^0, \mathbf{U}_h^\perp, \mathbf{p}_h) := (\mathbf{B}_\Gamma(\boldsymbol{\mu}_h^\perp), \mathbf{U}_h^0, \boldsymbol{\mu}_h^0, \mathbf{B}_\Omega(\mathbf{U}_h^\perp), \mathbf{p}_h),$$

for $\boldsymbol{\mu}_h^\perp \in \mathbf{X}_h(\operatorname{div}_\Gamma, \Gamma_h)$, $\boldsymbol{\mu}_h^0 \in \mathbf{N}_h(\operatorname{div}_\Gamma, \Gamma_h)$, $\mathbf{U}_h^\perp \in \mathbf{X}_h(\operatorname{curl}, \Omega_h)$, $\mathbf{U}_h^0 \in \mathbf{N}_h(\operatorname{curl}, \Omega_h)$, and $\mathbf{p} \in \mathcal{E}_1^1(\Gamma_h)$. Combining the estimates (1.32), (1.33) we end up with

$$\delta(\mathcal{W}, \mathcal{W}_h) \leq \sup_{\mathbf{w}_h \in \mathcal{W}_h} \frac{\|\mathbf{w}_h - \mathbf{B}(\mathbf{w}_h)\|_{\mathcal{W}}}{\|\mathbf{w}_h\|_{\mathcal{W}}} \leq Ch^{1/2} \rightarrow 0, \text{ as } h \rightarrow 0,$$

thus we have established the desired gap property for the space $\mathcal{W}_h$.

1.10 Convergence

The discrete inf-sup estimate established in Sect. 1.9 paves the way for a quasi optimal asymptotic estimate of the discretization error.

Theorem 1.7. *There exists a mesh width $h_0 \in \mathbb{H}$, depending only on Ω , κ , ν and the shape regularity of the meshes Ω_h , such that for every $h < h_0$ the discrete problem (1.29) has a unique solution $(\mathbf{E}_h, \boldsymbol{\vartheta}_h, \mathbf{p}_h) \in \mathcal{E}_{\nu+1}^1(\Omega_h) \times \mathcal{F}_\nu(\Gamma_h) \times \mathcal{E}_1^1(\Gamma_h)$, which is quasi optimal in the following sense*

$$\begin{aligned} &\|\mathbf{E} - \mathbf{E}_h\|_{\mathbf{H}(\operatorname{curl}, \Omega)} + \|\boldsymbol{\lambda} - \boldsymbol{\lambda}_h\|_{\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)} + \|\mathbf{p} - \mathbf{p}_h\|_{\mathbf{H}(\operatorname{curl}_\Gamma, \Gamma)} \\ &\leq C \inf \left\{ \begin{array}{l} \|\mathbf{E} - \mathbf{V}_h\|_{\mathbf{H}(\operatorname{curl}, \Omega)} + \|\boldsymbol{\lambda} - \boldsymbol{\mu}_h\|_{\mathbf{H}^{-1/2}(\operatorname{div}_\Gamma, \Gamma)}; \\ \mathbf{V}_h \in \mathcal{E}_{\nu+1}^1(\Omega_h), \boldsymbol{\mu}_h \in \mathcal{F}_\nu(\Gamma_h) \end{array} \right\}, \end{aligned}$$

with a constant $C > 0$ independent of $(\mathbf{E}, \boldsymbol{\vartheta}, \mathbf{p})$ and $h \in \mathbb{H}$.

Proof. In order to prove the quasi optimality estimate we have to verify all assumptions from Theorem 1.6. The roles of W, W_h are now played by $\mathcal{W}, \mathcal{W}_h$ and the spaces X, X_h and N, N_h have to be replaced by $\mathcal{X}, \mathcal{X}_h$ and $\mathcal{N}, \mathcal{N}_h$. Continuity, compactness and injectivity can be obtained directly from Sect. 1.6. The approximation and the gap property for $\mathcal{W}_h$ have already been established in Sect. 1.9. Eventually, we obtain h -uniform stability according to (1.30) for $\hat{\mathbf{a}}_\kappa^{\text{reg}}$ on the family $\mathcal{W}_h$, $h \in \mathbb{H}$, provided that h is sufficiently small.

Furthermore, from Lemmas 1.26 and 1.24 we obtain the following h -uniform equivalence of norms

$$\|(\mu_h^\perp, \mathbf{V}_h^0, \mu_h^0, \mathbf{V}_h^\perp, \mathbf{q}_h)\|_{\mathcal{W}} \asymp \|(\mathbf{V}_h^\perp + \mathbf{V}_h^0, \mu_h^\perp + \mu_h^0, \mathbf{q}_h)\|_{\mathcal{Y}},$$

for all $(\mu_h^\perp, \mathbf{V}_h^0, \mu_h^0, \mathbf{V}_h^\perp, \mathbf{q}_h) \in \mathcal{W}_h$, where the space $\mathcal{Y}$ is defined by

$$\mathcal{Y} := \mathbf{H}(\text{curl}, \Omega) \times \mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma) \times \mathbf{H}(\text{curl}_\Gamma, \Gamma)$$

and endowed with its natural graph norm. For later use we also define the following family of discrete subspaces $\mathcal{Y}_h := \mathcal{E}_{\nu+1}^1(\Omega_h) \times \mathcal{F}_\nu(\Gamma_h) \times \mathcal{E}_1^1(\Gamma_h)$.

Based on the discrete inf-sup estimate on the space $\mathcal{W}_h$, we get for $h_0 > h$

$$\begin{aligned} & \sup_{\mathbf{y}_h \in \mathcal{Y}_h} \frac{\left| \mathbf{a}_\kappa^{\text{reg}}((\mathbf{E}_h, \boldsymbol{\lambda}_h, \mathbf{p}_h), \mathbf{y}_h) \right|}{\|\mathbf{y}_h\|_{\mathcal{Y}}} \\ & \geq C \sup_{\mathbf{w}_h \in \mathcal{W}_h} \frac{\left| \hat{\mathbf{a}}_\kappa^{\text{reg}}((\boldsymbol{\lambda}_h^\perp, \mathbf{E}_h^0, \boldsymbol{\lambda}_h^0, \mathbf{E}_h^\perp, \mathbf{p}_h), \mathbf{w}_h) \right|}{\|\mathbf{w}_h\|_{\mathcal{W}}} \\ & \geq C \|(\boldsymbol{\lambda}_h^\perp, \mathbf{E}_h^0, \boldsymbol{\lambda}_h^0, \mathbf{E}_h^\perp, \mathbf{p}_h)\|_{\mathcal{W}} \geq C \|(\mathbf{E}_h, \boldsymbol{\lambda}_h, \mathbf{p}_h)\|_{\mathcal{Y}}, \end{aligned}$$

with constants independent of the functions and $h \in \mathbb{H}$. From Babuška's theory [6], we conclude the error estimate from the theorem. $\square$

Note that the auxiliary variable $\mathbf{p}$ does not show up on the right-hand side of the quasi optimality estimate. This is guaranteed by $\mathbf{p} = \mathbf{0} \in \mathcal{E}_1^1(\Gamma_h)$. However, we can not simply drop the auxiliary variable from (1.26), since the quasi-optimality estimate in Theorem 1.7 is an asymptotic estimate, which only holds under sufficient approximation properties of the space $\mathcal{W}_h$.

The main prerequisite for establishing orders of convergence of best approximations in finite element spaces are assumptions on the regularity of solutions of the continuous problem (1.26). We will assume that both the electric and the magnetic fields $\mathbf{E}, \mathbf{H} := (i\omega\mu_r)^{-1}\text{curl}\mathbf{E}$ belong to $H^s(\Omega)$ for some $s > 0$. We point out that the regularity of solutions of Maxwell's equations depends on the discontinuities of the material parameters ε_r and μ_r (cf. [29]).

It is reasonable to demand that the discontinuities of ε_r and μ_r be resolved by the meshes Ω_h . That is, if Ω_i , $i = 0, \dots, M$, $M \in \mathbb{M}$, are subdomains of Ω on which both material parameters are smooth, then $\Omega_h|_{\Omega_i}$ must supply a valid triangulation of Ω_i . Then we can exploit $\mathbf{curl} \mathbf{E} = i\kappa\mu_r \mathbf{H}$ to see that $\mathbf{curl} \mathbf{E}$ is locally in $H^s(\Omega_i)$, $i = 1, \dots, M$. Globally $\mathbf{curl} \mathbf{E}$ is at least contained in $H^{\min\{s, 1/4\}}(\Omega)$.

Lemma 1.27. *If $\mathbf{E}, \mathbf{H} \in H^s(\Omega)$ for some $s > 0$, and if the jumps of ε_r and μ_r are resolved by all triangulations, we find a constant $C > 0$ depending on only on ε_r , μ_r , Ω , ν and the shape regularity of the meshes Ω_h such that*

$$\|\mathbf{E} - \mathbf{I}_{\nu+1}^1(\mathbf{E})\|_{\mathbf{H}(\mathbf{curl}, \Omega)} \leq Ch^{\min\{\nu+1, s\}} \left(\|\mathbf{E}\|_{H^s(\Omega)} + \sum_{i=1}^M \|\mathbf{H}\|_{H^s(\Omega_i)} \right).$$

Proof. For a proof see [39, Lemma 12.2]. $\square$

Lemma 1.28. *Assume that the meshes Ω_h resolve the discontinuities of both ε_r and μ_r , that $\mathbf{H}, \mathbf{E} \in H^s(\Omega)$ and that $\mathbf{E}^{inc}$ is smooth. Then*

$$\begin{aligned} & \|\boldsymbol{\vartheta} - \boldsymbol{\Phi}_\nu^2(\boldsymbol{\vartheta})\|_{\mathbf{H}^{-1/2}(\text{div}_\Gamma, \Gamma)} \\ & \leq Ch^{\min\{\nu+1, s\}} \left(\|\mathbf{E}\|_{H^s(\Omega)} + \sum_{i=1}^M \|\mathbf{H}\|_{H^s(\Omega_i)} + \|\mathbf{E}^{inc}\|_{H^s(\Omega)} \right), \end{aligned}$$

where $C > 0$ depends neither on $\mathbf{H}$, $\mathbf{E}$, $\mathbf{E}^{inc}$ nor on $h \in \mathbb{H}$

Proof. For a proof see [39, Lemma 12.3]. $\square$

The two previous lemma along with the quasi optimality estimate from Theorem 1.7 imply the convergence of the Galerkin solutions in $\boldsymbol{\mathcal{E}}_\nu^1(\Omega_h) \times \boldsymbol{\mathcal{F}}_\nu(\Gamma_h) \times \boldsymbol{\mathcal{E}}_1^1(\Gamma_h)$ of the order $O(h^{\min\{\nu+1, s\}})$ in the natural energy norms as $h \rightarrow 0$.

References

- [1] H. AMMARI AND J.-C. NÉDÉLEC, Couplage éléments finis-équations intégrales pour la résolution des équations de Maxwell en milieu hétérogène, in Equations aux dérivées partielles et applications. Articles dédiées à Jacques-Louis Lions, Gauthier-Villars, Paris, France, 1998, pp. 19–33.
- [2] ———, Coupling of finite and boundary element methods for the time-harmonic Maxwell equations. II: A symmetric formulation, in The Maz'ya anniversary collection. Vol. 2, J. Rossmann, ed., vol. 110 of Oper. Theory, Adv. Appl., Birkhäuser, Basel, Switzerland, 1999, pp. 23–32.

- [3] ———, *Coupling integral equations method and finite volume elements for the resolution of the Leontovich boundary value problem for the time-harmonic Maxwell equations in three dimensional heterogeneous media*, in Mathematical aspects of boundary element methods. Minisymposium during the IABEM 98 conference, dedicated to Vladimir Maz'ya on the occasion of his 60th birthday on 31st December 1997, M. Bonnet, ed., vol. 41 of CRC Research Notes in Mathematics, CRC Press, Boca Raton, FL, USA, 2000, pp. 11–22.
- [4] ———, *Low-frequency electromagnetic scattering*, SIAM J. Math. Anal., 31 (2000), pp. 836–861.
- [5] C. AMROUCHE, C. BERNARDI, M. DAUGE, AND V. GIRAULT, *Vector potentials in three-dimensional non-smooth domains*, Math. Meth. Appl. Sci., 21 (1998), pp. 823–864.
- [6] I. BABUŠKA, *Error bounds for the finite element method*, Numer. Math., 16 (1971), pp. 322–333.
- [7] A. BENDALI, *Boundary element solution of scattering problems relative to a generalized impedance boundary condition*, in Partial differential equations: Theory and numerical solution. Proceedings of the ICM 98 satellite conference, Prague, Czech Republic, August 10–16, 1998., W. Jäger, ed., vol. 406 of CRC Res. Notes Math., Boca Raton, FL, USA, 2000, Chapman & Hall, CRC, pp. 10–24.
- [8] F. BREZZI AND M. FORTIN, *Mixed and hybrid finite element methods*, Springer, Heidelberg, Germany, 1991.
- [9] A. BUFFA, *Hodge decompositions on the boundary of a polyhedron: The multi-connected case*, Math. Meth. Appl. Sci., 11 (2001), pp. 1491–1504.
- [10] ———, *Remarks on the discretization of some non-coercive operator with applications to heterogeneous Maxwell equations*, SIAM J. Numer. Anal., 42 (2005), pp. 1–18.
- [11] A. BUFFA AND S. C. CHRISTIANSEN, *The electric field integral equation on Lipschitz screens: Definition and numerical approximation*, Numer. Math., 94 (2003), pp. 229–267.
- [12] A. BUFFA AND P. CIARLET JR., *On traces for functional spaces related to Maxwell's equations Part I: An integration by parts formula in Lipschitz polyhedra*, Math. Meth. Appl. Sci., 24 (2001), pp. 9–30.
- [13] ———, *On traces for functional spaces related to Maxwell's equations Part II: Hodge decompositions on the boundary of Lipschitz polyhedra and applications*, Math. Meth. Appl. Sci., 24 (2001), pp. 31–48.
- [14] A. BUFFA, M. COSTABEL, AND C. SCHWAB, *Boundary element methods for maxwell's equations on non-smooth domains*, Numer. Math., 92 (2002), pp. 679–710.
- [15] A. BUFFA, M. COSTABEL, AND D. SHEEN, *On traces for $\mathbf{H}(\text{curl}, \Omega)$ in Lipschitz domains*, J. Math. Anal. Appl., 276 (2002), pp. 845–867.
- [16] A. BUFFA AND R. HIPTMAIR, *Galerkin boundary element methods for electromagnetic scattering*, in Topics in computational wave propagation. Direct and inverse problems, M. Ainsworth, P. Davies, D. Duncan,

- P. Martin, and B. Rynne, eds., vol. 31 of Lecture notes in computational science and engineering, Springer, Heidelberg, Germany, 2003, pp. 83–124.
- [17] ———, *A coercive combined field integral equation for electromagnetic scattering*, SIAM J. Numer. Anal., 42 (2004), pp. 621–640.
 - [18] A. BUFFA, R. HIPTMAIR, T. VON PETERSDORFF, AND C. SCHWAB, *Boundary element methods for Maxwell equations on Lipschitz domains*, Numer. Math., 95 (2003), pp. 459–485.
 - [19] C. CARSTENSEN AND P. WRIGGERS, *On the symmetric boundary element method and the symmetric coupling of boundary elements and finite elements*, IMA J. Numer. Anal., 17 (1997), pp. 201–238.
 - [20] M. CESSENAT, *Mathematical methods in electromagnetism*, vol. 41 of Adv. Math. Appl. Sci., World Scientific, Singapore, 1996.
 - [21] G. CHEN AND J. ZHOU, *Boundary Element Methods*, Academic Press, New York, USA, 1992.
 - [22] S. H. CHRISTIANSEN, *Discrete Fredholm properties and convergence estimates for the electric field integral equations*, Numer. Math., 73 (2004), pp. 143–167.
 - [23] P. CIARLET, *The finite element method for elliptic problems*, vol. 4 of Stud. Math. Appl., North-Holland, Amsterdam, Netherlands, 1978.
 - [24] P. CIARLET AND J. ZOU, *Fully discrete finite element approaches for time-dependent Maxwell equations*, Numer. Math., 82 (1992), pp. 613–626.
 - [25] D. COLTON AND R. KRESS, *Inverse Acoustic and Electromagnetic Scattering Theory*, vol. 93 of Applied Mathematical Sciences, Springer, Heidelberg, Germany, 2nd ed., 1998.
 - [26] M. COSTABEL, *Symmetric methods for the coupling of finite elements and boundary elements*, in Boundary Elements IX, C. Brebbia, W. Wendland, and G. Kuhn, eds., Springer, Heidelberg, Germany, 1987, pp. 411–420.
 - [27] ———, *Boundary integral operators on Lipschitz domains: Elementary results*, SIAM J. Math. Anal., 19 (1988), pp. 613–626.
 - [28] M. COSTABEL AND M. DAUGE, *Maxwell and Lamé eigenvalues on polyhedra*, Math. Meth. Appl. Sci., 22 (1999), pp. 243–258.
 - [29] M. COSTABEL, M. DAUGE, AND S. NICAISE, *Singularities of Maxwell interface problems*, Math. Model. Numer. Anal., 33 (1999), pp. 627–649.
 - [30] M. COSTABEL AND W. WENDLAND, *Strong ellipticity of boundary integral operators*, J. Reine Angew. Math., 372 (1986), pp. 39–63.
 - [31] D. DAUTRAY AND J. L. LIONS, *Mathematical analysis and numerical methods for science and technology*, vol. 4, Springer, Heidelberg, Germany, 1990.
 - [32] A. DE LA BOURDONNAYE, *Some formulations coupling finite element and integral equation methods for Helmholtz equation and electromagnetism*, Numer. Math., (1995), pp. 257–268.

- [33] V. GIRAULT AND P. A. RAVIART, *Finite Element Methods for Navier-Stokes Equations*, Springer, Heidelberg, Germany, 1986.
- [34] P. GRISVARD, *Elliptic problems in non-smooth domains*, Pitman, Boston, USA, 1985.
- [35] R. HARRINGTON AND J. MAUTZ, *A combined-source solution for radiation and scattering from a perfectly conducting body*, IEEE Trans. Antennas Propagat., 21 (1979), pp. 445–454.
- [36] C. HAZARD AND M. LENOIR, *On the solution of time-harmonic scattering problems for Maxwell’s equations*, SIAM J. Math. Anal., 27 (1996), pp. 1597–1630.
- [37] R. HIPTMAIR, *Canonical construction of finite elements*, Math. Comp., 68 (1999), pp. 1325–1346.
- [38] ———, *Symmetric coupling for eddy current problems*, SIAM J. Numer. Anal., 40 (2002), pp. 41–65.
- [39] ———, *Coupling of finite elements and boundary elements in electromagnetic scattering*, SIAM J. Numer. Anal., 41 (2003), pp. 919–944.
- [40] R. HIPTMAIR AND P. MEURY, *Stabilized FEM-BEM coupling for Helmholtz transmission problems*, SIAM J. Numer. Anal., 44 (2006), pp. 2107–2130.
- [41] R. HIPTMAIR AND C. SCHWAB, *Natural boundary element methods for the electric field integral equation on polyhedra*, SIAM Journal on Numerical Analysis, 40 (2002), pp. 66–86.
- [42] R. HIPTMAIR AND W. ZHENG, *Local multigrid in $\mathbf{H}(\text{curl}, \Omega)$* , tech. rep., SAM, ETH Zürich, 2007.
- [43] G. C. HSIAO, *Mathematical foundations for the boundary field equation methods in acoustic and electromagnetic scattering*, in Analysis and Computational Methods in Scattering and Applied Mathematics. A volume in the memory of Ralph Ellis Kleinman, F. Santosa and I. Stakgold, eds., vol. 147 of Research Notes in Mathematics, Chapman & Hall, CRC, Boca Raton, FL, USA, 2000, pp. 149–163.
- [44] M. KUHN AND O. STEINBACH, *FEM-BEM coupling for 3d exterior magnetic fields*, Math. Meth. Appl. Sci., 25 (2002), pp. 357–371.
- [45] R. MCCAMY AND E. STEPHAN, *Solution procedures for three-dimensional eddy-current problems*, J. Math. Anal. Appl., 101 (1984), pp. 348–379.
- [46] W. MCLEAN, *Strongly Elliptic Systems and Boundary Integral Equations*, Cambridge University Press, Cambridge, UK, 2000.
- [47] P. MONK, *Finite element methods for Maxwell’s equations*, Oxford University Press, Oxford, UK, 2003.
- [48] J.-C. NÉDÉLEC, *Mixed finite elements in $\mathbb{R}^3$* , Numer. Math., 35 (1980), pp. 315–341.
- [49] ———, *Acoustic and Electromagnetic Equations: Integral Representations for Harmonic Problems*, vol. 144 of Appl. Math. Sci., Springer, Heidelberg, Germany, 2001.

- [50] P. A. RAVIART AND J. M. THOMAS, *A Mixed Finite Element Method for Second Order Elliptic Problems*, vol. 606 of Springer Lecture Notes in Mathematics, Springer, Heidelberg, Germany, 1977, pp. 292–315.
- [51] A. SCHATZ, *An observation concerning Ritz-Galerkin methods with indefinite bilinear forms*, Math. Comp., 28 (1974), pp. 959–962.
- [52] T. VON PETERSDORFF, *Boundary integral equations for mixed Dirichlet, Neumann and transmission problems*, Math. Meth. Appl. Sci., 11 (1989), pp. 185–213.
- [53] M. N. VOUVAKIS, S.-C. LEE, K. ZHAO, AND J.-F. LEE, *A symmetric FEM-IE formulation with a single-level IE-QR algorithm for solving electromagnetic radiation and scattering problems*, IEEE Trans. Antennas Propagat., 52 (2006), pp. 3060–3070.
- [54] M. N. VOUVAKIS, K. ZHAO, S.-M. SEO, AND J.-F. LEE, *A domain decomposition approach for non-conformal couplings between finite and boundary elements for unbounded electromagnetic scattering in $\mathbb{R}^3$* , J. Comp. Phys., (2007). submitted.
- [55] K. ZHAO, M. N. VOUVAKIS, AND J.-F. LEE, *Solving electromagnetic problems using a novel symmetric FEM-BEM approach*, IEEE Trans. Magn., 42 (2006), pp. 583–586.

A Posteriori Error Analysis and Adaptive Finite Element Methods for Electromagnetic and Acoustic Problems

Z. Chen

2.1 Introduction

The objective of this chapter is to report some of our recent efforts in exploring the possibility of extending the general framework of adaptive finite element methods based on a posteriori error estimates initiated in [BR78] to resolve Maxwell singularities. A posteriori error estimates are computable quantities in terms of the discrete solution and known data that measure the actual discrete errors without the knowledge of exact solutions. They are essential in designing algorithms for mesh modification which equi-distribute the computational effort and optimize the computation. The ability of error control and the asymptotically optimal approximation property make the adaptive finite element methods attractive for complicated physical and industrial processes.

The first problem we consider is the time-harmonic Maxwell equation in the bounded domain, that is, the time-harmonic Maxwell cavity problem. It is well-known that the solution of the time-harmonic Maxwell equations could have much stronger singularities than the corresponding Dirichlet or Neumann singular functions of the Laplace operator when the computational domain is non-convex or the coefficients of the equations are discontinuous. For example, for the domains that have “screen” or “crack” parts as indicated in Fig. 2.1, the regularity of the solution is only in $\mathbf{H}^s$ with $s < 1/2$. In this case the $\mathbf{H}^1$ -conforming discretization cannot be used directly to solve the time-harmonic cavity problem. One way to overcome the difficulty is to use the so-called singular field method which decomposes the solution into a regular part that can be treated by $\mathbf{H}^1$ -conforming Lagrangian finite elements and an explicit singular part [ACS98], [DHL99]. For the mathematical analysis of the singularities of the solutions of Maxwell equations, we refer to [BS87], [BS94], [CD00], and the references therein.

A posteriori error estimates for $\mathbf{H}(\text{curl})$ -conforming edge elements are obtained in [M98] for Maxwell scattering problems and in [BHHW00] for eddy current problems. The key ingredient in the analysis is the orthogonal Helmholtz decomposition $\mathbf{v} = \nabla\varphi + \Psi$, where for any $\mathbf{v} \in \mathbf{H}(\text{curl}; \Omega)$,

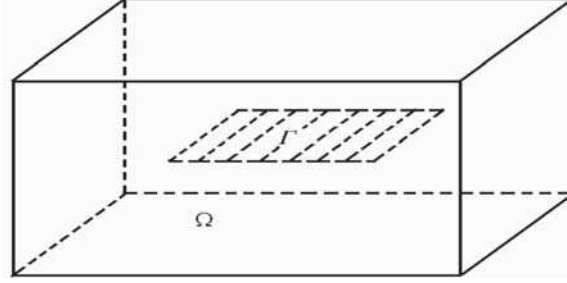


Fig. 2.1. A domain with screen Γ

$\varphi \in H^1(\Omega)$, and $\Psi \in \mathbf{H}(\mathbf{curl}; \Omega)$. Since a stable edge element interpolation operator is not available for functions in $\mathbf{H}(\mathbf{curl}; \Omega)$, some kind of regularity result for $\Psi \in \mathbf{H}(\mathbf{curl}; \Omega)$ is required. This regularity result is proved in [M98] for domains with smooth boundary and in [BHHW00] for convex polyhedral domains. The key observation in our analysis is that if one removes the orthogonality requirement in the Helmholtz decomposition, the regularity $\Psi \in \mathbf{H}^1(\Omega)$ can be proved in the decomposition $\mathbf{v} = \nabla\varphi + \Psi$ for a large class of non-convex polygonal domains or domains having screens [BS87], [BS94], see also [DHL99]. Our extensive numerical experiments for the lowest order edge element indicate that for the cavity problem with very strong singularities $\mathbf{H}^s$ ($s < 1/2$), the adaptive methods based on our a posteriori error estimates have the very desirable quasi-optimality property

$$\|\mathbf{E} - \mathbf{E}_k\|_{\mathbf{H}(\mathbf{curl}; \Omega)} \leq C N_k^{-1/3},$$

where N_k is the number of elements of the k th adaptive mesh $\mathcal{M}_k$, and $\mathbf{E}_k$ is the finite element solution over $\mathcal{M}_k$.

The second problem concerns an adaptive perfectly matched layer (PML) technique for solving the time harmonic electromagnetic scattering problem with the perfectly conducting boundary condition. Adaptive PML technique was first proposed in Chen and Wu [CW03] for scattering problem by periodic structures (the grating problem) and in Chen and Liu [CL05] for the acoustic scattering problem in which one uses the a posteriori error estimate to determine the PML parameters. Combined with the adaptive finite element method, the adaptive PML technique provides a complete numerical strategy to solve the scattering problems in the framework of finite element which produces automatically coarse mesh size away from the fixed domain and thus makes the total computational costs insensitive to the thickness of the PML absorbing layer.

In the third problem we consider the time-dependent eddy current problems which involve discontinuous coefficients, reentrant corners of material interfaces, and skin effect. Thus local singularities and internal layers of the solution arise. We develop an adaptive finite element method based on reliable and efficient a posteriori error estimates for the $\mathbf{H} - \psi$ formulation of

eddy current problems with multiply connected conductors. The numerical results indicate that our adaptive method has the following very desirable quasi-optimality property:

$$\eta_{\text{total}} \approx C N_{\text{total}}^{-1/4}$$

is valid asymptotically, where η_{total} is the total error estimate (see Theorem 2.5 below), and $N_{\text{total}} := \sum_{n=1}^M N_n$ with M being the number of time steps and N_n being the number of elements of the mesh $\mathcal{T}_n$ at the n th timestep.

In extending our general methodology of using adaptive PML technique for solving time-domain Maxwell scattering problems, we need to consider the convergence and stability of the time-domain PML methods for Maxwell scattering problems. As a first step we consider here the stability and convergence of the time-domain PML method for acoustic scattering problems. We will consider the well-posedness and the stability of the time-dependent acoustic scattering problem with the radiation condition at infinity, the well-posedness of the unsplit-field PML method for the acoustic scattering problems, and the exponential convergence of the non-splitting PML method in terms of the thickness and medium property of the artificial PML layer. The stability of the time-domain PML method can be proved by combining the stability of original scattering problem and the convergence of the PML method.

2.2 The Time-Harmonic Maxwell Cavity Problem

Let $\Omega \subset \mathbb{R}^3$ be a bounded polygonal domain with two disjoint connected boundaries Γ and Σ . Given a current density $\mathbf{f}$, we seek a time-harmonic electric field $\mathbf{E}$ subject to the perfectly conducting boundary condition on Γ and the impedance boundary condition on Σ

$$\nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}) - k^2 \varepsilon_r \mathbf{E} = \mathbf{f} \quad \text{in } \Omega, \quad (2.1)$$

$$\mu_r^{-1} (\nabla \times \mathbf{E}) \times \mathbf{n} - \mathbf{i} k \lambda \mathbf{E}_t = \mathbf{g} \quad \text{on } \Sigma, \quad (2.2)$$

$$\mathbf{E} \times \mathbf{n} = 0 \quad \text{on } \Gamma, \quad (2.3)$$

where $\mathbf{n}$ is the unit outer normal of the boundary, $\mathbf{E}_t := (\mathbf{n} \times \mathbf{E}|_{\Sigma}) \times \mathbf{n}$, ε_r is the complex relative dielectric coefficient, $\mu_r > 0$ is the relative magnetic permeability of the material in Ω , $k > 0$ is the wave number, and $\lambda > 0$ is the impedance on Σ .

Let $\mathbf{f} \in \mathbf{L}^2(\Omega)$ and $\mathbf{g} \in \mathbf{L}^2(\Sigma)$ satisfying $\mathbf{g} \cdot \mathbf{n} = 0$ on Σ . The weak formulation of (2.1)–(2.3) is: Find $\mathbf{E} \in H_{\Gamma}(\mathbf{curl}; \Omega)$ such that

$$a(\mathbf{E}, \mathbf{v}) = \int_{\Omega} \mathbf{f} \cdot \bar{\mathbf{v}} + \int_{\Sigma} \mathbf{g} \cdot \bar{\mathbf{v}}_t \quad \forall \mathbf{v} \in H_{\Gamma}(\mathbf{curl}; \Omega), \quad (2.4)$$

where $H_\Gamma(\mathbf{curl}; \Omega) = \{\mathbf{v} \in H(\mathbf{curl}; \Omega) \mid \mathbf{v} \times \mathbf{n} = 0 \text{ on } \Gamma \text{ and } \mathbf{v}_t \in \mathbf{L}^2(\Sigma)\}$ and

$$a(\mathbf{E}, \mathbf{v}) := (\mu_r^{-1} \nabla \times \mathbf{E}, \nabla \times \mathbf{v}) - (k^2 \varepsilon_r \mathbf{E}, \mathbf{v}) - i \int_{\Sigma} k \lambda \mathbf{E}_t \cdot \bar{\mathbf{v}}_t.$$

The existence and uniqueness of the solution of the problem (2.4) under various conditions on the domain Ω , the coefficients ε_r , μ_r have been studied in [M03]. Here for the sake of simplicity we simply assume that the problem (2.4) has a unique solution. Thus there exists a constant $\beta > 0$ depending only on Ω , ε_r , μ_r , λ and the wave number k such that [BA73, Chap. 5]

$$\sup_{0 \neq \mathbf{v} \in H_\Gamma(\mathbf{curl}; \Omega)} \frac{a(\mathbf{E}, \mathbf{v})}{\|\mathbf{v}\|_{H_\Gamma(\mathbf{curl}; \Omega)}} \geq \beta \|\mathbf{E}\|_{H_\Gamma(\mathbf{curl}; \Omega)}. \quad (2.5)$$

For definiteness we assume in this section that Γ is a Lipschitz screen such that $\Omega \cup \Gamma$ is a Lipschitz domain (see Fig. 2.1) and refer to the discussion of general cases to [CWZ07]. We recall that a surface F is called a Lipschitz screen, if it is a bounded open part of some two-dimensional C^2 -smooth manifold such that its boundary ∂F is Lipschitz continuous and F is on one side of ∂F . The following decomposition theorem whose proof can be found in [BS87], [BS94], [DHL99], [CWZ07] plays an important role in the forthcoming a posteriori error analysis.

Theorem 2.1. *For any $\mathbf{v} \in H(\mathbf{curl}; \Omega)$ satisfying $\mathbf{v} \times \mathbf{n} = 0$ on Γ , there exists a function $\mathbf{v}_s \in \mathbf{H}^1(\Omega)$ satisfying $\mathbf{v}_s \times \mathbf{n} = 0$ on Γ and $\varphi \in H_F^1(\Omega)$ such that*

$$\begin{aligned} \mathbf{v} &= \nabla \varphi + \mathbf{v}_s \quad \text{in } \Omega, \\ \|\mathbf{v}_s\|_{1, \Omega} + \|\varphi\|_{1, \Omega} &\leq C \|\mathbf{v}\|_{H(\mathbf{curl}; \Omega)}. \end{aligned}$$

Here $H_F^1(\Omega)$ is the subspace of $H^1(\Omega)$ whose functions have zero traces on Γ .

Let $\mathcal{M}_h$ be a regular tetrahedral triangulation of Ω and $\mathcal{F}_h$ be the set of faces not lying on Γ . The finite element space $\mathbf{U}_h$ over $\mathcal{M}_h$ is defined by

$$\begin{aligned} \mathbf{U}_h &:= \{\mathbf{u} \in H(\mathbf{curl}; \Omega) : \mathbf{u} \times \mathbf{n}|_\Gamma = \mathbf{0} \text{ and} \\ &\quad \mathbf{u}|_T = \mathbf{a}_T + \mathbf{b}_T \times \mathbf{x} \text{ with } \mathbf{a}_T, \mathbf{b}_T \in \mathbb{R}^3, \quad \forall T \in \mathcal{M}_h\}. \end{aligned}$$

Degrees of freedom on every $T \in \mathcal{M}_h$ are $\int_{E_i} \mathbf{u} \cdot d\mathbf{l}$, $i = 1, \dots, 6$, where $E_1, \dots, E_6$ are six edges of T . For any $T \in \mathcal{M}_h$ and $F \in \mathcal{F}_h$, we denote the diameters of T and F by h_T and h_F , respectively.

The finite element approximation to (2.4) is: Find $\mathbf{E}_h \in \mathbf{U}_h$ such that

$$a(\mathbf{E}_h, \mathbf{v}) = \int_{\Omega} \mathbf{f} \cdot \bar{\mathbf{v}} + \int_{\Sigma} \mathbf{g} \cdot \bar{\mathbf{v}}_t, \quad \forall \mathbf{v} \in \mathbf{U}_h. \quad (2.6)$$

Let $\mathbf{E}$ and $\mathbf{E}_h$ be the solutions of (2.4) and (2.6), respectively. Define the total error function by $\mathbf{e}_h := \mathbf{E} - \mathbf{E}_h$. By (2.5), we know that

$$\|\mathbf{e}_h\|_{H_\Gamma(\mathbf{curl}; \Omega)} \leq \beta^{-1} \sup_{\mathbf{v} \in H_\Gamma(\mathbf{curl}; \Omega)} \frac{a(\mathbf{e}_h, \mathbf{v})}{\|\mathbf{v}\|_{H_\Gamma(\mathbf{curl}; \Omega)}}.$$

To derive a posteriori error estimates, we require the Scott–Zhang interpolant $\mathcal{I}_h : H_\Gamma^1(\Omega) \rightarrow V_h$ [SC94] and the Beck–Hiptmair–Hoppe–Wohlmuth interpolant $\Pi_h : \mathbf{H}^1(\Omega) \cap \mathbf{H}_\Gamma(\mathbf{curl}; \Omega) \rightarrow \mathbf{U}_h$ [BHHW00], where V_h is the standard piecewise linear H_Γ^1 -conforming finite element space over $\mathcal{M}_h$. It is known that $\mathcal{I}_h$ and Π_h satisfy the following approximation and stability properties: for any $T \in \mathcal{M}_h$, $F \in \mathcal{F}_h$, $\varphi_h \in V_h$, $\varphi \in H_\Gamma^1(\Omega)$,

$$\begin{aligned} \mathcal{I}_h \varphi_h &= \varphi_h, \quad \|\nabla \mathcal{I}_h \varphi\|_{0,T} \leq C |\varphi|_{1,D_T} \\ \|\varphi - \mathcal{I}_h \varphi\|_{0,T} &\leq C h_T |\varphi|_{1,D_T}, \quad \|\varphi - \mathcal{I}_h \varphi\|_{0,F} \leq C h_F^{1/2} |\varphi|_{1,D_F} \end{aligned}$$

and for any $T \in \mathcal{M}_h$, $F \in \mathcal{F}_h$, $\mathbf{w}_h \in \mathbf{U}_h$, $\mathbf{w} \in H_\Gamma(\mathbf{curl}; \Omega)$

$$\begin{aligned} \Pi_h \mathbf{w}_h &= \mathbf{w}_h, \quad \|\Pi_h \mathbf{w}\|_{H(\mathbf{curl}; T)} \leq C \|\mathbf{w}\|_{1,D_T}, \\ \|\mathbf{w} - \Pi_h \mathbf{w}\|_{0,T} &\leq C h_T \|\mathbf{w}\|_{1,D_T}, \quad \|\mathbf{w} - \Pi_h \mathbf{w}\|_{0,F} \leq C h_F^{1/2} \|\mathbf{w}\|_{1,D_F}, \end{aligned}$$

where D_A is the union of elements in $\mathcal{M}_h$ with non-empty intersection with A , $A = T$ or F .

By Theorem 2.1, for any $\mathbf{v} \in H_\Gamma(\mathbf{curl}; \Omega)$, there exist a $\varphi \in H_\Gamma^1(\Omega)$ and a $\mathbf{v}_s \in \mathbf{H}^1(\Omega) \cap H_\Gamma(\mathbf{curl}; \Omega)$ such that

$$\begin{aligned} \mathbf{v} &= \nabla \varphi + \mathbf{v}_s, \\ \|\varphi\|_{1,\Omega} + \|\mathbf{v}_s\|_{1,\Omega} &\leq C \|\mathbf{v}\|_{H(\mathbf{curl}; \Omega)}, \end{aligned}$$

where the constant C depends only on Ω . Since $\nabla \mathcal{I}_h \varphi$ and $\Pi_h \mathbf{v}_s$ belong to $\mathbf{U}_h$, by the Galerkin orthogonality, we have

$$a(\mathbf{e}_h, \mathbf{v}) = a(\mathbf{e}_h, \nabla \varphi - \nabla \mathcal{I}_h \varphi) + a(\mathbf{e}_h, \mathbf{v}_s - \Pi_h \mathbf{v}_s) \quad \forall \mathbf{v} \in H_\Gamma(\mathbf{curl}; \Omega).$$

For any face $F \in \mathcal{F}_h$, assuming $F = T_1 \cap T_2$, $T_1, T_2 \in \mathcal{M}_h$ and the unit normal $\mathbf{n}$ points from T_2 to T_1 , we denote the jump of a function v across F by $[v]_F := v|_{T_1} - v|_{T_2}$. The following theorem is proved in [CWZ07].

Theorem 2.2. *Let $\mathbf{g} \in \mathbf{L}^2(\Sigma)$ satisfying $\operatorname{div}_\Sigma \mathbf{g} \in L^2(\Sigma)$ and $\mathbf{g} \cdot \mathbf{n} = 0$ on Σ . Then there exists a constant C depending on β and the mesh $\mathcal{M}_h$ such that*

$$\begin{aligned} \|\mathbf{e}_h\|_{H_\Gamma(\mathbf{curl}; \Omega)}^2 &\leq C \sum_{T \in \mathcal{M}_h} h_T^2 \|\mathbf{f} + k^2 \varepsilon_r \mathbf{E}_h - \nabla \times (\mu_r^{-1} \nabla \times \mathbf{E}_h)\|_{0,T}^2 \\ &\quad + C \sum_{T \in \mathcal{M}_h} h_T^2 \|\operatorname{div} (k^2 \varepsilon_r \mathbf{E}_h)\|_{0,T}^2 \\ &\quad + C \sum_{F \in \mathcal{F}_h} h_F \|\mu_r^{-1} (\nabla \times \mathbf{E})_h \times \mathbf{n}\|_F^2 \\ &\quad + C \sum_{F \in \mathcal{F}_h} h_F \|k^2 \varepsilon_r \mathbf{E}_h \cdot \mathbf{n}\|_F^2 \end{aligned}$$

$$\begin{aligned}
& + C \sum_{F \subset \Sigma} h_F \|\mathbf{g} + \mathbf{i} k \lambda \mathbf{E}_{k,t} + \mathbf{n} \times \mu_r^{-1} (\nabla \times \mathbf{E})_h\|_{0,F}^2 \\
& + C \sum_{F \subset \Sigma} h_F \|\operatorname{div}_\Sigma(\mathbf{g} + \mathbf{i} k \lambda \mathbf{E}_{k,t})\|_{0,F}^2.
\end{aligned}$$

Based on the a posteriori error estimates in above theorem, an adaptive multilevel method for solving (2.1)–(2.3) is designed and implemented. The extensive numerical experiments in [CWZ07] for the lowest order edge element indicate that the adaptive methods based on our a posteriori error estimates can efficiently capture the Maxwell singularity and achieve the following very desirable quasi-optimality property

$$\|\mathbf{E} - \mathbf{E}_h\|_{H(\operatorname{curl}; \Omega)} \leq C N^{-1/3},$$

where N is the number of elements of the mesh $\mathcal{M}_h$. Fig. 2.2 shows an adaptive mesh of 2,947,848 elements after 11 adaptive iterations for solving a time-harmonic problem containing an inner screen $\Gamma := \{(x, y, z) : -0.5 \leq x, z \leq 0.5, y = 0\}$. In the example $\Omega = (-1, 1)^3 \setminus \Gamma$, $\Sigma = \partial\Omega \setminus \Gamma$, $\mu_r = \varepsilon_r = \lambda = 1$, and

$$\mathbf{f} := \mathbf{0}, \quad \mathbf{g} := (\nabla \times \mathbf{E}_i) \times \mathbf{n} - \mathbf{i} k \mathbf{E}_{i,t},$$

where $\mathbf{E}_i = (e^{iy}, 0, e^{iy})^T / \sqrt{2}$ perpendicular to the perfect conducting “screen”. Thus (2.1)–(2.3) models the scattering by Γ under the incident field $\mathbf{E}_i$. In this case, only $\mathbf{H}^s$ -regularity ($s < 1/2$) of the solution is guaranteed. We observe that the mesh is locally refined near the boundary of

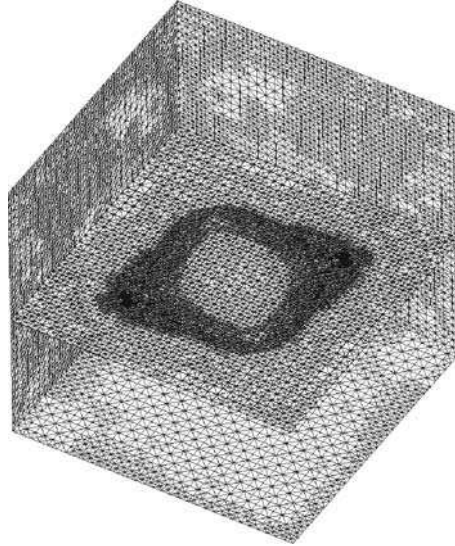


Fig. 2.2. An adaptively refined mesh of 2,947,848 elements after 11 adaptive iterations

the “screen”. We refer to [CWZ07] for more information on the adaptive multilevel algorithm and more numerical examples.

2.3 The Time-Harmonic Electromagnetic Scattering Problem

In this section we consider the time-harmonic electromagnetic scattering problem with the perfectly conducting boundary condition

$$\nabla \times \nabla \times \mathbf{E} - k^2 \mathbf{E} = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{D}, \quad (2.7)$$

$$\mathbf{n} \times \mathbf{E} = \mathbf{g} \quad \text{on } \Gamma_D, \quad (2.8)$$

$$|\mathbf{x}| \left[(\nabla \times \mathbf{E}) \times \hat{\mathbf{x}} - ik\mathbf{E} \right] \rightarrow 0 \quad \text{as } |\mathbf{x}| \rightarrow \infty. \quad (2.9)$$

Here $D \subset \mathbb{R}^3$ is a bounded domain with Lipschitz polyhedral boundary Γ_D , $\mathbf{E}$ is the electric field, $\mathbf{g}$ is determined by the incoming wave, $\hat{\mathbf{x}} = \mathbf{x}/|\mathbf{x}|$, and $\mathbf{n}$ is the unit outer normal to Γ_D . We assume the wave number $k \in \mathbb{R}$ is a constant.

2.3.1 The PML Equation

Let D be contained in the interior of the ball $B_R = \{\mathbf{x} \in \mathbb{R}^3, |\mathbf{x}| < R\}$ with boundary Γ_R . We first recall the series solution of the scattering problem (2.7)–(2.9) outside the ball B_R by following the development in Monk [M03]. Let $Y_n^m(\hat{\mathbf{x}})$, $m = -n, \dots, n$, $n = 1, 2, \dots$, be the *spherical harmonics* which satisfies

$$\Delta_{\partial B_1} Y_n^m(\hat{\mathbf{x}}) + n(n+1)Y_n^m(\hat{\mathbf{x}}) = 0 \quad \text{on } \partial B_1, \quad (2.10)$$

where $\Delta_{\partial B_1} = \frac{1}{\sin \vartheta} \frac{\partial}{\partial \vartheta} (\sin \vartheta \frac{\partial}{\partial \vartheta}) + \frac{1}{\sin^2 \vartheta} \frac{\partial^2}{\partial \varphi^2}$ is the Laplace–Beltrami operator for the surface of the unit sphere ∂B_1 . The set of all spherical harmonics $\{Y_n^m(\hat{\mathbf{x}}) : m = -n, \dots, n, n = 1, 2, \dots\}$ forms a complete orthonormal basis of $L^2(\partial B_1)$.

Denote the *vector spherical harmonics*

$$\mathbf{U}_n^m = \frac{1}{\sqrt{n(n+1)}} \nabla_{\partial B_1} Y_n^m, \quad \mathbf{V}_n^m = \hat{\mathbf{x}} \times \mathbf{U}_n^m,$$

where $\nabla_{\partial B_1} Y_n^m = \frac{\partial Y_n^m}{\partial \vartheta} \mathbf{e}_\vartheta + \frac{1}{\sin \vartheta} \frac{\partial Y_n^m}{\partial \varphi} \mathbf{e}_\varphi$, and $\{\mathbf{e}_r, \mathbf{e}_\vartheta, \mathbf{e}_\varphi\}$ are the unit vectors of the spherical coordinates. The set of all vector spherical harmonics $\{\mathbf{U}_n^m, \mathbf{V}_n^m : m = -n, \dots, n, n = 1, 2, \dots\}$ forms a complete orthonormal basis of $\mathbf{L}_t^2(\partial B_1) = \{\mathbf{u} \in L^2(\partial B_1)^3 : \mathbf{u} \cdot \hat{\mathbf{x}} = 0 \text{ on } \partial B_1\}$.

Let $h_n^{(1)}(z)$ be the spherical Hankel function of the first kind of order n . We introduce the *vector wave functions*

$$\mathbf{M}_n^m(r, \hat{\mathbf{x}}) = \nabla \times \{\mathbf{x} h_n^{(1)}(kr) Y_n^m(\hat{\mathbf{x}})\}, \quad \mathbf{N}_n^m(r, \hat{\mathbf{x}}) = \frac{1}{ik} \nabla \times \mathbf{M}_n^m(r, \hat{\mathbf{x}}),$$

which are the radiation solutions of the Maxwell equation (2.7) in $\mathbb{R}^3 \setminus \{0\}$. In the domain $\mathbb{R}^3 \setminus \bar{B}_R$, the solution $\mathbf{E}$ of (2.7)–(2.9) can be written as, for $r > R$,

$$\mathbf{E}(r, \hat{\mathbf{x}}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n \frac{a_{nm} \mathbf{M}_n^m(r, \hat{\mathbf{x}})}{h_n^{(1)}(kR) \sqrt{n(n+1)}} + \frac{ikR b_{nm} \mathbf{N}_n^m(r, \hat{\mathbf{x}})}{z_n^{(1)}(kR) \sqrt{n(n+1)}}, \quad (2.11)$$

where $z_n^{(1)}(kR) = h_n^{(1)}(kR) + kR h_n^{(1)'}(kR)$, and a_{nm}, b_{nm} are determined by the trace of $\mathbf{E}$ on Γ_R through $\hat{\mathbf{x}} \times \mathbf{E}|_{\Gamma_R} = \sum_{n=1}^{\infty} \sum_{m=-n}^n a_{nm} \mathbf{U}_n^m + b_{nm} \mathbf{V}_n^m$. The series in (2.11) converges uniformly of $r > R$.

Now we turn to the introduction of the absorbing PML layer. We surround the domain $\Omega_R = B_R \setminus \bar{D}$ with a PML layer $\Omega^{\text{PML}} = \{\mathbf{x} \in \mathbb{R}^3 : R < |\mathbf{x}| < \rho\}$. Let $\alpha(r) = 1 + i\sigma(r)$ be the model medium property which satisfies

$$\sigma \in C(\mathbb{R}), \quad \sigma \geq 0, \quad \text{and } \sigma = 0 \text{ for } r \leq R.$$

Denote by $\tilde{r}$ the complex radius defined by

$$\tilde{r} = \tilde{r}(r) = \begin{cases} r & \text{if } r \leq R, \\ \int_0^r \alpha(t) dt = r\beta(r) & \text{if } r \geq R. \end{cases}$$

It is easy to check that the vector wave functions satisfy

$$\begin{aligned} \mathbf{M}_n^m(r, \hat{\mathbf{x}}) &= h_n^{(1)}(kr) \nabla_{\partial B_1} Y_n^m(\hat{\mathbf{x}}) \times \hat{\mathbf{x}}, \\ \mathbf{N}_n^m(r, \hat{\mathbf{x}}) &= \frac{1}{ik} \nabla \times \mathbf{M}_n^m \\ &= \frac{\sqrt{n(n+1)}}{ikr} z_n^{(1)}(kr) \mathbf{U}_n^m(\hat{\mathbf{x}}) + \frac{n(n+1)}{ikr} h_n^{(1)}(kr) Y_n^m(\hat{\mathbf{x}}) \hat{\mathbf{x}}. \end{aligned}$$

We introduce

$$\begin{aligned} \tilde{\mathbf{M}}_n^m(\tilde{r}, \hat{\mathbf{x}}) &= h_n^{(1)}(k\tilde{r}) \nabla_{\partial B_1} Y_n^m(\hat{\mathbf{x}}) \times \hat{\mathbf{x}}, \\ \tilde{\mathbf{N}}_n^m(\tilde{r}, \hat{\mathbf{x}}) &= \frac{1}{ik} \tilde{\nabla} \times \tilde{\mathbf{M}}_n^m \\ &= \frac{\sqrt{n(n+1)}}{ik\tilde{r}} z_n^{(1)}(k\tilde{r}) \mathbf{U}_n^m(\hat{\mathbf{x}}) + \frac{n(n+1)}{ik\tilde{r}} h_n^{(1)}(k\tilde{r}) Y_n^m(\hat{\mathbf{x}}) \hat{\mathbf{x}}, \end{aligned}$$

where $\tilde{\nabla} \times$ is the curl operator with respect to the complex spherical variables $(\tilde{r}, \vartheta, \varphi)$, that is, for $\Phi = \Phi_r \mathbf{e}_r + \Phi_\vartheta \mathbf{e}_\vartheta + \Phi_\varphi \mathbf{e}_\varphi$,

$$\begin{aligned} \tilde{\nabla} \times \Phi &= \frac{1}{\tilde{r} \sin \vartheta} \left(\frac{\partial}{\partial \vartheta} (\sin \vartheta \Phi_\varphi) - \frac{\partial \Phi_\vartheta}{\partial \varphi} \right) \mathbf{e}_r \\ &\quad + \frac{1}{\tilde{r}} \left(\frac{1}{\sin \vartheta} \frac{\partial \Phi_r}{\partial \varphi} - \frac{\partial (\tilde{r} \Phi_\varphi)}{\partial \tilde{r}} \right) \mathbf{e}_\vartheta \\ &\quad + \frac{1}{\tilde{r}} \left(\frac{\partial (\tilde{r} \Phi_\vartheta)}{\partial \tilde{r}} - \frac{\partial \Phi_\varphi}{\partial \vartheta} \right) \mathbf{e}_\varphi. \end{aligned}$$

It is easy to check that $\tilde{\nabla} \times \Phi = A \nabla \times B \Phi$, where $A = \text{diag}(\beta^{-2}, \alpha^{-1}\beta^{-1}, \alpha^{-1}\beta^{-1})$ and $B = \text{diag}(\alpha, \beta, \beta)$ are 3×3 diagonal matrices.

We follow [M03] to derive the PML equation. For any

$$\lambda = \sum_{n=1}^{\infty} \sum_{m=-n}^n a_{nm} \mathbf{U}_n^m + b_{nm} \mathbf{V}_n^m \in \mathbf{H}^{-1/2}(\text{Div}; \Gamma_R),$$

let $\mathbb{E}(\lambda)(\tilde{r}, \hat{\mathbf{x}})$ be the PML extension given by

$$\mathbb{E}(\lambda)(\tilde{r}, \hat{\mathbf{x}}) = \sum_{n=1}^{\infty} \sum_{m=-n}^n \frac{a_{nm} \tilde{\mathbf{M}}_n^m(\tilde{r}, \hat{\mathbf{x}})}{h_n^{(1)}(kR) \sqrt{n(n+1)}} + \frac{ikR b_{nm} \tilde{\mathbf{N}}_n^m(\tilde{r}, \hat{\mathbf{x}})}{z_n^{(1)}(kR) \sqrt{n(n+1)}}. \quad (2.12)$$

For the solution $\mathbf{E}$ of the scattering problem (2.7)-(2.9), let $\tilde{\mathbf{E}} = \mathbb{E}(\hat{\mathbf{x}} \times \mathbf{E}|_{\Gamma_R})$ be the PML extension of $\hat{\mathbf{x}} \times \mathbf{E}|_{\Gamma_R}$. Since $\tilde{r} = r$ on Γ_R , we know that $\hat{\mathbf{x}} \times \tilde{\mathbf{E}} = \hat{\mathbf{x}} \times \mathbf{E}$ on Γ_R . On the other hand, since $h_n^{(1)}(z) \sim \frac{1}{z} e^{i(z - \frac{1}{2}n\pi - \frac{1}{2}\pi)}$ asymptotically as $|z| \rightarrow \infty$, heuristically $\tilde{\mathbf{E}}(\tilde{r}, \hat{\mathbf{x}})$ will decay exponentially for $r > R$. It is obvious that $\tilde{\mathbf{E}}$ satisfies

$$\tilde{\nabla} \times \tilde{\nabla} \times \tilde{\mathbf{E}} - k^2 \tilde{\mathbf{E}} = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{B}_R,$$

which gives the desired PML equation in the spherical coordinates

$$\nabla \times B(A \nabla \times B \tilde{\mathbf{E}}) - k^2 A^{-1} \tilde{\mathbf{E}} = 0 \quad \text{in } \mathbb{R}^3 \setminus \bar{B}_R.$$

The PML problem is then to find $\hat{\mathbf{E}}$, which approximates $\mathbf{E}$ in Ω_R and $B\tilde{\mathbf{E}}$ in $\Omega^{\text{PML}} = B_\rho \setminus \bar{B}_R$, as the solution of the following system

$$\nabla \times BA(\nabla \times \hat{\mathbf{E}}) - k^2 (BA)^{-1} \hat{\mathbf{E}} = 0 \quad \text{in } \Omega_\rho = B_\rho \setminus \bar{D}, \quad (2.13)$$

$$\mathbf{n} \times \hat{\mathbf{E}} = \mathbf{g} \quad \text{on } \Gamma_D, \quad \hat{\mathbf{x}} \times \hat{\mathbf{E}} = 0 \quad \text{on } \Gamma_\rho. \quad (2.14)$$

The first hint of why the PML method should work is the following estimate for the PML extension.

Lemma 2.1. *For any $\lambda \in \mathbf{H}^{-1/2}(\text{Div}; \Gamma_R)$, let $\mathbb{E}(\lambda)$ be the PML extension in (2.12). Then, for any $r > R$, we have*

$$\|\hat{\mathbf{x}} \times \mathbb{E}(\lambda)\|_{\mathbf{H}^{-1/2}(\text{Div}; \Gamma_r)} \leq C(1 + kR) e^{-\text{Im}(k\tilde{r})(1 - \frac{R^2}{|\tilde{r}|^2})^{1/2}} \|\lambda\|_{\mathbf{H}^{-1/2}(\text{Div}; \Gamma_R)}.$$

We give a brief description of the proof of the lemma. The full proof can be found in [CC06]. We first recall the following exponential decay estimate of the first Hankel function proved in [CL05] based on the Macdonald formula.

Lemma 2.2. *For any $\nu \in \mathbb{R}$, $z \in \mathbb{C}_{++} = \{z \in \mathbb{C} : \text{Im}(z) \geq 0, \text{Re}(z) \geq 0\}$ and $\Theta \in \mathbb{R}$ such that $0 < \Theta < |z|$, we have*

$$|H_\nu^{(1)}(z)| \leq e^{-\text{Im}(z)(1 - (\Theta^2/|z|^2))^{1/2}} |H_\nu^{(1)}(\Theta)|.$$

Next by simple calculation we have

$$\hat{\mathbf{x}} \times \mathbb{E}(\lambda) = \sum_{n=1}^{\infty} \sum_{m=-n}^n \frac{h_n^{(1)}(k\tilde{r})}{h_n^{(1)}(kR)} a_{nm} \mathbf{U}_n^m + \frac{R}{\tilde{r}} \frac{z_n^{(1)}(k\tilde{r})}{z_n^{(1)}(kR)} b_{nm} \mathbf{V}_n^m$$

which together with following estimate for the spherical Hankel functions due to Nédélec [N80, p.195] implies Lemma 2.1.

Lemma 2.3. *For any $\Theta > 0$, $\delta_n(\Theta) = \frac{z_n^{(1)}(\Theta)}{h_n^{(1)}(\Theta)}$ satisfies $|\delta_n(\Theta)| \geq \frac{n(n+1)}{2\Theta^2+n+1}$.*

2.3.2 Finite Element Discretization

We start by introducing the weak formulation of the PML problem (2.13)–(2.14). Let

$$b(\Psi, \Phi) = \int_{\Omega_\rho} (BA \nabla \times \Psi \cdot \nabla \times \bar{\Phi} - k^2 (BA)^{-1} \Psi \cdot \bar{\Phi}) d\mathbf{x}.$$

Then the weak formulation of (2.13)–(2.14) is: Given $\mathbf{g} \in \mathbf{H}^{-1/2}(\text{Div}; \Gamma_D)$, find $\hat{\mathbf{E}} \in \mathbf{H}(\mathbf{curl}, \Omega_\rho)$, such that $\mathbf{n} \times \hat{\mathbf{E}} = \mathbf{g}$ on Γ_D , $\hat{\mathbf{x}} \times \hat{\mathbf{E}} = 0$ on Γ_ρ , and

$$b(\hat{\mathbf{E}}, \Phi) = 0, \quad \forall \Phi \in \mathbf{H}_0(\mathbf{curl}; \Omega_\rho). \quad (2.15)$$

Let Γ_ρ^h , which consists of piecewise triangles whose vertices lie on Γ_ρ , be an approximation of Γ_ρ . Let Ω_ρ^h be the subdomain of Ω_ρ bounded by Γ_D and Γ_ρ^h . Let $\mathcal{M}_h$ be a regular triangulation of the domain Ω_ρ^h . We will use the lowest order Nédélec edge element [N80] for which the finite element space $\mathbf{U}_h$ over $\mathcal{M}_h$ is defined by

$$\mathbf{U}_h = \{\mathbf{u} \in \mathbf{H}(\mathbf{curl}; \Omega_\rho^h) : \mathbf{u}|_K = \mathbf{a}_K + \mathbf{b}_K \times \mathbf{x}, \forall \mathbf{a}_K, \mathbf{b}_K \in \mathbb{R}^3, \forall K \in \mathcal{M}_h\}.$$

Degrees of freedom of functions $\mathbf{u} \in \mathbf{U}_h$ on every $K \in \mathcal{M}_h$ are $\int_{e_i} \mathbf{u} \cdot d\mathbf{l}$, $i = 1, \dots, 6$, where $e_1, \dots, e_6$ are six edges of K . Denote by $\mathring{\mathbf{U}}_h = \mathbf{U}_h \cap \mathbf{H}_0(\mathbf{curl}; \Omega_\rho^h)$. In the following, we will always assume that the functions in $\mathring{\mathbf{U}}_h$ are extended to the domain Ω_ρ by zero so that any function $\mathbf{u} \in \mathring{\mathbf{U}}_h$ is also a function in $\mathbf{H}_0(\mathbf{curl}; \Omega_\rho)$. The finite element approximation to (2.15) reads as follows: Find $\mathbf{E}_h \in \mathbf{U}_h$ such that $\mathbf{n} \times \mathbf{E}_h = \mathbf{g}_h$ on Γ_D , $\mathbf{n} \times \mathbf{E}_h = 0$ on Γ_ρ^h , and

$$b(\mathbf{E}_h, \Phi_h) = 0, \quad \forall \Phi_h \in \mathring{\mathbf{U}}_h.$$

Here $\mathbf{g}_h$ is some edge element approximation of $\mathbf{g}$ on Γ_D . Notice that the integral in $b(\mathbf{E}_h, \Phi_h)$ is actually over Ω_ρ^h since $\Phi_h = 0$ in $\Omega_\rho \setminus \Omega_\rho^h$ by our convention.

For any $K \in \mathcal{M}_h$, we denote by h_K its diameter. Let $\mathcal{F}_h$ be the set of all faces of the mesh $\mathcal{M}_h$ that do not lie on Γ_D and Γ_ρ^h . For any $F \in \mathcal{F}_h$, h_F

stands for its diameter. For any interior face F which is a common face of K_1 and K_2 in $\mathcal{M}_h$, we define the following jump residuals across F

$$\begin{aligned} [\mathbf{n} \times (BA \nabla \times \mathbf{E}_h)] &= \mathbf{n}_F \times (BA \nabla \times (\mathbf{E}_h|_{K_1} - \mathbf{E}_h|_{K_2})), \\ [k^2(BA)^{-1} \mathbf{E}_h \cdot \mathbf{n}] &= k^2(BA)^{-1}(\mathbf{E}_h|_{K_1} - \mathbf{E}_h|_{K_2}) \cdot \mathbf{n}_F, \end{aligned}$$

using the convention that the unit norm vector $\mathbf{n}_F$ to F points from K_2 to K_1 . The local error indicator η_K for any $K \in \mathcal{M}_h$ is defined as

$$\begin{aligned} \eta_K^2 &= h_K^2 \|k^2(BA)^{-1} \mathbf{E}_h - \nabla \times BA \nabla \times \mathbf{E}_h\|_{\mathbf{L}^2(K)}^2 \\ &\quad + h_K^2 \|\operatorname{div}(k^2(BA)^{-1} \mathbf{E}_h)\|_{L^2(K)}^2 \\ &\quad + h_K \|[\mathbf{n} \times (BA \nabla \times \mathbf{E}_h)]\|_{\mathbf{L}^2(\partial K)}^2 + h_K \| [k^2(BA)^{-1} \mathbf{E}_h \cdot \mathbf{n}] \|_{L^2(\partial K)}^2. \end{aligned}$$

The following theorem is the main result of this section whose proof can be found in [CC06].

Theorem 2.3. *There exists a constant C depending only on the minimum angle of the mesh $\mathcal{M}_h$ and $\sigma_0 = \max_{\tau \in \mathbb{R}} \sigma(\tau)$ such that the following a posteriori error estimate is valid:*

$$\begin{aligned} &\|\mathbf{E} - \mathbf{E}_h\|_{\mathbf{H}(\operatorname{curl}; \Omega_R)} \\ &\leq C \|\mathbf{g} - \mathbf{g}_h\|_{\mathbf{H}^{-1/2}(\operatorname{Div}; \Gamma_D)} + C(1 + kR)^3 R^{1/2} \left(\sum_{K \in \mathcal{M}_h} \eta_K^2 \right)^{1/2} \\ &\quad + C(1 + kR)^3 e^{-\operatorname{Im}(k\bar{\rho})(1 - (R^2/|\bar{\rho}|^2))^{1/2}} \|\hat{\mathbf{x}} \times \mathbf{E}_h\|_{\mathbf{H}^{-1/2}(\operatorname{Div}; \Gamma_R)}. \end{aligned}$$

2.3.3 A Numerical Example

The implementation of the adaptive algorithm in this section is based on the adaptive finite element package ALBERT [SS00] and its adaptation to the edge element by Dr. Long Wang. We use the a posteriori error estimate in Theorem 2.3 to determine the PML parameters. We choose the PML medium property as the power function and thus we need only to specify the thickness $\rho - R$ of the layer and the medium parameter σ_0 . Recall from Theorem 2.3 that the a posteriori error estimate consists of two parts: the PML error and the finite element discretization error. In our implementation we first choose ρ and σ_0 such that the exponentially decaying factor:

$$e^{-k \operatorname{Im}(\bar{\rho})(1 - (R^2/|\bar{\rho}|^2))^{1/2}} \leq 10^{-8},$$

which makes the PML error negligible compared with the finite element discretization errors. Once the PML region and the medium property are fixed, we use the standard finite element adaptive strategy to modify the mesh according to the a posteriori error estimate (cf. e.g. [CL05]).

The following numerical example concerns the scattering of the plane wave $\mathbf{E}_i$ perpendicular to the screen described in last section. Figure 2.3 shows the

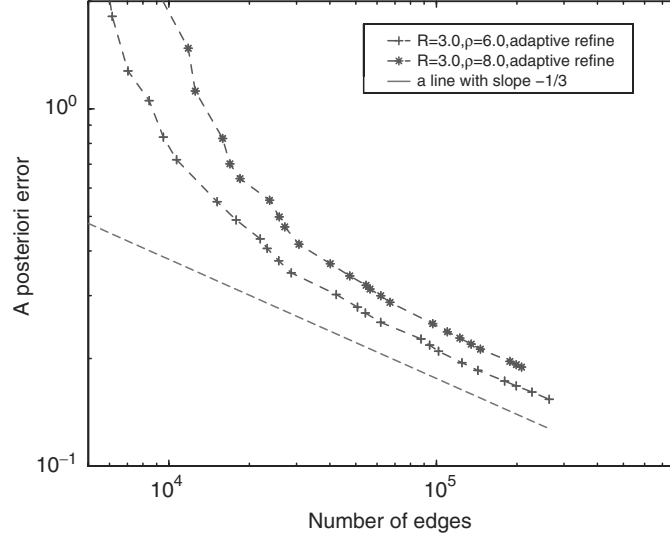


Fig. 2.3. Quasi-optimality of the adaptive mesh refinements of the a posteriori error estimator

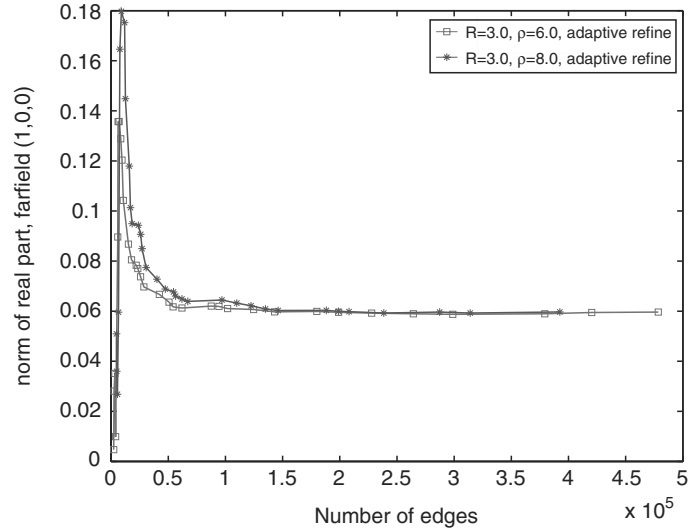


Fig. 2.4. The module of the real part of the far fields in the direction $(1, 0, 0)$

$\log N_k$ - $\log \mathcal{E}_k$ curves, where $\mathcal{E}_k = (\sum_{K \in \mathcal{M}_k} \eta_K^2)^{1/2}$ is the associated a posteriori error estimate. It indicates that the meshes and the associated numerical complexity are quasi-optimal: $\mathcal{E}_k \approx C N_k^{-1/3}$ is valid asymptotically.

Figure 2.4 shows the far fields in the direction $(1, 0, 0)$ for different choices of the PML parameters. We observe that the far fields are insensitive to the choices of PML parameters. More numerical examples can be found in [CC06].

2.4 The Eddy Current Problem

Three dimensional eddy current problems describe very low-frequency electromagnetic phenomena by quasi-static Maxwell's equations. In this case, displacement currents may be neglected and thus Maxwell's equations become

$$\begin{cases} \mathbf{curl} \mathbf{H} = \mathbf{J} & \text{in } \mathbb{R}^3, & (\text{Ampere's law}) \\ \mu \frac{\partial \mathbf{H}}{\partial t} + \mathbf{curl} \mathbf{E} = 0 & \text{in } \mathbb{R}^3, & (\text{Farady's law}) \\ \text{div}(\mu \mathbf{H}) = 0 & \text{in } \mathbb{R}^3, \end{cases} \quad (2.16)$$

where $\mathbf{E}$ is the electric field, $\mathbf{H}$ is the magnetic field, and $\mathbf{J}$ is the total current defined by:

$$\mathbf{J} = \begin{cases} \sigma \mathbf{E} & \text{in } \Omega_c, & (\text{conducting region}) \\ \mathbf{J}_s & \text{in } \mathbb{R}^3 \setminus \overline{\Omega_c}. & (\text{nonconducting region}) \end{cases}$$

Here μ is the magnetic permeability, σ is the electric conductivity, $\mathbf{J}_s$ is the solenoidal source current carried by some coils in the air, and Ω_c is the conducting region which carries eddy currents. To avoid extra complicated constraints on $\mathbf{J}_s$, we assume $\text{supp}(\mathbf{J}_s) \cap \Omega_c = \emptyset$.

Let $\Omega \subset \mathbb{R}^3$ be a sufficiently large convex polyhedral domain containing all conductors and coils (see Fig. 2.5 for a typical model with one conductor and one coil). We assume that μ and σ are real valued $L^\infty(\Omega)$ functions and there exist two positive constants $\mu_{\min}$ and $\sigma_{\min}$ such that $\mu \geq \mu_{\min}$ in Ω and $\sigma \geq \sigma_{\min}$ in Ω_c . Furthermore, we assume $\sigma \equiv 0$ outside of Ω_c .

Since $\text{div} \mathbf{J}_s \equiv 0$, there exists a source magnetic field $\mathbf{H}_s$ such that

$$\mathbf{J}_s = \mathbf{curl} \mathbf{H}_s \quad \text{in } \mathbb{R}^3. \quad (2.17)$$

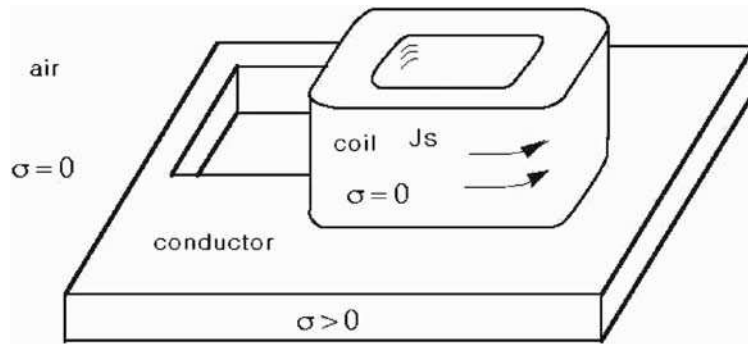


Fig. 2.5. Setting of the eddy current problems: A conductor with a hole and a coil

The field $\mathbf{H}_s$ can be written explicitly by the Biot–Savart Law for general coils:

$$\mathbf{H}_s := \mathbf{curl} \mathbf{A}_s \quad \text{where} \quad \mathbf{A}_s(\mathbf{x}) := \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{\mathbf{J}_s(\mathbf{y})}{|\mathbf{x} - \mathbf{y}|} d\mathbf{y}.$$

In the following we are going to find the residual $\mathbf{H}_0 := \mathbf{H} - \mathbf{H}_s$. Clearly, by (2.16) and (2.4), we have

$$\mathbf{curl} \mathbf{H}_0 = 0 \quad \text{in } \Omega \setminus \overline{\Omega_c}.$$

Our goal is to write $\mathbf{H}_0$ as $\nabla\psi$ for some scalar potential ψ . Since $\Omega \setminus \overline{\Omega_c}$ may not be simply connected, ψ may not be unique. To deal with this difficulty, we introduce the following assumption (see [ABDG98, Hypothesis 3.3]).

Hypothesis. There exist I connected open surfaces $\Sigma_0, \dots, \Sigma_I$, called “cuts”, contained in $\Omega \setminus \overline{\Omega_c}$, such that

1. Each cut Σ_i is an open part of some smooth two-dimensional manifold with Lipschitz-continuous boundary, $i = 1, \dots, I$
2. The boundary of Σ_i is contained in $\partial\Omega_c$ and $\overline{\Sigma_i} \cap \overline{\Sigma_j} = \emptyset$ for $i \neq j$
3. The open set $\Omega^\circ := (\Omega \setminus \overline{\Omega_c}) \setminus (\cup_{i=1}^I \Sigma_i)$ is simply connected and pseudo-Lipschitz (see [ABDG98, Definition 3.1] for the definition of pseudo-Lipschitz domain)

For each Σ_i , we fix its unit normal vector $\mathbf{n}$ pointing to one side. Define

$$\Theta := \{\varphi \in H^1(\Omega^\circ) : [\varphi]_{\Sigma_j} = \text{const.}, \quad 1 \leq j \leq I\},$$

where $[\varphi]_{\Sigma_j}$ is the jump of φ across the cut Σ_j . For any $\varphi \in \Theta$, we can extend $\nabla\varphi \in \mathbf{L}^2(\Omega^\circ)$ continuously to a function $\tilde{\nabla}\varphi \in \mathbf{L}^2(\Omega \setminus \overline{\Omega_c})$ such that

$$\tilde{\nabla}\varphi = \nabla\varphi \quad \text{in } \Omega^\circ.$$

It is known [ABDG98, Lemma 3.11] that for any $\varphi \in H^1(\Omega^\circ)$, $\varphi \in \Theta$ if and only if $\mathbf{curl}(\tilde{\nabla}\varphi) = 0$ in $\Omega \setminus \overline{\Omega_c}$.

Since Ω° is simply connected, there exists a unique potential $\psi \in \Theta/\mathbb{R}^1$ such that

$$\mathbf{H}_0 = \nabla\psi \quad \text{in } \Omega^\circ.$$

Thus the second equation in (2.16) becomes

$$\begin{cases} \mu \frac{\partial (\mathbf{H}_s + \nabla\psi)}{\partial t} + \mathbf{curl} \mathbf{E} = 0 & \text{in } \Omega^\circ, \\ \mu \frac{\partial (\mathbf{H}_s + \mathbf{H}_0)}{\partial t} + \mathbf{curl} \mathbf{E} = 0 & \text{in } \Omega_c. \end{cases} \quad (2.18)$$

For the initial conditions, we set

$$\psi(\cdot, 0) = 0, \quad \mathbf{H}_0(\cdot, 0) = \mathbf{0}. \quad (2.19)$$

Since the total electro-magnetic energy is finite, we may assume $\mathbf{H} \in \mathbf{L}^2(\mathbb{R}^3)$ which implies $\mathbf{curl} \mathbf{E} \in \mathbf{L}^2(\mathbb{R}^3)$. Assuming Ω large enough, we set the following boundary condition on $\partial\Omega$:

$$\nabla\psi \cdot \mathbf{n} = -\mathbf{H}_s \cdot \mathbf{n} \quad \text{on } \partial\Omega. \quad (2.20)$$

Our next goal is going to derive a weak formula for (2.16), starting from (2.18). Since the tangential field $\mathbf{H}_0 \times \mathbf{n}$ is continuous through $\partial\Omega_c$, we add this constraint to the test functions and define

$$\begin{aligned} \mathbf{X} = \Big\{ \mathbf{v} : \mathbf{v} = \tilde{\nabla}\varphi \text{ in } \Omega \setminus \overline{\Omega_c} \text{ for some } \varphi \in \Theta/\mathbb{R}^1 \text{ and } \mathbf{v} = \mathbf{w} \text{ in } \Omega_c \\ \text{for some } \mathbf{w} \in \mathbf{H}(\mathbf{curl}; \Omega_c) \text{ such that } \tilde{\nabla}\varphi \times \mathbf{n} = \mathbf{w} \times \mathbf{n} \text{ on } \partial\Omega_c \Big\}. \end{aligned}$$

It is clear that $\mathbf{X} \subset \mathbf{H}(\mathbf{curl}; \Omega)$. For any $\varphi \in \Theta/\mathbb{R}^1$, we multiply the first equation of (2.18) by $\nabla\varphi$, integrate by part to obtain

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega^\circ} \mu (\nabla\psi + \mathbf{H}_s) \cdot \nabla\varphi &= - \int_{\Omega^\circ} \mathbf{curl} \mathbf{E} \cdot \nabla\varphi \\ &= - \int_{\partial\Omega^\circ} \mathbf{curl} \mathbf{E} \cdot \mathbf{n} \varphi. \end{aligned} \quad (2.21)$$

Note that $\partial\Omega^\circ = \partial\Omega \cup \partial\Omega_c \cup (\cup_{j=1}^I \Sigma_j)$. By (2.18) and (2.20) we have $\mathbf{curl} \mathbf{E} \cdot \mathbf{n} = 0$ on $\partial\Omega$. Thus

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega^\circ} \mu (\nabla\psi + \mathbf{H}_s) \cdot \nabla\varphi &= \sum_{j=1}^I \int_{\Sigma_j} \mathbf{E} \cdot [\mathbf{n} \times \nabla\varphi]_{\Sigma_j} \\ &\quad + \int_{\partial\Omega_c} \mathbf{E} \cdot (\mathbf{n} \times \tilde{\nabla}\varphi) \\ &= \int_{\partial\Omega_c} \mathbf{E} \cdot (\mathbf{n} \times \tilde{\nabla}\varphi), \end{aligned} \quad (2.22)$$

where $\mathbf{n}$ is the unit outer normal to $\partial\Omega_c$, and we have used the fact that $[\nabla\varphi \times \mathbf{n}]_{\Sigma_j} = \mathbf{0}$ on Σ_j because of $\varphi \in \Theta$. For any $\mathbf{w} \in \mathbf{H}(\mathbf{curl}; \Omega_c)$, we multiply the second equation of (2.18) by $\mathbf{w}$ and integrate by part to obtain

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega_c} \mu (\mathbf{H}_s + \mathbf{H}_0) \cdot \mathbf{w} &= - \int_{\Omega_c} \mathbf{curl} \mathbf{E} \cdot \mathbf{w} \\ &= \int_{\partial\Omega_c} \mathbf{E} \cdot (\mathbf{n} \times \mathbf{w}) - \int_{\Omega_c} \mathbf{E} \cdot \mathbf{curl} \mathbf{w}. \end{aligned}$$

By (2.2) and the first equation of (2.16), we have

$$\frac{\partial}{\partial t} \int_{\Omega_c} \mu (\mathbf{H}_s + \mathbf{H}_0) \cdot \mathbf{w} + \int_{\Omega_c} \sigma^{-1} \mathbf{curl} \mathbf{H}_0 \cdot \mathbf{curl} \mathbf{w} = \int_{\partial\Omega_c} \mathbf{E} \cdot (\mathbf{n} \times \mathbf{w}), \quad (2.23)$$

where $\mathbf{n}$ is the unit normal on $\partial\Omega_c$ pointing to the exterior of Ω_c , and we have used (2.17) and the fact that $\mathbf{J}_s \equiv \mathbf{0}$ in Ω_c . By the tangential continuity of the electric field $\mathbf{E}$, we add (2.21) to (2.23) and obtain, for any $\mathbf{v} \in \mathbf{X}$ such that $\mathbf{v} = \tilde{\nabla}\varphi$ in $\Omega \setminus \overline{\Omega_c}$ and $\mathbf{v} = \mathbf{w}$ in Ω_c ,

$$\begin{aligned} \frac{\partial}{\partial t} \int_{\Omega^\circ} \mu \nabla \psi \cdot \nabla \varphi + \frac{\partial}{\partial t} \int_{\Omega_c} \mu \mathbf{H}_0 \cdot \mathbf{w} + \int_{\Omega_c} \sigma^{-1} \mathbf{curl} \mathbf{H}_0 \cdot \mathbf{curl} \mathbf{w} \\ = - \frac{\partial}{\partial t} \int_{\Omega} \mu \mathbf{H}_s \cdot \mathbf{v}. \end{aligned}$$

For the convenience in notation, we drop the subscript of $\mathbf{H}_0$ and denote the reaction field by $\mathbf{H}$ in the rest of this section. Thus we are led to the following variational problem based on the magnetic reaction field and magnetic scalar potential: Find $\mathbf{H} \in \mathbf{L}^2((0, T); \mathbf{X})$ such that $\mathbf{H}(\cdot, 0) \equiv \mathbf{0}$ and

$$\frac{\partial}{\partial t} \int_{\Omega} \mu \mathbf{H} \cdot \mathbf{v} + \int_{\Omega_c} \sigma^{-1} \mathbf{curl} \mathbf{H} \cdot \mathbf{curl} \mathbf{v} = - \frac{\partial}{\partial t} \int_{\Omega} \mu \mathbf{H}_s \cdot \mathbf{v} \quad \forall \mathbf{v} \in \mathbf{X}. \quad (2.24)$$

We use a fully discrete scheme to approximate (2.24). Let $\{t_0, \dots, t_M\}$ form a partition of the time interval $[0, T]$ and $\tau_n = t_n - t_{n-1}$ be the n th timestep. Let $\mathcal{T}_n$ be a regular tetrahedral triangulation of Ω such that $\mathcal{T}_n^c := \mathcal{T}_n|_{\Omega_c}$ and $\mathcal{T}_n^\circ := \mathcal{T}_n|_{\Omega^\circ}$ are triangulations of Ω_c and Ω° respectively. Let $\mathcal{T}_{\text{init}}$ be the initial regular triangulation of Ω such that each $\mathcal{T}_n$, $n = 0, \dots, M$, is a refinement of $\mathcal{T}_{\text{init}}$.

Let $V_n \subset H^1(\Omega)$ and $V_n^\circ \subset H^1(\Omega^\circ)$ be the conforming linear Lagrangian finite element spaces over $\mathcal{T}_n$ and $\mathcal{T}_n^\circ$ respectively, and $\mathbf{V}_n^c \subset \mathbf{H}(\mathbf{curl}; \Omega_c)$ be the Nédélec edge element space of the lowest order over $\mathcal{T}_n^c$ [N80]. We introduce the finite element space $\mathbf{X}_n \subset \mathbf{X}$ by

$$\begin{aligned} \mathbf{X}_n = \left\{ \mathbf{v} : \mathbf{v} = \tilde{\nabla}\varphi_n \text{ in } \Omega \setminus \overline{\Omega_c} \text{ for some } \varphi_n \in \Theta \cap V_n^\circ/\mathbb{R}^1 \text{ and } \mathbf{v} = \mathbf{w}_n \text{ in } \Omega_c \right. \\ \left. \text{for some } \mathbf{w}_n \in \mathbf{V}_n^c \text{ such that } \tilde{\nabla}\varphi_n \times \mathbf{n} = \mathbf{w}_n \times \mathbf{n} \text{ on } \partial\Omega_c \right\}. \end{aligned}$$

Thus a fully discrete scheme of (2.24) is: Find $\mathbf{H}_n \in \mathbf{X}_n$ such that $\mathbf{H}_0 \equiv \mathbf{0}$ and

$$\int_{\Omega} \mu \frac{\mathbf{H}_n - \mathbf{H}_{n-1}}{\tau_n} \cdot \mathbf{v} + \int_{\Omega_c} \sigma^{-1} \mathbf{curl} \mathbf{H}_n \cdot \mathbf{curl} \mathbf{v} = \int_{\Omega} \bar{\mathbf{f}}_n \cdot \mathbf{v} \quad \forall \mathbf{v} \in \mathbf{X}_n, \quad (2.25)$$

where $\mathbf{f} := -\mu \partial \mathbf{H}_s / \partial t$ and $\bar{\mathbf{f}}_n := \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \mathbf{f}$ is the mean value of $\mathbf{f}$ over $[t_{n-1}, t_n]$. The uniqueness and existence of solutions to (2.25) follows directly from the Lax–Milgram Lemma.

As in the second section, the key ingredient in the analysis of a posteriori error estimates for Maxwell's equations is Helmholtz-type decompositions for functions in $\mathbf{H}(\mathbf{curl}; \Omega)$. In the next, we will introduce an $\mathbf{H}(\mathbf{curl})$ -stable decomposition for $\mathbf{X}$. Since both Ω_c and $\Omega \setminus \overline{\Omega_c}$ are multiply connected, it is

difficult to find a scalar function ψ with constant jumps across all “cuts” to define the irrotational part. Instead, we represent these discontinuities by the help of some finite element function [ZCW06].

Theorem 2.4. *Let $\mathbf{X}_{\text{init}}$ be the finite element space over $\mathcal{T}_{\text{init}}$. For any $\mathbf{v} \in \mathbf{X}$, there exists a $\varphi \in H^1(\Omega)/\mathbb{R}^1$, a $\mathbf{v}_{\text{init}} \in \mathbf{X}_{\text{init}}$, and a $\mathbf{v}_s \in \mathbf{H}(\mathbf{curl}; \Omega) \cap \mathbf{H}^1(\Omega_c)$ such that $\mathbf{v}_s = \mathbf{0}$ in $\Omega \setminus \Omega_c$ and*

$$\mathbf{v} = \nabla \varphi + \mathbf{v}_{\text{init}} + \mathbf{v}_s.$$

Furthermore, there exists a positive C depending only on Ω and $\mathcal{T}_{\text{init}}$ such that

$$\|\varphi\|_{1,\Omega} + \|\mathbf{v}_s\|_{1,\Omega_c} + \|\mathbf{v}_{\text{init}}\|_{\mathbf{H}(\mathbf{curl}; \Omega)} \leq C \|\mathbf{v}\|_{\mathbf{H}(\mathbf{curl}; \Omega)}.$$

The following residual based a posteriori error estimate is proved in [ZCW06].

Theorem 2.5. *There exists a positive constant C depending only on Ω , μ , and σ such that for any $0 \leq m \leq M$,*

$$\|\sqrt{\mu} \mathbf{e}(t_m)\|_{0,\Omega}^2 + \|\mathbf{curl} \mathbf{e}\|_{\mathbf{L}^2((0,T); \mathbf{L}^2(\Omega))}^2 \leq C \sum_{n=1}^m \tau_n \left\{ (\eta_{\text{time}}^n)^2 + (\eta_{\text{space}}^n)^2 \right\},$$

where the a posteriori error estimates are given by

$$\begin{aligned} (\eta_{\text{time}}^n)^2 &= \|\mathbf{curl}(\mathbf{H}_n - \mathbf{H}_{n-1})\|_{0,\Omega_c}^2 + \tau_n^{-1} \|\mathbf{f} - \bar{\mathbf{f}}_n\|_{\mathbf{L}^2((t_{n-1}, t_n); \mathbf{L}^2(\Omega))}^2, \\ (\eta_{\text{space}}^n)^2 &= \sum_{T \in \mathcal{T}_n} h_T^2 \left\| \text{div} \left(\bar{\mathbf{f}}_n - \mu \frac{\partial \mathbf{H}_h}{\partial t} \right) \right\|_{0,T}^2 \\ &\quad + \sum_{T \in \mathcal{T}_n^c} h_T^2 \left\| \bar{\mathbf{f}}_n - \mu \frac{\partial \mathbf{H}_h}{\partial t} - \mathbf{curl}(\sigma^{-1} \mathbf{curl} \mathbf{H}_n) \right\|_{0,T}^2 \\ &\quad + \sum_{F \in \mathcal{F}_n^\Omega} h_F \left\| \left[\left(\bar{\mathbf{f}}_n - \mu \frac{\partial \mathbf{H}_h}{\partial t} \right) \cdot \mathbf{n} \right]_F \right\|_{0,F}^2 \\ &\quad + \sum_{F \in \mathcal{F}_n^{\Omega_c}} h_F \left\| [\sigma^{-1} \mathbf{curl} \mathbf{H}_n \times \mathbf{n}]_{J,F} \right\|_{0,F}^2 \\ &\quad + \sum_{F \in \mathcal{F}_n^{\partial\Omega}} h_F \left\| \left(\bar{\mathbf{f}}_n - \mu \frac{\partial \mathbf{H}_h}{\partial t} \right) \cdot \mathbf{n} \right\|_{0,F}^2. \end{aligned}$$

Here $\mathcal{F}_n^\Omega$, $\mathcal{F}_n^{\Omega_c}$, and $\mathcal{F}_n^{\partial\Omega}$ denote the edges in Ω , in Ω_c , and on $\partial\Omega$, respectively.

Based on the a posteriori error estimates in above theorem, an adaptive finite element method with variable time-steps and designed and implemented

in [ZCW06]. The results indicate that our adaptive method has the following very desirable quasi-optimality property:

$$\eta_{\text{total}} \approx C N_{\text{total}}^{-1/4}$$

is valid asymptotically, where η_{total} is the total error estimate (see Theorem 2.5), and $N_{\text{total}} := \sum_{n=1}^M N_n$ with M being the number of time steps and N_n being the number of elements of the mesh $\mathcal{T}_n$ at the n th timestep. We refer to [ZCW06] for more details.

2.5 The Time-Domain Acoustic Scattering Problem

We consider the acoustic scattering problem with the sound-hard boundary condition on the obstacle

$$\frac{\partial u}{\partial t} = -\operatorname{div} \mathbf{p}, \quad \frac{\partial \mathbf{p}}{\partial t} = -\nabla u \quad \text{in } [\mathbb{R}^2 \setminus \bar{D}] \times (0, T), \quad (2.26)$$

$$\mathbf{p} \cdot \mathbf{n}_D = g \quad \text{on } \Gamma_D \times (0, T), \quad (2.27)$$

$$\sqrt{r}(u - \mathbf{p} \cdot \hat{\mathbf{x}}) \rightarrow 0, \quad \text{as } r = |x| \rightarrow \infty, \quad \text{a.e. } t \in (0, T), \quad (2.28)$$

$$u|_{t=0} = u_0, \quad \mathbf{p}|_{t=0} = \mathbf{p}_0. \quad (2.29)$$

Here u is the pressure and $\mathbf{p}$ is the velocity field of the wave. $D \subset \mathbb{R}^2$ is a bounded domain with Lipschitz boundary Γ_D , g is determined by the incoming wave, $\hat{x} = x/|x|$, and $\mathbf{n}_D$ is the unit outer normal to Γ_D . $u_0, \mathbf{p}_0$ are assumed to be supported in some circle $B_R = \{x \in \mathbb{R}^2 : |x| < R\}$ for some $R > 0$. Equation (2.9) is the radiation condition which corresponds to the well-known Sommerfeld radiation condition in the frequency domain. We remark that the results in this chapter can be easily extended to solve the scattering problems with other boundary conditions such as the sound-soft or the impedance boundary condition on Γ_D .

One of the fundamental problem in the efficient simulation of the wave propagation is the reduction of the exterior problem which is defined in the unbounded domain to the problem in the bounded domain. For any $s \in \mathbb{C}$ such that $\operatorname{Re}(s) > 0$, let $u_L = \mathcal{L}(u)$ and $\mathbf{p}_L = \mathcal{L}(\mathbf{p})$ be the Laplace transform of u and $\mathbf{p}$ in time

$$u_L(x, s) = \int_0^\infty e^{-st} u(x, t) dt, \quad \mathbf{p}_L(x, s) = \int_0^\infty e^{-st} \mathbf{p}(x, t) dt.$$

Since u_0 and $\mathbf{p}_0$ are supported inside the circle B_R , we know that u_L satisfies the following Helmholtz equation outside B_R

$$-\Delta u_L + s^2 u_L = 0.$$

Moreover, (2.9) implies that u_L satisfies the radiation condition

$$\sqrt{r} \left(\frac{\partial u_L}{\partial r} + s u_L \right) \rightarrow 0, \quad \text{as } r \rightarrow \infty.$$

Thus we have the following series representation for u_L outside B_R

$$u_L = \sum_{n=-\infty}^{\infty} \frac{K_n(sr)}{K_n(sR)} u_L^n(R, s) e^{in\vartheta}, \quad (2.30)$$

where $u_L^n(R, s) = \frac{1}{2\pi} \int_0^{2\pi} u_L(R, \vartheta, s) e^{-in\vartheta} d\vartheta$, and $K_n(z)$ is the modified Bessel function of order n . Since $\mathbf{p}_0$ is supported in B_R , we have

$$\mathbf{p}_L \cdot \hat{\mathbf{x}} + \sum_{n=-\infty}^{\infty} \frac{K'_n(sR)}{K_n(sR)} u_L^n(R, s) e^{in\vartheta} = 0 \quad \text{on } \Gamma_R.$$

By taking the inverse Laplace transform we obtain the following Dirichlet-to-Neumann boundary condition for the solution of the scattering problem (2.26)–(2.29) on $\Gamma_R \times (0, T)$

$$\mathbf{p} \cdot \hat{\mathbf{x}} + \sum_{n=-\infty}^{\infty} \left[\mathcal{L}^{-1} \left(\frac{K'_n(sR)}{K_n(sR)} \right) * u_n(R, t) \right] e^{in\vartheta} = 0, \quad (2.31)$$

where $u_n(R, t) = \frac{1}{2\pi} \int_0^{2\pi} u(R, \vartheta, t) e^{-in\vartheta} d\vartheta$ is the Fourier coefficient of u on Γ_R .

Theorem 2.6. Assume that $u_0 \in H^2(\Omega_R)$, $\mathbf{p}_0 \in H(\text{div}; \Omega_R)$, $\text{div} \mathbf{p}_0 \in H^2(\Omega_R)$ so that $\text{supp}(u_0) \subset B_R$, $\text{supp}(\mathbf{p}_0) \subset B_R$, and $g \in H^2(0, T; H^{-1/2}(\Gamma_D))$. Let the following compatibility conditions are satisfied $g|_{t=0} = \mathbf{p}_0 \cdot \mathbf{n}_D$, $\partial_t g|_{t=0} = -\nabla u_0 \cdot \mathbf{n}_D$ on Γ_D . Then the problem (2.26)–(2.27), (2.31), (2.29) has a unique solution $u \in L^2(0, T; H^1(\Omega_R)) \cap H^1(0, T; L^2(\Omega_R))$, $\mathbf{p} \in L^2(0, T; H(\text{div}, \Omega_R)) \cap H^1(0, T; L^2(\Omega_R))$ such that $u|_{t=0} = u_0$, $\mathbf{p}|_{t=0} = \mathbf{p}_0$, and for any $v \in L^2(0, T; H^1(\Omega_R))$, $\mathbf{q} \in L^2(0, T; L^2(\Omega_R))$,

$$\begin{aligned} \int_0^T \left[\left(\frac{\partial u}{\partial t}, v \right) - (p, \nabla v) - \langle (\mathcal{L}^{-1} \circ G \circ \mathcal{L})(u), v \rangle_{\Gamma_R} \right] dt &= \int_0^T \langle g, v \rangle_{\Gamma_D} dt, \\ \int_0^T \left[\left(\frac{\partial \mathbf{p}}{\partial t} \cdot \mathbf{q} \right) + (\nabla u \cdot \mathbf{q}) \right] dt &= 0. \end{aligned}$$

Here $(\mathcal{L}^{-1} \circ G \circ \mathcal{L})(u) \in L^2(0, T; H^{-1/2}(\Gamma_R))$. Moreover, $(u, \mathbf{p})$ satisfies the following stability estimate

$$\begin{aligned} & \left[\int_0^T \left(\|\partial_t u\|_{L^2(\Omega_R)}^2 + \|\nabla u\|_{L^2(\Omega_R)}^2 + \|\partial_t \mathbf{p}\|_{L^2(\Omega_R)}^2 + \|\text{div} \mathbf{p}\|_{L^2(\Omega_R)}^2 \right) dt \right]^{1/2} \\ & \leq C \max(1, T^{3/2}) \|(u_0, \mathbf{p}_0)\|_{\Omega_R} + C \max(1, T) \|g\|_{H^2(0, T; H^{-1/2}(\Gamma_D))}, \\ & \text{where } \|(u_0, \mathbf{p}_0)\|_{\Omega_R} = \|u_0\|_{H^2(\Omega_R)} + \|\text{div} \mathbf{p}_0\|_{H^2(\Omega_R)}. \end{aligned}$$

The proof of the theorem can be found in [C07], which depends on the abstract inversion theorem of the Laplace transform and sharp a priori estimate for the Helmholtz equations. To the author's best knowledge, this is the first result of that kind for the time-domain scattering problems in the literature.

The exact non-local boundary condition (2.31) is the starting point of various approximate absorbing boundary conditions which have been proposed and studied in the literature, see the review paper Hagstrom [H99] and the references therein. An interesting alternative to the method of absorbing boundary conditions is the method of perfectly matched layer (PML). Since the work of Berenger [B94] which proposed a PML technique for solving the time-dependent Maxwell equations in the Cartesian coordinates, various constructions of PML absorbing layers have been proposed and studied in the literature (cf. e.g. Turkel and Yefet [TY98], Teixeira and Chew [TC01] for the reviews). Under the assumption that the exterior solution is composed of outgoing waves only, the basic idea of the PML technique is to surround the computational domain by a layer of finite thickness with specially designed model medium that would either slow down or attenuate all the waves that propagate from inside the computational domain.

There are two classes of time-domain PML methods for the wave scattering problems. The first class, called "split-field PML method" in the engineering literature, includes the original Berenger PML method. It is shown in Abarbanel and Gottlieb [AG97] that the Berenger PML method is only weakly well-posed and thus may suffer instability in practical applications. The second class, the so-called "unsplit-field PML formulations" in the engineering literature, is, however, strongly well-posed. One such successful method is the uniaxial PML method developed in Sacks et al [SKLL95] and Gedney [G96] for the Maxwell equations in the Cartesian coordinates. The unsplit-field PML methods in the curvilinear coordinates are introduced in Petropoulos [P00] and Teixeira and Chew [TC01] for Maxwell equations.

Now we describe briefly the unsplit-field PML method for (2.26)–(2.29) to be studied in this chapter. Let $\alpha(r) = \eta(r) + s^{-1}\sigma(r)$ be the artificial medium property, where $\eta = 1 + \sigma$ and $\sigma \in C(\mathbb{R})$ such that $\sigma \geq 0$ for $r \in \mathbb{R}$ and $\sigma = 0$ for $r \leq R$. Denote by $\tilde{r}$ the complex radius

$$\tilde{r} = \tilde{r}(r) = \begin{cases} r & \text{if } r \leq R, \\ \int_0^r \alpha(\tau) d\tau = r\beta(r) & \text{if } r \geq R, \end{cases}$$

where $\beta(r) = \hat{\eta}(r) + s^{-1}\hat{\sigma}(r)$, and $\hat{\eta}(r) = \frac{1}{r} \int_R^r \eta(\tau) d\tau$, $\hat{\sigma}(r) = \frac{1}{r} \int_R^r \sigma(\tau) d\tau$.

The starting point is the series representation of $u_L = \mathcal{L}(u)$ for $r > R$ in (2.30). Based on the observation that $K_n(s\tilde{r}) = K_n(sr\hat{\eta} + r\hat{\sigma})$ decays exponentially for $\hat{\sigma}$ since $K_n(z) \sim \left(\frac{\pi}{2z}\right)^{1/2} e^{-z}$ as $|z| \rightarrow \infty$, we define the PML extension $(\tilde{u}_L, \tilde{\mathbf{p}}_L)$ of $(u_L, \mathbf{p}_L)$ as

$$\begin{aligned}\tilde{u}_L(r, \vartheta, s) &= \sum_{n=-\infty}^{\infty} \frac{K_n(s\tilde{r})}{K_n(sR)} u_L^n(R, s) e^{in\vartheta}, \quad \forall r > R, \\ s\tilde{\mathbf{p}}_L &= -\tilde{\nabla}\tilde{u}_L = -\left(\frac{\partial\tilde{u}_L}{\partial\tilde{r}}\mathbf{e}_r + \frac{1}{\tilde{r}}\frac{\partial\tilde{u}_L}{\partial\vartheta}\mathbf{e}_\vartheta\right), \quad \forall r > R,\end{aligned}$$

where $\mathbf{e}_r$ and $\mathbf{e}_\vartheta$ are the unit vectors of the polar coordinates. Since $\tilde{u}_L$ satisfies $-\tilde{\Delta}\tilde{u}_L + s^2\tilde{u}_L = 0$ outside B_R , where $\tilde{\Delta} = \frac{1}{\tilde{r}}\frac{\partial}{\partial\tilde{r}}\left(\tilde{r}\frac{\partial}{\partial\tilde{r}}\right) + \frac{1}{\tilde{r}^2}\frac{\partial^2}{\partial\vartheta^2}$ is the Laplace operator with respect to $(\tilde{r}, \vartheta)$, we know that, where $\tilde{\mathbf{p}}_L = \tilde{\mathbf{p}}_{L,r}\mathbf{e}_r + \tilde{\mathbf{p}}_{L,\vartheta}\mathbf{e}_\vartheta$,

$$s\tilde{u}_L = -\tilde{\nabla} \cdot \tilde{\mathbf{p}}_L = -\left[\frac{1}{\tilde{r}}\frac{\partial}{\partial\tilde{r}}(\tilde{r}\tilde{\mathbf{p}}_{L,r}) + \frac{1}{\tilde{r}}\frac{\partial\tilde{\mathbf{p}}_{L,\vartheta}}{\partial\vartheta}\right].$$

Since $\tilde{r} = r\beta$ and $\frac{d\tilde{r}}{dr} = \alpha$, for $r \geq R$, by using the chain rule, we obtain

$$s\tilde{u}_L = -\left(\frac{1}{\alpha\beta r}\frac{\partial}{\partial r}(\beta r\tilde{\mathbf{p}}_{L,r}) + \frac{1}{\beta r}\frac{\partial\tilde{\mathbf{p}}_{L,\vartheta}}{\partial\vartheta}\right), \quad s\tilde{\mathbf{p}}_{L,r} = -\frac{1}{\alpha}\frac{\partial\tilde{u}_L}{\partial r}, \quad s\tilde{\mathbf{p}}_{L,\vartheta} = -\frac{1}{\beta r}\frac{\partial\tilde{u}_L}{\partial\vartheta}.$$

Heuristically $(\tilde{u}_L, \tilde{\mathbf{p}}_L)$ decays exponentially for $r > R$ and its inverse Laplace transform $(\tilde{u}, \tilde{\mathbf{p}})$ will also decay exponentially in the time domain. The desired time-domain PML system will be obtained by taking the inverse Laplace transform of above equations.

$$\begin{aligned}\eta\hat{\eta}\frac{\partial\hat{u}}{\partial t} + \operatorname{div}\hat{\mathbf{p}} + (\sigma\hat{\eta} + \hat{\sigma}\eta)\hat{u} + \sigma\hat{u}_\Delta &= 0 \quad \text{in } \Omega_\rho \times (0, T), \\ M\frac{\partial\hat{\mathbf{p}}}{\partial t} + \nabla\hat{u} + \Lambda_\Delta(\hat{\mathbf{p}} - \hat{\mathbf{p}}_\Delta) &= 0 \quad \text{in } \Omega_\rho \times (0, T), \\ \frac{\partial\hat{u}_\Delta}{\partial t} - \hat{\sigma}\hat{u} &= 0, \quad \frac{\partial\hat{\mathbf{p}}_\Delta}{\partial t} + \Lambda(\hat{\mathbf{p}}_\Delta - \hat{\mathbf{p}}) = 0 \quad \text{in } \Omega_\rho \times (0, T), \\ \hat{\mathbf{p}} \cdot \mathbf{n}_D &= g \quad \text{on } \Gamma_D \times (0, T), \quad \hat{u} = 0 \quad \text{on } \Gamma_\rho \times (0, T), \\ \hat{u}|_{t=0} &= u_0, \quad \hat{\mathbf{p}}|_{t=0} = \mathbf{p}_0, \quad \hat{u}_\Delta|_{t=0} = 0, \quad \hat{\mathbf{p}}_\Delta|_{t=0} = 0 \quad \text{in } \Omega_\rho.\end{aligned}$$

By the construction of the PML problem, $(\hat{u}, \hat{\mathbf{p}})$ is designed to approximate the solution of the original scattering problem $(u, \mathbf{p})$ in the domain $\Omega_R \times (0, T)$.

Although the tremendous attention and success in the application of PML methods in the engineering literature, there are few mathematical results on the convergence of the PML methods. For the Helmholtz equation in the frequency domain, it is proved in Lassas and Somersalo [LS98], Hohage et al. [HSZ03] that the PML solution converges exponentially to the solution of the original scattering problem as the thickness of the PML layer tends to infinity. In Chen and Wu [CW03], Chen and Liu [CL05], an adaptive PML technique is proposed and studied in which a posteriori error estimate is used to determine the PML parameters. In particular, it is shown that exponential convergence can be achieved for fixed thickness of the PML layer by enlarging

PML medium properties. For the time-domain PML method, not much mathematical convergence analysis is known except the work in Hagstrom [H99] in which the planar PML method in one space direction is considered for the wave equation. In de Hoop et al. [DBR02] and Diaz and Joly [DJ06] the PML system with point source is analyzed based on the Cagniard–de Hoop method.

Our convergence analysis makes use of the following uniform exponential decay property of the modified Bessel function $K_n(z)$.

Lemma 2.4. *For any $\nu \in \mathbb{R}$, $s \in \mathbb{C}$ with $\operatorname{Re}(s) > 0$, $\rho > R > 0$, and $\tau > 0$, we have*

$$\frac{|K_\nu(s\rho + \tau)|}{|K_\nu(sR)|} \leq e^{-\tau(1-\frac{R^2}{\rho^2})}.$$

The proof which can be found in [C07] depends on the Macdonald formula for the integral representation of the product of modified Bessel functions and extends our earlier uniform estimate in [CL05] for the first Hankel function $H_\nu^1(z)$, $\nu \in \mathbb{R}$.

Now for $r > R$, let $\tilde{u} = \mathcal{L}^{-1}(\tilde{u}_L)$, where $\tilde{u}_L$ is the PML extension

$$\tilde{u}(r, \vartheta, t) = \sum_{n=-\infty}^{\infty} \left[\mathcal{L}^{-1} \left(\frac{K_n(s\tilde{r})}{K_n(sR)} \right) * u_n(R, t) \right] e^{in\vartheta},$$

where $u_n(R, t) = \mathcal{L}^{-1}(u_L^n(R, s)) = \frac{1}{2\pi} \int_0^{2\pi} u_L(R, \vartheta, t) e^{-in\vartheta} d\vartheta$. Since $s\tilde{\rho} = s\rho\hat{\eta}(\rho) + \rho\hat{\sigma}(\rho)$, by using the convolution estimate,

$$\begin{aligned} & \|\tilde{u}\|_{L^2(0,T;H^{1/2}(\Gamma_\rho))}^2 \\ &= \rho \sum_{n=-\infty}^{\infty} (1+n^2)^{1/2} \left\| \mathcal{L}^{-1} \left(\frac{K_n(s\tilde{\rho})}{K_n(sR)} \right) * u_n(R, t) \right\|_{L^2(0,T)}^2 \\ &\leq \rho e^{2s_1 T} \sum_{n=-\infty}^{\infty} (1+n^2)^{1/2} \max_{-\infty < s_2 < \infty} \left| \frac{K_n(s\tilde{\rho})}{K_n(sR)} \right|^2 \|u_n(R, t)\|_{L^2(0,T)}^2 \\ &\leq \frac{\rho}{R} e^{2s_1 T} \max_{-\infty < n < \infty} \max_{-\infty < s_2 < \infty} \left| \frac{K_n(s\tilde{\rho})}{K_n(sR)} \right|^2 \|u\|_{L^2(0,T;H^{1/2}(\Gamma_R))}^2 \\ &\leq \frac{\rho}{R} e^{2s_1 T} e^{-2\rho\hat{\sigma}(\rho)(1-\frac{R^2}{\rho^2\hat{\eta}(\rho)^2})} \|u\|_{L^2(0,T;H^{1/2}(\Gamma_R))}^2. \end{aligned}$$

This implies

$$\|\tilde{u}\|_{L^2(0,T;H^{1/2}(\Gamma_\rho))} \leq \left(\frac{\rho}{R}\right)^{1/2} e^{s_1 T - \rho\hat{\sigma}(\rho)(1-(R^2/\rho^2\hat{\eta}(\rho)^2))} \|u\|_{L^2(0,T;H^{1/2}(\Gamma_R))}.$$

Since the above estimate is valid for any $s_1 > 0$, we conclude by letting $s_1 \rightarrow 0$ that

$$\|\tilde{u}\|_{L^2(0,T;H^{1/2}(\Gamma_\rho))} \leq \left(\frac{\rho}{R}\right)^{1/2} e^{-\rho\hat{\sigma}(\rho)(1-(R^2/\rho^2\hat{\eta}(\rho)^2))} \|u\|_{L^2(0,T;H^{1/2}(\Gamma_R))}.$$

We have the following theorem on the convergence of the PML system.

Theorem 2.7. *Let $(u, \mathbf{p})$ be the solution of the original scattering problem and $(\hat{u}, \hat{\mathbf{p}}, \hat{u}_\Delta, \hat{\mathbf{p}}_\Delta)$ be the solution of the PML problem. Then there exists a constant $C > 0$ depending only on ρ/R but independent of σ, η, R, ρ , and T such that*

$$\begin{aligned} & \|u - \hat{u}\|_{L^2(0,T;L^2(\Omega_R))} + \|\mathbf{p} - \hat{\mathbf{p}}\|_{L^2(0,T;L^2(\Omega_R))} \\ & \leq C(\eta_m T) e^{-\rho \hat{\sigma}(\rho) \left(1 - \frac{R^2}{\rho^2 \hat{\eta}(\rho)^2}\right) + T} \|u\|_{H^1(0,T;H^{1/2}(\Gamma_R))}. \end{aligned}$$

where $\eta_m = \max_{R \leq r \leq \rho} \eta(r)$.

Long time stability of the PML methods is also a much studied topic in the literature (see e.g. Bécache and Joly [BJ02], Bécache et al. [BPG04], Appelö et al. [AHK06]). For a PML method to be practically useful, it must be stable in time, that is, the solution should not grow exponentially in time. We remark that the well-posedness of the PML system which follows from the theory of symmetric hyperbolic systems allows the exponential growth of the solutions. In [BJ02, BPG04, AHK06] the stability of the PML systems is considered under the assumption of constant PML medium property which, however, violates the property of perfect matchness of the associated PML system. Thus those studies do not fully explain the success of practical applications of the PML methods. The strategy to prove the stability of the PML method is based on the combination of the stability of the original scattering problem in Theorem 2.6 and the convergence of the PML method in Theorem 2.7. We refer to [C07] for more details.

Acknowledgement

The author is grateful to Mr. Junqing Chen, Dr. Long Wang and Dr. Weiying Zheng for the joint works on which some part of this chapter is based. The author is also grateful to the support of China NSF under the grant 10428105 and of the National Basic Research Project under the grant 2005CB321701.

References

- [AHK06] Appelö, D., Hagstrom, T., Kreiss, G.: Perfectly matched layers for hyperbolic systems: General formulation, well-posedness and stability. Preprint, University of New Mexico (2006)
- [AG97] Abarbanel S., Gottlieb, D.: A Mathematical Analysis of the PML Method. J. Comput. Phys. **134**, 357-363 (1997)
- [ABDG98] Amrouche, C., Bernardi, C., Dauge, M., Girault, V.: Vector potentials in three-dimensional non-smooth domains. Math. Meth. Appl. Sci. **21** 823-864 (1998)
- [ACS98] Assous, F., Ciarlet, Jr. P., Sonnendrücker E.: Resolution of the Maxwell equations in a domain with reentrant corners. Math. Model. Numer. Anal. **32**, 359-389 (1998)

- [BA73] Babuška, I., Aziz, A.: Survey Lectures on Mathematical Foundations of the Finite Element Method. In: Aziz, A. (ed) *The Mathematical Foundations of the Finite Element Method with Application to Partial Differential Equations*. Academic Press, New York (1973)
- [BR78] Babuška, I., Rheinboldt, C.: Error estimates for adaptive finite element computations. *SIAM J. Numer. Anal.* **15**, 736–754 (1978)
- [BW05] Bao G., Wu, H.J.: On the convergence of the solutions of PML equations for Maxwell’s equations. *SIAM J. Numer. Anal.* **43** 2121–2143, (2005)
- [BHHW00] Beck, R., Hiptmair, R., Hoppe R.H.W., Wohlmuth, B.: Residual based a posteriori estimators for eddy current computation. *M2AN Math. Modeling and Numer. Anal.* **34**, 159–182 (2000)
- [BJ02] Bécache E., Joly P.: On the analysis of Berenger’s perfectly matched layers for Maxwell equations. *Math. Modelling Numer. Anal.* **36**, 87–119 (2002)
- [BPG04] Bécache, E., Petropoulos, P.G., Gedney, D.: On the long-time behavior of unsplit perfectly matched layers. *IEEE Trans. Antennas and Propagation* **52**, 1335–1342 (2004)
- [B94] Bérenger, J.-P.: A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.* **114** 185–200, (1994)
- [BS87] Birman, M.Sh., Solomyak, M.Z.: L^2 -Theory of the Maxwell operator in arbitrary domains. *Uspekhi Mat. Nauk* **42**, 61–76 (1987) (in Russian); *Russian Math. Surveys* **43**, 75–96 (1987) (in English)
- [BS94] Birman, M.Sh., Solomyak, M.Z.: On the main singularities of the electric component of the electro-magnetic field in regions with screens. *St. Petersburg Math. J.* **5**, 125–139 (1994)
- [BP06] Bramble, J.H., Pasciak, J.E.: Analysis of a finite PML approximation for the three dimensional time-harmonic Maxwell and acoustic scattering problems. *Math. Comp.* (to appear)
- [CC06] Chen, J.Q., Chen, Z.: An adaptive perfectly matched layer technique for 3D time-harmonic electromagnetic scattering problem. (to appear)
- [C07] Chen, Z.: Stability and convergence of the time-domain perfectly matched layer method for acoustic scattering problems. (to appear)
- [CL05] Chen, Z., Liu, X.Z.: An adaptive perfectly matched layer technique for time-harmonic scattering problems. *SIAM J. Numer. Anal.* **43**, 645–671, (2005)
- [CWZ07] Chen, Z., Wang, L., Zheng, W.: An adaptive multilevel method for time-harmonic Maxwell equations with singularities, *SIAM J. Sci. Comput.* **29**, 118–138, (2007)

- [CW03] Chen, Z., Wu, H.J.: An adaptive finite element method with perfectly matched absorbing layers for the wave scattering by periodic structures. *SIAM J. Numer. Anal.* **41**, 799–826, (2003)
- [CD00] Costabel, M., Dauge, M.: Singularities of electromagnetic fields in polyhedral domains. *Arch. Ration. Mech. Anal.* **151**, 221–276 (2000)
- [DBR02] de Hoop, A.T., van den Berg, P.M., Remis R.F.: Absorbing boundary conditions and perfectly matched layers – An analytic time-domain performance analysis. *IEEE Trans. Mag.* **38** 657–660 (2002)
- [DJ06] Diaz J., Joly P.: A time domain analysis of PML models in acoustics, *Comput. Methods Appl. Mech. Engrg.* **195** 3820–2853 (2006)
- [DHL99] Dhia, A.B., Hazard, C., Lohrengel, S.: A singular field method for the solution of Maxwell’s equations in polyhedral domains. *SIAM J. Appl. Math.* **59** 2028–2044, (1999)
- [G96] Gedney, S.D.: An anisotropic perfectly matched layer absorbing media for the truncation of FDTD lattices. *IEEE Trans. Antennas Propagat.* **AP-44** 1630–1639 (1995)
- [H99] Hagstrom, T.: Radiation boundary conditions for the numerical simulation of waves. *Acta Numerica* 47–106 (1999)
- [HSZ03] Hohage, T., Schmidt, F., Zschiedrich, L.: Solving time-harmonic scattering problems based on the pole condition. II: Convergence of the PML method. *SIAM J. Math. Anal.* **35** 547–560, (2003)
- [LS98] Lassas M., Somersalo, E.: On the existence and convergence of the solution of PML equations. *Computing* **60** 229–241, (1998)
- [M98] Monk, P.: A posteriori error indicators for Maxwell’s equations. *J. Comp. Appl. Math.* **100**, 173–190 (1998)
- [M03] Monk, P.: *Finite Element Methods for Maxwell’s Equations*. Clarendon Press, Oxford (2003)
- [N80] Nédélec, J.: Mixed finite elements in R^3 . *Numer. Math.* **35**, 315–341 (1980)
- [P00] Petropoulos. P.G.: Reflectionless sponge layers as absorbing boundary conditions for the numerical solution of Maxwell equations in Rectangular, cylindrical, and spherical coordinates. *SIAM J. Appl. Math.* **60**, 1037–1058 (2000)
- [SKLL95] Sacks, Z.S., Kingsland, D.M., Lee, D.M., Lee. J.F.: A perfectly matched anisotropic absorber for use as an absorbing boundary condition. *IEEE Trans. Antennas Propagat.* **AP-43** 1460–1463 (1995)
- [SS00] Schmidt, A., Siebert K.G.: *Design of adaptive finite element software: The finite element Toolbox ALBERTA*. Lecture Notes in Computational Science and Engineering 2, Springer Verlag, Berlin (2005)

- [SC94] Scott, L.R., Zhang, Z.: Finite element interpolation of non-smooth functions satisfying boundary conditions. *Math. Comp.* **54**, 483–493 (1994)
- [TC01] Teixeira, F.L., Chew, W.C.: Advances in the theory of perfectly matched layers. In: W.C. Chew et al, (ed), *Fast and Efficient Algorithms in Computational Electromagnetics*. Artech House, Boston, (2001)
- [TY98] Turkel, E., Yefet, A.: Absorbing PML boundary layers for wave-like equations. *Appl. Numer. Math.* **27** 533–557 (1998)
- [ZCW06] Zheng, W.Y., Chen, Z., Wang, L.: An adaptive finite element method for the H - ψ formulation of time-dependent eddy current problems. *Numer. Math.* **103**, 667–689, (2006)

Time Domain Adaptive Integral Method for Surface Integral Equations

H. Bağcı, A.E. Yılmaz, J.-M. Jin, and E. Michielssen

3.1 Introduction

To ensure the interoperability of modern broadband and integrated navigation and communication systems, engineers need simulation tools capable of tracking electromagnetic transients on electrically large and complex, multiscale and potentially nonlinearly loaded structures. In this context, marching-on-in-time based time-domain integral-equation (MOT-TDIE) solvers provide an increasingly appealing alternative to finite difference/element based simulation engines [1, 2]. Indeed, compared to the latter, MOT-TDIE solvers automatically impose radiation conditions, do not require fields to be discretized throughout homogeneous volumes, and are highly immune to numerical dispersion [3, 4]. Moreover, recent algorithmic advances have rendered these solvers (a) well-conditioned and stable, (b) computationally efficient, and (c) applicable to the analysis transients on geometrically complex structures. (d) Finally, MOT-TDIE solvers have been hybridized with various subsystem simulators, thereby vastly expanding their application range.

1. *Stability and conditioning:* Modern MOT-TDIE solvers, in contrast to their predecessors, are (almost always) stable. Indeed, during the past decade, the stability of these solvers has steadily improved due to the application of averaging/filtering techniques [5, 6], implicit time stepping methods [7, 8], smooth and carefully tailored temporal basis functions [7, 9, 10], and space-time Galerkin schemes [11]. Recently, time-domain Calderón identities [12] and spatially-hierarchical schemes [13] were leveraged to precondition MOT-TDIE systems, thereby accelerating the convergence of their iterative solution. These developments have enabled the robust application of MOT-TDIE solvers to the analysis of transients on structures modeled in terms of high-density/multiscale unstructured meshes.
2. *Acceleration algorithms:* The computational complexity and memory requirements of classical MOT-TDIE solvers scale very poorly. To remedy

this solution, two accelerators were developed: the (multilevel) plane wave time-domain algorithm (PWTD) [14–16] and the time-domain adaptive integral method (TD-AIM) [17]. These accelerators permit the rapid evaluation of transient fields due to wideband source constellations, viz. the fast computation of all space-time convolutions required by MOT-TDIE solvers, thereby have enabled the MOT-TDIE analysis of transients on structures involving in excess of one million spatial basis functions lasting thousands of time steps, and this on readily available parallel computers.

3. *Complex structures:* Modern MOT-TDIE solvers, unlike their predecessors which target simple perfect electrically conducting (PEC) structures, apply to the analysis of electromagnetic transients on surfaces characterized by impedance boundary conditions [18], surfaces buried in half-space backgrounds [19, 20], dielectric/lossy/dispersive penetrable volumes [21–23], and surfaces with wire attachments [24, 25]. These solvers permit modeling of electromagnetic transients on real-world structures, e.g., complex platform-mounted and dielectric backed antennas and their feeds, and quasi-optical devices.
4. *Hybridization with subsystem simulators:* Whereas historically MOT-TDIE solvers were used primarily as stand-alone electromagnetic analysis engines, recently they have been hybridized with various subsystem simulators including circuit and [26, 27] cable solvers [25, 28–31], and macromodeling tools [32]. This hybridization has rendered MOT-TDIE solvers useful for analyzing field interactions with platforms carrying cable-interconnected circuits, electronic components, and printed circuit boards.

Without a doubt, fast MOT-TDIE solver technology is rapidly approaching a stage of maturity permitting its widespread application to complex and real-world engineering problems. This chapter summarizes some of the authors' recent work in the field, much of which is rooted in the work of J.C. Nédélec and co-workers [11, 33, 34]. Specifically, it describes recent progress in the formulation and implementation of TD-AIM accelerated MOT-TDIE solvers, viz. extensions of the frequency-domain adaptive integral method (AIM) [35] and pre-corrected FFT algorithm [36] to the time domain, and demonstrates the technology's applicability to a host of real-world electromagnetic interference (EMI) problems.

The remainder of the chapter is organized as follows. Section 3.2 introduces the reader to FFT-accelerated MOT-TDIE solvers by contrasting the technology to FFT-accelerated frequency-domain and PWTD-accelerated time-domain solvers. Section 3.3 describes several time-domain surface integral equations, outlines classical MOT schemes for solving them, and describes the TD-AIM accelerator (including its parallel implementation). Section 3.4 elucidates the hybridization of TD-AIM-accelerated MOT-TDIE solvers with several subsystem simulators and demonstrates the versatility of the resulting hybrid simulators through their application to several real-world EMI problems.

3.2 FFT-Accelerated MOT-TDIE Solvers: A Perspective

The aforementioned PWTD scheme constitutes the extension of the Helmholtz-equation fast multipole scheme [37–40] to the time domain. Its development preceded that of the TD-AIM discussed here. How do these schemes compare and why is there a need for a second accelerator? This section answers some of these questions and places the development of the TD-AIM into its historical perspective.

FFT schemes for accelerating the solution of frequency-domain (time-harmonic) integral equations, such as the conjugate gradient FFT (CG-FFT) method [41], frequency-domain AIM [35], and pre-corrected FFT algorithm [36], provide an appealing avenue for tackling a broad class of surface scattering problems. The classical iterative solution of frequency-domain integral equations requires $O(N_s^2)$ operations per matrix-vector multiplication and $O(N_s^2)$ bytes of memory; here, and in what follows, N_s denotes the number of spatial basis functions that discretize the scatterer current density. Both the CG-FFT algorithm and AIM reduce the computational complexity of a matrix-vector multiplication by employing uniform spatial grids that facilitate the use of (spatial) FFTs for rapidly convolving source distributions with Green functions. To this end, the CG-FFT algorithm assumes a uniform scatterer discretization, whereas the AIM introduces a uniform auxiliary grid that does not constrain the primary surface discretization. The AIM reduces the above matrix-vector multiplication cost to $O(N_c \log N_c)$ operations and the associated memory requirements to $O(N_c)$ bytes, where N_c is the number of nodes of the auxiliary grid. For general three-dimensional (3D) surfaces devoid of geometric details, $N_c \sim N_s^{1.5}$; for quasi-planar surfaces whose transverse dimensions are much larger than their (fixed) height, $N_c \sim N_s$. The computational complexity and memory requirements of AIM-accelerated solvers generally scale less favorably than those of multilevel fast multipole ones [39, 40]. Nonetheless, the AIM often remains a viable alternative, especially when the structure under study is relatively small, quasi-planar, or densely packed. The AIM also has the advantage of being immediately applicable to all problems involving Green functions that exhibit translational, rotational, or reflection invariance [40]. Recently proposed higher-order methods [42, 43], which employ auxiliary uniform grids on facets to reduce N_c , and effective parallelization strategies based on either domain decomposition [35] or parallel spatial FFTs [44] further improve the viability of AIM-like solvers for large-scale frequency-domain analysis.

The above picture carries over virtually entirely to the time domain. The classical MOT solution of TDIEs requires $O(N_t N_s^2)$ operations and $O(N_s^2)$ bytes of memory; here N_t is the number of time steps in the simulation. Recently, various extensions of the CG-FFT algorithm to the time domain have been proposed [45–48]. Similar to their frequency-domain counterpart, these algorithms assume a uniform discretization of the scatterer surface and therefore are of limited use. This chapter describes the TD-AIM, i.e., the

time-domain counterpart of the AIM; its predecessors and related methods were outlined in [35, 49–53]. The TD-AIM has computational complexity and memory requirements of $O(N_t N_c (\log N_c + \log^2 N_g))$ and $O(N_g N_c)$, respectively. Here, N_g denotes the maximum number of time steps for a pulsed field to travel across the scatterer; for surface scatterers, N_g is generally proportional to $N_s^{0.5}$ [48]. TD-AIM attains these efficiency gains by accelerating the field computations as briefly described next and detailed in Sect. 3.3:

1. All space-time sources on the scatterer surface, which produce transient fields, are locally projected onto a uniform auxiliary grid for each time step.
2. The fields due to the resulting auxiliary-grid sources are computed everywhere on the grid via global, multilevel/blocked, space-time FFTs.
3. These fields are locally interpolated back onto the scatterer surface.
4. As this procedure is inaccurate when source and observer points reside close to each other, near fields are computed classically and (pre-) corrected for errors introduced through the use of global FFTs.

Just as the frequency-domain AIM is asymptotically less efficient than the multilevel fast multipole method, the TD-AIM is asymptotically inferior to the multilevel PWTD scheme. That said, as the TD-AIM relies solely on the translational invariance of the Green function to achieve computational savings, it is applicable with little modification to problems involving lossy [53], layered [19, 20], or dispersive media [54]. Furthermore, as subsequent sections will show, it is relatively easy to implement and parallelize. Finally, TD-AIM accelerated MOT-TDIE solvers trivially lend themselves to hybridization with various subsystem simulators. In conclusion, for many problems of practical interest, the TD-AIM is computationally efficient and effective; the method is an attractive alternative to the PWTD algorithm.

3.3 FFT-Accelerated MOT-TDIE Solvers: Formulation and Implementation

This section details the construction of FFT-accelerated MOT-TDIE solvers. First, time-domain electric-, magnetic-, and combined-field integral equations for analyzing electromagnetic scattering from PEC structures residing in an unbounded homogenous medium are presented and their classical MOT-based solution is reviewed. Next, the TD-AIM is introduced and its theoretical computational complexity and memory requirements are explored. Also, a parallel implementation of the scheme is described. The section concludes by describing numerical experiments that demonstrate the accuracy and parallel efficiency of the TD-AIM accelerated MOT-TDIE solver.

3.3.1 Time-Domain Integral Equations and Their Solution via Marching-on-fin-Time

Let S denote the surface of a closed PEC body that resides in an unbounded, lossless, homogenous dielectric medium with permittivity ε and permeability μ . A transient electromagnetic field $\{\mathbf{E}^{\text{inc}}(\mathbf{r}, t), \mathbf{H}^{\text{inc}}(\mathbf{r}, t)\}$ is incident on S ; it is assumed that this field is (approximately) temporally bandlimited to f_{max} and that it vanishes $\forall \mathbf{r} \in S$ for $t < 0$. A surface current is induced on S that in turn generates the scattered field

$$\mathbf{E}^{\text{sca}}(\mathbf{r}, t) = -\partial_t \mathbf{A}(\mathbf{r}, t) - \nabla \Phi(\mathbf{r}, t), \quad (3.1a)$$

$$\mathbf{H}^{\text{sca}}(\mathbf{r}, t) = \nabla \times \mathbf{A}(\mathbf{r}, t)/\mu, \quad (3.1b)$$

where ∂_t represents the time derivative and $\mathbf{A}(\mathbf{r}, t)$ and $\Phi(\mathbf{r}, t)$ are the vector and scalar potentials

$$\mathbf{A}(\mathbf{r}, t) = \mu \iint_S \frac{\mathbf{J}(\mathbf{r}', t - R/c)}{4\pi R} ds', \quad (3.2a)$$

$$\Phi(\mathbf{r}, t) = -\frac{1}{\varepsilon} \iint_S \int_0^{t-R/c} \frac{\nabla' \cdot \mathbf{J}(\mathbf{r}', t')}{4\pi R} dt' ds'. \quad (3.2b)$$

Here, $\mathbf{J}(\mathbf{r}, t)$ is the surface current density, $R = |\mathbf{r} - \mathbf{r}'|$ is the distance between source point $\mathbf{r}'$ and observation point $\mathbf{r}$, and $c = 1/\sqrt{\mu\varepsilon}$ is the speed of light. Enforcing the temporal derivatives of the fundamental boundary conditions on the electric and magnetic fields tangential to S yields time-domain electric- and magnetic-field integral equations (EFIE and MFIE). The combined-field integral equation (CFIE) is a linear combination of the EFIE and the MFIE [55, 56]. The time-domain EFIE, MFIE, and CFIE read

$$\begin{aligned} \text{EFIE : } & -\hat{\mathbf{n}}(\mathbf{r}) \times (\hat{\mathbf{n}}(\mathbf{r}) \times \partial_t \mathbf{E}^{\text{inc}}(\mathbf{r}, t)) = \\ & -\hat{\mathbf{n}}(\mathbf{r}) \times (\hat{\mathbf{n}}(\mathbf{r}) \times (\partial_t^2 \mathbf{A}(\mathbf{r}, t) + \nabla \partial_t \Phi(\mathbf{r}, t))), \end{aligned} \quad (3.3a)$$

$$\begin{aligned} \text{MFIE : } & \hat{\mathbf{n}}(\mathbf{r}) \times \partial_t \mathbf{H}^{\text{inc}}(\mathbf{r}, t) = \\ & \partial_t \mathbf{J}(\mathbf{r}, t) - \hat{\mathbf{n}}(\mathbf{r}) \times \nabla \times \partial_t \mathbf{A}(\mathbf{r}, t)/\mu, \end{aligned} \quad (3.3b)$$

$$\text{CFIE : } \text{CFIE} = \eta(1 - \alpha) \text{MFIE} + \alpha \text{EFIE}. \quad (3.3c)$$

Here, $\hat{\mathbf{n}}(\mathbf{r})$ is an outward directed unit vector normal to S and $\eta = \sqrt{\mu\varepsilon}$ is the intrinsic impedance of the medium. The discussions hereafter will focus on the CFIE; equations pertaining to the EFIE and the MFIE can be derived from those for the CFIE by setting $\alpha = 1$ and $\alpha = 0$, respectively. The EFIE is valid for open surfaces as well, whereas the MFIE and the CFIE are pertinent to closed surfaces.

To numerically solve the CFIE, $\mathbf{J}(\mathbf{r}, t)$ is discretized using $N_s N_t$ spatio-temporal basis functions as

$$\mathbf{J}(\mathbf{r}, t) \cong \sum_{k'=1}^{N_s} \sum_{l'=1}^{N_t} I_{k',l'} \mathbf{S}_{k'}(\mathbf{r}) T(t - l' \Delta t). \quad (3.4)$$

Here $I_{k',l'}$ is an unknown expansion coefficient and $\Delta t = \beta / f_{\max}$ is the time-step size with typically $0.02 \leq \beta \leq 0.1$. In what follows, the spatial and temporal basis functions $\mathbf{S}_{k'}(\mathbf{r})$ and $T(t)$ are assumed local. For example, the $\mathbf{S}_{k'}(\mathbf{r})$ and $T(t)$ can be Rao–Wilton–Glisson (RWG) functions [57] or their higher-order extensions [58] and shifted Lagrange interpolants [7], respectively. Furthermore, it is assumed that $T(t) = 0$ for $t \leq -\Delta t$ and $t > T^{\max}$, i.e., that the temporal basis functions are (discretely) causal and of duration $T^{\max} + \Delta t$. Finally, spatial discretization lengths on S are assumed to be of $O(c\Delta t)$; this assumption is valid whenever S is electrically large and devoid of small geometric details. Upon substituting (3.4) into the CFIE (3.3c) and testing the resulting equation with the spatial functions $\mathbf{S}_k(\mathbf{r})$ at times $t = l\Delta t$, $N_s N_t$ equations for the $N_s N_t$ expansion coefficients result:

$$\mathbf{Z}_0 \mathbf{I}_l = \mathbf{V}_l^{\text{inc}} - \mathbf{V}_l^{\text{scat}} = \mathbf{V}_l^{\text{inc}} - \sum_{l'=\max(1, l-N_g)}^{l-1} \mathbf{Z}_{l-l'} \mathbf{I}_{l'} \quad \text{for } l = 1, 2, \dots, N_t. \quad (3.5)$$

The entries of the vectors $\mathbf{I}_{l'}$ and $\mathbf{V}_l^{\text{inc}}$ and those of the matrices $\mathbf{Z}_{l-l'}$ are

$$\mathbf{I}_{l'}(k') = I_{k',l'}, \quad (3.6a)$$

$$\begin{aligned} \mathbf{V}_l^{\text{inc}}(k) = & \iint_S \eta(1-\alpha) \mathbf{S}_k(\mathbf{r}) \cdot \hat{\mathbf{n}}(\mathbf{r}) \times \partial_t \mathbf{H}^{\text{inc}}(\mathbf{r}, t) \\ & + \alpha \mathbf{S}_k(\mathbf{r}) \cdot \partial_t \mathbf{E}^{\text{inc}}(\mathbf{r}, t) \, ds \Big|_{t=(l-l')\Delta t}, \end{aligned} \quad (3.6b)$$

$$\begin{aligned} \mathbf{Z}_{l-l'}(k, k') = & \eta(1-\alpha) \iint_S \mathbf{S}_k(\mathbf{r}) \cdot \mathbf{S}_{k'}(\mathbf{r}') \, \partial_t T(t) \, ds \\ & + \eta(1-\alpha) \iint_S (\hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{S}_k(\mathbf{r})) \\ & \times \nabla \mu \iint_S \frac{\partial_t T(t - R/c) \mathbf{S}_{k'}(\mathbf{r}')}{4\pi R} \, ds' \, ds \\ & + \alpha \iint_S \mathbf{S}_k(\mathbf{r}) \cdot \mu \iint_S \frac{\partial_t^2 T(t - R/c) \mathbf{S}_{k'}(\mathbf{r}')}{4\pi R} \, ds' \, ds \\ & + \alpha \iint_S \nabla \cdot \mathbf{S}_k(\mathbf{r}) \frac{1}{\varepsilon} \iint_S \frac{T(t - R/c) \nabla' \cdot \mathbf{S}_{k'}(\mathbf{r}')}{4\pi R} \, ds' \, ds \Big|_{t=(l-l')\Delta t}. \end{aligned} \quad (3.6c)$$

The integer N_g in (3.5) is defined such that $N_g \Delta t$ approximates the longest possible transit time of the field produced by a temporal basis function across S : $N_g = \lfloor (R^{\max}/c + T^{\max}) \rfloor$ where $R^{\max}$ is the maximum distance between any two points on S and $\lfloor \cdot \rfloor$ rounds to the smaller integer. It follows that only

the matrices $\mathbf{Z}_0$ through $\mathbf{Z}_{N_g}$ are nonzero because the basis functions are local and the Green function implicit in (3.5) is impulsive in time [53]. That is, the fields radiated by currents on various parts of the scatterer at a given time step interact with the scatterer for at most N_g time steps. Once the spatial and temporal basis functions and the time-step size that support the frequency content of the incident field are determined, the unknown coefficients in (3.5) can be found recursively. First, $\mathbf{I}_1$ at time $t = \Delta t$ is found; this, in turn, permits computation of $\mathbf{V}_2^{\text{scat}}$. This vector is then added to the tested incident field $\mathbf{V}_2^{\text{inc}}$ and (3.5) is solved for the current $\mathbf{I}_2$ at time $t = 2\Delta t$. At the next time step, $\mathbf{I}_1$ and $\mathbf{I}_2$ are used to compute $\mathbf{V}_3^{\text{scat}}$, which together with $\mathbf{V}_3^{\text{inc}}$ permits the computation of $\mathbf{I}_3$, and so forth. This recursive solution algorithm is known as the MOT scheme [59].

The dominant cost of the MOT method is the computation of the vectors $\mathbf{V}_l^{\text{scat}}$, which involves a space-time convolution of the currents with the Green function for each time step l . Indeed, under the above assumptions, for $l > N_g$, that is, as soon as the retarded fields from every part of the scatterer reach all the other parts, the computation of a single $\mathbf{V}_l^{\text{scat}}$ requires $O(N_s^2)$ operations. Compared to the cost of computing $\mathbf{V}_l^{\text{scat}}$, the cost of iteratively solving (3.5) typically is insignificant because $\mathbf{Z}_0$ contains only $O(N_s)$ nonzero elements, i.e., it is highly sparse, and the iterative solution typically converges in very few (<15) iterations. Thus, the goal of the TD-AIM is to accelerate the computation of the fields on the right-hand side of (3.5), the classical evaluation of which requires $O(N_t N_s^2)$ operations for all time steps.

3.3.2 Time Domain Adaptive Integral Method (TD-AIM)

The space-time translational invariance of the Green function inherent in (3.6c) can be exploited to rapidly evaluate $\mathbf{V}_l^{\text{scat}}$ for $1 \leq l \leq N_t$. The scheme presented here is a marriage between the fast time- and frequency-domain integral-equation solvers in [53] and [35]. In [53], a fast scheme for evaluating the temporal convolution of the impedance matrices $\mathbf{Z}_{l-l'}$ with space-time currents was introduced assuming that S was a uniformly meshed plate. Temporal convolutions were evaluated via blocked (multilevel) FFTs while spatial convolutions could be evaluated by a CG-FFT like scheme because of the uniform surface mesh used. In [35], a fast scheme for evaluating fields generated by time-harmonic sources residing on an arbitrarily shaped and meshed surface was described. The use of FFTs to evaluate these fields was facilitated by introducing an auxiliary grid. Here, the extension of the scheme in [53] to nonuniformly meshed surfaces using ideas similar to [35] is elucidated.

The TD-AIM embeds S within an auxiliary 3D Cartesian grid with $N_c = N_{cx} \times N_{cy} \times N_{cz}$ nodes. Node separation along the three Cartesian directions Δs_x , Δs_y , and Δs_z are assumed identical and equal to Δs for ease of presentation; the effects of node separation on accuracy are investigated in Sect. 3.3.6 but Δs is always of $O(c\Delta t)$. The TD-AIM computes $\mathbf{V}_l^{\text{scat}}$ in four stages:

1. At each time step, all primary sources on S are locally projected onto the auxiliary grid. The auxiliary sources that are associated with a given primary source are chosen to reproduce the transient fields of the primary source with high accuracy, at least for observation points that are separated by more than a pre-specified distance from the primary source.
2. Future transient fields produced by these auxiliary sources are computed at all the nodes on the auxiliary grid; this is achieved via global, blocked, space-time FFTs.
3. The fields at the next time step are locally interpolated from the auxiliary grid onto the primary surface mesh.
4. Near fields due to all primary sources on S are computed wherever needed and (pre-) corrected for errors induced through the use of global FFTs in Stage (2).

Specifically, the TD-AIM approximates each of the impedance matrices $\mathbf{Z}_1$ through $\mathbf{Z}_{N_g}$ as $\mathbf{Z}_{l-l'} \approx \mathbf{Z}_{l-l'}^{\text{FFT}} + \mathbf{Z}_{l-l'}^{\text{near}}$, where $\mathbf{Z}_{l-l'}^{\text{FFT}}$ and $\mathbf{Z}_{l-l'}^{\text{near}}$ account for Stages (1)–(3) and Stage (4) of the algorithm, respectively. The matrices $\mathbf{Z}_{l-l'}^{\text{FFT}}$ can be expressed as

$$\begin{aligned}
 \mathbf{Z}_{l-l'}^{\text{FFT}} = & \eta(1 - \alpha) \left[\mathbf{\Gamma}_x^\dagger(t) \mathbf{\Gamma}_y^\dagger(t) \mathbf{\Gamma}_z^\dagger(t) \right] \\
 & * \begin{bmatrix} \mathbf{0} & \mathbf{G}^{Hy}(t) & -\mathbf{G}^{Hz}(t) \\ -\mathbf{G}^{Hx}(t) & \mathbf{0} & \mathbf{G}^{Hz}(t) \\ \mathbf{G}^{Hx}(t) & -\mathbf{G}^{Hy}(t) & \mathbf{0} \end{bmatrix} * \begin{bmatrix} \mathbf{\Lambda}_x(t) \\ \mathbf{\Lambda}_y(t) \\ \mathbf{\Lambda}_z(t) \end{bmatrix} \\
 & + \alpha \left[\mathbf{\Lambda}_x^\dagger(t) \mathbf{\Lambda}_y^\dagger(t) \mathbf{\Lambda}_z^\dagger(t) \right] * \begin{bmatrix} \mathbf{G}^A(t) * \mathbf{\Lambda}_x(t) \\ \mathbf{G}^A(t) * \mathbf{\Lambda}_y(t) \\ \mathbf{G}^A(t) * \mathbf{\Lambda}_z(t) \end{bmatrix} \\
 & + \alpha \mathbf{\Lambda}_\nabla^\dagger(t) * \mathbf{G}^\varphi(t) * \mathbf{\Lambda}_\nabla(t) \Big|_{t=(l-l')\Delta t}, \tag{3.7}
 \end{aligned}$$

where $\mathbf{\Lambda}_{x,y,z,\nabla}(t)$ and $\mathbf{\Gamma}_{x,y,z}(t)$ are sparse and time-dependent matricial projection operators, $\dagger$ represents a transpose, $*$ denotes a combined temporal convolution/matrix multiplication, and the matricial $\mathbf{G}^{\mathbf{H},A,\varphi}(t)$ propagate onto all of the auxiliary-grid nodes (temporal derivatives of) magnetic fields, magnetic vector potentials, and electric scalar potentials due to sources on the auxiliary grid. In (3.7), the curl operator of (3.6c) is transferred onto neither the spatial basis functions [60] nor the spatial testing functions [35]; rather, is left on the Green functions to facilitate its numerical computation as described in Sect. 3.3.4 and [61]. The various entities in (3.7) are discussed in more detail below.

The matricial projection operators are constructed by choosing M_k points on the auxiliary grid that each function $\mathbf{S}_k(\mathbf{r})$ is projected onto; denote this set of points by C_k . These points can be chosen to reside inside or on the surface of the smallest cube that snaps to the auxiliary grid and that encloses $\mathbf{S}_k(\mathbf{r})$. Then, for each $\mathbf{S}_k(\mathbf{r})$, the M_k entries of the seven matricial projection

operators $\mathbf{\Lambda}_{x,y,z,\nabla}(t)$ and $\mathbf{\Gamma}_{x,y,z}(t)$ are selected such that the scalar fields produced by $\hat{\mathbf{x}} \cdot \mathbf{S}_k(\mathbf{r}) T(t)$, $\hat{\mathbf{y}} \cdot \mathbf{S}_k(\mathbf{r}) T(t)$, $\hat{\mathbf{z}} \cdot \mathbf{S}_k(\mathbf{r}) T(t)$, $\nabla \cdot \mathbf{S}_k(\mathbf{r}) T(t)$, $\hat{\mathbf{x}} \cdot \hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{S}_k(\mathbf{r}) T(t)$, $\hat{\mathbf{y}} \cdot \hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{S}_k(\mathbf{r}) T(t)$, and $\hat{\mathbf{z}} \cdot \hat{\mathbf{n}}(\mathbf{r}) \times \mathbf{S}_k(\mathbf{r}) T(t)$, “match” those of the auxiliary sources for observers separated from the $\mathbf{S}_k(\mathbf{r})$ by several grid lengths Δs .

Two of the most commonly used criteria in determining the auxiliary source amplitudes in frequency-domain AIM are moment matching [35] and field matching [62]. The field-matching approach often results in better accuracy with little extra cost. The two approaches differ significantly, however, when applied in a TD-AIM framework.

In the moment-matching approach, the auxiliary source strengths and temporal signatures are chosen to reproduce the M_k multipole moments of the original basis function. Because the moments are frequency independent, the temporal signatures of the equivalent sources coincide with those of the temporal basis functions. Moreover, because the temporal basis functions are, in general, zero at sampling instants (except at $t = 0$), all $*$ operations in (3.7) reduce to matrix multiplications. While the resulting coefficients are frequency independent, the accuracy of the representation is frequency dependent.

In the field-matching approach, the coefficients and time signatures of the auxiliary sources are chosen to replicate the transient fields radiated by the original basis function on a near-field sphere. To this end, the discrete Fourier transform of the radiated field is computed at a set of frequencies, and at each of these frequencies the coefficients are found via least-squares approximation. Then, samples of $\mathbf{\Lambda}_{x,y,z,\nabla}(t)$ and $\mathbf{\Gamma}_{x,y,z}(t)$ are found by inverse discrete Fourier transformation. Because the best-fit coefficients are frequency-dependent, the temporal signatures of the auxiliary sources may differ from basis function to basis function and from auxiliary source point to auxiliary source point. In addition, they are, in general, nonzero at sampling instants. While the coefficients are frequency dependent, the accuracy of the representation can potentially be made frequency independent.

Although the field-matching approach usually produces more accurate results for a given $M_{k'}$, moment matching is more suitable for practical applications because it (a) automatically yields time-limited $\mathbf{\Lambda}_{x,y,z,\nabla}(t)$ and $\mathbf{\Gamma}_{x,y,z}(t)$, (b) allows more matrix-elements to be approximated accurately via (3.7) (see below), and (c) needs fewer operations for multiplying $\mathbf{Z}_{l-l'}^{\text{FFT}}$.

In (3.7), the entries of the sparse propagation matricial $\mathbf{G}^{\mathbf{H},A,\varphi}(t)$ are

$$\{\mathbf{G}^{Hx}(t, u, u'), \mathbf{G}^{Hy}(t, u, u'), \mathbf{G}^{Hz}(t, u, u'), \mathbf{G}^A(t, u, u'), \mathbf{G}^\varphi(t, u, u')\} \quad (3.8)$$

$$= \{\mu\partial_x\partial_t, \mu\partial_y\partial_t, \mu\partial_z\partial_t, \mu\partial_t^2, 1/\varepsilon\} \frac{\delta(t - |\mathbf{r} - \mathbf{r}_{u'}|/c)}{4\pi|\mathbf{r} - \mathbf{r}_{u'}|} \Big|_{\mathbf{r}=\mathbf{r}_u}. \quad (3.9)$$

where $\mathbf{r}_u$ denotes node u on the auxiliary grid. Note that, to avoid singularities, $\mathbf{G}^{\mathbf{H},A,\varphi}(t, u, u') \equiv 0$. The efficient action of these matricial propagators on equivalent source signatures via blocked FFTs is discussed in Sect. 3.3.3.

The M_k point sources on the auxiliary grid can accurately reproduce the transient fields of $\mathbf{S}_k(\mathbf{r})$ only for observers separated from the source by several grid lengths Δs . Their erroneous contributions to the fields at nearby observers are corrected with the help of $\mathbf{Z}_{l-l'}^{\text{near}}$ matrices. The matrices $\mathbf{Z}_{l-l'}^{\text{near}}$ are sparse approximations to $\mathbf{Z}_{l-l'} - \mathbf{Z}_{l-l'}^{\text{FFT}}$ and are defined as

$$\mathbf{Z}_{l-l'}^{\text{near}}(k, k') = \begin{cases} 0 & \text{if } R_{k,k'} > \gamma \Delta s, \\ \mathbf{Z}_{l-l'}(k, k') - \mathbf{Z}_{l-l'}^{\text{FFT}}(k, k') & \text{if } R_{k,k'} \leq \gamma \Delta s, \end{cases} \quad (3.10)$$

where, $R_{k,k'}$ is the minimum “grid-distance” between the auxiliary points representing the functions $\mathbf{S}_k(\mathbf{r})$ and $\mathbf{S}_{k'}(\mathbf{r})$ [35], i.e.,

$$\begin{aligned} R_{k,k'} &= \min_{u \in C_k, u' \in C_{k'}} \|\mathbf{r}_u - \mathbf{r}_{u'}\|_\infty \\ &= \min_{u \in C_k, u' \in C_{k'}} \max(|x_u - x_{u'}|, |y_u - y_{u'}|, |z_u - z_{u'}|), \end{aligned} \quad (3.11)$$

and $\gamma \Delta s$ is a threshold distance beyond which $\mathbf{Z}_{l-l'}^{\text{FFT}}$ represents the scattered fields with the desired accuracy; in practice, $1 \leq \gamma \leq 6$. In general, the larger γ is the more costly and the more accurate the TD-AIM becomes.

3.3.3 Multilevel/Blocked Space–Time FFTs

In practice, the entries of the matrices $\mathbf{Z}_{l-l'}^{\text{FFT}}$ defined above are never evaluated. Rather, discrete convolutions of the form

$$\sum_{l'=\max(1, l-N_g)}^{l-1} \mathbf{Z}_{l-l'}^{\text{FFT}} \mathbf{I}_{l'} \quad (3.12)$$

are evaluated by discretizing the temporal convolutions inherent in (3.7). It then becomes clear that Stage (2) of the TD-AIM calls for the evaluation of discrete convolutions of the form

$$\sum_{l'=\max(1, l-N_g)}^{l-1} \mathbf{G}_{l-l'}^{\mathbf{H}, A, \varphi} \tilde{\mathbf{I}}_{l'}^{\mathbf{H}, A, \varphi}. \quad (3.13)$$

Here $\mathbf{G}_{l-l'}^{\mathbf{H}, A, \varphi} = \mathbf{G}^{\mathbf{H}, A, \varphi}(t) * \tilde{T}(t) \Big|_{t=(l-l')\Delta t}$ and $\tilde{T}(t)$ is a function that interpolates the auxiliary source samples $\tilde{\mathbf{I}}_{l'}^{\mathbf{H}, A, \varphi}$ (typically, although not necessarily, $\tilde{T}(t) = T(t)$). The FFT-acceleration scheme for evaluating these discrete temporal convolutions exploits the spatial Toeplitz structure of the above operators as well as that of their temporal arrangement implicit in (3.5) to accelerate these multiplications via blocked four-dimensional (4D) FFTs. In what follows, the mechanics of this operation are demonstrated; for the sake of brevity, only scalar potential contributions are considered.

$$\begin{bmatrix}
0 & & & & & & & & & & & & & & & & \\
\boxed{G_1^\phi} & 0 & & & & & & & & & & & & & & & \\
G_2^\phi & G_1^\phi & 0 & & & & & & & & & & & & & & \\
G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & & & & & & & & & & & \\
G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & & & & & & & & & & & \\
G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & & & & & & & & & \\
G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & & & \bar{0} & & & & & & \\
G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & & & & & & & \\
G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & & & & & & & \\
G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & & & & & \\
G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & & & & & \\
G_{11}^\phi & G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & & & \\
G_{12}^\phi & G_{11}^\phi & G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & & & \\
G_{13}^\phi & G_{12}^\phi & G_{11}^\phi & G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & & & \\
G_{14}^\phi & G_{13}^\phi & G_{12}^\phi & G_{11}^\phi & G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & G_1^\phi & 0 & & \\
G_{15}^\phi & G_{14}^\phi & G_{13}^\phi & G_{12}^\phi & G_{11}^\phi & G_{10}^\phi & G_9^\phi & G_8^\phi & G_7^\phi & G_6^\phi & G_5^\phi & G_4^\phi & G_3^\phi & G_2^\phi & \boxed{G_1^\phi} & 0 & \\
\end{bmatrix}
\begin{bmatrix}
\tilde{I}_1^\phi \\
\tilde{I}_2^\phi \\
\tilde{I}_3^\phi \\
\tilde{I}_4^\phi \\
\tilde{I}_5^\phi \\
\tilde{I}_6^\phi \\
\tilde{I}_7^\phi \\
\tilde{I}_8^\phi \\
\tilde{I}_9^\phi \\
\tilde{I}_{10}^\phi \\
\tilde{I}_{11}^\phi \\
\tilde{I}_{12}^\phi \\
\tilde{I}_{13}^\phi \\
\tilde{I}_{14}^\phi \\
\tilde{I}_{15}^\phi \\
\tilde{I}_{16}^\phi
\end{bmatrix}$$

Fig. 3.1. Computation of the scalar potential contribution in (3.13). At each time step l , row l of the matrix-vector multiplication has to be computed. Rather than computing the multiplication row-by-row as in the MOT method, one of the blocked aggregates indicated by *squares* is multiplied at each time step. Causality is not violated: only past currents are used to find the present and future fields

To our knowledge, the use of space-time FFTs for solving time-domain integral equations was first proposed in the context of a global solution scheme, i.e., one that does not march in time but instead solves for all space-time unknowns simultaneously [45]. Nevertheless, space-time FFTs can also be used while marching in time by employing the multilevel/blocking framework of [48] or [53]; the latter was originally proposed in [63]. In this chapter, the scheme of [53] is adopted because of its simplicity. Figure 3.1 illustrates the mechanics of computing the scalar potential on the auxiliary grid for the first 16 time steps. Denote the matrix in Fig. 3.1 by $\mathbf{G}^\phi$; for future reference, denote the corresponding magnetic field and vector potential matrices by $\mathbf{G}^H$ and $\mathbf{G}^A$, respectively. To compute, for example at time step eight, the scalar potentials generated by $\mathbf{J}(\mathbf{r}, t)$ on S , the block matrix comprising the leftmost seven matrices on row eight of $\mathbf{G}^\phi$, i.e., $[G_7^\phi, G_6^\phi, \dots, G_1^\phi]$, has to be multiplied by the vector $[\tilde{I}_1^\phi, \tilde{I}_2^\phi, \dots, \tilde{I}_7^\phi]^\top$. Note that $\mathbf{G}^\phi$ (and its extension to all N_t time steps) is block-Toeplitz on four levels; the temporal Toeplitz structure is immediately visible in Fig. 3.1 and the 3D spatial Toeplitz structure of each of the matrices $\mathbf{G}_{l-l'}$ follows trivially from their construction. Therefore, $\mathbf{G}^\phi$ can be rapidly multiplied by a vector using 4D FFTs. When operating within

an MOT framework, however, the current vectors $\tilde{\mathbf{I}}_8^\varphi, \tilde{\mathbf{I}}_9^\varphi, \dots, \tilde{\mathbf{I}}_{N_t}^\varphi$ are unknown at time step seven; moreover, multiplication of the entire $\mathbf{G}^\varphi$ by the vector $[\tilde{\mathbf{I}}_1^\varphi, \tilde{\mathbf{I}}_2^\varphi, \dots, \tilde{\mathbf{I}}_7^\varphi, \tilde{\mathbf{I}}_8^\varphi, \dots, \tilde{\mathbf{I}}_{N_t}^\varphi]^\dagger$ (with $\tilde{\mathbf{I}}_8^\varphi, \tilde{\mathbf{I}}_9^\varphi, \dots, \tilde{\mathbf{I}}_{N_t}^\varphi$ filled with zeros) to compute the scattered fields at time step eight is clearly inefficient (as a similar procedure would have to be repeated each and every time step). Nevertheless, there exist various space–time submatrices of $\mathbf{G}^\varphi$ that are themselves block-Toeplitz on four levels and that can be multiplied by current coefficients without violating causality. That is, only currents that are already known are required to multiply these submatrices when marching in time. These submatrices are the aggregates of the individual matrices $\mathbf{G}_{l-l'}^\varphi$ indicated by the square boxes superimposed on $\mathbf{G}^\varphi$ in Fig. 3.1 and are further referred to as block aggregates. Stage (2) of the TD-AIM computes future scattered fields by multiplying these block aggregates with current vectors.

The cost of multiplying the block aggregates varies from time step to time step. For example, at time step nine, the scheme calls for the multiplication of a block aggregate of size $8N_c \times 8N_c$, whereas at time step ten only a matrix of size $N_c \times N_c$ is multiplied. Furthermore, larger block aggregates are multiplied less frequently. For example, the $4N_c \times 4N_c$ block aggregate in $\mathbf{G}^\varphi$ is multiplied only once for every eight time steps, whereas the $N_c \times N_c$ block is multiplied once for every two time steps (Fig. 3.1). Using this scheme, future scattered fields are constructed *partially* at each time step, and the *complete* scattered field at a given time step is available only at that time step. That is, at each time step, temporal chunks of past auxiliary current coefficients are transformed to the spectral-frequency domain, multiplied with (the 4D FFTs of) the corresponding block aggregate in Fig. 3.1, and then inverse transformed to produce temporal chunks of future scattered fields.

It is important to note that the largest nonzero block aggregate in $\mathbf{G}^\varphi$ contains only $O(N_g)$ block rows and columns. That is, Fig. 3.1 should not be interpreted to imply that the size of the largest block aggregate in $\mathbf{G}^\varphi$ scales as $O(N_t)$; indeed, the impulsive nature of the Green function renders the very large block aggregates zero. This implies that the number of different square boxes is only $\lfloor \log_2 N_g \rfloor + 1$, with the largest one of size $2^{\lfloor \log_2 N_g \rfloor} N_c \times 2^{\lfloor \log_2 N_g \rfloor} N_c$. Thus, the largest temporal FFT size is proportional not to the duration of the analysis but to the maximum transit time across the scatterer.

3.3.4 Computational Cost and Complexity/Comparison to Other Time Domain Methods

Stages (1), (3), and (4) of the algorithm require $O(N_t N_s)$ operations because each of the seven projection matrixials $\mathbf{\Lambda}_{x,y,z,\nabla}(t)$ and $\mathbf{\Gamma}_{x,y,z}(t)$ as well as each near-field matrix $\mathbf{Z}_{l-l'}^{\text{near}}$ contains at most $O(N_s)$ nonzero elements, and because $\mathbf{Z}_{l-l'}^{\text{near}}$ matrices are zero for $l - l' > l^{\text{near}}$, with $l^{\text{near}} \sim (\gamma \Delta s)/(c \Delta t)$. The sparsity of the projection matrices follows directly from the fact that each basis function $\mathbf{S}_k(\mathbf{r})$ is represented by a fixed number of M_k nodes on

the auxiliary grid where M_k is independent of N_s . That each near-field correction matrix contains no more than $O(N_s)$ nonzero entries and that only a fixed and small number of the $\mathbf{Z}_{l-l'}^{\text{near}}$ matrices are nonzero follows from the following facts: (a) γ is independent of N_s , (b) the temporal functions $\tilde{T}(t)$ are localized, with $c\Delta t$ on the order of the discretization length on S , and (c) the free-space Green function is impulsive in nature. Therefore, each basis function communicates with at most $O(1)$ of its neighbors through the near-field correction matrices. Because the projection and near-field matrices are so sparse, the computational cost of the algorithm is dominated by that of Stage (2), i.e., the multiplication of the matrices $\mathbf{G}_{l-l'}^{\mathbf{H},A,\varphi}$ by vectors of past coefficients of auxiliary sources.

To estimate the computational cost of Stage (2), recall that there are $\lfloor \log_2 N_g \rfloor + 1$ different nonzero block aggregates in $\mathbf{G}^{\mathbf{H},A,\varphi}$. The i th block aggregate, $i = 0, 1, \dots, \lfloor \log_2 N_g \rfloor$, is of size $2^i N_c \times 2^i N_c$ and can be multiplied in $O(N_c (\log N_c + 2^i \log 2^i))$ operations using space-time FFTs by storing the currents and fields in the spectral domain (k space). Notice that the above complexity estimate is significantly lower than that resulting from a straightforward application of a 4D FFT, which would require $O(2^i N_c \log(2^i N_c))$ operations. The complexity is reduced by observing that the spatial FFTs need not be repeatedly computed. (This observation is also important for parallel efficiency as discussed in Sect. 3.3.5.) For example, at time step nine, spatial FFTs of auxiliary current coefficients at time steps one through eight are needed, but those of steps one through seven are already computed at previous time steps. Hence, the number of spatial FFTs can be minimized by pre-computing the 3D forward spatial FFTs of each matrix $\mathbf{G}_{l-l'}^{\mathbf{H},A,\varphi}$, by computing 3D forward spatial FFTs of the currents *only* at the previous time step, and by computing 3D inverse spatial FFTs of the fields *only* at the next time step. Because the i th block aggregate is multiplied once every 2^{i+1} time steps, the *per-time step* cost of multiplication is $O(N_c (\log N_c^{0.5^{i+1}} + \log 2^{i/2}))$. Thus, the total computational complexity of Stage (2) is

$$\begin{aligned} N_t \sum_{i=0}^{\lfloor \log_2 N_g \rfloor} O(N_c (\log N_c^{0.5^{i+1}} + \log 2^{i/2})) \\ = O(N_t N_c (\log N_c + \lfloor \log_2 N_g \rfloor^2)). \end{aligned} \quad (3.14)$$

For quasi-planar surfaces, $N_c \sim N_s$, while for general 3D surface scatterers $N_c \sim N_s^{1.5}$. Therefore, because $N_g \sim N_s^{0.5}$, the total number of operations of TD-AIM scales as $O(N_t N_s \log^2 N_s)$ for quasi-planar surfaces and as $O(N_t N_s^{1.5} \log^2 N_s)$ for general surfaces. The memory requirements of the TD-AIM is dictated by the largest block to be FFTed, which requires $O(N_g N_c)$ bytes of storage space, i.e., $O(N_s^{1.5})$ bytes for quasi-planar surfaces and $O(N_s^2)$ bytes for general 3D surfaces.

Next, to quantify the performance of TD-AIM for the three surface integral equations in (3.3), the number of spatial FFTs required for solving each one is counted. By computing and storing the spatial FFTs of the propagation matrices $\mathbf{G}_1^{A,\varphi}, \dots, \mathbf{G}_{N_g}^{A,\varphi}$ prior to time marching, a total of $2N_g + 4N_t$ forward and $4N_t$ inverse spatial FFTs are computed for the EFIE. Similarly, $3N_g + 3N_t$ forward and $3N_t$ inverse spatial FFTs are required for the MFIE. A straightforward combination for the CFIE would thus require $5N_g + 4N_t$ forward and $7N_t$ inverse spatial FFTs. In our implementation, the number of spatial FFTs required for the CFIE is reduced to $2N_g + 4N_t$ forward and $4N_t$ inverse spatial FFTs using an approach similar to that in [61]. The CFIE cost is reduced by observing that both the EFIE and the MFIE kernels are formulated in terms of the vector potential $\mathbf{A}(\mathbf{r}, t)$, and that each Cartesian component of the temporal derivatives of $\mathbf{A}(\mathbf{r}, t)$ are available on the uniform mesh at the end of Stage (2). Consequently, the MFIE contributions can be obtained from the EFIE computations without any additional FFTs, i.e., space-time samples of $\nabla \times \partial_t \mathbf{A}(\mathbf{r}, t)$ are computed from the space-time samples of $\partial_t^2 \mathbf{A}(\mathbf{r}, t)$ using a higher-order finite difference approach and numerical time integration. (The time integration translates to a trivial complex scalar multiplication in the time-harmonic formulations.) The time integral is evaluated efficiently in the time-marching context by storing the value of the integral at each auxiliary point at the previous time step and adding to it at each time step. Hence, the CFIE computation requires the same number of spatial (and temporal) FFTs as that of the EFIE and a total of $O(N_t N_c)$ extra operations and $O(N_c)$ extra storage.

A comparison with other time-domain schemes is in order. Irrespective of the nature of the scatterer, the CPU cost and memory requirements of classical MOT solvers scale as $O(N_t N_s^2)$ and $O(N_s^2)$, respectively. Therefore, the CPU and memory costs of the TD-AIM scheme always scale better than those of classical solvers, with the exception of the TD-AIM memory cost for 3D surfaces, which scales only on par with that of classical MOT solvers. In [46, 47] algorithms that ignore the temporal Toeplitz structure of (3.5) and employ only spatial FFTs were considered. The computational complexity of those schemes when applied to Stage (2) scales as $O(N_t N_c N_g)$, i.e., as $O(N_t N_s^{1.5})$ for quasi-planar surfaces and as $O(N_t N_s^2)$ for general surfaces (under the above delineated conditions). Therefore, the CPU cost of the present algorithm always scales better than time-domain schemes that use only spatial FFTs. The memory requirements of those schemes, however, are of the same order as those of the present algorithm. Finally, the CPU and memory requirements of general purpose, multilevel PWTD schemes scale as $O(N_t N_s \log^2 N_s)$ and $O(N_g N_s)$, respectively [16]. Therefore, when compared to multilevel PWTD acceleration, the TD-AIM asymptotically scales worse for general 3D surfaces and has the same computational cost for quasi-planar structures. Nonetheless, in our experience, TD-AIM remains competitive with multilevel PWTD for 3D surfaces up to tens of thousands of spatial unknowns, and generally outperforms it for quasi-planar structures.

3.3.5 Parallelization

The practical bottleneck of the TD-AIM is its memory requirements. Compared to its frequency-domain counterpart, the TD-AIM requires $O(N_g)$ times more memory because it needs to store the temporal history of sources to compute retarded fields throughout the auxiliary mesh. To moderate the impact of this memory bottleneck, this section presents a TD-AIM parallelization strategy targeting distributed memory computers that communicate via message passing. While the TD-AIM scheme's memory appetite serves as the main motivation behind the parallelization effort, parallel efficiency is not ignored and load balancing and scalability issues are also addressed.

The following approach to parallelization is based on the balanced distribution of the uniform grid and the FFT operations related to it among the P available processors. Because zero-padding (doubling) is required to multiply a (block-)Toeplitz matrix via FFTs, all 4D FFTs are done on arrays of size *at most* $2N_{cx} \times 2N_{cy} \times 2N_{cz} \times 2N_g$ (the temporal array size varies from time step to time step), which are either derived from the blocked aggregates in $\mathbf{G}^{\mathbf{H},A,\varphi}$ or are the zero-padded currents and fields on the auxiliary grid. To reduce the memory demand per processor, the arrays are distributed among the processors by one-dimensional (1D) slab-decomposition: each processor stores $2N_{cx}/P \times 2N_{cy} \times 2N_{cz} = 8N_c/P$ spatial entries over time as depicted in Fig. 3.2. Because now only part of the auxiliary grid is available to each

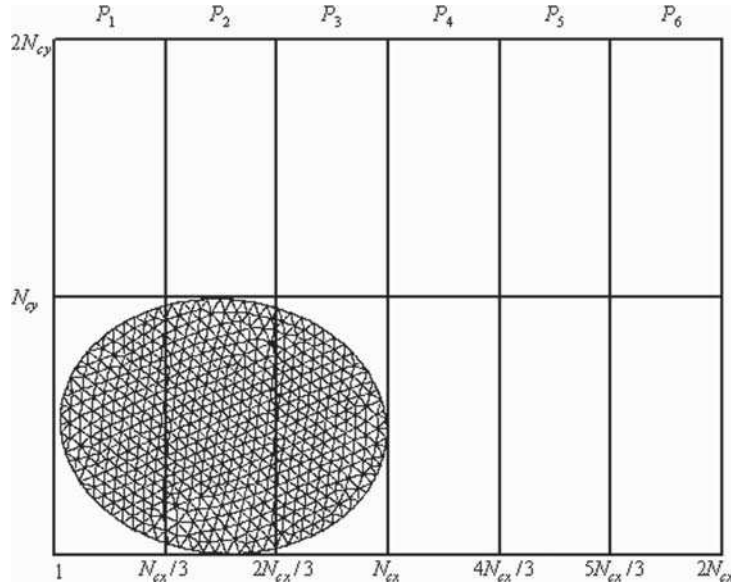


Fig. 3.2. One-dimensional slab-decomposition for $P = 6$. The auxiliary mesh is of size $N_{cx} \times N_{cy} \times N_{cz}$ (z dimension is not shown) and is distributed by dividing the x dimension into slabs. Due to doubling, each processor stores $N_{cx}/3 \times 2N_{cy} \times 2N_{cz}$ spatial entries over time

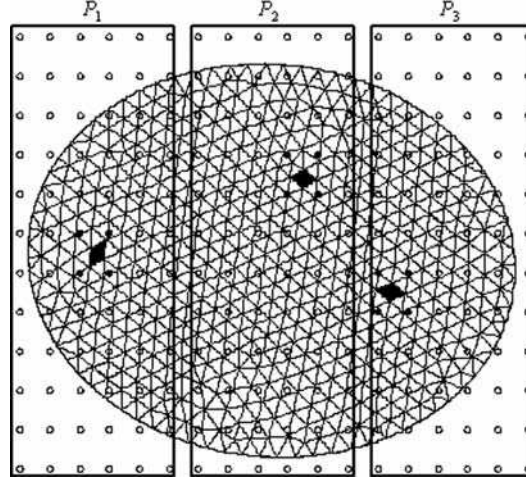
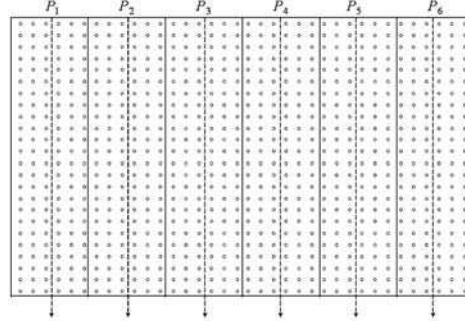


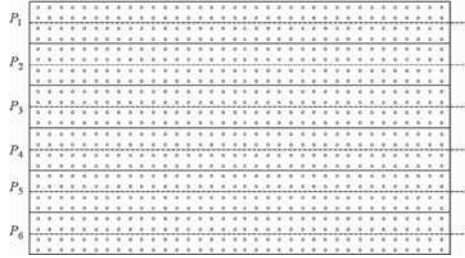
Fig. 3.3. Stage (1) of the algorithm: parallel projection onto the uniform mesh. Here, $P = 6$, $N_{cx} = 18$, and $N_{cy} = 12$ (z dimension is not shown). Only the part of the uniform mesh that is projected to by the active processors is shown. Three RWG functions and the related nodes are highlighted. Each processor projects all the RWG functions that affect its section of the mesh

processor, all four stages of the algorithm should be modified accordingly as illustrated in Figs. 3.3 and 3.4 and described below.

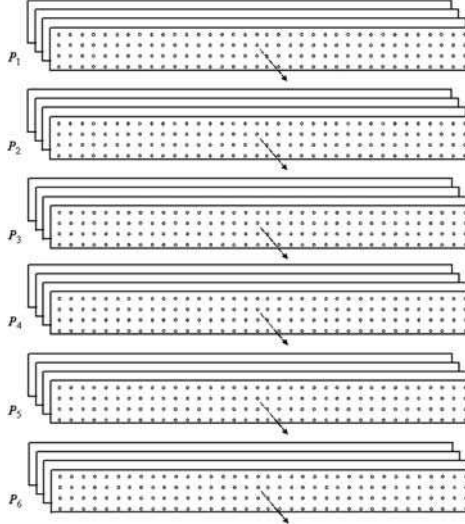
1. At time step l , each processor projects the current density $\mathbf{I}_{l-1}$ onto its section of the auxiliary grid (Fig. 3.3). Because approximately half of the processors do the projection and because the primary mesh is not uniform, the distribution of this effort among processors is unbalanced. Nonetheless, this does not significantly affect the parallel efficiency because of the minute amount of CPU resources required to compute local projections as compared to FFTs.
2. The space-time FFTs are computed in parallel using the FFTW library [64]. Specifically, each processor computes two-dimensional (2D) FFTs in the y and z dimensions of its section of the zero-padded current-arrays (Fig. 3.4a). Next, all arrays are transposed, which requires an all-to-all processor communication. Finally, each processor computes FFTs in the x dimension to complete the spatial FFTs [44, 52, 64] (Fig. 3.4b). Hence, the auxiliary current coefficients at time $(l-1)\Delta t$ is transformed to the spectral domain (k space). These spectral-domain arrays are stored to minimize repeated computations and communication. Then, the processors concurrently compute temporal FFTs at each of their $8N_c/P$ spatial nodes according to the blocking scheme of Sect. 3.3.3 to transform the current to the spectral-frequency domain (Fig. 3.4c). Next, each processor multiplies its part of the transformed currents and block aggregates to obtain a part of fields in the spectral-frequency domain. Once these



(a)



(b)



(c)

Fig. 3.4. Stage (2) of the algorithm: parallel space-time FFTs. Here, $P = 6$, $N_{cx} = 18$, and $N_{cy} = 12$ (z dimension is not shown). **(a)** Each processor computes six FFTs of size 24 in the y dimension. This is followed by an all-to-all communication step that transposes the arrays. **(b)** Each processor then computes four FFTs of size 36 in the x dimension for the transposed arrays. **(c)** Temporal FFTs, the size of which depends on the time step, are computed. Here, each processor computes 144 FFTs of size 4

fields are found, the above steps are reversed: Each processor computes inverse temporal FFTs to find temporal chunks of future fields in the spectral domain (k space), and these *partial* future fields are added to those obtained from previous time steps at each one of the $8N_c/P$ spatial points. Finally, the inverse spatial FFTs of the fields *only* at the next time step are computed to obtain the *complete* field in the space-time domain at time $l\Delta t$. As described here, the computational cost of Stage (2) is $O(N_t N_c (\log N_c + \log^2 N_g)/P)$ and its per-processor memory requirement is $O(N_g N_c/P)$. Because there are only two global communications for transposing the arrays at each time step, the total communication cost is $O(N_t N_c)$. The work in this stage is equally distributed if N_{cx}/P and N_{cy}/P are integers.

3. Similar to Stage (1), each processor interpolates the fields on its section of the auxiliary grid to the surface mesh, that is, the processors consider all the unknowns on the primary mesh that are affected by their sections of the arrays.
4. The near-field interactions are corrected in parallel. Let aN_s denote the number of nonzero elements of the $\mathbf{Z}_{l-l'}^{\text{near}}$ matrices, i.e., the number of near-field corrections. To multiply the $\mathbf{Z}_{l-l'}^{\text{near}}$ matrices in parallel, the nonzero elements are distributed among the processors using a column-based decomposition, i.e., each processor stores and multiplies approximately aN_s/P matrix elements plus or minus one column of the matrices. Hence, each processor stores a short history (l^{near} time steps) of parts of the primary currents that correspond to its columns of $\mathbf{Z}_{l-l'}^{\text{near}}$.

Once all four stages of the TD-AIM algorithm are completed at a given time step l and $\mathbf{V}_l^{\text{scat}}$ is formed, (3.5) is solved in parallel for the current density at the next time step. Because $\mathbf{Z}_0$ matrix in general has $O(N_s)$ nonzero elements, the communication cost dominates the parallel solution time, which does not exhibit good scalability, and hampers the overall parallel efficiency [65]. The solution time becomes sub-dominant, however, as the problem becomes electrically large, i.e., as N_s , N_c , and N_g increase.

3.3.6 Accuracy and Computational Complexity Verification

This section presents numerical examples that demonstrate the operation of the TD-AIM accelerated MOT-TDIE solver. First, two matching approaches are compared. Then, the computational complexity, memory requirements, and parallel efficiency of the accelerated solver are examined by simulating two types of scatterers that represent the best- and worst-case scenarios for the algorithm, viz. plates and spheres. In all simulations, the temporal basis functions are fourth-order Lagrange interpolants [7], and the MFIE contributions, when needed, are computed using the numerical scheme presented in Sect. 3.3.4, with a fifth-order accurate temporal integration and a fourth-order accurate central differencing scheme. All the results in this section were obtained on cluster of 1-GHz Pentium III processors with 1 GB of memory.

Matching Accuracy

To investigate the accuracy of the moment- and field-matching approaches, the interaction between two RWG functions is computed and the error incurred by the TD-AIM is examined. A flat RWG basis function $\mathbf{S}_{k'}(\mathbf{r})$ that is anchored at the origin supports an impressed current $\mathbf{S}_{k'}(\mathbf{r}) e^{-2(\pi f_{\max} t - 12)^2/9}$, where $f_{\max}$ quantifies the maximum frequency of interest and more than 99.997% of the Gaussian pulse's power is at frequencies below $f_{\max}$. The fields radiated by this basis function are measured on another flat RWG function $\mathbf{S}_k(\mathbf{r})$ (Fig. 3.5). The auxiliary grid is centered at $x = 0.5\Delta s_x$, $y = 0.5\Delta s_y$, and $z = 0.5\Delta s_z$, where Δs_x , Δs_y , and Δs_z are the grid spacings. The relative energy error in the tested fields is defined as

$$\Delta^{\text{AIM}} = \left[\sum_{l=1}^{N_t} \left(\mathbf{V}_l^{\text{scat}}(k) - \mathbf{V}_l^{\text{scat,AIM}}(k) \right)^2 / \sum_{l=1}^{N_t} \left(\mathbf{V}_l^{\text{scat}}(k) \right)^2 \right]^{0.5}, \quad (3.15)$$

where $\mathbf{V}_l^{\text{scat}}$ is given in (3.5) and

$$\mathbf{V}_l^{\text{scat,AIM}} = \sum_{l'=\max(1, l-N_g)}^{l-1} \mathbf{Z}_{l-l'}^{\text{FFT}}(k, k') \mathbf{I}_{l'}(k'). \quad (3.16)$$

Figures 3.6 and 3.7 present Δ^{AIM} as a function of the center-to-center distance between $\mathbf{S}_{k'}(\mathbf{r})$ and $\mathbf{S}_k(\mathbf{r})$. For the results presented in both figures, $f_{\max} = c$ ($\lambda_{\min} = c/f_{\max} = 1$ m), $\Delta t = 1/(30c)$ ($\beta = 1/15$), in order to capture the significant part of the pulse for even the farthest interaction, $N_t = 250$, and the number of dipoles is 8 and 64. In Fig. 3.6, $\Delta s_x = \Delta s_y = \Delta s_z = \lambda_{\min}/20 = 5$ cm while in Fig. 3.7, $\Delta s_x = \Delta s_y = \Delta s_z = \lambda_{\min}/40 = 2.5$ cm. In both figures, the time-basis functions are approximate prolate functions [9, 10] that exhibit excellent time- and band-limitedness properties allowing accurate evaluations of the integrals in (3.6c). In the field-matching approach these functions are also used to interpolate the samples of the time signatures. In Figs. 3.6b and 3.7b, the near-field sphere on which the fields are matched is chosen to be at 50 cm. Taken as a whole, Figs. 3.6 and 3.7 show that the error made by (3.7) for both moment- and field-matching approaches decreases as the auxiliary-grid

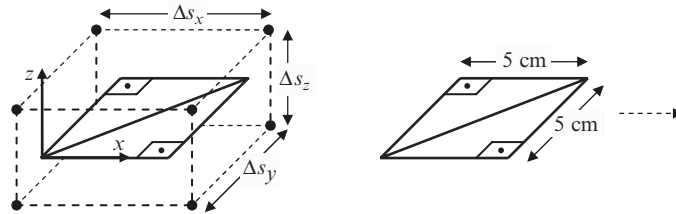


Fig. 3.5. The RWG functions and some of the auxiliary points used

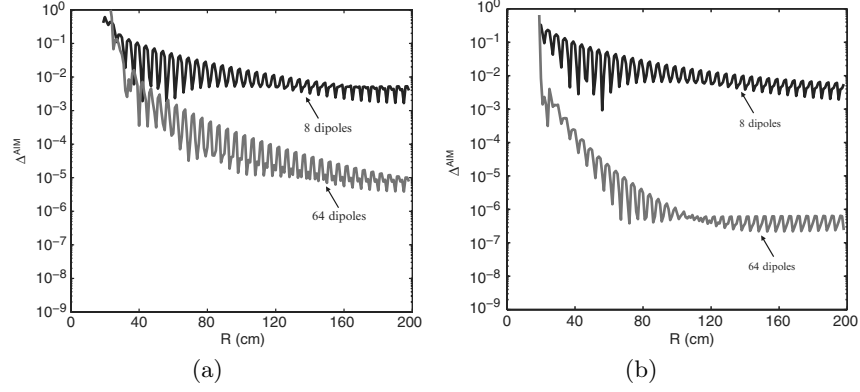


Fig. 3.6. Relative energy error Δ^{AIM} for the RWG functions in Fig. 3.5 as a function of their center-to-center distance for $\Delta s_x = \Delta s_y = \Delta s_z = \lambda_{\min}/20 = 5$ cm. (a) The multipole moments are matched from zero up to order one (8 dipoles) and up to order three (using 64 dipoles). (b) The fields are matched on a near-field sphere at 50 cm using 8 and 64 dipoles

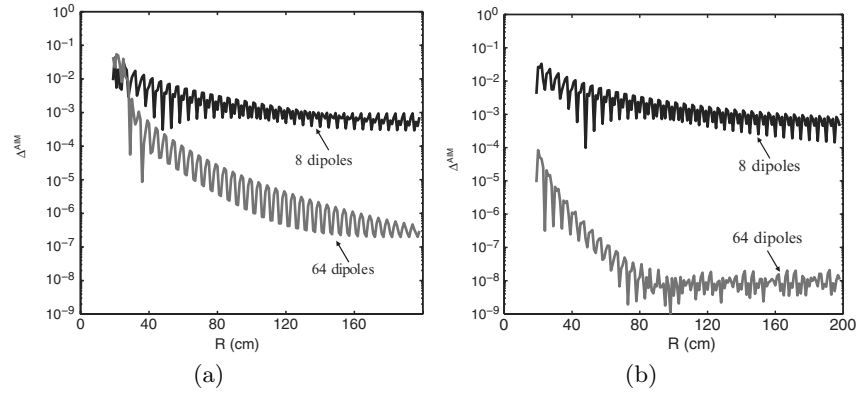


Fig. 3.7. Relative energy error Δ^{AIM} for the RWG functions in Fig. 3.5 as a function of their center-to-center distance for $\Delta s_x = \Delta s_y = \Delta s_z = \lambda_{\min}/40 = 2.5$ cm. (a) The multipole moments are matched from zero up to order one (using 8 dipoles) and up to order three (using 64 dipoles). (b) The fields are matched on a near-field sphere at 50 cm using 8 and 64 dipoles

spacing becomes smaller. These figures also show that the moment-matching approach produces results accurate enough for practical applications. Even though field-matching results in more accurate matrix elements, because of the reasons detailed in Sect. 3.3.2, moment-matching is utilized in the hybrid solver for simulations presented in Sect. 3.4. A more detailed error analysis of moment-matching approach for time-domain surface integral equations (including CFIE) can be found in [17].

Computational Complexity Verification

The theoretical computational complexity, memory requirements, and parallel efficiency of the TD-AIM were derived in Sects. 3.3.4 and 3.3.5. Here, the scheme's practical efficiency is evaluated by analyzing scattering plates and spheres. In what follows, all scatterers are centered at the origin of the coordinate system, and plate side-lengths and sphere diameters are denoted L_p and L_s , respectively. Scattering from square plates is analyzed using the EFIE, whereas scattering from spheres is analyzed using the CFIE ($\alpha = 0.4$). The TD-AIM parameters are chosen to minimize the CPU time and memory product while ensuring that a relative root-mean-square RCS error with respect to a frequency-domain method-of-moments (MOM) solver, which uses the same mesh as the TD-AIM accelerated MOT-TDIE solver, is less than 0.01.

Figure 3.8a,b plot the average TD-AIM wall-clock time per time step (i.e., the total wall-clock time spent to construct $\mathbf{V}_l^{\text{scat}}$ divided by N_t). Figure 3.9a,b plot the corresponding *measured* peak memory requirement of the algorithm which also includes operating system overhead. The figures show the parallel efficiency of the algorithm as the surface areas of the plates and spheres are increased 625 and 144 times, respectively, i.e., L_p varies from 1 to 25 m and L_s varies from 1 to 12 m. Both the CPU time and the memory requirements of the algorithm exhibit good parallel efficiency as the size of the scatterers increase. The computational complexity of TD-AIM with respect to the number of surface unknowns N_s is verified in Fig. 3.10a,b using the data points in Fig. 3.10a,b: The total CPU time per time step and the memory requirements of TD-AIM are computed by multiplying the data points in Fig. 3.10a,b with the corresponding number of processors P . Thus, if the implementation had ideal parallel efficiency all the data points for a given N_s would coincide in Fig. 3.10. The computational complexity of the implementation is in good

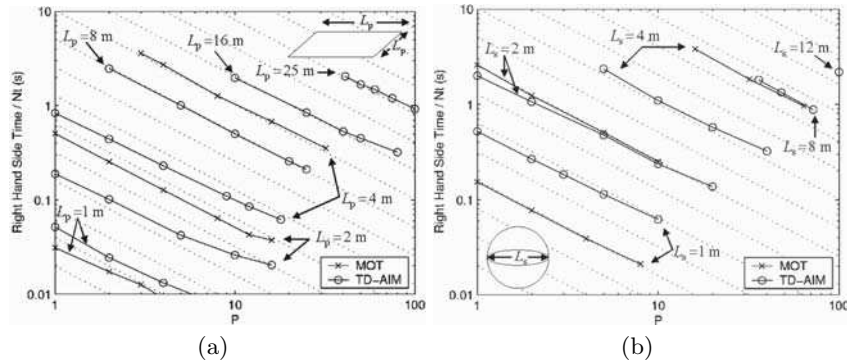


Fig. 3.8. Average wall-clock time to compute $\mathbf{V}_l^{\text{scat}}$ at each time step for (a) plates and (b) spheres. *Dashed lines* are ideal speed-up tangents

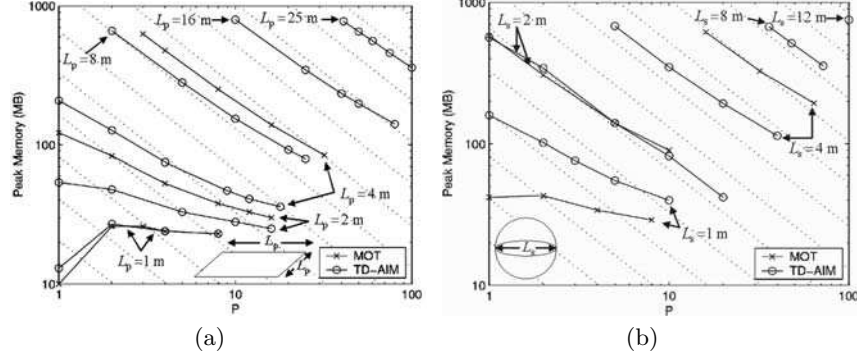


Fig. 3.9. Observed peak storage requirement among all processors for (a) plates and (b) spheres. *Dashed lines* are ideal speed-up tangents

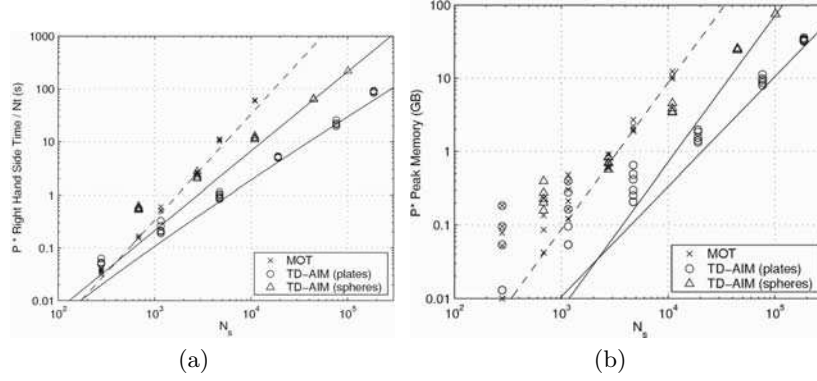


Fig. 3.10. TD-AIM versus MOT for plates and spheres. (a) Computational complexity. The lines are parallel to N_s^2 , $N_s^{1.5}$, and $N_s \log^2 N_s$. (b) Memory requirement. The lines are parallel to N_s^2 , N_s^2 , and $N_s^{1.5}$

agreement with the trends predicted in Sect. 3.3. Figure 3.10a,b also compare the computational demands of TD-AIM with those of a classical (parallel) MOT scheme: The TD-AIM accelerated MOT-TDIE solver outperforms the classical one for as little as $N_s \approx 500$ for plate and $N_s \approx 2,500$ for sphere simulations.

3.4 Hybridization and Applications to Challenging EMI Problems

Even though the TD-AIM accelerator renders stand-alone MOT-TDIE field solvers useful for analyzing transient fields on electrically large and multi-scale platforms, these solvers are of little use when these platforms carry

cable-interconnected subwavelength scale, and potentially nonlinear electronic subsystems. To characterize field interactions with such structures, the hybridization of MOT-TDIE field solvers with specialized subsystem simulators is called for. For example, to facilitate the efficient analysis of real-world EMI problems, MOT-TDIE field solvers should be hybridized with a circuit solver that computes node voltages and branch currents in nonlinear lumped-element circuits, a cable solver that computes voltages and currents along multiconductor transmission lines, and modules that facilitate the macromodel description of electronic subsystems.

This section elucidates the hybridization of MOT-TDIE field solvers with subsystem modelers and demonstrates the versatility of the resulting hybrid simulator through its application to real-world EMI problems.

3.4.1 Hybridization with Circuit Solvers

It is well-known that electrically small components can be effectively and accurately modeled as (nonlinear) lumped-element circuits using modified nodal analysis (MNA)-SPICE solvers [66–68]. MNA enforces Kirchhoff’s equations on non-ground nodes and solves the resulting nonlinear system of equations for non-ground node voltages and voltage source currents.

Recently, TDIE-field solvers were hybridized with MNA-circuit solvers and applied to the analysis of transient field interactions with electrically large platforms loaded with nonlinear lumped-element circuits [26, 27]. Hybridization of field and circuit solvers (i.e., combining the MOT and MNA systems) results in a coupled nonlinear system of equations that is solved simultaneously for all field and circuit solver unknowns via Newton–Raphson. The parallel scalability of the hybrid simulator is maintained by distributing the field and circuit solvers’ computational work to two separate groups of processors [27]. This simple but effective parallelization strategy results in near-ideal scalability since these groups of processors communicate only during the iterative solution of the coupled system. Additionally, this separation strategy allows for the separate development and optimization of field and circuit solvers.

3.4.2 Hybridization with Cable Solvers

Under transverse electromagnetic (TEM)-like propagation assumption, fields along multiconductor transmission lines are represented by voltage and current waves satisfying the well-known transmission-line equations [69, 70]. A 1D TDIE is obtained by enforcing the boundary conditions relating voltages and currents at the transmission-line terminations. The standard MOT recipe, which originally was developed for solving 3D TDIEs pertinent to scattering problems, is used to solve the 1D TDIEs describing transmission-line signal propagation. The lossy and dispersive nature of the guided-wave propagation along the transmission line is accounted for by using the pertinent Green function. The TDIE-cable solver’s computational bottleneck is the evaluation

of excitation voltages and currents, which requires the convolution of Green functions with the “past” voltages and currents. The computational complexity of this operation, which scales as $O(N_t^2)$, is reduced to $O(N_t \log^2 N_t)$ using the FFT acceleration algorithm of [53]. The main advantage of this acceleration scheme is that it applies regardless of the method used for obtaining the Green function (measurements, direct time-domain computation, Fourier transformation of frequency-domain models).

The TDIE-field solver was hybridized with TDIE-cable and MNA-circuit solvers and applied to the EMI analysis of electrically large, real-world problems involving coaxial and unshielded multiconductor cables [25, 30]. Connectors and loads that terminate the cables are assumed to be electrically small and modeled with lumped element circuit networks; node voltages and branch currents on these circuits are computed using the circuit solver. The hybrid simulator solves the coupled system of equations, which is obtained by combining the two MOT and the MNA systems, simultaneously for all field, cable, and circuit unknowns. The same parallelization strategy is followed; the cable solver’s computational work is assigned to the circuit solver’s group of processors.

3.4.3 Incorporation of Macromodelers

Macromodels are reduced multiport transfer function representations of electronic subsystems that would require large circuit networks if modeled using lumped elements [71, 72]. They have long been employed in circuit solvers to reduce computational costs and avoid loss of accuracy in system-level analysis. Gains in CPU time and memory are attained by using recursive convolution algorithms and reduced-order model generation techniques [73–77].

In practice, macromodels can be connected to ports of subsystems modeled either by the circuit- or field-solver component of the hybrid simulator; hence, they need to be interfaced with both solvers simultaneously. However, the integration of the commonly used admittance parameter macromodels – or any other macromodel defined by a single set of network parameters – with each solver requires a separate treatment, because the field-solver unknowns are current quantities, while the circuit-solver unknowns are voltage quantities. The effective incorporation of the macromodels with fast hybrid simulators requires the identification of associated computational bottlenecks in the solution of the resulting coupled system of equations and the use of fast recursive convolution schemes to overcome these bottlenecks [32].

3.4.4 Applications

In the applications presented below, all the structures are excited by plane waves and/or “delta-gap” voltage sources. Electric fields $\mathbf{E}^{\text{inc}}(\mathbf{r}, t)$ of $\hat{\mathbf{p}}$ -polarized plane waves propagating in the $\hat{\mathbf{k}}$ direction and voltages $V^{\text{inc}}(t)$ of localized sources are expressed as

$$\mathbf{E}^{\text{inc}}(\mathbf{r}, t) = \hat{\mathbf{p}} E_0 G_{\text{mod}}(t - \mathbf{r} \cdot \hat{\mathbf{k}}/c), \quad (3.17a)$$

$$V^{\text{inc}}(t) = V_0 G_{\text{mod}}(t), \quad (3.17b)$$

where E_0 and V_0 are the electric field peak and voltage amplitudes, and $G_{\text{mod}}(t) = e^{-(t-t_p)^2/2\sigma^2} \cos(2\pi f_c(t-t_p))$ is a modulated Gaussian signature function with modulation frequency f_c , delay $t_p = 8\sigma$, duration $\sigma = 3/(2\pi f_{\text{bw}})$, and bandwidth f_{bw} . This choice of parameters guarantees that more than 99.997% of $G_{\text{mod}}(t)$'s power resides inside the frequency band $[f_{\text{min}} = f_c - f_{\text{bw}}, f_{\text{max}} = f_c + f_{\text{bw}}]$. All simulations were carried on a cluster of 2-GHz Apple G5 processors.

Monopole Antennas Mounted on a Car

The hybrid simulator is used in the EMI analysis of three antennas mounted on a 1984 Chevrolet Camaro Z28 (Fig. 3.11a): Two 10 cm long monopole antennas M_1 and M_2 and one 50 cm long monopole antenna M_3 are mounted on the mirrors and near the rear of the car, respectively (Fig. 3.11b). Antennas M_1 and M_2 are connected to voltage sources using 15 cm long cables T_1 and T_2 , and antenna M_3 is connected to a 50- Ω load located inside an electronic shielding box in the trunk using a 1.20 m long cable T_3 (Fig. 3.11b). Cables T_1 , T_2 , and T_3 are RG-58 coaxial cables with foam polyethylene dielectric filling, outer shield radius $a_o = 0.1524$ cm, inner shield radius $a_i = 0.1397$ cm, and wave speed $c_{\text{CBL}} = 0.78c$. Cables T_1 and T_2 are embedded within the mirror cavities; hence, they only interact with external fields via their terminations. Cable T_3 interacts with external fields along its shield as well as via its terminations. Cable T_3 's shield transfer impedance is given by $\hat{T}^i(f) = R_0 [(1+j)(a_o - a_i)/\delta] / \sinh[(1+j)(a_o - a_i)/\delta] + j2\pi f L_a$, where $\delta = \sqrt{1/(\pi f \sigma \mu)}$ is the skin depth, $\sigma = 5.0 \times 10^7 \text{ S m}^{-1}$ is the conductivity, $\mu = \mu_0$ is the permeability, $R_0 = 14.3 \text{ m}\Omega \text{ m}^{-1}$, and $L_a = 1.0 \text{ nH m}^{-1}$ [78]. The two voltage sources connected to cables T_1 and T_2 have $V_0 = 1 \text{ V}$, $f_{\text{min}} = 0.4 \text{ GHz}$, $f_c = 0.8 \text{ GHz}$, and $f_{\text{max}} = 1.2 \text{ GHz}$. The simulation is carried out for $N_t = 2,000$ time steps with $\Delta t = 55 \text{ ps}$. The current density on the surfaces modeling the car, the electronic shielding box, the exposed cable T_3 and the voltages on the cable loads are modeled by 128 976 surface, 667 wire, 44 junction basis functions and 6 circuit unknowns, respectively. The number of cable unknowns is six. Coupling of the external and guided fields is realized at 55 points. The temporal basis functions used for discretizing the 3D and 1D TDIEs are prolate-based band-limited interpolant with $8\Delta t$ half-width [9, 10], and third-order Lagrange polynomial [7], respectively. The TD-AIM kernel matches up to third-order moments, $\gamma = 6$, $\Delta s_x = 40.84 \text{ cm}$, $\Delta s_y = 40.84 \text{ cm}$, and $\Delta s_z = 53.37 \text{ cm}$; this choice of TD-AIM parameters results in $N_c = 192 \times 81 \times 35$ auxiliary grid points. Figure 3.12 presents the transient coupled voltages observed at node 1 (Fig. 3.11b) due to radiation

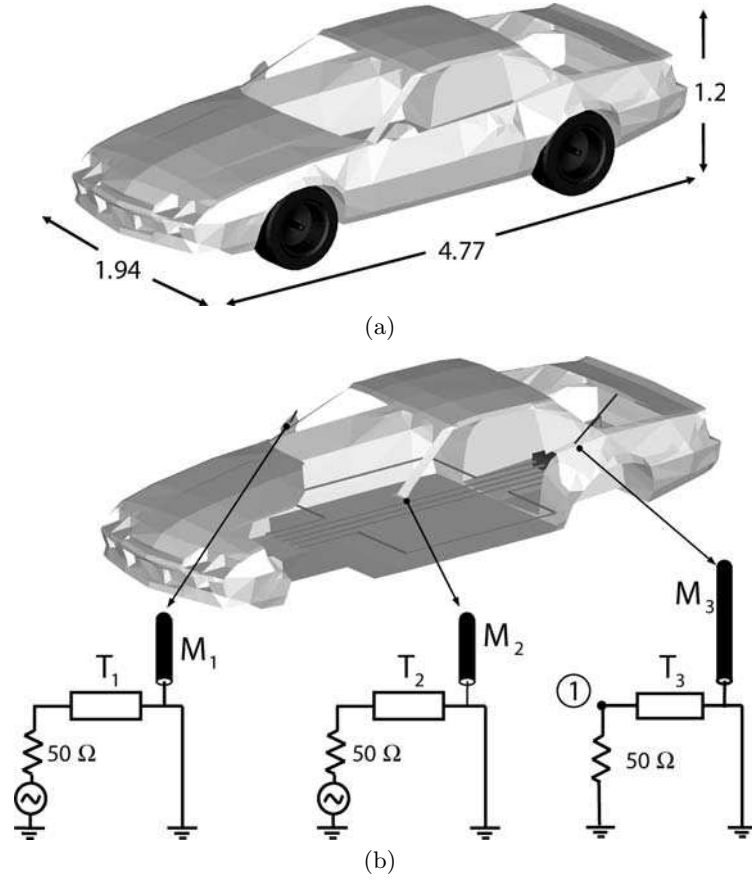


Fig. 3.11. Monopole antennas mounted on a car. (a) Dimensions of the car. (All dimensions are in meters.) (b) Locations of the monopole antennas and descriptions of their feed networks

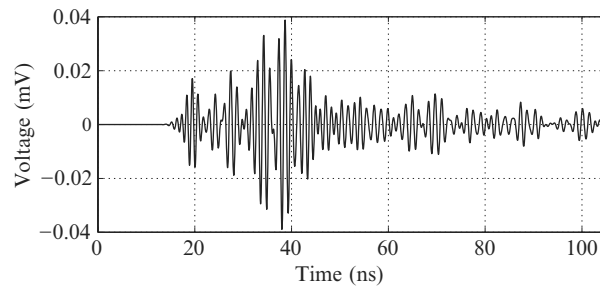


Fig. 3.12. Transient voltage observed at node 1 (Fig. 3.11b) due to external fields radiated by the short monopole antennas

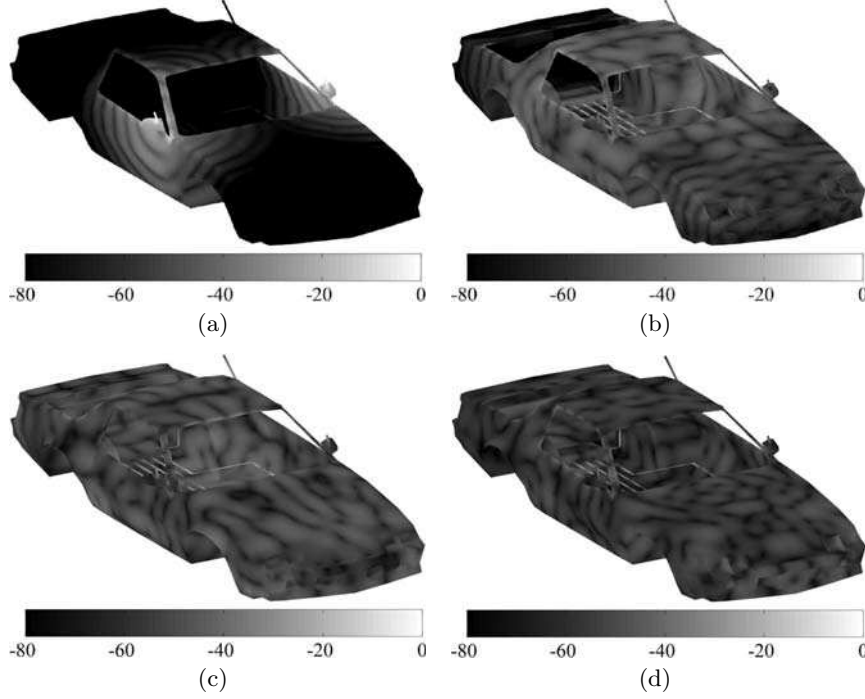


Fig. 3.13. Snapshots of the transient currents on the surfaces modeling the car, the antennas, and the exposed coaxial cable (in dB scale) at (a) $\Delta t = 6.6$ ns, (b) $\Delta t = 9.9$ ns, (c) $\Delta t = 13.2$ ns, and (d) $\Delta t = 26.4$ ns

from monopoles M_1 and M_2 . Figure 3.13a–d present snapshots of the current density on the surfaces modeling the car, the antennas, and the exposed coaxial cable at different time instances. The hybrid simulator required 120 GB of memory and 40 m to fill the matrices and 1.46 h to find the solution using 121 processors (120 for the field solver, 1 for the circuit and cable solvers).

PC Enclosures in a Cockpit

The hybrid simulator is used in the EMI analysis of three RG-58 coaxial cables connecting three PCs located inside an airplane cockpit. All of the PCs have identical outer dimensions and two of them, which are close to the floor of the cockpit, contain a mother board and two daughter cards (Fig. 3.14a,b). The two daughter cards are identical in size; the daughter card, which is closer to the back of the cockpit (first card), is connected to the mother board via eight pins, and the other one (second card) is connected via one pin (see [79] for detailed description of the card configuration). One coaxial cable T_1 connects the feed points (pins) of the second card in the two PCs. Two cables T_2 and T_3 connect the two PCs on the right and are terminated with $75\text{-}\Omega$

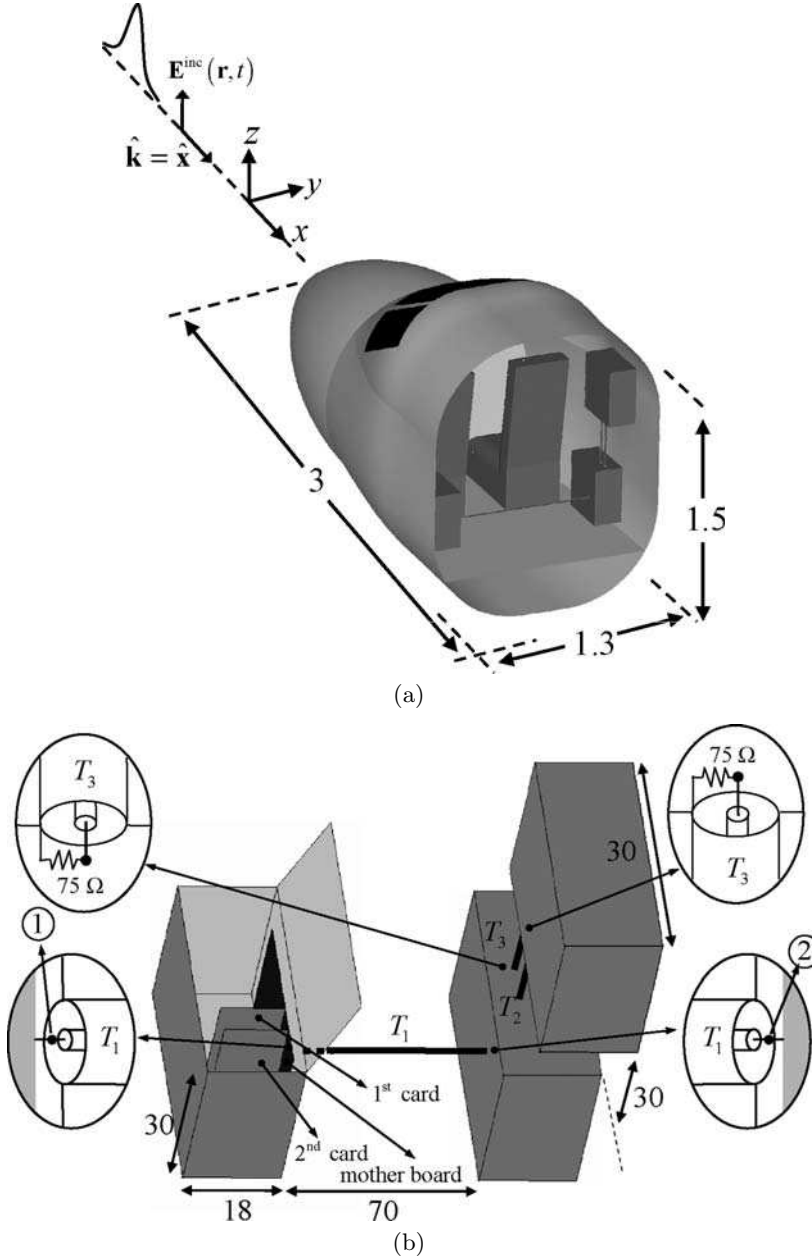


Fig. 3.14. PCs located in a cockpit. (a) Dimensions of the cockpit and the external plane wave excitation. (All dimensions are in meters.) Although not shown in the figure, the back of the cockpit is closed during the simulations. (b) Dimensions of the PC boxes (all have identical sizes) and the coaxial cables. (All dimensions are in centimeters.)

resistors (Fig. 3.14b). The lengths of cables T_1 , T_2 , and T_3 are 74, 30, and 30 cm, respectively. Surfaces modeling the floor and the seats, the surface separating the nose cavity from the rest of the cockpit, the surface at the back of the cockpit, and the surfaces modeling the daughter cards inside the PCs are assumed resistive with $377\text{-}\Omega$ impedance. The structure is illuminated by a plane wave incident on the cockpit nose with $E_0 = 3,000 \text{ V m}^{-1}$, $\hat{\mathbf{k}} = \hat{\mathbf{x}}$, $\hat{\mathbf{p}} = \hat{\mathbf{z}}$, $f_{\min} = 0.9 \text{ GHz}$, $f_c = 1.7 \text{ GHz}$, and $f_{\max} = 2.5 \text{ GHz}$ (Fig. 3.14a). The simulation is carried out for $N_t = 1,600$ time steps with $\Delta t = 33 \text{ ps}$. The current density on the surfaces modeling the cockpit, the PCs, the card configurations and the voltages on the cable loads are modeled by 284 179 surface, 152 wire, 136 junction basis functions and 6 circuit unknowns, respectively. The number of cable unknowns is six. Coupling of the external and guided fields is realized at 158 points. The temporal basis functions used for discretizing the 3D and 1D TDIEs are prolate-based band-limited interpolant with $8\Delta t$ half-width [9, 10] and third-order Lagrange polynomial [7], respectively. The TD-AIM kernel matches up to third-order moments, $\gamma = 5$, $\Delta s_x = 15.43 \text{ mm}$, $\Delta s_y = 15.93 \text{ mm}$, and $\Delta s_z = 15.93 \text{ mm}$; this choice of TD-AIM parameters results in $N_c = 200 \times 100 \times 90$ auxiliary grid points. Figure 3.15a,b present the transient coupled voltages observed at nodes 1 and 2 (Fig. 3.14b) due to the plane wave excitation and Fig. 3.16a,b show that

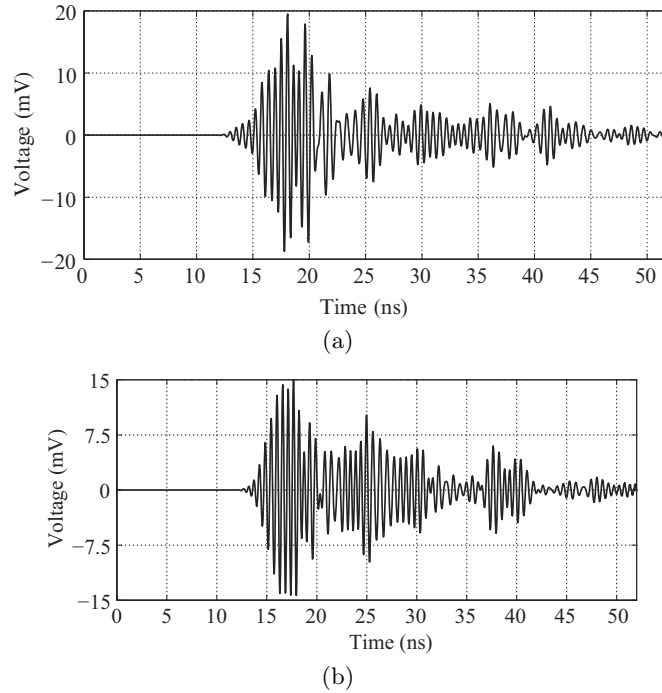


Fig. 3.15. Transient voltages observed at nodes (a) 1 and (b) 2 due to plane wave excitation

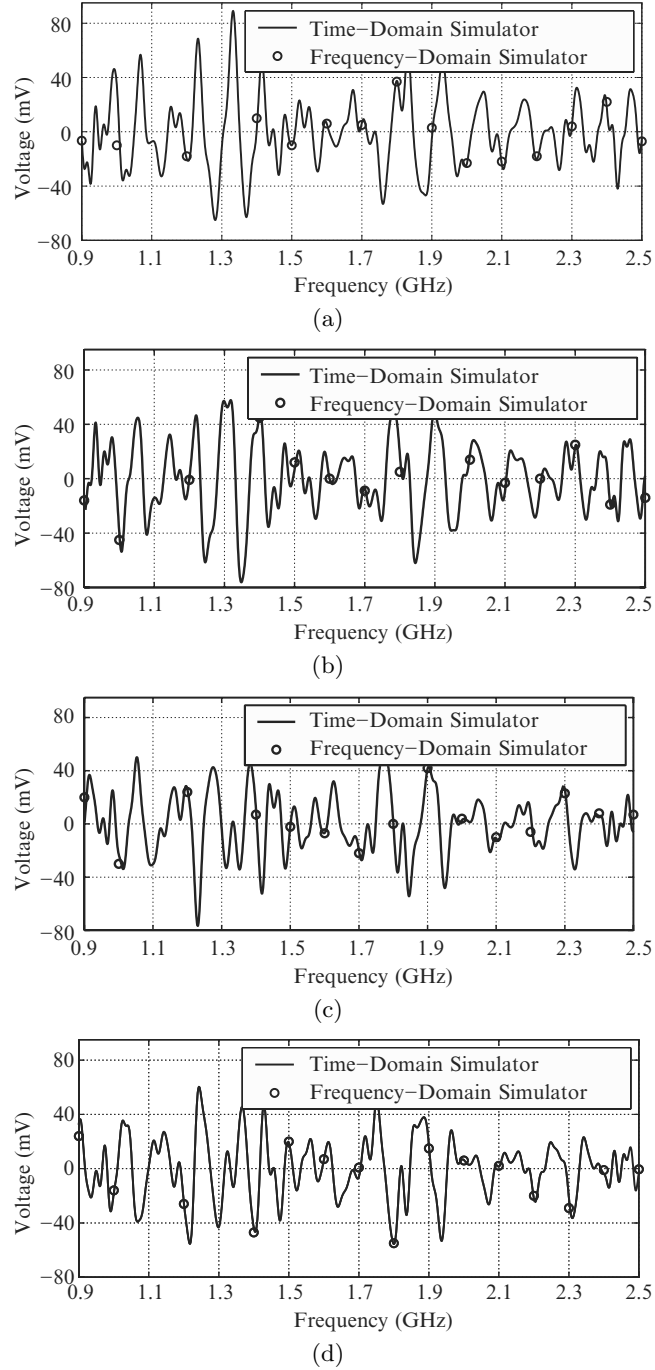


Fig. 3.16. Frequency-domain voltages observed at nodes 1 and 2: (a) real and (b) imaginary parts of voltage at node 1; (c) real and (d) imaginary parts of the voltage at node 2

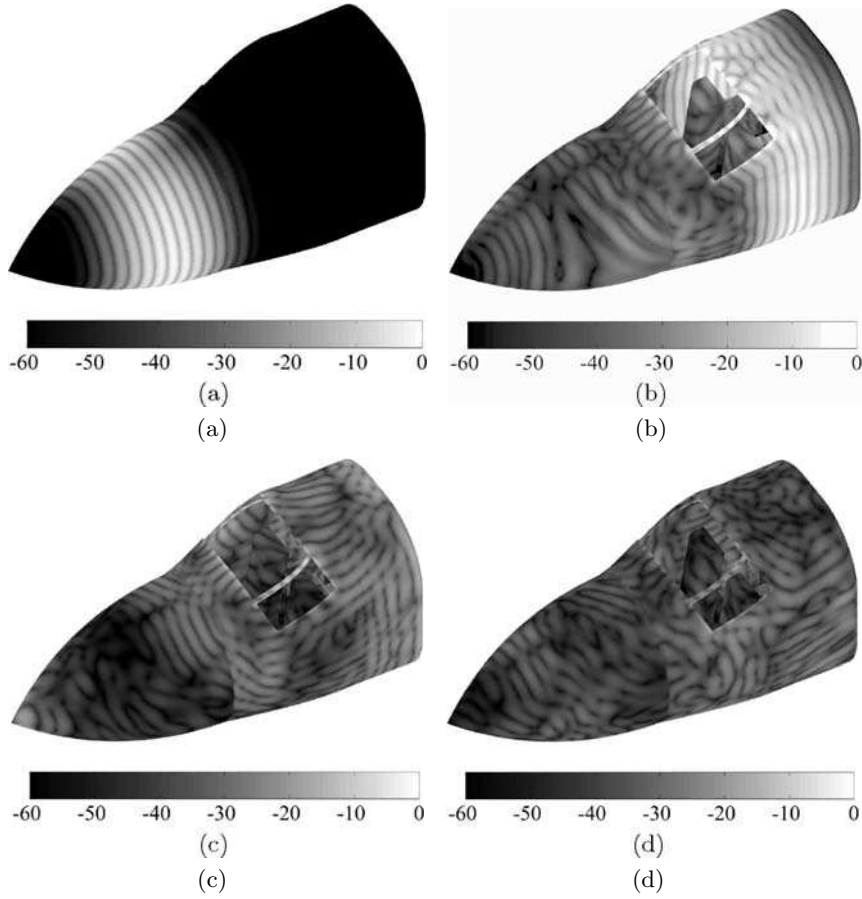


Fig. 3.17. Snapshots of the transient currents on the surfaces modeling the cockpit, the PCs, the card configurations, and the coaxial cables (in dB scale) at (a) $\Delta t = 8.25$ ns, (b) $\Delta t = 13.2$ ns, (c) $\Delta t = 15.675$ ns, and (d) $\Delta t = 18.15$ ns

frequency-domain voltages observed at these obtained by the hybrid simulator agree well with those obtained by a similar frequency-domain simulator. Figure 3.17a–d presents snapshots of the current density on the surfaces modeling the cockpit, the PCs, the card configurations, and the coaxial cables at different time instances. The hybrid simulator required 310 GB of memory and 31 m to fill the matrices and 2.14 h to find the solution using 201 processors (200 for the field solver, 1 for the circuit and cable solvers).

RG-58 and UTP-CAT5 Cables Located on an Aircraft

The hybrid simulator is used in the EMI analysis of RG-58 and UTP-CAT5 cables located on a Beechcraft King Air 250 aircraft (Fig. 3.18a). A 1 m long

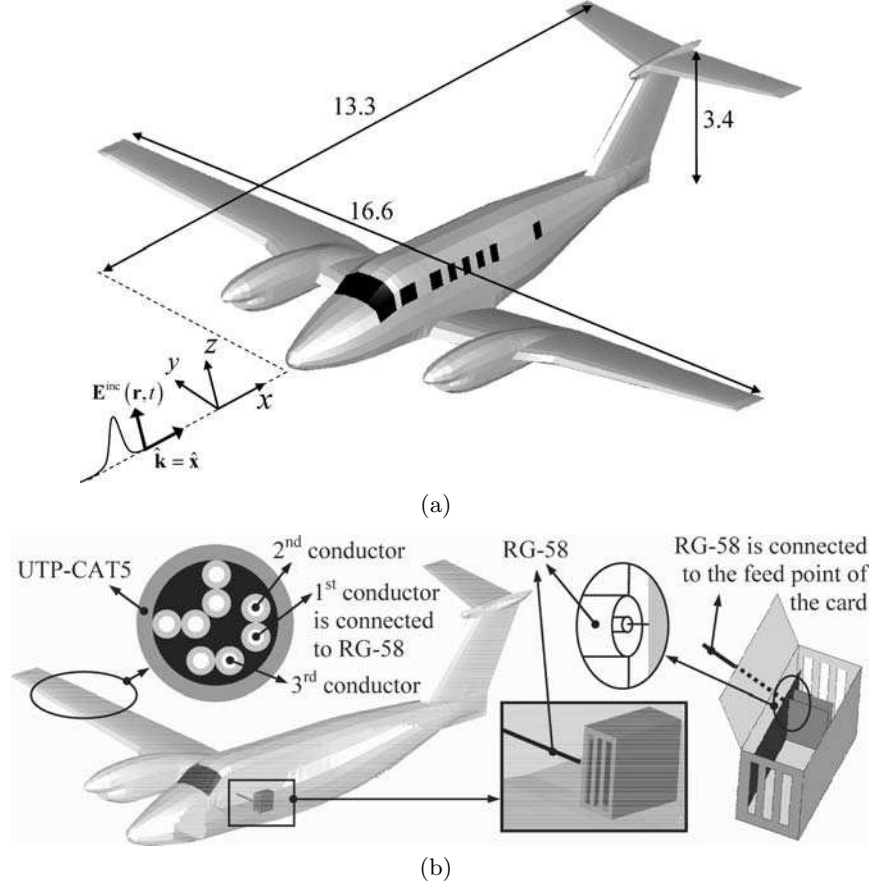


Fig. 3.18. RG-58 and UTP-CAT5 cables on an aircraft. (a) Dimensions of the aircraft and the plane-wave excitation. (All dimensions are in meters.) (b) Description of the cable-cable-card connections

RG-58 coaxial cable connects the feed pin of the PC's second daughter card and the first conductor of the 5 m long UTP-CAT5 cable located inside the wing cavity (Fig. 3.18b). The PC box enclosing the card configuration has six ventilation slots permitting the interaction of external fields with the card configuration. The UTP-CAT5 cable consists of four pairs of dielectric-coated conductors, which are held together by a dielectric cable jacket. The cable's per-unit-length parameters were extracted using a 2D MOM solver [80] and detailed in [81]. The exposed RG-58 coaxial cable interacts with the external fields via its terminations and along its shield while the UTP-CAT5 cable is embedded within the wing cavity and interacts with the external fields only via its terminations. All UTP-CAT5 cable's conductors (except the first conductor, which is connected to the RG-58 cable) are terminated with 50- Ω

resistors. The structure is illuminated by a plane wave incident on the nose of the aircraft with $E_0 = 3,000 \text{ V m}^{-1}$, $\hat{\mathbf{k}} = \hat{\mathbf{x}}$, $\hat{\mathbf{p}} = \hat{\mathbf{z}}$, $f_{\min} = 20 \text{ MHz}$, $f_c = 135 \text{ MHz}$, and $f_{\max} = 250 \text{ MHz}$ (Fig. 3.18b). The simulation is carried out for $N_t = 1500$ time steps with $\Delta t = 0.3 \text{ ns}$. The current density on the surfaces modeling the aircraft, the PC, the card configuration, the coaxial cable and the voltages on the cable loads are modeled by 45 175 surface, 23 wire, 64 junction basis functions and 20 circuit unknowns, respectively. The number of cable unknowns is 18 (2 for the RG-58 and 16 for the UTP-CAT5). Coupling of the external and guided fields (of the RG-58 cable) is realized at 10 points. The temporal basis functions used for discretizing the 3D and 1D TDIEs are prolate-based band-limited interpolant with $8\Delta t$ half-width [9, 10] and third-order Lagrange polynomial [7], respectively. The TD-AIM kernel matches up to fifth-order moments, $\gamma = 5$, $\Delta s_x = 10.52 \text{ cm}$, $\Delta s_y = 9.59 \text{ cm}$, and $\Delta s_z = 10.52 \text{ cm}$; this choice of TD-AIM parameters results in $N_c = 135 \times 180 \times 42$ auxiliary grid points. Figure 3.19a,b present the transient coupled voltages at the source-end terminations of the UTP-CAT5's second and third conductors due to the plane wave excitation. Figure 3.20a–d present snapshots of the current density on the surfaces modeling the aircraft, the PC box, the card configuration, and the coaxial cable at different time

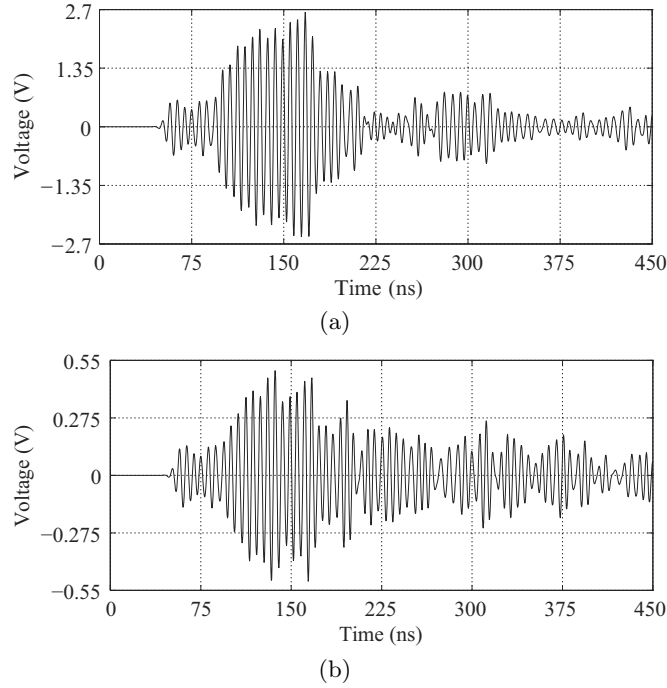


Fig. 3.19. Transient voltages at the source-end terminations of the UTP-CAT5 cable's (a) second and (b) third conductors

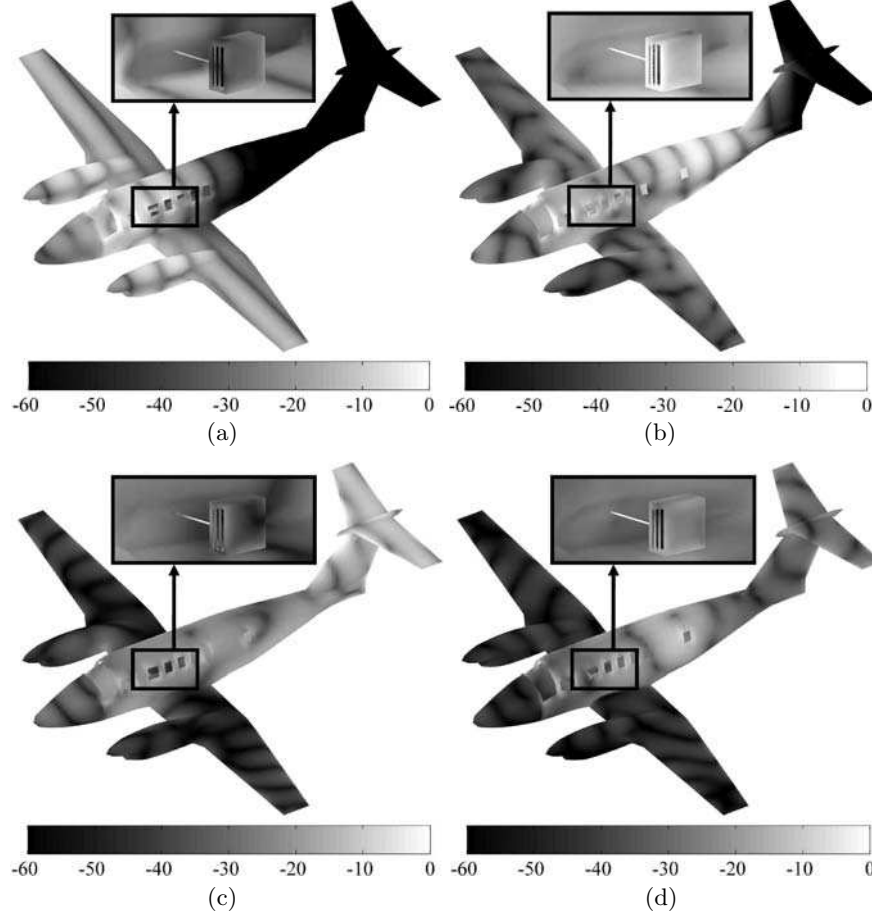


Fig. 3.20. Snapshots of the transient currents on the surfaces modeling the aircraft, the PC box, the card configuration, and the coaxial cable (in dB scale) at (a) $\Delta t = 45$ ns, (b) $\Delta t = 60$ ns, (c) $\Delta t = 75$ ns, and (d) $\Delta t = 90$ ns

instances. The hybrid simulator required 70 GB of memory and 30 m to fill the matrices and 2.85 h to find the solution using 46 (45 for the field solver, 1 for the circuit and cable solvers) processors.

3.5 Conclusions

This chapter presented a review of progress in fast MOT-TDIE solver technologies for analyzing electromagnetic transients with a specific focus on the application of TD-AIM accelerators. A parallel version of the TD-AIM accelerated MOT-TDIE solver that was hybridized with circuit, cable, and

macromodel simulators was applied to several real-world EMI problems. Our simulations demonstrate that MOT-TDIE solvers are approaching a stage of maturity and becoming an appealing alternative to finite difference/element based simulation technologies.

Acknowledgments

The authors would like to thank the Computational Science and Engineering (CSE) Department at the University of Illinois at Urbana-Champaign for the access to their parallel computer cluster. This work was supported in part by the MURI Grant 2003-07178-01-11, “Modeling antenna feeds,” by the DARPA Grant FA9550-06-1-0251, by the AFRL/DE SBIR grant “Time-domain BLT solver for electromagnetic coupling to cables and circuits,” and by the CSE fellowship at the University of Illinois.

References

- [1] A. Taflove and S. C. Hagness. *Computational Electrodynamics: The Finite-Difference Time-Domain Method*. Artech House, Boston, 2000.
- [2] J. Jianming. *The Finite Element Method in Electromagnetics*. Wiley, New York, 2002.
- [3] E. K. Miller. A selective survey of computational electromagnetics. *IEEE Trans. Antennas Propagat.*, 36(9):1281–1305, 1988.
- [4] A. F. Peterson, L. R. Scott, and R. Mittra. *Computational Methods for Electromagnetics*. Wiley, New York, 1997.
- [5] A. Sadigh and E. Arvas. Treating the instabilities in marching on-in-time method from a different perspective. *IEEE Trans. Antennas Propagat.*, 41(12):1695–1702, 1993.
- [6] P. J. Davies and D. B. Duncan. Averaging techniques for time-marching schemes for retarded potential integral equations. *Appl. Numer. Math.*, 23:291–310, 1997.
- [7] G. Manara, A. Monorchio, and R. Reggiannini. A space-time discretization criterion for a stable time-marching solution of the electric field integral equation. *IEEE Trans. Antennas Propagat.*, 45(3):527–532, 1997.
- [8] S. Dodson, S. P. Walker, and M. J. Bluck. Implicitness and stability of time domain integral equation scattering analyses. *ACES J.*, 13(3): 291–301, 1998.
- [9] D. S. Weile, G. Pisharody, N. W. Chen, B. Shanker, and E. Michielssen. A novel scheme for the solution of the time-domain integral equations of electromagnetics. *IEEE Trans. Antennas Propagat.*, 52(1):283–295, 2004.
- [10] R.A. Wildman, G. Pisharody, D.S. Weile, S. Balasubramaniam, and E. Michielssen. An accurate scheme for the solution of the time-domain integral equations of electromagnetics using higher order vector bases

- and bandlimited extrapolation. *IEEE Trans. Antennas Propagat.*, 52(11):2973–2984, 2004.
- [11] T. Abboud, J. C. Nédélec, and J. Volakis. Stable solution of retarded potential equations. In *ACES Conf.*, volume 1, pages 146–151, 2001.
 - [12] K. Cools, F. P. Andriulli, and E. Michielssen. Time-domain Calderón identities and preconditioning of the time-domain EFIE. In *IEEE AP-S. Int. Symp.*, pages 2975–2978, 2006.
 - [13] F. P. Andriulli, H. Bağcı, F. Vipiana, G. Vecchi, and Michielssen E. A marching-on-in-time hierarchical scheme for the time domain electric field integral equation. *submitted for publication*, 2007.
 - [14] A. A. Ergin, B. Shanker, and E. Michielssen. The plane-wave time-domain algorithm for the fast analysis of transient wave phenomena. *IEEE Antennas Propag. Mag.*, 41(4):39–52, 1999.
 - [15] A. A. Ergin, B. Shanker, and E. Michielssen. Fast analysis of transient acoustic wave scattering from rigid bodies using the multilevel plane wave time domain algorithm. *J. Acous. Soc. Am.*, 107(3):1168–1178, 2000.
 - [16] B. Shanker, A. A. Ergin, M. Lu, and E. Michielssen. Fast analysis of transient electromagnetic scattering phenomena using the multilevel plane wave time domain algorithm. *IEEE Trans. Antennas Propagat.*, 51(3):628–641, 2003.
 - [17] A. E. Yilmaz, J.-M. Jin, and E. Michielssen. Time domain adaptive integral method for surface integral equations. *IEEE Trans. Antennas Propagat.*, 52(10):2692–2708, 2004.
 - [18] Q. Chen, M. Lu, and E. Michielssen. Integral-equation-based analysis of transient scattering from surfaces with an impedance boundary condition. *Microwave Opt. Tech. Lett.*, 42(3):213–220, 2004.
 - [19] H. Bağcı, A. E. Yilmaz, V. Lomakin, and E. Michielssen. Fast and accurate solution of time domain electric field integral equation for dielectric half-space. In *IEEE AP-S. Int. Symp.*, volume 3, pages 583–586, 2003.
 - [20] H. Bağcı, A. E. Yilmaz, V. Lomakin, and E. Michielssen. Fast solution of mixed-potential time-domain integral equations for half-space environments. *IEEE Trans. Geosci. Remote Sensing*, 43(2):269–279, 2005.
 - [21] N. T. Gres, A. A. Ergin, and E. Michielssen. Volume-integral-equation-based analysis of transient electromagnetic scattering from three-dimensional inhomogeneous dielectric objects. *Radio Sci.*, 36(3):379–386, 2001.
 - [22] B. Shanker, A. A. Ergin, and E. Michielssen. Plane-wave-time-domain-enhanced marching-on-in-time scheme for analyzing scattering from homogeneous dielectric structures. *J. Opt. Soc. Am.*, 19(4):716–726, 2002.
 - [23] G. Kobidze, J. Gao, B. Shanker, and E. Michielssen. A fast time domain integral equation based scheme for analyzing scattering from dispersive objects. *IEEE Trans. Antennas Propagat.*, 53(3):1215–1226, 2005.
 - [24] K. Aygün, S. E. Fisher, A. A. Ergin, B. Shanker, and E. Michielssen. Transient analysis of multielement wire antennas mounted on arbitrarily shaped perfectly conducting bodies. *Radio Sci.*, 34(4):225–232, 1999.

- [25] H. Bağcı, A. E. Yilmaz, J. M. Jin, and E. Michielssen. Fast and rigorous analysis of EMC/EMI phenomena on electrically large and complex cable-loaded structures. *accepted for publication in IEEE Trans. Electromagn. Compat.*, 2006.
- [26] K. Aygün, B. C. Fischer, J. Meng, B. Shanker, and E. Michielssen. A fast hybrid field-circuit simulator for transient analysis of microwave circuits. *IEEE Trans. Microwave Theory Tech.*, 52(2):573–583, 2004.
- [27] A. E. Yilmaz, J. M. Jin, and E. Michielssen. A parallel FFT accelerated transient field-circuit simulator. *IEEE Trans. Microwave Theory Tech.*, 53(9):2851–2865, 2005.
- [28] H. Bağcı, A. E. Yilmaz, and E. Michielssen. EMC/EMI analysis of electrically large and multiscale structures loaded with coaxial cables by a hybrid TDIE-FDTD-MNA approach. In *IEEE AP-S. Int. Symp.*, volume 2B, pages 14–17, 2005.
- [29] H. Bağcı, A. E. Yilmaz, and E. Michielssen. A fast hybrid TDIE-FDTD-MNA scheme for analyzing cable-induced transient coupling into shielding enclosures. In *IEEE Int. Symp. EMC*, volume 3, pages 828–833, 2005.
- [30] H. Bağcı, A. E. Yilmaz, and E. Michielssen. FFT-accelerated MOT-based solution of time-domain BLT equations. In *IEEE AP-S. Int. Symp.*, pages 1175–1184, 2006.
- [31] H. Bağcı, A. E. Yilmaz, and E. Michielssen. Full TDIE-based modeling of electromagnetic coupling into lossy multiconductor cables on electrically large platforms. In *USNC/URSI National Radio Sci. Meet.*, 2005.
- [32] A. E. Yilmaz, M. J. Choi, A. C. Cangellaris, J.-M. Jin, and E. Michielssen. Incorporation of frequency-dependent multiport macromodels into a fast time-domain integral equation solver. In *IEEE AP-S. Int. Symp.*, volume 3A, pages 151–154, 2005.
- [33] I. Terrasse. *Résolution mathématique et numérique des équations de Maxwell instationnaires par une méthode de potentiels retardés*. PhD thesis, École Polytechnique, 1993.
- [34] T. Ha-Duong. On retarded potential boundary integral equations and their discretisation. In M. Ainsworth, P. J. Davies, D. B. Duncan, P.A. Martin, and B.P. Rynne, editors, *Topics in Computational Wave Propagation: Direct and Inverse Problems*, pages 301–336. Springer, Berlin, 2003.
- [35] E. Bleszynski, M. Bleszynski, and T. Jaroszewic. AIM: Adaptive integral method for solving large-scale electromagnetic scattering and radiation problems. *Radio Sci.*, 31(5):1225–1251, 1996.
- [36] J. R. Phillips and J. K. White. A precorrected-FFT method for electrostatic analysis of complicated 3D structures. *IEEE Trans. Computer-Aided Design*, 16(10):1059–1072, 1997.
- [37] V. Rokhlin. Diagonal forms of translational operators for the Helmholtz equation in three dimensions. *Appl. Comput. Harmon. Anal.*, 1(1):82–93, 1993.

- [38] V. Rokhlin. Rapid solution of integral equations of classical potential theory. *J. Comp. Phys.*, 60(2):187–207, 1985.
- [39] J. M. Song and W. C. Chew. Multilevel fast-multipole algorithm for solving combined field integral equations of electromagnetic scattering. *Microwave Opt. Tech. Lett.*, 10(1):14–19, 1995.
- [40] W. C. Chew, J. M. Jin, C. C. Lu, E. Michielssen, and J. M. Song. Fast solution methods in electromagnetics. *IEEE Trans. Antennas Propagat.*, 45(3):533–543, 1997.
- [41] M. F. Catedra, R. F. Torres, J. Basterrechea, and E. Gago. *The CG-FFT Method: Application of Signal Processing Techniques to Electromagnetics*. Artech House, Norwood, MA, 1995.
- [42] O. P. Bruno. Fast, high-order, high-frequency accurate Fourier methods for scattering problems. In *IEEE AP-S. Int. Symp.*, volume 3, pages 180–183, 2002.
- [43] O. P. Bruno and L. A. Kunyansky. A fast, high-order algorithm for the solution of surface scattering problems: basics implementation, tests, and applications. *J. Comp. Phys.*, 169(1):80–110, 2001.
- [44] H. T. Anastassiou, M. Smelyanskiy, S. Bindiganavale, and J. L. Volakis. Scattering from relatively flat surfaces using the adaptive integral method. *Radio Sci.*, 33(1):7–16, 1998.
- [45] R. F. Bloemenkamp and P. M. Van Den Berg. A conjugate gradient FFT method for transient scattering by dielectric cylinders. In *IEEE AP-S. Int. Symp.*, volume 2, pages 1374–1377, 1999.
- [46] A. E. Yilmaz, D. S. Weile, J. M. Jin, and E. Michielssen. A fast Fourier transform accelerated marching-on-in-time algorithm for electromagnetic analysis. *Electromagn.*, 21(3):181–197, 2001.
- [47] J. L. Hu, C. H. Chan, and Y. Xu. A fast solution of time domain integral equation using fast Fourier transformation. *Microwave Opt. Tech. Lett.*, 25(3):172–175, 2000.
- [48] A. E. Yilmaz, D. S. Weile, J. M. Jin, and E. Michielssen. A hierarchical FFT algorithm (HIL-FFT) for the fast analysis of transient electromagnetic scattering phenomena. *IEEE Trans. Antennas Propagat.*, 50(7):971–982, 2002.
- [49] A. E. Yilmaz, K. Aygün, J. M. Jin, and E. Michielssen. Matching criteria and the accuracy of time domain adaptive integral method. In *IEEE AP-S. Int. Symp.*, volume 2, pages 166–169, 2002.
- [50] A. E. Yilmaz, K. Aygün, J. M. Jin, and E. Michielssen. Fast analysis of heatsink emissions with time-domain AIM. In *IEEE Int. Symp. EMC*, Istanbul, Turkey, 2003.
- [51] A. E. Yilmaz, J. M. Jin, and E. Michielssen. Time domain adaptive integral method for the combined field integral equation. In *IEEE AP-S. Int. Symp.*, volume 3, pages 543–546, 2003.
- [52] A. E. Yilmaz, S. Q. Li, J. M. Jin, and E. Michielssen. A parallel framework for FFT-accelerated time-marching algorithms. In *USNC/URSI National Radio Sci. Meet.*, page 319, 2002.

- [53] A. E. Yilmaz, D. S. Weile, B. Shanker, J. M. Jin, and E. Michielssen. Fast analysis of transient scattering in lossy media. *IEEE Antennas Wireless Propagat. Lett.*, 1(1):14–17, 2002.
- [54] E. Bleszynski, M. Bleszynski, and T. Jaroszewicz. A new fast time domain integral equation solution algorithm. In *IEEE AP-S. Int. Symp.*, volume 4, pages 176–179, 2001.
- [55] A. F. Peterson. The interior resonance problem associated with surface integral equations of electromagnetics: numerical consequences and a survey of remedies. *Electromagn.*, 10(3):293–312, 1990.
- [56] B. Shanker, A. A. Ergin, K. Aygün, and E. Michielssen. Analysis of transient electromagnetic scattering from closed surfaces using the combined field integral equation. *IEEE Trans. Antennas Propagat.*, 48(7):1064–1074, 2000.
- [57] S. M. Rao, D. R. Wilton, and A. W. Glisson. Electromagnetic scattering by surfaces of arbitrary shape. *IEEE Trans. Antennas Propagat.*, 30(3):409–418, 1982.
- [58] R. D. Graglia, D. R. Wilton, and A. F. Peterson. Higher order interpolatory vector bases for computational electromagnetics. *IEEE Trans. Antennas Propagat.*, 45(3):329–342, 1997.
- [59] C. L. Bennett and H. Mieras. Time-domain scattering from open thin conducting surfaces. *Radio Sci.*, 10(6):1231–1239, 1981.
- [60] E. Topsakal, M. Carr, J. Volakis, and M. Bleszynski. Galerkin operators in adaptive integral method implementations. *Proc. Microwaves Antennas Propagat.*, 148(2):79–84, 2001.
- [61] X. C. Nie, L. W. Li, and N. Yuan. Precorrected-FFT algorithm for solving combined field integral equations in electromagnetic scattering. In *IEEE AP-S. Int. Symp.*, volume 3, pages 574–577, 2002.
- [62] F. Ling, C. F. Wang, and J. M. Jin. Application of adaptive integral method to scattering and radiation analysis of arbitrarily shaped planar structures. *J. Electromagn. Waves Appl.*, 12(8):1021–1037, 1998.
- [63] E. Hairer, C. H. Lubich, and M. Schlichte. Fast numerical solution of nonlinear Volterra convolution equations. *SIAM J. Sci. Stat. Comput.*, 6(3):532–541, 1985.
- [64] M. Frigo and S. G. Johnson. FFTW: An adaptive software architecture for the FFT. In *IEEE ICASSP*, volume 3, pages 1381–1384, 1998.
- [65] S. P. Walker and C. Y. Leung. Parallel computation of time-domain integral equation analyses of electromagnetic scattering and RCS. *IEEE Trans. Antennas Propagat.*, 45(4):614–619, 1997.
- [66] C.-W. Ho, A. Ruehli, and P. Brennan. The modified nodal approach to network analysis. *IEEE Trans. Circuits Syst.*, 22(6):504–509, 1975.
- [67] L. Kijun and S.-Bai Prak. Reduced modified nodal approach to circuit analysis. *IEEE Trans. Circuits Syst.*, 32(10):1056–1060, 1985.
- [68] A. Vladimirescu. *The Spice Book*. Wiley, New York, 1994.
- [69] C. R. Paul. *Analysis of Multiconductor Transmission Lines*. Wiley, New York, 1994.

- [70] F. Olyslager. *Electromagnetic Waveguides and Transmission Lines*. Oxford University Press, Oxford, U.K., 1999.
- [71] N. B. Rabbat, Ruehli A. E., Mahoney G. W., and Coleman J. J. A survey on macromodeling. In *IEEE Int. Symp. Circuits Syst.*, 1975.
- [72] N. B. Rabbat, Ruehli A. E., Mahoney G. W., and Coleman J. J. A review of macromodeling techniques. *IEEE Circuit Syst. Newsletter*, 9: 3–9, 1975.
- [73] A. Semlyen and A. Dabuleanu. Fast and accurate switching transient calculations on transmission lines with ground return using recursive convolution. *IEEE Trans. Power Appar. Syst.*, 94(2):561–571, 1975.
- [74] W. Janke and G. Blakiewicz. Semi-analytical recursive algorithms for convolution calculations. *IEE Proc.-Circuit Devices Syst.*, 42(2):125–130, 1995.
- [75] T. Hu, B. Zhong, S. L. Dvorak, and J. L. Prince. Application of recursive convolution to transient simulation of interconnects using a hybrid phase-pole macromodel. *IEEE Trans. Adv. Pack.*, 27(4):603–610, 2004.
- [76] A. C. Cangellaris, M. Celik, S. Pasha, and L. Zhao. Electromagnetic model order reduction for system-level modeling. *IEEE Trans. Microwave Theory Tech.*, 47(6):840–850, 1999.
- [77] A. C. Cangellaris and L. Zhao. Model order reduction techniques for electromagnetic macromodelling based on finite methods. *Int. J. Num. Modeling: Electronic Networks, Devices and Fields*, 3(2-3):181–197, 2000.
- [78] E. F. Vance. *Coupling to Shielded Cables*. Wiley, New York, 1978.
- [79] K. Aygün, B. Shanker, A. A. Ergin, and E. Michielssen. A two-level plane wave time-domain algorithm for fast analysis of EMC/EMI problems. *IEEE Trans. Electromagn. Compat.*, 44(1):152–164, 2002.
- [80] J. C. Clements, C. R. Paul, and A. T. Adams. Computation of the capacitance matrix for systems of dielectric-coated cylindrical conductors. *IEEE Trans. Electromagn. Compat.*, 17(4):238–248, 1975.
- [81] P. Kirawanich, N. E. Islam, and S. J. Yakura. An electromagnetic topology approach: Crosstalk characterization of the unshielded twisted-pair cable. *PIER*, 58:285–299, 2006.

Local and Nonlocal Nonreflecting Boundary Conditions for Electromagnetic Scattering

M.J. Grote

4.1 Introduction

Mathematical models of natural phenomena usually consist of partial differential equations, whose derivation is based on physical conservation laws (conservation of energy, etc.). Many standard numerical methods, such as finite differences and finite elements, can approximately solve partial differential equations. In fact, they can even handle complicated geometries, inhomogeneous media, and nonlinearity. However, they typically require an artificial boundary, which truncates the unbounded exterior domain, to fit the infinite region on a finite computer. This immediately raises the purely mathematical question:

Which boundary condition guarantees that the solution to the initial-boundary value problem inside the artificial boundary coincides with the solution of the original problem in the unbounded region?

If we exhibit a boundary condition, such that the fictitious boundary appears perfectly transparent, we shall call it “exact.” Otherwise it will correspond to an *approximate boundary condition*¹ and generate some spurious reflection, which travels back and spoils the solution everywhere in the computational domain. The resulting error in the computer simulation then consists of two independent error components: the discretization error of the numerical method used in the interior and the spurious reflection generated at the fictitious boundary. Unless both error components are reduced systematically, the numerical solution will not converge to the solution of the original problem in the unbounded region. Instead, if one fails to reduce the error introduced at the artificial boundary while refining the underlying mesh, the numerical solution will converge to the solution of a different initial-boundary value problem with the approximate boundary condition.

¹ “... also called radiating, absorbing, silent, transmitting, transparent, open, free-space, and one-way boundary conditions,” Givoli, 1991.

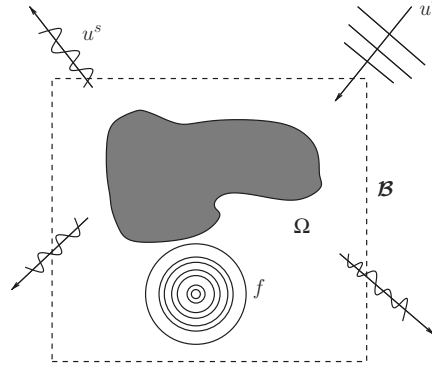


Fig. 4.1. A typical scattering problem consists of an obstacle, a source term f , an incoming wave u^i , and a scattered wave u^s . The artificial boundary $\mathcal{B}$ defines the outer boundary of the computational domain Ω

In this chapter, we shall restrict ourselves to time dependent electromagnetic scattering problems in unbounded three-dimensional space. Typically, a scattering problem consists of an obstacle, a source term f , and possibly an incident wave u^i – see Fig. 4.1. Our goal is to calculate numerically the time-dependent wave field u^s scattered from the complex, possibly nonlinear, but bounded scattering region.

To make the computational domain finite, we surround the region of interest by an artificial boundary, $\mathcal{B}$, and we denote by Ω the computational domain inside $\mathcal{B}$. At $\mathcal{B}$ we seek an exact nonreflecting boundary condition upon the scattered field.

Usually various approximate boundary conditions are used, which are local differential operators on $\mathcal{B}$. Examples are the Mur [Mur81] and the Peterson [Pet88] conditions, which are the generalizations to Maxwell's equations of the absorbing boundary conditions derived for the scalar wave equation by Engquist and Majda [EM77] and by Bayliss and Turkel [BT80]. In principle, these boundary conditions can be made arbitrarily accurate. Yet in practice, probably because their formulations involve increasingly higher derivatives, these boundary conditions are not used beyond second order; then, they remain only approximate conditions. Although their low (first and second) order versions usually perform well at nearly normal incidence, their performance degrades rapidly as grazing incidence is approached. In complex situations the scattered waves arrive at the artificial boundary from all interior angles and at all frequencies, so these approximate boundary conditions then yield some spurious reflection. Moreover, these errors tend to accumulate with time and prevent accurate long-time integration.

An exact nonreflecting boundary condition for the wave equation was proposed by Ting and Miksis [TM86]. It is based on a Kirchhoff integral representation of the solution on $\mathcal{B}$ and requires storing the solution at a

surface inside $\mathcal{B}$ for the length of time it takes a wave to propagate across Ω . This approach was generalized to Maxwell's equations by De Moerloose and De Zutter [MZ93]. The update of the solution value at any point on the two-dimensional artificial boundary $\mathcal{B}$ requires a two-dimensional convolution in time and space. As a consequence, using this boundary condition may be more expensive than using the numerical scheme itself inside Ω .

Since the mid-1990s highly accurate and efficient new approaches for computational electromagnetics have been found, such as the perfectly matched layer (PML) approach by Bérenger [Ber94] and the exact, temporally local, nonreflecting boundary conditions of Grote and Keller [GrKe98, Gro00]. Because the latter provides an analytic expression for the exterior wave field, it is advantageous for far-field evaluation [GrKi03] and in situations of multiple scattering [GrKi04, GrKi07]. A comparison of the PML technique [Ber94] with the nonreflecting boundary conditions [GrKe98, Gro00] was performed by Kantartzis et al. in [KPT98].

By introducing auxiliary functions, Hagstrom and Hariharan [HH98] derived a new formulation of the (local) Bayliss and Turkel [BT80] conditions, which enables arbitrary-order implementations without high order derivatives. This alternative local boundary condition for the wave equation is exact in the same sense as the conditions proposed in [GrKe98, Gro00, GrKe95, GrKe96]. Recently, Hagstrom and Warburton [HW03] combined their boundary condition with a DG-finite element method and applied it to the two-dimensional TM-Maxwell equations. Similarly, Givoli and Neta [GN03] and Hagstrom and Warburton [HW04] proposed a reformulation of the Higdon [Hig87] conditions without high order derivatives – see [Giv04] for a recent review.

Since the Cartesian xyz -components of any three-dimensional electromagnetic field in free space each satisfy the scalar wave equation, one can apply the boundary condition derived in [HH98, HW03] to each individual field component. Such a formulation, however, requires three auxiliary variables at the artificial boundary. Yet by combining ideas from [GrKe98] and [HH98], it is possible to derive a new nonreflecting boundary condition for Maxwell's equations, which is local both in space and time, and involves time and tangential derivatives of only two scalar auxiliary functions defined on the artificial boundary $\mathcal{B}$ [Gro06]. Since at least two scalar potentials are necessary to represent the general three-dimensional electro-magnetic field in free space, this boundary condition is optimal, in the sense that the number of auxiliary variables required is minimal. In contrast, the PML approach with the same number of grid points across the damping layer would require at least three times that amount, since the full (modified) Maxwell equations need to be discretized there.

After introducing in Sect. 4.2 some general results for Maxwell's equations in spherical geometry, we review in Sect. 4.3 the derivation of the nonlocal boundary condition from [GrKe98]. In Sect. 4.4, we recall the main steps in the derivation of the local boundary condition from [Gro06]. Then, in Sect. 4.5, we show how to combine these two nonreflecting boundary conditions with

the popular finite-difference time-domain (FDTD) scheme by Yee [Yee66]. Finally in Sect. 4.6, we present numerical results which confirm the expected high accuracy of the local and nonlocal nonreflecting boundary conditions.

4.2 Maxwell's Equations

We choose $\mathcal{B}$ to be a sphere of radius R . In $\mathcal{B}^{\text{ext}}$, the region outside $\mathcal{B}$, the medium is assumed to be linear, homogeneous, isotropic, of constant electric permittivity ε , of constant magnetic permeability μ , and of zero conductivity. In addition, we assume that at $t = 0$ the scattered field is confined to the computational domain Ω . In $\mathcal{B}^{\text{ext}}$ the electric field $\mathbf{E}$ and the magnetic field $\mathbf{H}$ then satisfy Maxwell's equations

$$\overrightarrow{\text{curl}} \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t}, \quad \overrightarrow{\text{curl}} \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t}. \quad (4.1)$$

Both $\mathbf{E}$ and $\mathbf{H}$ vanish at $t = 0$ in $\mathcal{B}^{\text{ext}}$, so $\text{div} \mathbf{E} = \text{div} \mathbf{H} = 0$ at $t = 0$. From (4.1) it follows that they remain solenoidal there for all time:

$$\text{div} \mathbf{E} = \text{div} \mathbf{H} = 0. \quad (4.2)$$

From (4.1) it also follows that both $\mathbf{E}$ and $\mathbf{H}$ satisfy the vector wave equation in $\mathcal{B}^{\text{ext}}$:

$$\frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} + \overrightarrow{\text{curl}} \overrightarrow{\text{curl}} \mathbf{E} = 0, \quad \frac{1}{c^2} \frac{\partial^2 \mathbf{H}}{\partial t^2} + \overrightarrow{\text{curl}} \overrightarrow{\text{curl}} \mathbf{H} = 0. \quad (4.3)$$

Here $c = 1/\sqrt{\varepsilon\mu}$.

Next, we introduce the polar coordinates r, ϑ, φ , the unit vectors $\hat{\mathbf{r}}, \hat{\boldsymbol{\vartheta}}, \hat{\boldsymbol{\varphi}}$, and let Y_{nm} denote the nm th spherical harmonic

$$Y_{nm}(\vartheta, \varphi) = \sqrt{\frac{(2n+1)(n-|m|)!}{4\pi(n+|m|)!}} P_n^{|m|}(\cos \vartheta) e^{im\varphi}, \quad n \geq 0, |m| \leq n. \quad (4.4)$$

The Y_{nm} are orthonormal with respect to the L_2 inner product on the *unit* sphere. If the problem considered is real, it is advantageous to use the real spherical harmonics, given by the real and imaginary parts of (4.4) with a modified normalization constant.

Following [CK92, p. 170], we let $\mathbf{U}_{nm}$ and $\mathbf{V}_{nm}$ denote the vector spherical harmonics

$$\mathbf{U}_{nm}(\vartheta, \varphi) = \frac{r \nabla Y_{nm}}{\sqrt{n(n+1)}} = \frac{1}{\sqrt{n(n+1)}} \left[\frac{\partial Y_{nm}}{\partial \vartheta} \hat{\boldsymbol{\vartheta}} + \frac{1}{\sin \vartheta} \frac{\partial Y_{nm}}{\partial \varphi} \hat{\boldsymbol{\varphi}} \right], \quad (4.5)$$

$$\mathbf{V}_{nm}(\vartheta, \varphi) = \hat{\mathbf{r}} \times \mathbf{U}_{nm} = \frac{1}{\sqrt{n(n+1)}} \left[\frac{-1}{\sin \vartheta} \frac{\partial Y_{nm}}{\partial \varphi} \hat{\boldsymbol{\vartheta}} + \frac{\partial Y_{nm}}{\partial \vartheta} \hat{\boldsymbol{\varphi}} \right]. \quad (4.6)$$

They form an orthonormal basis for the space of tangential L_2 fields on the unit sphere with respect to the L_2 inner product.

The vector spherical harmonics are eigenfunctions of the vector Laplace–Beltrami operator,

$$\vec{\Delta}_S \mathbf{u} \equiv \nabla_S \operatorname{div}_S \mathbf{u} - \overrightarrow{\operatorname{curl}}_S \operatorname{curl}_S \mathbf{u}, \quad (4.7)$$

and thus satisfy

$$\vec{\Delta}_S \mathbf{V}_{nm} = -n(n+1)\mathbf{V}_{nm}, \quad \vec{\Delta}_S \mathbf{U}_{nm} = -n(n+1)\mathbf{U}_{nm}, \quad n \geq 1. \quad (4.8)$$

Here ∇_S , div_S , $\overrightarrow{\operatorname{curl}}_S$, and curl_S denote the surface gradient, divergence, and curl operators [Ned00]:

$$\nabla_S u = \frac{\partial u}{\partial \vartheta} \hat{\boldsymbol{\vartheta}} + \frac{1}{\sin \vartheta} \frac{\partial u}{\partial \varphi} \hat{\boldsymbol{\varphi}}, \quad (4.9)$$

$$\operatorname{div}_S \mathbf{u} = \frac{1}{\sin \vartheta} \left(\frac{\partial}{\partial \vartheta} (\sin \vartheta u_\vartheta) + \frac{\partial}{\partial \varphi} u_\varphi \right), \quad (4.10)$$

$$\overrightarrow{\operatorname{curl}}_S u = \frac{1}{\sin \vartheta} \frac{\partial u}{\partial \varphi} \hat{\boldsymbol{\vartheta}} - \frac{\partial u}{\partial \vartheta} \hat{\boldsymbol{\varphi}}, \quad (4.11)$$

$$\operatorname{curl}_S \mathbf{u} = \frac{1}{\sin \vartheta} \left(\frac{\partial}{\partial \vartheta} (\sin \vartheta u_\varphi) - \frac{\partial}{\partial \varphi} u_\vartheta \right). \quad (4.12)$$

Note that

$$\operatorname{div}_S \mathbf{V}_{nm} = 0, \quad \operatorname{curl}_S \mathbf{U}_{nm} = 0, \quad (4.13)$$

so that in fact we have

$$\overrightarrow{\operatorname{curl}}_S \operatorname{curl}_S \mathbf{V}_{nm} = n(n+1)\mathbf{V}_{nm}, \quad \nabla_S \operatorname{div}_S \mathbf{U}_{nm} = -n(n+1)\mathbf{U}_{nm}. \quad (4.14)$$

The vector spherical harmonics also satisfy the following useful equations for arbitrary $f(r)$:

$$\overrightarrow{\operatorname{curl}}(f(r)\mathbf{V}_{nm}) = -\frac{\sqrt{n(n+1)}f(r)}{r}Y_{nm}\hat{\mathbf{r}} - \frac{1}{r}\frac{\partial(rf(r))}{\partial r}\mathbf{U}_{nm}, \quad (4.15)$$

$$\hat{\mathbf{r}} \times \overrightarrow{\operatorname{curl}}(f(r)\mathbf{V}_{nm}) = -\frac{1}{r}\frac{\partial(rf(r))}{\partial r}\mathbf{V}_{nm}, \quad (4.16)$$

$$\hat{\mathbf{r}} \times \overrightarrow{\operatorname{curl}}(f(r)Y_{nm}\hat{\mathbf{r}}) = \frac{\sqrt{n(n+1)}f(r)}{r}\mathbf{U}_{nm}, \quad (4.17)$$

$$\operatorname{div}(f(r)\mathbf{U}_{nm}) = -\frac{\sqrt{n(n+1)}f(r)}{r}Y_{nm}. \quad (4.18)$$

To solve (4.1) in $\mathcal{B}^{\text{ext}}$, we decompose the electromagnetic field into transverse electric (TE) and transverse magnetic (TM) fields. The electric component of the TE multipole field of order (n, m) is given by

$$\mathbf{E}_{nm}^{TE}(r, \vartheta, \varphi, t) = f_{nm}(r, t)\mathbf{V}_{nm}(\vartheta, \varphi), \quad (4.19)$$

where f_{nm} satisfies

$$L_n[f_{nm}] \equiv \left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{n(n+1)}{r^2} \right) f_{nm} = 0, \quad r \geq R. \quad (4.20)$$

The magnetic component of the TM multipole field of order (n, m) is given by

$$\mathbf{H}_{nm}^{TM}(r, \vartheta, \varphi, t) = g_{nm}(r, t) \mathbf{V}_{nm}(\vartheta, \varphi), \quad (4.21)$$

where $L_n[g_{nm}] = 0$.

The TE and TM solutions form a complete set of solutions of Maxwell's equations in a source-free region ([Jac75, p. 746]). Therefore the general electric and magnetic multipole fields of order (n, m) are obtained by combining (4.19) with the electric field associated with (4.21), and by combining (4.21) with the magnetic field associated with (4.19), respectively:

$$\mathbf{E}_{nm}(r, \vartheta, \varphi, t) = f_{nm}(r, t) \mathbf{V}_{nm} + \frac{1}{\varepsilon} \overrightarrow{\text{curl}}[\mathbf{V}_{nm} \int_0^t g_{nm}(r, s) ds], \quad (4.22)$$

$$\mathbf{H}_{nm}(r, \vartheta, \varphi, t) = -\frac{1}{\mu} \overrightarrow{\text{curl}}[\mathbf{V}_{nm} \int_0^t f_{nm}(r, s) ds] + g_{nm}(r, t) \mathbf{V}_{nm}. \quad (4.23)$$

In $\mathcal{B}^{\text{ext}}$, the total electromagnetic field is a superposition of multipole fields:

$$\mathbf{E} = \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{E}_{nm}, \quad \mathbf{H} = \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{H}_{nm}. \quad (4.24)$$

We remark that in contrast to the acoustic wave equation, the time dependent Maxwell equations with initial data supported in a bounded domain do not admit spherically symmetric solutions; hence all sums start at $n = 1$.

From (4.15) we infer that the terms in (4.22) and (4.23) that involve $\overrightarrow{\text{curl}}(\mathbf{V}_{nm} \dots)$ are orthogonal to $\mathbf{V}_{nm}$. Thus, from (4.24) we conclude that

$$f_{nm} = (\mathbf{E}, \mathbf{V}_{nm}), \quad g_{nm} = (\mathbf{H}, \mathbf{V}_{nm}). \quad (4.25)$$

The inner product involves integration with respect to ϑ and φ on the sphere of radius r .

4.3 Nonlocal Boundary Condition

To obtain a boundary condition for $\mathbf{H}_{nm}$, we first apply $\hat{\mathbf{r}} \times \overrightarrow{\text{curl}}$ to (4.23). We use (4.16) and the fact that $\mathbf{V}_{nm} \int_0^t f_{nm}$ is also a solution of (4.3) to get

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{H}_{nm} = -\sqrt{\frac{\varepsilon}{\mu}} \frac{1}{c} \frac{\partial f_{nm}}{\partial t} \mathbf{U}_{nm} - \frac{1}{r} \frac{\partial(r g_{nm})}{\partial r} \mathbf{V}_{nm}. \quad (4.26)$$

Next we differentiate (4.23) with respect to t and simplify the result using (4.15). The tangential components of the resulting equation yield

$$\frac{1}{c} \frac{\partial \mathbf{H}_{nm}^{\text{tan}}}{\partial t} = \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{r} \frac{\partial (r f_{nm})}{\partial r} \mathbf{U}_{nm} + \frac{1}{c} \frac{\partial g_{nm}}{\partial t} \mathbf{V}_{nm}. \quad (4.27)$$

Now we subtract (4.27) from (4.26) to get

$$\begin{aligned} \hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{H}_{nm} - \frac{1}{c} \frac{\partial \mathbf{H}_{nm}^{\text{tan}}}{\partial t} = \\ - \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r f_{nm}] \mathbf{U}_{nm} - \frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r g_{nm}] \mathbf{V}_{nm}. \end{aligned} \quad (4.28)$$

Similarly from (4.22) we derive the equation

$$\begin{aligned} \hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E}_{nm} - \frac{1}{c} \frac{\partial \mathbf{E}_{nm}^{\text{tan}}}{\partial t} = \\ - \frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r f_{nm}] \mathbf{V}_{nm} + \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r g_{nm}] \mathbf{U}_{nm}. \end{aligned} \quad (4.29)$$

Equations (4.28) and (4.29) cannot yet be used as boundary conditions because their right-hand sides involve radial derivatives of the unknown functions f_{nm} and g_{nm} . To eliminate these derivatives we note that f_{nm} and g_{nm} satisfy the differential equation (4.20), and that they both vanish at $t = 0$ for $r \geq R$. Equation (4.20) is the equation satisfied by the coefficient of Y_{nm} in the expansion of a solution of the scalar wave equation.

In [GrKe95] an exact nonreflecting boundary condition was derived for solutions of (4.20), which is local in time. We shall not repeat this derivation in its full generality here, but instead present the main ideas by discussing in detail the simplest cases with $n = 1$.

We seek an exact boundary condition for $f_{1m}(r, t)$, which satisfies (4.20) with $n = 1$:

$$\left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial r^2} - \frac{2}{r} \frac{\partial}{\partial r} + \frac{2}{r^2} \right) f_{1m} = 0, \quad r \geq R. \quad (4.30)$$

First, we shall transform f_{1m} to a new variable v , which satisfies the one-dimensional wave equation. To do so, we recall that if $v = v(r, t)$ satisfies

$$\frac{\partial^2 v}{\partial t^2} - c^2 \frac{\partial^2 v}{\partial r^2} = 0, \quad (4.31)$$

then

$$f = \frac{\partial}{\partial r} \frac{v}{r}$$

satisfies (4.30). Next, we drop the indices on $f = f_{1m}(r, t)$, and invert the result above. Let

$$v(r, t) = r \int_r^\infty f(s, t) \, ds. \quad (4.32)$$

Then v satisfies (4.31), whose general solution is

$$v(r, t) = F(r + ct) + G(r - ct),$$

where F and G are arbitrary functions, which are determined by initial and boundary conditions. Hence, F is constant on the characteristics $r + ct = \text{const.}$, whereas G remains constant on the characteristics $r - ct = \text{const.}$ Thus F corresponds to incoming waves, whereas G corresponds to outgoing waves.

As both v and $\partial_t v$ vanish outside $\mathcal{B}$ at $t = 0$, there are no incoming waves in $r \geq R$, and we have

$$F(r) = 0, \quad r \geq R. \quad (4.33)$$

Moreover, both v and $\partial_t v$ vanish outside $\mathcal{B}$ at $t = 0$. Therefore, the exact boundary condition for v is

$$\left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) v(r, t) = 0, \quad r = R. \quad (4.34)$$

We remark that the integral in (4.32) is finite for every t , because $f(r, t)$ vanishes for $r \geq R + ct$.

To use (4.34) in computation, we shall reformulate it and derive an equivalent but more tractable form, which does not involve integrals or high-order derivatives. To do so, we first calculate

$$\frac{\partial v}{\partial r} = \int_r^\infty f(s, t) \, ds - rf = \frac{v}{r} - rf. \quad (4.35)$$

We now use (4.34) to obtain

$$\frac{1}{c} \frac{\partial v}{\partial t} = -\frac{\partial v}{\partial r} = -\frac{v}{r} + rf. \quad (4.36)$$

Next, we apply $\partial_r + c^{-1}\partial_t$ to (4.36) and again use (4.34), which leads to

$$\left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) rf(r, t) = \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) \left[\frac{1}{c} \frac{\partial}{\partial t} v + \frac{v}{r} \right] = -\frac{v}{r^2}. \quad (4.37)$$

We now set $r = R$ and let $\psi(t) = v(R, t)/R$ in (4.37) to obtain

$$\left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) rf = -\frac{\psi(t)}{R}, \quad r = R. \quad (4.38)$$

Equation (4.38) is an exact boundary condition for f , but it still involves the a priori unknown quantity $\psi(t)$. To determine it, we set $r = R$ in (4.36), which after division by R yields the *ordinary differential equation*

$$\frac{1}{c} \frac{d\psi(t)}{dt} = -\frac{\psi(t)}{R} + f(R, t), \quad \psi(0) = 0. \quad (4.39)$$

We note that $\psi(0) = 0$ because $v(r, t)$ vanishes for $r \geq R$ at $t = 0$.

Equations (4.38) and (4.39) yield the exact boundary condition for $f_{1m}(r, t)$, which is local in time. In general, f_{nm} satisfies the following boundary condition at $r = R$, which was derived in [GrKe95] for the wave equation, and used for computation in [GrKe96]:

$$\left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r f_{nm}] = -\mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^E(t), \quad r = R. \quad (4.40)$$

This is the nm -th component of (2.6) in [GrKe96] with $\mathbf{c} = \mathbf{d}$ and $\mathbf{z} = \boldsymbol{\psi}$. Here $\mathbf{d}_n$ and $\boldsymbol{\psi}_{nm}^E(t)$ are n -component vectors.

The vector function $\boldsymbol{\psi}_{nm}^E(t) = \{\psi_{nm}^{E,j}(t)\}, j = 1, \dots, n$, satisfies the *linear first-order ordinary* differential equation

$$\frac{1}{c} \frac{d}{dt} \boldsymbol{\psi}_{nm}^E(t) = \mathbf{A}_n \boldsymbol{\psi}_{nm}^E(t) + f_{nm}(R, t) \mathbf{e}_n, \quad \boldsymbol{\psi}_{nm}^E(0) = 0. \quad (4.41)$$

Here $\mathbf{A}_n = \{A_n^{ij}\}$ is the constant $n \times n$ matrix

$$A_n^{ij} = \begin{cases} -n(n+1)/(2R^j) & \text{if } i = 1, \\ (n+i)(n+1-i)/(2i) & \text{if } i = j+1, \\ 0 & \text{otherwise.} \end{cases} \quad (4.42)$$

The constant n -component vectors $\mathbf{d}_n = \{d_n^j\}$ and $\mathbf{e}_n = \{e_n^j\}$ are defined as

$$d_n^j = \frac{n(n+1)j}{2R^j}, \quad j = 1, \dots, n, \quad (4.43)$$

$$\mathbf{e}_n = [1, 0, \dots, 0]^\top. \quad (4.44)$$

Clearly, the same procedure applies to $g_{nm}(r, t)$, since $L_n[g_{nm}] = 0$. Thus, we also have

$$\left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r g_{nm}] = -\mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^H(t), \quad r = R, \quad (4.45)$$

where the n -component vector function $\boldsymbol{\psi}_{nm}^H(t)$ satisfies the ordinary differential equation

$$\frac{1}{c} \frac{d}{dt} \boldsymbol{\psi}_{nm}^H(t) = \mathbf{A}_n \boldsymbol{\psi}_{nm}^H(t) + g_{nm}(R, t) \mathbf{e}_n, \quad \boldsymbol{\psi}_{nm}^H(0) = 0. \quad (4.46)$$

Now, we use (4.40) and (4.45) to eliminate the radial derivatives of f_{nm} and g_{nm} from (4.28) and (4.29). Thus, we rewrite (4.28) and (4.29) at $r = R$ as

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{H}_{nm} - \frac{1}{c} \frac{\partial \mathbf{H}_{nm}^{\text{tan}}}{\partial t} = \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{R} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^E(t) \mathbf{U}_{nm} + \frac{1}{R} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^H(t) \mathbf{V}_{nm}, \quad r = R, \quad (4.47)$$

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E}_{nm} - \frac{1}{c} \frac{\partial \mathbf{E}_{nm}^{\text{tan}}}{\partial t} = \frac{1}{R} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^E(t) \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{R} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^H(t) \mathbf{U}_{nm}, \quad r = R. \quad (4.48)$$

Finally, we obtain the boundary condition at $r = R$ by summing over n and m in (4.47) and (4.48):

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{H} - \frac{1}{c} \frac{\partial \mathbf{H}^{\text{tan}}}{\partial t} = \sqrt{\frac{\varepsilon}{\mu}} \frac{1}{R} \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^E(t) \mathbf{U}_{nm} + \frac{1}{R} \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^H(t) \mathbf{V}_{nm}, \quad r = R, \quad (4.49)$$

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E} - \frac{1}{c} \frac{\partial \mathbf{E}^{\text{tan}}}{\partial t} = \frac{1}{R} \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^E(t) \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{R} \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{d}_n \cdot \boldsymbol{\psi}_{nm}^H(t) \mathbf{U}_{nm}, \quad r = R. \quad (4.50)$$

The vector functions $\boldsymbol{\psi}_{nm}^E(t)$ and $\boldsymbol{\psi}_{nm}^H(t)$ in (4.49) and (4.50) satisfy the linear ordinary differential equations (4.41) and (4.46), which can be written as follows by using (4.25):

$$\frac{1}{c} \frac{d}{dt} \boldsymbol{\psi}_{nm}^E(t) = \mathbf{A}_n \boldsymbol{\psi}_{nm}^E(t) + (\mathbf{E}^{\text{tan}}|_{r=R}, \mathbf{V}_{nm}) \mathbf{e}_n, \quad \boldsymbol{\psi}_{nm}^E(0) = 0. \quad (4.51)$$

$$\frac{1}{c} \frac{d}{dt} \boldsymbol{\psi}_{nm}^H(t) = \mathbf{A}_n \boldsymbol{\psi}_{nm}^H(t) + (\mathbf{H}^{\text{tan}}|_{r=R}, \mathbf{V}_{nm}) \mathbf{e}_n, \quad \boldsymbol{\psi}_{nm}^H(0) = 0. \quad (4.52)$$

Each inner product in (4.51) and (4.52) involves two, not three, scalar inner products since $\mathbf{V}_{nm}$ is purely tangential. Equations (4.49) and (4.50) are the boundary conditions which we sought. They are exact and ensure that no spurious reflections occur at $\mathcal{B}$. They involve only first-order derivatives and can be incorporated easily into numerical methods.

The functions f_{nm} and g_{nm} satisfy the scalar wave equation and determine the electromagnetic field uniquely outside $\mathcal{B}$. It was shown in [GrKe96] that for smooth solutions of the scalar wave equation, imposing the exact boundary condition at $\mathcal{B}$ guarantees that the solution in Ω coincides with the restriction to Ω of the solution to the Cauchy problem in the unbounded domain. Therefore for smooth data, the solution to the initial boundary value problem inside Ω with (4.49) or (4.50) imposed at $\mathcal{B}$, is unique and coincides with the

restriction to Ω of the electromagnetic field in the unbounded domain. It is also well-posed with respect to perturbations in the initial conditions.

In practice, the infinite sums in (4.49), (4.50) are truncated at some finite value N . On the modes $n > N$, the nonreflecting boundary condition then reduces to the first-order Peterson condition [Pet88]:

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E} - \frac{1}{c} \frac{\partial \mathbf{E}^{\text{tan}}}{\partial t} = 0, \quad (4.53)$$

and similarly for $\mathbf{H}$. By choosing higher values of N , the boundary conditions can be made arbitrarily accurate at a fixed distance $r = R$. In particular, the error at the artificial boundary due to the truncation at N can always be reduced below the discretization error inside Ω ; in that sense, these boundary conditions are exact.

The boundary conditions (4.49), (4.50) do not require saving past values of $\mathbf{E}$ or $\mathbf{H}$. Instead they involve the two functions $\psi_{nm}^E(t)$ and $\psi_{nm}^H(t)$. The amount of memory needed to store them, about $4/3 N^3$ scalar values, is negligible when compared to the storage required for $\mathbf{E}$ and $\mathbf{H}$. Most of the extra work involved in applying the boundary condition results from computing the inner products of $\mathbf{E}$ and $\mathbf{H}$ with $\mathbf{V}_{nm}$ in (4.51) and (4.52), and from computing the right-hand sides of (4.49) and (4.50).

To compute the Fourier components in (4.51) or (4.52), it is not necessary to compute $O(N^2)$ inner products over the entire sphere. Indeed, since the vector spherical harmonics $\mathbf{V}_{nm}$ separate in ϑ and φ , it is sufficient to compute $O(N)$ inner products with $\cos(m\varphi)$ and $\sin(m\varphi)$ over the sphere, and then to compute $O(N^2)$ *one-dimensional* inner products in ϑ over $[0, \pi]$. The same trick can be used to calculate the sums over n and m on the right of (4.49) and (4.50). Recently, Rohklin and Tygert proposed a numerically stable fast spherical harmonic transform [RT06], which reduces even further the cost involved in the inner products.

4.4 Local Boundary Condition

The nonreflecting boundary conditions (4.49), (4.50) are exact and local in time, but they are nonlocal over $\mathcal{B}$, as they involve inner products of the solution with spherical harmonics. In this section, we shall recall the derivation of a second different formulation [Gro06], which is *local both in space and time*.

By using (4.15) to expand the second term on the right of (4.22) and applying both (4.13) and (4.14) to the resulting expressions, we conclude that

$$\overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{E}_{nm} = n(n+1) f_{nm}(r, t) \mathbf{V}_{nm}. \quad (4.54)$$

Similarly we find

$$\overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{H}_{nm} = n(n+1) g_{nm}(r, t) \mathbf{V}_{nm}. \quad (4.55)$$

By using Laplace transform techniques, and the fact that f_{nm} and $\partial_t f_{nm}$ vanish at $t = 0$, one can easily derive the general solution of (4.20) for the Fourier coefficients f_{nm} :

$$f_{nm}(r, t) = \sum_{k=0}^n r^{-k-1} f_{nm}^k(r - ct), \quad n \geq 1 \quad (4.56)$$

with $f_{nm}^k(r) = 0$ for $r \geq R$, and similarly for g_{nm} – see also [HH98, Kir05].

We now introduce expansion (4.56) into (4.20) to calculate

$$L_n[f_{nm}] = \sum_{k=0}^{n-1} \frac{1}{r^{k+3}} \left[2(k+1) (f_{nm}^{k+1})' + (n(n+1) - k(k+1)) f_{nm}^k \right]. \quad (4.57)$$

Since $L_n[f_{nm}]$ vanishes identically for $r \geq R$, we immediately obtain the recurrence relation

$$(f_{nm}^{k+1})' = \frac{k(k+1) - n(n+1)}{2(k+1)} f_{nm}^k, \quad 0 \leq k \leq n-1, \quad (4.58)$$

and similarly for g_{nm}^k .

Next, we apply the differential operator $\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} - c^{-1} \partial_t$ to $\mathbf{E}$, and denote by $\mathbf{w}^1$ the *tangential part* of the resulting expression:

$$\mathbf{w}^1(r, \vartheta, \varphi, t) = \hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E} - \frac{1}{c} \frac{\partial}{\partial t} \mathbf{E}^{\text{tan}}. \quad (4.59)$$

Clearly $\mathbf{w}^1$ is unknown, or else we would be done. One of the simplest absorbing boundary condition consists in setting $\mathbf{w}^1$ identically to zero. We shall now derive a system of differential equations, whose solution approximates $\mathbf{w}^1$. The accuracy will increase with the order of the system, and also with the distance of the artificial boundary from the obstacle.

Since $\mathbf{w}^1$ is purely tangential, we can expand it in vector spherical harmonics as

$$\mathbf{w}^1(r, \vartheta, \varphi, t) = \sum_{n \geq 1} \sum_{|m| \leq n} \mathbf{w}_{nm}^1(r, \vartheta, \varphi, t), \quad (4.60)$$

where

$$\mathbf{w}_{nm}^1(r, \vartheta, \varphi, t) = \xi_{nm}^1(r, t) \mathbf{V}_{nm}(\vartheta, \varphi) - \sqrt{\frac{\mu}{\varepsilon}} \eta_{nm}^1(r, t) \mathbf{U}_{nm}(\vartheta, \varphi). \quad (4.61)$$

We now differentiate (4.22) with respect to t and simplify the result using (4.15). The tangential components of the resulting expression yield

$$\frac{1}{c} \frac{\partial \mathbf{E}_{nm}^{\text{tan}}}{\partial t} = \frac{1}{c} \frac{\partial f_{nm}}{\partial t} \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{r} \frac{\partial (r g_{nm})}{\partial r} \mathbf{U}_{nm}. \quad (4.62)$$

Next, we use (4.15) and the fact that $\mathbf{V}_{nm} \int_0^t g_{nm}$ is also a solution of (4.3) to get

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E}_{nm} = -\frac{1}{r} \frac{\partial(r f_{nm})}{\partial r} \mathbf{V}_{nm} + \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{c} \frac{\partial g_{nm}}{\partial t} \mathbf{U}_{nm}. \quad (4.63)$$

As we subtract (4.62) from (4.63) we get

$$\mathbf{w}_{nm}^1 = -\frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r f_{nm}] \mathbf{V}_{nm} + \sqrt{\frac{\mu}{\varepsilon}} \frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) [r g_{nm}] \mathbf{U}_{nm}. \quad (4.64)$$

If we apply the differential operator $r^{-1}(\partial_r + c^{-1}\partial_t)r$ to (4.56) we obtain

$$\frac{1}{r} \left(\frac{\partial}{\partial r} + \frac{1}{c} \frac{\partial}{\partial t} \right) r f_{nm}(r, t) = \sum_{k=1}^n (-k) r^{-k-2} f_{nm}^k(r - ct), \quad (4.65)$$

and similarly for $g_{nm}(r, t)$. From the orthogonality of the functions $\mathbf{V}_{nm}$ and $\mathbf{U}_{nm}$ we immediately find that

$$\begin{aligned} \xi_{nm}^1(r, t) &= \sum_{k=1}^n k r^{-k-2} f_{nm}^k(r - ct), \\ \eta_{nm}^1(r, t) &= \sum_{k=1}^n k r^{-k-2} g_{nm}^k(r - ct). \end{aligned} \quad (4.66)$$

Since $\mathbf{w}^1$ consists of a superposition of ξ_{nm}^1 and η_{nm}^1 , we conclude that $\mathbf{w}^1 = O(r^{-3})$.

To derive an evolution equation for $\mathbf{w}^1$, we first calculate

$$\frac{1}{c} \frac{\partial \xi_{nm}^1}{\partial t} + \frac{\xi_{nm}^1}{r} = - \sum_{k=1}^n k r^{-k-2} (f_{nm}^k)' + \sum_{k=1}^n k r^{-k-3} f_{nm}^k. \quad (4.67)$$

Next, we use (4.58) to rewrite the first sum on the right of (4.67) as

$$\sum_{k=0}^{n-1} (k+1) r^{-k-3} (f_{nm}^{k+1})' = \sum_{k=0}^{n-1} \left[\frac{k(k+1) - n(n+1)}{2} \right] r^{-k-3} f_{nm}^k. \quad (4.68)$$

We now combine the two terms on the right of (4.67) using (4.68) to obtain

$$\frac{1}{c} \frac{\partial \xi_{nm}^1}{\partial t} + \frac{\xi_{nm}^1}{r} = \frac{n(n+1)}{2} \sum_{k=0}^n r^{-k-3} f_{nm}^k - \sum_{k=2}^n \frac{k(k-1)}{2} r^{-k-3} f_{nm}^k. \quad (4.69)$$

The same calculations with f_{nm}^k replaced by g_{nm}^k yield

$$\frac{1}{c} \frac{\partial \eta_{nm}^1}{\partial t} + \frac{\eta_{nm}^1}{r} = \frac{n(n+1)}{2} \sum_{k=0}^n r^{-k-3} g_{nm}^k - \sum_{k=2}^n \frac{k(k-1)}{2} r^{-k-3} g_{nm}^k. \quad (4.70)$$

Next, we multiply (4.69) by $\mathbf{V}_{nm}$ and (4.70) by $-\sqrt{\mu/\varepsilon}\mathbf{U}_{nm}$, use (4.56), and add the two resulting expressions to find

$$\begin{aligned} \frac{1}{c} \frac{\partial \mathbf{w}_{nm}^1}{\partial t} + \frac{\mathbf{w}_{nm}^1}{r} &= \frac{n(n+1)}{2r^2} \left[f_{nm} \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} g_{nm} \mathbf{U}_{nm} \right] \\ &\quad - \sum_{k=2}^n \frac{k(k-1)}{2} r^{-k-3} \left[f_{nm}^k \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} g_{nm}^k \mathbf{U}_{nm} \right]. \end{aligned} \quad (4.71)$$

From (4.54) and (4.55), together with the fact that $\hat{\mathbf{r}} \times \mathbf{V}_{nm} = -\mathbf{U}_{nm}$, we observe that the first two terms on the right of (4.71) reduce to

$$\frac{1}{2r^2} \left[\overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{E}_{nm} + \sqrt{\frac{\mu}{\varepsilon}} \hat{\mathbf{r}} \times \overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{H}_{nm} \right]. \quad (4.72)$$

Summation over (n, m) finally yields

$$\frac{1}{c} \frac{\partial \mathbf{w}^1}{\partial t} + \frac{\mathbf{w}^1}{r} = \frac{1}{2r^2} \left[\overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{E} + \sqrt{\frac{\mu}{\varepsilon}} \hat{\mathbf{r}} \times \overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{H} \right] + \mathbf{w}^2, \quad (4.73)$$

with

$$\mathbf{w}^2 = - \sum_{n \geq 2} \sum_{|m| \leq n} \sum_{k=2}^n \frac{k(k-1)}{2} r^{-k-3} \left[f_{nm}^k(r-ct) \mathbf{V}_{nm} - \sqrt{\frac{\mu}{\varepsilon}} g_{nm}^k(r-ct) \mathbf{U}_{nm} \right]. \quad (4.74)$$

Since $\mathbf{w}^2 = O(r^{-5})$, we have succeeded in writing an evolution equation for $\mathbf{w}^1$, which involves only (known) tangential derivatives of the tangential components of $\mathbf{E}$ and $\mathbf{H}$, together with an increasingly smaller remainder, $\mathbf{w}^2$, which may be set to zero in a first approximation. In the special case of a solution that consists of a linear combination of $\{\mathbf{V}_{nm}, \mathbf{U}_{nm}\}$, $n = 1, m = -1, 0, 1$, we have $\mathbf{w}^2 = 0$ and the boundary condition will be exact.

The procedure used above to find an evolution equation for $\mathbf{w}^1$ can be extended to $\mathbf{w}^2$, and subsequently to higher order correction terms – see [Gro06] for further details. This eventually yields the following exact nonreflecting boundary condition:

$$\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E} - \frac{1}{c} \frac{\partial \mathbf{E}^{\text{tan}}}{\partial t} = \mathbf{w}^1, \quad (4.75)$$

$$\frac{1}{c} \frac{\partial \mathbf{w}^1}{\partial t} + \frac{\mathbf{w}^1}{r} = \frac{1}{2r^2} \left[\overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{E} + \sqrt{\frac{\mu}{\varepsilon}} \hat{\mathbf{r}} \times \overrightarrow{\text{curl}}_S \text{curl}_S \mathbf{H} \right] + \mathbf{w}^2, \quad (4.76)$$

$$\frac{1}{c} \frac{\partial \mathbf{w}^p}{\partial t} + \frac{p}{r} \mathbf{w}^p = \frac{1}{4r^2} (\overrightarrow{\Delta}_S + p(p-1)) \mathbf{w}^{p-1} + \mathbf{w}^{p+1}, \quad p \geq 2. \quad (4.77)$$

The boundary condition (4.75)–(4.77) is local both in space and time. It only involves first time derivatives and second tangential derivatives of $\mathbf{E}$ and of the (unknown) auxiliary functions $\mathbf{w}^p$, $p \geq 1$, which satisfy (4.76) and (4.77).

In practice, only a finite number of auxiliary functions $\mathbf{w}^p$, $p = 1, \dots, P$ is used setting $w^{P+1} = 0$. Then, in general the boundary condition is no longer exact, but it *remains exact* for solutions which consist of a *finite* combination of vector spherical harmonics up to order $n = P$, that is $f_{nm} = g_{nm} = 0, n > P$. Imposition of the boundary condition at any fixed radius R thus yields at least spectral accuracy for smooth wave fields with increasing P . Therefore (4.75)–(4.77) is exact in the same sense as the nonlocal conditions presented in Sect. 4.3, namely that P can always be chosen sufficiently large so that the error introduced at $\mathcal{B}$ is smaller than the discretization error inside Ω , without moving $\mathcal{B}$ farther away from the scatterer. However, this new boundary condition does not require any vector spherical harmonics or inner products with them; hence, it is somewhat easier and cheaper to implement.

In general, the error due to the truncation behaves like $O(r^{-2P-2})$ – in fact $\mathbf{w}^{P+1} = O(r^{-2(P+1)-1})$, but then one inverse power in r cancels out in (4.75) because $E = O(r^{-1})$. If we set $P = 0$, that is $\mathbf{w}^p = 0$ for all $p \geq 1$, the boundary condition (4.75) reduces to the first-order Peterson condition (4.53), the time dependent counterpart of the Silver–Müller radiation condition for time-harmonic waves [CK92].

Equation (4.75) provides a boundary condition for $\mathbf{E}$. By duality a similar boundary condition can easily be derived for $\mathbf{H}$. In (4.75) the term $\hat{\mathbf{r}} \times \overrightarrow{\text{curl}} \mathbf{E}$ naturally appears when multiplying (4.3) by a test function and integrating by parts. Hence (4.75) easily fits into a variational formulation of (4.3). Although Maxwell’s equations involve six electromagnetic field components at every location $(\mathbf{x}, t)$ in space and time, it is remarkable that this nonreflecting boundary condition requires only two scalar quantities, which correspond to the two tangential components of $\mathbf{w}^p$.

4.5 Finite Difference Time Domain (FDTD) Implementation

We shall now show how the two nonreflecting boundary conditions (4.50)–(4.52) and (4.75)–(4.77) fit into the finite-difference time-domain (FDTD) method. First proposed by Yee [Yee66], this popular method staggers both $\mathbf{E}$ and $\mathbf{H}$ in time and space, and thereby achieves second order accuracy using current values only. Due to the nature of the Yee scheme, the boundary condition is needed only for one of the two electromagnetic field components. Here we choose to apply it to $\mathbf{E}$. Thus $\mathbf{E}^{\text{tan}}$ is known at $r = R - \Delta r$ and $r = R$, whereas $\mathbf{H}^{\text{tan}}$ is known at $r = R - \Delta r/2$. The boundary condition is necessary to advance $\mathbf{E}^{\text{tan}}$ at $r = R$, since Maxwell’s equations (4.1) would require radial derivatives of $\mathbf{H}^{\text{tan}}$, whose finite difference approximation involves unknown values of $\mathbf{H}^{\text{tan}}$ outside $\mathcal{B}$. Thus, we shall use either (4.50) or (4.75) to advance $\mathbf{E}^{\text{tan}}$ at $r = R$ from time t to time $t + \Delta t$. To do so, we apply either (4.50) or (4.75) at $t = t + \Delta t/2$ and $r = R - \Delta r/2$, and approximate the first order derivatives on the left by centered finite differences ([KL93, Sect. 3.7]). Further

details of the implementation and a full algorithmic description are presented separately for the boundary conditions (4.50)–(4.52) and (4.75)–(4.77) below.

4.5.1 Nonlocal Boundary Condition

The right side of (4.50) involves infinite sums, which are truncated at a finite value N . It requires the values of $\psi_{nm}^E(t)$ and $\psi_{nm}^H(t)$ at $t = t + \Delta t/2$. These are computed concurrently with the solution inside Ω , using the linear ordinary differential equations (4.51) and (4.52). The inner products in (4.51) and (4.52) are computed over the sphere $r = R - \Delta r/2$ using the fourth order Simpson rule. To solve (4.51) and (4.52) numerically, we opt for the trapezoidal rule because the eigenvalues of the matrices $\mathbf{A}_n$ lie in the left half of the complex plane [GrKe96]. Since the trapezoidal rule is unconditionally stable, there is no restriction on the time-step in the integration of (4.51) and (4.52). The work required in solving the linear systems (4.51) and (4.52) is negligible, because the matrices $\mathbf{A}_n$ are very small and remain constant. The trapezoidal rule approximation of (4.51) is

$$\begin{aligned} \left(I - \frac{\Delta t}{2} \mathbf{A}_n\right) \psi_{nm}^E(t_{k+1/2}) &= \left(I + \frac{\Delta t}{2} \mathbf{A}_n\right) \psi_{nm}^E(t_{k-1/2}) \\ &+ \Delta t \left(\mathbf{E}^k \big|_{R-\Delta r/2}, \mathbf{V}_{nm}\right) \mathbf{e}_n, \end{aligned} \quad (4.78)$$

where $\mathbf{E}^k$ at $r = R - \Delta r/2$ is the average of $\mathbf{E}^k$ at $r = R - \Delta r$ and $r = R$. The trapezoidal rule approximation of (4.52) is

$$\begin{aligned} \left(I - \frac{\Delta t}{2} \mathbf{A}_n\right) \psi_{nm}^H(t_{k+1/2}) &= \left(I + \frac{\Delta t}{2} \mathbf{A}_n\right) \psi_{nm}^H(t_{k-1/2}) \\ &+ \frac{\Delta t}{2} \left(\mathbf{H}^{k-1/2} \big|_{R-\Delta r/2} + \mathbf{H}^{k+1/2} \big|_{R-\Delta r/2}, \mathbf{V}_{nm}\right) \mathbf{e}_n. \end{aligned} \quad (4.79)$$

The complete algorithm proceeds as follows:

0. Initialize $\mathbf{E}$ at $t = 0$ and $\mathbf{H}$ at $t = \Delta t/2$, and set $\psi_{nm}^E = 0$ and $\psi_{nm}^H = 0$ at $t = \Delta t/2$.
1. Compute $\mathbf{E}$ at $t_k = t_{k-1} + \Delta t$ at all inner points of Ω using (4.1).
2. Compute $\mathbf{E}^{\text{tan}}$ at t_k and $r = R$ using (4.50) applied at $r = R - \Delta r/2$ and $t_{k-1/2} = t_{k-1} + \Delta t/2$.
3. Compute $\mathbf{H}$ at $t_{k+1/2}$ using (4.1).
4. Compute ψ_{nm}^E and ψ_{nm}^H at $t_{k+1/2}$ using (4.78) and (4.79), respectively; return to 1.

4.5.2 Local Boundary Condition

In (4.75), the values of $\mathbf{w}^1(r, \vartheta, \varphi, t)$ are required at $t = t + \Delta t/2$ and $r = R - \Delta r/2$ as well. In fact, the grid locations for $\mathbf{w}^j$ coincide with those of $\mathbf{H}^{\text{tan}}$ on

the outer sphere at $r = R - \Delta r/2$. Following [HH98] we advance the auxiliary functions w^j , $j = 1, \dots, P$ with the Crank–Nicolson scheme to avoid any additional restriction on the time step beyond that imposed by the Yee scheme in the interior. However, to keep the computation explicit in time, the values of w^{j+1} at $t = t + \Delta t$ in the evolution equation for w^j are simply obtained by (explicit) extrapolation from the two previous values at $t = t + \Delta t/2$ and $t = t - \Delta t/2$. The resulting explicit–implicit time discretization yields a *fully explicit scheme*, when the w^j are advanced sequentially in increasing order, while circumventing any additional restriction on the time step.

The complete algorithm proceeds as follows:

0. Initialize $\mathbf{E}$ at $t = 0$ and $\mathbf{H}$ at $t = \Delta t/2$, and set $w^j = 0$, $j = 1, \dots, P$, at $t = -\Delta t/2$, $t = \Delta t/2$ and $r = R - \Delta r/2$.
1. Compute $\mathbf{E}$ at $t_k = t_{k-1} + \Delta t$ at all inner points of Ω using (4.1).
2. Compute $\mathbf{E}^{\text{tan}}$ at t_k and $r = R$ using (4.75) applied at $r = R - \Delta r/2$ and $t_{k-1/2} = t_{k-1} + \Delta t/2$.
3. Compute $\mathbf{H}$ at $t_{k+1/2}$ using (4.1).
4. Compute $w^1, w^2, \dots, w^P$ at $t_{k+1/2}$ in that order using (4.75); return to 1.

4.6 Numerical Results

To illustrate the high accuracy of the nonlocal and local nonreflecting boundary conditions, (4.50)–(4.52) and (4.75)–(4.77), respectively, we now combine them with the FDTD method, as described in Sect. 4.5. We apply the resulting numerical schemes to compute the scattered field of a perfectly conducting sphere of radius r_0 , denoted by Γ , illuminated by a nearby Hertzian dipole.

The radiating electric dipole is located outside the spherical obstacle at $S = (0, 0, z_0)$, $z_0 > r_0$, at distance z_0 from the origin. It is aligned along z , so that its moment points along the positive z -axis. Its time dependence is a Gaussian pulse centered about $t = t_0$:

$$P(t) = \begin{cases} 0 & t < 0, \\ \alpha e^{-(t-t_0)^2/\sigma^2} & 0 \leq t \leq 2t_0, \\ 0 & t > 2t_0. \end{cases} \quad (4.80)$$

We set $\alpha = 10^{-9}$ and choose σ so that $P(t)$ is equal to the smallest machine number at $t = 0$ and $t = 2t_0$.

Since this problem is symmetric about the z -axis, the electromagnetic field has only three nonvanishing components: $\mathbf{E}(r, \vartheta, t) = E^r \hat{\mathbf{r}} + E^\vartheta \hat{\boldsymbol{\vartheta}}$, and $\mathbf{H}(r, \vartheta, t) = H^\varphi \hat{\boldsymbol{\varphi}}$. Next, we split the total electromagnetic field $(\mathbf{E}, \mathbf{H})$ into the incident field $(\mathbf{E}^i, \mathbf{H}^i)$ and the scattered field $(\mathbf{E}^s, \mathbf{H}^s)$. Hence $\mathbf{E} = \mathbf{E}^i + \mathbf{E}^s$ and $\mathbf{H} = \mathbf{H}^i + \mathbf{H}^s$. The incident field is known and can be found in ([Jon64, p. 152]). On Γ , the tangential component of the total electric field vanishes. In the infinite region outside Γ , the scattered field satisfies Maxwell's equations (4.3).

Because of the inherent symmetry, the computational domain Ω can be reduced to the two-dimensional region $r_0 \leq r \leq R$, $0 \leq \vartheta \leq \pi$, shown in Fig. 4.2. Inside Ω we use the FDTD method in polar coordinates on a 32×352 uniform mesh in r and ϑ . We set $r_0 = 0.5$ m, $R = 0.7$ m, $z_0 = 0.6$ m, $c = 2.998 \times 10^8$ m/s, and $t_0 = 3$ ns. Hence the obstacle is 1 m in diameter and the source is located 0.1 m away from it.

We shall compare the numerical solutions obtained by using either (4.50), where the sums are truncated at N , or (4.75), where $p \leq P$, with that obtained using the standard first order Peterson condition (4.53). We recall that (4.53) is identical to (4.50) with $N = 0$, or equivalently to (4.75) with $P = 0$. The boundary condition (4.50) is implemented as described in Sect. 4.5, albeit due to the radial symmetry, $\psi_{nm}^E(t)$ is identically zero. Our reference solution is the numerical solution in the infinite domain, which we refer to as the *exact solution*. To compute it inside Ω we use a much larger domain which extends as far as $r = 3.7$ m. This enables us to compute the solution of the initial-boundary value problem in the infinite region outside Γ for $0 \leq t \leq 20$ ns. We shall now compare the numerical solutions, obtained by using the three different boundary conditions at $r = R$, with the exact solution at two different locations inside Ω at $r = 0.6$ m : Q_1 ($\vartheta = 45^\circ$) and Q_2 ($\vartheta = 170^\circ$) – see Fig. 4.2.

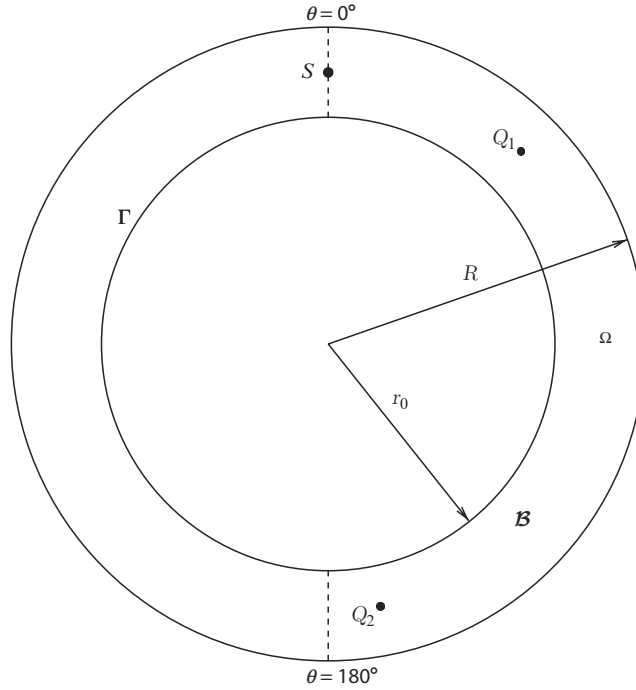


Fig. 4.2. The computational domain Ω is shown drawn to scale, with $r_0 = 0.5$ m and $R = 0.7$ m. The dipole source is located at $S = (0, 0, z_0)$, with $z_0 = 0.6$ m

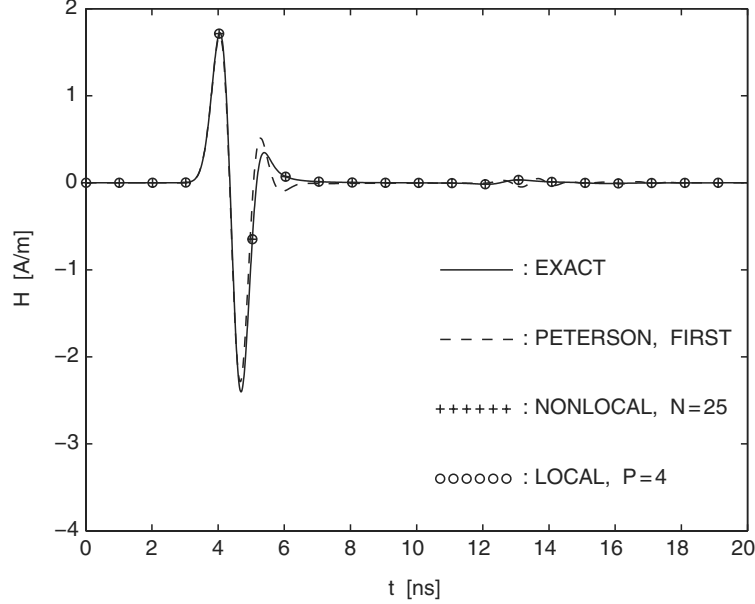


Fig. 4.3. The numerical solutions for H^φ , computed using the Peterson condition (4.53), the nonlocal condition (4.50), and the local condition (4.75) are compared with the exact solution at Q_1

In Fig. 4.3, the φ -component of the magnetic field is shown at the first location Q_1 . The numerical solutions obtained either with (4.50) truncated at $N = 25$ or with (4.75) truncated at $P = 4$, are hardly distinguishable from the exact solution. While the relative error due to the first Peterson condition is only a few percent, this seemingly accurate behavior is deceptive. Indeed these *locally* small reflections travel back into the computational domain, and contaminate the solution everywhere inside Ω , in particular in regions where the solution is of lesser magnitude. To demonstrate this point, we select the next location behind the obstacle at Q_2 , where the electromagnetic field is weaker.

The φ -component of the magnetic field at Q_2 is shown in Fig. 4.4, and again it agrees completely with the numerical solution obtained using the two nonreflecting boundary conditions. The solution obtained using the first Peterson condition agrees with the exact solution for a finite time. It then diverges from it, as the spurious reflection due to its imposition reaches this location. Since these spurious reflections are *larger than the true solution*, the numerical solution with the first Peterson condition imposed at $\mathcal{B}$ is meaningless in the shadow region of the sphere.

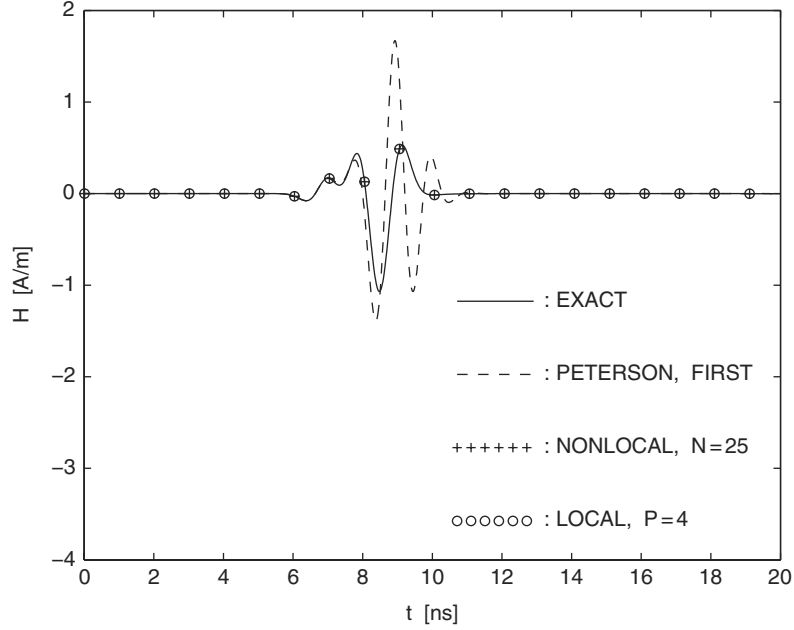


Fig. 4.4. The numerical solutions for H^φ , computed using the Peterson condition (4.53), the nonlocal condition (4.50), and the local condition (4.75) are compared with the exact solution at Q_2

4.7 Conclusion

The exact nonreflecting boundary conditions (4.50)–(4.52) or (4.75)–(4.77) have been found to be very accurate in numerical computations. They involve only first time derivatives and second tangential derivatives of the electromagnetic field and of certain auxiliary functions. Both boundary conditions fit naturally into the finite-difference time-domain method (FDTD) and allow the artificial boundary to be brought as close as desired to the scatterer. They are easy to implement and require little extra storage and computer time. In [Gro00] an alternative nonlocal formulation was derived, which does not involve any derivatives of $\mathbf{E}$ or $\mathbf{H}$; hence, it fits easily into the variational formulation of Maxwell's equations and is well-suited for use with finite element methods.

In practice, only a finite number P (resp. N) of auxiliary functions is used. Then, in general the boundary conditions are no longer exact, but they remain exact for any combination of spherical harmonics up to order P (resp. N). Imposition of the boundary condition at any fixed radius R thus yields at least spectral accuracy for smooth wave fields with increasing N or P . Therefore (4.50) and (4.75) are both exact in the sense that N or P can always be chosen sufficiently large so that the error introduced at the artificial boundary

remains below the discretization error inside the computational domain, for any fixed R . Both the nonlocal and the local formulations are explicit, in the sense that they do not require the solution of any large linear system on the artificial boundary. With the exact boundary condition the overall numerical scheme retains its optimal rate of convergence, as the error introduced at the artificial boundary can always be reduced below the discretization error due to the numerical method in the interior computational domain.

Although the artificial boundary must be spherical, the boundary conditions are not tied to any coordinate system, and the computational grid used inside Ω can be arbitrary. Because the local boundary condition (4.75) does not require any vector spherical harmonics or inner products with them, it is somewhat easier and cheaper to implement.

Both the local and nonlocal nonreflecting boundary conditions inherently provide an analytic expression for evaluating the electromagnetic field everywhere outside Ω . Therefore, they are advantageous for far-field evaluation [GrKi03] and multiple scattering problems [GrKi04, GrKi07].

References

- [BT80] Bayliss, A., Turkel, E.: Radiation boundary conditions for wave-like equations. *Comm. Pure Appl. Math.*, **33**, 707–725 (1980)
- [Ber94] Bérenger, J.-P.: A perfectly matched layer for the absorption of electromagnetic waves. *J. Comput. Phys.*, **114**, 185–200 (1994)
- [CK92] Colton, D., Kress, R.: *Inverse Acoustic and Electromagnetic Scattering Theory*. Springer, Berlin Heidelberg New York (1992)
- [EM77] Engquist, B., Majda, A. J.: Absorbing boundary conditions for the numerical simulation of waves. *Math. Comp.*, **31**, 629–651 (1977)
- [Giv04] D. Givoli, High-order local non-reflecting boundary conditions: a review. *Wave Motion*, **39**, 319–326 (2004)
- [GN03] Givoli, D., Neta, B.: High-order nonreflecting boundary scheme for time-dependent waves. *J. Comput. Phys.*, **186**, 24–46 (2003)
- [Gro00] Grote, M. J.: Nonreflecting boundary conditions for electromagnetic scattering. *Int. J. Num. Model.*, **13**, 397–416 (2000)
- [Gro06] Grote, M. J.: Local nonreflecting boundary condition for Maxwell's equations. *Comput. Methods Appl. Mech. Engrg.*, **195**, 3691–3708 (2006)
- [GrKe95] Grote, M. J., Keller, J. B.: Exact nonreflecting boundary conditions for the time dependent wave equation. *SIAM J. Appl. Math.*, **55**, 280–297 (1995)
- [GrKe96] Grote, M. J., Keller, J. B.: Nonreflecting boundary conditions for time dependent scattering. *J. Comput. Phys.*, **127**, 52–65 (1996)
- [GrKe98] Grote, M. J., Keller, J. B.: Nonreflecting boundary conditions for Maxwell's equations. *J. Comput. Phys.*, **139**, 327–342 (1998)

- [GrKi03] Grote, M. J., Kirsch, C.: Far-field evaluation via nonreflecting boundary conditions. In: Hou, T. Y., Tadmor, E. (eds) *Hyperbolic Problems: Theory, Numerics, Applications*. Springer, Berlin Heidelberg New York (2003)
- [GrKi04] Grote, M. J., Kirsch, C.: Dirichlet-to-Neumann boundary conditions for multiple scattering problems. *J. Comput. Phys.*, **201**, 630–650 (2004)
- [GrKi07] Grote, M. J., Kirsch, C.: Nonreflecting boundary conditions for time-dependent multiple scattering. *J. Comput. Phys.*, **221**, 41–62 (2007)
- [HH98] Hagstrom, T., Hariharan, S. I.: A formulation of asymptotic and exact boundary conditions using local operators. *Appl. Numer. Math.*, **27**, 403–416 (1998)
- [HW03] Hagstrom, T., Warburton, T.: High-order radiation boundary conditions for time-domain electromagnetics using an unstructured discontinuous Galerkin method. In: K. J. Bathe (ed) *Computational Fluid and Solid Mechanics*. Elsevier, Amsterdam (2003)
- [HW04] Hagstrom, T., Warburton, T.: A new auxiliary variable formulation of high-order local radiation conditions: corner compatibility conditions and extensions to first-order systems. *Wave Motion*, **39**, 327–338 (2004)
- [Hig87] R. Higdon, Numerical absorbing boundary conditions for the wave equation. *Math. Comp.*, **49**, 65–90 (1987).
- [Jac75] Jackson, J. D.: *Classical Electrodynamics*, 2nd edition. Wiley, New York (1975)
- [Jon64] Jones, D. S.: *The Theory of Electromagnetism*. Pergamon Press, New York, Macmillan (1964)
- [KPT98] Kantartzis, N. V., Petropoulos, P. G., Tsiboukis, T. D.: A Comparison of the Grote-Keller Exact ABC and the Well-Posed PML for Maxwell's Equations in Spherical Coordinates. *IEEE Trans. on Magnetics*, **35**, 1418–1422 (1999)
- [Kir05] Kirsch, C.: *Nonreflecting Boundary Conditions for the Numerical Solution of Wave Propagation Problems in Unbounded Domains*. Ph.D. Thesis, University of Basel, Basel (2005)
- [KL93] Kunz, K. S., Luebbers, R. J.: *Finite Difference Time Domain Methods for Electromagnetics*. CRC Press (1993)
- [MZ93] De Moerloose, J., De Zutter, D.: Surface integral representation radiation boundary condition for the FDTD method. *IEEE Trans. Antenn. Propag.*, **41**, 890–895 (1993)
- [Mur81] Mur, G.: Absorbing boundary conditions for the finite-difference approximation of the time-domain electromagnetic-field equations. *IEEE Trans. Electromagn. Compat.*, **23**, 377–382 (1981)
- [Ned00] Nédélec, J.-C.: *Acoustic and Electromagnetic Equations*. Springer, Berlin Heidelberg New York (2000)

- [Pet88] Peterson, A. F.: Absorbing boundary conditions for the vector wave equation. *Microwave and Optical Techn. Letters*, **1**, 62–64 (1988)
- [RT06] Rokhlin, V., Tygert, M.: Fast algorithms for spherical harmonic expansions. *SIAM J. Sci. Comput.*, **27**, 1903–1928 (2006)
- [TM86] Ting, L., Miksis, M. J.: Exact boundary conditions for scattering problems. *J. Acoust. Soc. Amer.*, **80**, 1825–1827 (1986)
- [Yee66] Yee, K.-S.: Numerical solution of initial boundary value problems involving Maxwell’s equations in isotropic media. *IEEE Trans. Antennas Propag.*, **14**, 302–307 (1966)

High-Order Methods for High-Frequency Scattering Applications

O.P. Bruno and F. Reitich

5.1 Introduction

The problem of simulating the scattering of (acoustic, electromagnetic, elastic) waves has provided a particularly sustained, demanding and motivating challenge for the development of efficient and accurate numerical methods since the advent of computers. The classical issues present in most other applications, such as those related to the environmental and/or geometrical intricacies of the media in which quantities of interest are defined, are augmented in the context of wave propagation by the intrinsic complexities (i.e. oscillations) of the quantities themselves. Still, very efficient methodologies have been devised, particularly in the last twenty years, to simulate wave processes in rather complex settings. These techniques can be based, for instance, on finite elements (see e.g. [34, 35, 46] and the references therein), finite differences [40, 49] or boundary integral equations [4, 8, 11, 16, 25], and they can, today, effectively address these problems, with a high degree of accuracy, in domains that can span tens or perhaps even a few hundred wavelengths. The very nature of these classical approaches, however, limits their applicability at higher frequencies since the numerical resolution of field oscillations translates in a commensurately higher number of degrees of freedom and this, in turn, can easily lead to impractical computational times. In this chapter we review some recently proposed methodologies [5, 13–15, 29] that can overcome these limitations while retaining the mathematical rigor of classical numerical procedures.

As a result of the inability of standard simulation techniques to resolve full-wave models (e.g. the Helmholtz, Maxwell or Navier equations) at high frequencies, the state-of-the-art must rely on *asymptotic high-frequency theories*, most notably geometrical optics (GO) [12, 37]. The most advantageous characteristic that these theories display is their ability to bypass the need to resolve field oscillations on the scale of the wavelength of radiation (see Sect. 5.2.2). This is, however, attained at the expense of a loss of error-controllability, which follows from the approximation that the theories entail at the level of

the models (e.g. replacing the Helmholtz or Maxwell model by the eikonal equation, see Sect. 5.2.2). As a consequence these methods can incur in significant inaccuracies when applied at large but finite frequencies, leaving a sizeable gap in the range of frequencies wherein engineering or industrial design can rely on simulation [43].

The methods we review in this chapter arose, in fact, in response to the need to close this gap. As we detail below the schemes result from a thoughtful incorporation of asymptotic theories into rigorous solution methods. The initial developments, and those we review herein, deal with such combinations in the context of integral-equation based solvers though, as shall be clear from the discussion, the basic ideas can be extended to other solution techniques (e.g. those based on finite elements). As we shall show, by design, the resulting algorithms do indeed combine the advantages of rigorous approaches, namely error-controllability, with those inherent in asymptotic theories, that is, computational times that do not increase with increasing frequency. Moreover, the procedures we review have the additional benefit that they seamlessly reduce to standard solvers as the frequency decreases.

The rest of the chapter is organized as follows. First, for the sake of completeness, in Sect. 5.2 we collect some preliminary results on which we build the ensuing developments. Specifically, in Sect. 5.2.1 we first review the basic integral-equation formulations of the scattering problems; for the sake of simplicity of presentation we focus on the scalar Helmholtz (acoustic) model, though all considerations clearly extend to more complex vector models. The basic concepts of geometrical optics, on the other hand, are summarized in Sect. 5.2.2. Section 5.3 constitutes the core of the chapter, as it is where we describe the integration of the concepts in Sect. 5.2 and the resulting numerical implementation. As we explain there, a basic algorithm can be derived in the context of single-scattering geometries (Sect. 5.3.1), and iteratively applied to treat multiple scattering effects in general configurations (Sect. 5.3.2). Examples of application of the resulting schemes are presented in Sect. 5.4, and conclusions are summarized in Sect. 5.5.

5.2 Preliminaries

In this section, we collect some preliminary derivations and results that will be used to derive our high-frequency schemes. As we mentioned, we shall present the ideas in the context of scalar scattering models. More precisely, we consider the problem of evaluating the scattered field $u = u(x)$ generated by an incident (acoustic) plane wave $u^{\text{inc}}(x) = e^{ik\alpha \cdot x}$, $|\alpha| = 1$, as it impinges on a smooth impenetrable obstacle $K \subset \mathbb{R}^d$ ($d = 2, 3$). For the sake of definiteness we assume that the obstacle is “sound soft” in which case the mathematical model takes on the form of a field equation

$$\Delta u(x) + k^2 u(x) = 0, \quad x \in \Omega = \mathbb{R}^d \setminus \overline{K}, \quad (5.1)$$

subject to a boundary condition

$$u(x) = -u^{\text{inc}}(x) = -e^{ik\alpha \cdot x}, \quad x \in \partial K; \quad (5.2)$$

as will be clear from the derivations that follow, the extension of the basic principles and numerical schemes to other boundary conditions is rather straightforward. To uniquely identify the physically relevant solution, equations (5.1) and (5.2) must be supplemented with the classical Sommerfeld radiation condition [26]

$$\lim_{|x| \rightarrow \infty} |x|^{(d-1)/2} \left[\left(\frac{x}{|x|}, \nabla u(x) \right) - ik u(x) \right] = 0. \quad (5.3)$$

In the next two sections we review two fundamental solution procedures for the problem (5.1)–(5.2). First, in Sect. 5.2.1, we recall the basic ideas behind the rigorous reformulation of the problem in the form of an integral equation. The final subsection, in turn, is devoted to a discussion of *asymptotic* high-frequency models and, particularly, of the geometrical optics formulation.

5.2.1 Integral Equation Formulations

The problem (5.1)–(5.2) can be recast in the form of an integral equation in a variety of ways (see e.g. [26]). The so-called “indirect approach”, for instance, seeks a solution u in the form of a double-layer potential

$$u(x) = \int_{\partial K} \frac{\Phi(x, y)}{\partial \nu(y)} \mu(y) \, d\sigma(y), \quad x \in \Omega, \quad (5.4)$$

where $\nu(x)$ denotes the vector normal to ∂K and exterior to K and

$$\Phi(x, y) = \begin{cases} \frac{i}{4} H_0^{(1)}(k|x-y|) & \text{if } d = 2, \\ \frac{1}{4\pi} \frac{e^{ik|x-y|}}{|x-y|} & \text{if } d = 3 \end{cases} \quad (5.5)$$

stands for the outgoing fundamental solution of the Helmholtz operator. Letting x in (5.4) converge to a boundary point on ∂K , using the classical “jump relations” for the double-layer potential [26] and the boundary condition (5.2) we obtain the second kind integral equation

$$\mu(x) - \int_{\partial K} \frac{\partial G(x, y)}{\partial \nu(y)} \mu(y) \, d\sigma(y) = -2e^{ik\alpha \cdot x}, \quad x \in \partial K \quad (5.6)$$

where we have set $G = -2\Phi$.

Alternatively, integral equations can be derived using a “direct approach” based on Green’s identities. In detail, for $x \in \Omega$, we have

$$-u(x) = \int_{\partial K} \left(\frac{\partial u(y)}{\partial \nu(y)} \Phi(x, y) - u(y) \frac{\partial \Phi(x, y)}{\partial \nu(y)} \right) \, ds(y) \quad (5.7)$$

and

$$0 = \int_{\partial K} \left(\frac{\partial u^{\text{inc}}(y)}{\partial \nu(y)} \Phi(x, y) - u^{\text{inc}}(y) \frac{\partial \Phi(x, y)}{\partial \nu(y)} \right) ds(y). \quad (5.8)$$

Adding (5.7) and (5.8), and using (5.2), it follows that

$$u(x) = - \int_{\partial K} \Phi(x, y) \eta(y) ds(y), \quad x \in \Omega, \quad (5.9)$$

where

$$\eta(y) = \frac{\partial (u(y) + u^{\text{inc}}(y))}{\partial \nu(y)}. \quad (5.10)$$

Using (5.9), (5.10) and the jump relations for the derivatives of single-layer potentials [26] we obtain the integral equation

$$\eta(x) - \int_{\partial K} \frac{\partial G(x, y)}{\partial \nu(x)} \eta(y) ds(y) = 2 \frac{\partial u^{\text{inc}}(x)}{\partial \nu(x)}, \quad x \in \partial K. \quad (5.11)$$

For future reference we note here that while equations (5.6) and (5.11) are very similar from a mathematical standpoint, they differ significantly from a physical perspective. Indeed, while the latter entails a physically realizable unknown (e.g. the total surface current in electromagnetics), no natural physical interpretation can be attached to the former. Mathematically, on the other hand, both are Fredholm equations of the second kind with weakly singular kernels. In particular, for instance, in both cases the solutions are not unique when the wavenumber k is an internal resonance and thus, in practical implementations, a “combined field” integral equation (CFIE) formulation is traditionally used [26]. The ideas that follow, however, clearly extend to the CFIE formulation (see e.g. [14]) and, thus, for the sake of simplicity in presentation, we shall assume that the wave number k is not an internal resonance and work with the integral equations (5.6) and (5.11).

5.2.2 Asymptotic Expansions and Geometrical Optics

While the solution of equations (5.6) and (5.11) can, in principle, provide approximations to the field u of arbitrary accuracy, the cost of their numerical inversion grows rather dramatically with increasing frequency. Indeed, clearly, the Green function (5.5) oscillates on the scale of the wavelength of radiation $\lambda = 2\pi/k$ and, moreover, so do the densities μ and η , as a simple analysis of the equations they satisfy reveals. This, in turn, imposes stringent demands on (1) the requisite number of degrees of freedom to represent the unknown surface functions; and (2) the number of points needed to accurately evaluate the integrals in the right-hand sides of (5.6) and (5.11). Indeed, the simple evaluation of such integrals incurs a cost that is proportional to $((ka)^{d-1})^2$ in $d = 2$ or $d = 3$ dimensions, where a denotes a typical length-scale of the scatterer K , and it thus quickly becomes prohibitive at short wavelengths

(even if accelerated evaluations, e.g. based of fast multipole methods [4, 25] or FFTs [11, 16], that reduce the cost to $((ka)^{d-1})^\alpha$, $1 \leq \alpha < 2$, are used).

These dimensional considerations are not, of course, restricted to integral equation formulations but rather they apply to any rigorous solution strategy. The high-frequency character of the sought returns, on the other hand, does suggest an alternative approach based on asymptotics near the limit of vanishing wavelength. Specifically, such asymptotics begin with the Luneberg–Kline expansion [12]

$$u(x) + u^{\text{inc}}(x) \sim e^{ik\varphi(x)} \sum_{n=0}^{\infty} \frac{A_n(x)}{k^n} \quad (5.12)$$

for an unknown phase φ and amplitudes A_n . Substituting this expression into (5.1) and letting $k \rightarrow \infty$ we readily obtain the eikonal equation

$$|\nabla\varphi| = 1 \quad (5.13)$$

for the phase, while the amplitudes solve a sequence of transport equations whose solutions can be found iteratively starting from

$$A_0(x)\Delta\varphi(x) + 2\nabla\varphi(x) \cdot \nabla A_0(x) = 0. \quad (5.14)$$

In spite of the apparent simplicity of the geometric equation (5.13) its non-linear character, and possible multi-valuedness, poses significant challenges for the numerical approximation of its solutions and, as a result, the design of advanced algorithms for geometrical optics continues to be a very active area of research in computational science. Clearly a simple procedure can be based on the “method of characteristics” (so-called “ray-tracing” in this context, see e.g. [7]) but, as has been long recognized, a number of problems arise when applying this technique (e.g. related to its computational cost, and issues of ray divergence and wavefront reconstruction [30]). The consequent limitations have prompted the recent development of new computational methods based on (Eulerian) solution of partial differential equations. Early versions of this approach concentrated on the design of upwind [51, 52] and ENO schemes [32] for the direct solution of the eikonal equation (5.13), leading to accurate approximations of the viscosity solution [27]. This (single-valued) solution, however, represents only the wave of first arrival at any given point [27] and it may thus be insufficient for certain applications wherein significant effects arise as a consequence of multiple scattering. For this reason, a number of algorithms have more recently been developed to upgrade the viscosity solution to the multi-valued solution relevant in these cases. Among these we encounter, for instance, the “big ray tracing method” [3], the “method of decomposition along caustics” [9] and the “slowness matching method” [50].

All of these procedures are based on domain decomposition and local approximations of viscosity solutions, which are then combined into a multi-valued quantity. In this connection, a particularly promising scheme has been recently introduced [6] based on spectral methodologies that result in uniquely

accurate evaluations. The procedure was specifically designed to work with spectral solution techniques for boundary integral equation formulations (in a manner such as that described below in Sect. 5.3) and it thus provides an efficient and accurate mechanism to approximate the values of the phase φ in (5.13) on the surface of the scatterers at each successive reflection. Briefly, to this end the method relies on a sort of “inverse ray tracing” (to avoid ray divergence) that, at each reflection, finds the points $Q(P_j)$ on the surface from where rays emanate to arrive onto a *fixed grid* P_j . The latter grids can be constructed (locally in three space dimensions) so as to allow for a spectral interpolation of the function $Q(P)$ and thus for the iterative application of these ideas; see Figs. 5.1 and 5.2.

Finally, an alternative approach to the approximation of multi-valued solutions is based on a “kinetic” formulation that views rays as trajectories of particles following a Hamiltonian dynamics; see [30] and the references therein. In this approach, multi-valued solutions are naturally “unfolded” through the introduction of conjugate phase variables. This, however, is achieved at the

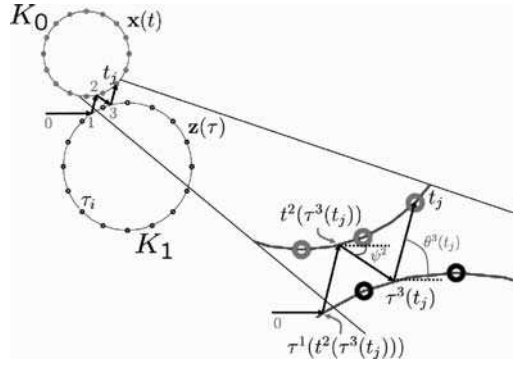


Fig. 5.1. Spectral geometrical optics solver. In this geometry, at reflection n the functions $\tau^n(t_j)$ on K_0 and $t^n(\tau_j)$ on K_1 are defined on fixed grids and interpolated spectrally to allow for the evaluation of the corresponding functions in the following reflection. The total phase is reconstructed from suitable composition of these functions

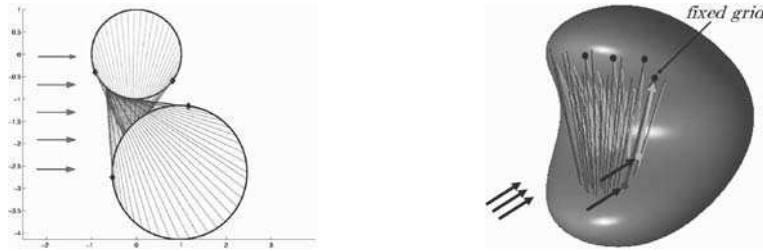


Fig. 5.2. Examples of application of the spectral geometrical solver of [6]; see also Fig. 5.1

expense of doubling the number of independent variables, with the consequent potential for increased computational cost. To deal with this problem, two alternative strategies have been developed, leading to “wavefront” and “moment-based” methods respectively [30]. In the former, an interface representing a wavefront is evolved following the Liouville formulation, while the latter is based on the derivation of new equations (for the moments of the density) with fewer unknowns. A recent scheme [22] has sought to combine elements from these two approaches by relying on the evolution of an interface (defined in terms of level-set functions [41]) while avoiding the direct discretization of the phase variables. Instead, the procedure is based on suitable (spectral) representations of the unknown field quantities and, as such, it can be related to moment methods where the moments are not chosen to be integrals against monomials in phase variables (needing a “closure hypothesis”), but rather against basis functions that guarantee accurate representations of general phase variations; see Fig. 5.3.

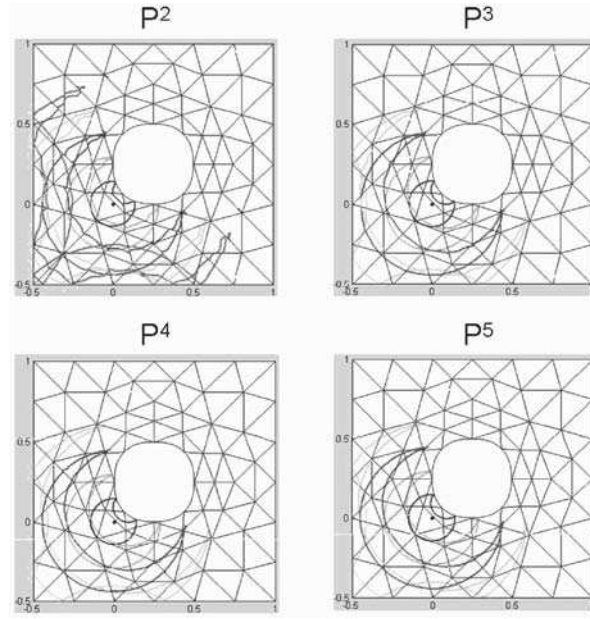


Fig. 5.3. Sample scattering computation based on a spectral approach to geometrical optics in phase space, from [21] (see also [22]). Phase variations are represented in the form of Fourier (or spherical harmonics) series; spatial approximations, in turn, are attained via high-order discontinuous Galerkin finite element methods [23, 24]. The time integration is based on strong stability preserving Runge–Kutta (SSP-RK) schemes [20, 33]. The panels show the results using the space P^ℓ of polynomials of degree ℓ for the space variables and the SSP-RK procedure of order $\ell + 1$ for increasing values of ℓ

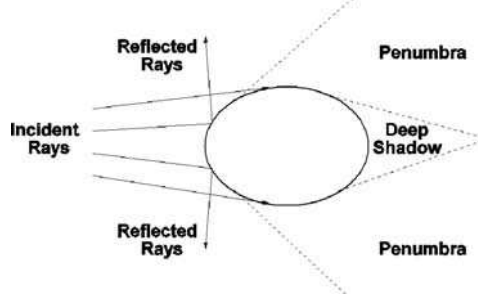


Fig. 5.4. Rays and zones defined by high-frequency radiation incident on a scatterer

Although the geometrical optics approximation described above, in any of its implementations, does simplify the solution of the scattering problem at high frequencies by *explicitly* encoding oscillations into the approximation (5.12) it is, as we have mentioned, of limited utility at large but finite frequencies. This is due to the short-wavelength limiting procedure which results in the neglect of important effects (e.g. diffraction and creeping waves). In fact, a rigorous form of the expansion (5.12) takes on a significantly more complex form (which reduces to (5.12) in the “illuminated region”; see Fig. 5.4). Clearly, this form can be described in terms of that corresponding to the normal derivative $\eta(x)$ (cf. (5.10)) of the total field evaluated on the ∂K , since the field at any point can be recovered from (5.9). For instance, if K is convex (so that, in particular, no multiple-scattering can occur) an accurate representation is given by the following theorem.

Theorem 5.1 ([39]). *If K is convex then, for all $P, Q \geq 0$, the density η in (5.11) admits the representation*

$$\begin{aligned} \eta(x) &= \eta(x, k, \alpha) \\ &= e^{ik\alpha \cdot x} \sum_{p=0}^P \sum_{q=0}^Q k^{2/3-2p/3-q} b_{p,q}(\alpha, x) \Psi^{(p)}(k^{1/3} Z(\alpha, x)) + R_{P,Q}(k, \alpha, x) \end{aligned} \quad (5.15)$$

where the complex-valued functions $b_{p,q}$ and the real-valued function Z are smooth, and Ψ is entire in the complex plane. Moreover, Z is positive in the illuminated region, negative in the shadow region, and vanishes precisely to first order at the shadow boundary (see Fig. 5.4). The function Ψ behaves asymptotically as

$$\Psi(\tau) = \begin{cases} \sum_{p=0}^n a_p \tau^{1-3p} + \mathcal{O}(\tau^{1-3(n+1)}) & \text{as } \tau \rightarrow \infty, \\ c_0 e^{-i\tau^3/3 - i\tau\beta} (1 + \mathcal{O}(e^{\tau c_1})) & \text{as } \tau \rightarrow -\infty, \end{cases} \quad (5.16)$$

for some constants c_0 and $c_1 > 0$, where $\beta = e^{-2\pi i/3} \beta_1$ and β_1 is the right-most root of Ai . The remainder $R_{P,Q}$ satisfies

$$|D_x^\gamma R_{P,Q}(k, \alpha, x)| \leq C_{P,Q,\gamma} (1+k)^{-\min\{2P/3, Q+1/3\}+1/3|\gamma|}$$

for some constants $C_{P,Q,\gamma}$.

5.3 A High-Order High-Frequency Method

As we anticipated in the Introduction, here we present the details of an approach to the simulation of high-frequency scattering processes that combines the virtues of the rigorous integral-equation formulations of Sect. 5.2.1 with those of the asymptotic methods of Sect. 5.2.2. More precisely, we present a procedure to attain solutions to the former formulations with any prescribed accuracy, while retaining the frequency-independent computational cost that characterizes the latter methods. As we said, the basic strategy is one that relies on the iterative account of geometrical reflections. The simplest instance is, of course, one where a single reflection occurs (i.e. single-scattering configurations, such as those provided by convex scatterers) which we describe and treat first in Sect. 5.3.1. In Sect. 5.3.2 then we review the iterative procedure that allows us to evaluate multiple scattering effects through a sequential application of ideas based on those in Sect. 5.3.1.

5.3.1 Single-Scattering Configurations

Our numerical approach within single-scattering configurations results from the recognition and suitable treatment of the two main characteristics of integral equations such as those in (5.6) and (5.11) that result in impractical computational times at high frequencies. Specifically, these correspond to (1) the highly oscillatory behavior of the (unknown) densities, which thus require a large number of degrees of freedom to accurately represent them; and (2) the equally fast variations of the (known) kernel which, even if the densities varied slowly, demands a large number integration points.

The basic idea behind the resolution of the issue in (1) above relies on the possibility to *pre-determine* the nature of the oscillations in the densities, so that these are represented by *slow* unknown modulations of *known* rapidly varying exponentials. In detail, we seek a decomposition

$$\eta(x) = \eta^{\text{slow}}(x)e^{ik\varphi(x)} \quad (5.17)$$

and/or

$$\mu(x) = \mu^{\text{slow}}(x)e^{ik\varphi(x)} \quad (5.18)$$

for some phase function φ that can be determined a priori. Interestingly, while (5.15) guarantees that the decomposition (5.17) is possible, in the illuminated region, for the “physical” density η with

$$\varphi(x) = \alpha \cdot x$$

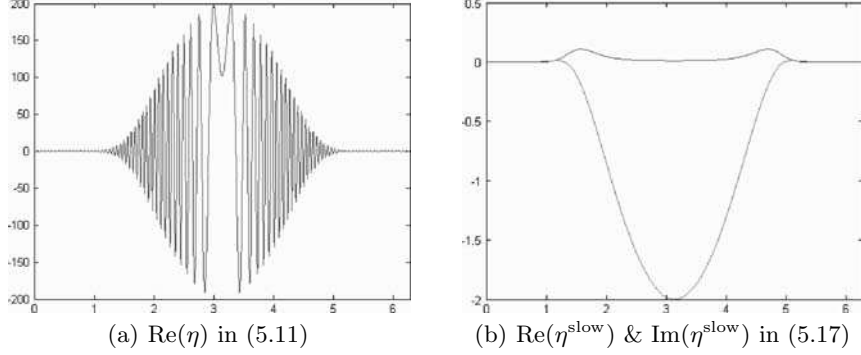


Fig. 5.5. (a) Real part of the solution $\eta(x)$ to (5.11) corresponding to scattering off a circular cylinder of radius a with $ka = 100$. (b) Real and imaginary parts of the corresponding slow density $\eta^{\text{slow}}(x)$ defined as in (5.17)

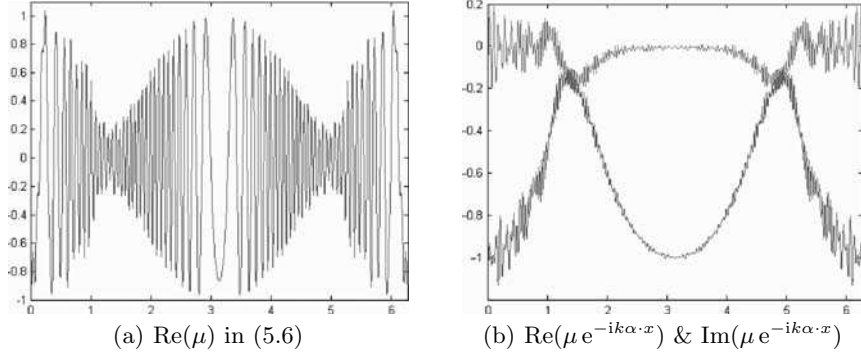


Fig. 5.6. (a) Real part of the solution $\mu(x)$ to (5.6) corresponding to scattering off a circular cylinder of radius a with $ka = 100$. (b) Real and imaginary parts of the corresponding densities $\mu^{\text{slow}}(x)$ defined as in (5.18)

it turns out that this does not hold for the density μ in (5.6); see Figs. 5.5 and 5.6. For this reason, at high frequencies the formulation (5.11) is preferable to that in (5.6) and we shall henceforth concentrate on the solution of the former.

The extraction of the phase of the incident radiation as described above has, in fact, been used extensively in the past (see e.g. [1, 2, 19, 28, 31, 36, 38, 42, 47, 53] and the references therein), but its utility was consistently limited by two factors: on the one hand, as we have said, the factorization (5.17) is only valid in the illuminated region (cf. Theorem 5.1); and, on the other hand, even after phase extraction the need to accurately evaluate the highly oscillatory integrals in the formulation remains a challenge (cf. item 2) in the first paragraph of this section). Indeed, the decomposition (5.17) allows for a recasting of equation (5.11) in the form

$$\eta^{\text{slow}}(x) - \int_{\partial K} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik\alpha \cdot (y-x)} \eta^{\text{slow}}(y) \, ds(y) = 2ik\alpha \cdot \nu(x), \quad x \in \partial K \quad (5.19)$$

where the oscillatory behavior of η^{slow} does not accentuate in the illuminated region, but the integrals in the left-hand side require quadratures with step sizes that are proportional to and smaller than the wavelength.

In the particular case wherein the entire scattering surface is illuminated (e.g. a shallow infinite rough surface under near-to-normal incidence) and thus the density η^{slow} solving (5.19) is truly slowly varying throughout, the resulting high-frequency integration problem can be solved, to arbitrarily high order, via explicit asymptotic expansions. More precisely, it can be shown (see e.g. [18, 44, 45]) that the function η admits a representation such as that in (5.12) in inverse powers of the wavenumber

$$\eta(x) = e^{ik\varphi(x)} \eta^{\text{slow}}(x) = e^{ik\varphi(x)} \sum_{n=0}^{\infty} \frac{\eta_n^{\text{slow}}(x)}{k^n} \quad (5.20)$$

and the integral equation (5.19) can be used to recursively obtain the functions η_n^{slow} by appealing to the classical theory of oscillatory integrals [10]; see Table 5.2, Sect. 5.4.2.

Under more general illumination conditions where shadowing can occur, however, the expansion (5.20) ceases to be valid. As Theorem 5.1 suggests, fractional powers of the wavenumber could be used in this case, though the appearance of boundary layers at shadowing transitions would further require a singular expansion; see (5.15) and Fig. 5.7. To deal with these issues an alternative integration method was proposed in [14] which does not rely on such asymptotic expansions. Instead, the approach proposed therein is based on the design of rigorous quadrature formulas that allow for the evaluation of the integrals in (5.19) in frequency-independent computational times; clearly, once this is enabled, the actual solution can be attained through an iterative procedure (e.g. GMRES [48]).

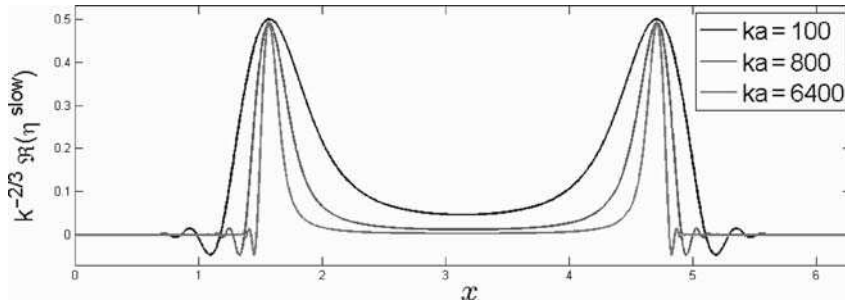


Fig. 5.7. Example of boundary layers at shadowing transitions. Results correspond to scattering by a circular cylinder of radius a , under plane wave incidence with $\alpha = (1, 0)$

To enable an accurate representation of the unknown density η^{slow} in (5.19) in this case, our approach relies on the use of non-equispaced grids which are suitably refined at shadowing transitions. For instance, if the curvature in these regions does not vanish, the boundary layers can be shown to be of size proportional to $\lambda^{1/3}$, and the density to vanish exponentially as these are transversed towards the deep shadow (cf. (5.15) and Fig. 5.7). Thus, to attain a prescribed accuracy, we choose a sufficiently fine distribution of grid points that is frequency independent throughout except at shadow boundaries where the inter-node separation is a fraction of and proportional to $\lambda^{1/3}$. Beyond these transitions the density can be assumed to vanish (and, thus, no degrees of freedom are necessary therein), with an error that can be controlled by varying the constant of proportionality in their $O(\lambda^{1/3})$ size; see Fig. 5.8. For the integration rule, on the other hand, our starting point is the observation that the process of phase extraction leading to the integral equation (5.19) has a beneficial effect that is additional to that of transforming the unknown into a slowly oscillatory one. Indeed, it follows from (5.19) that the relevant integrals can be written in the form

$$\int_{\partial K} G^{\text{slow}}(x, y) e^{ik\psi(x, y)} \eta^{\text{slow}}(y) \, ds(y), \quad (5.21)$$

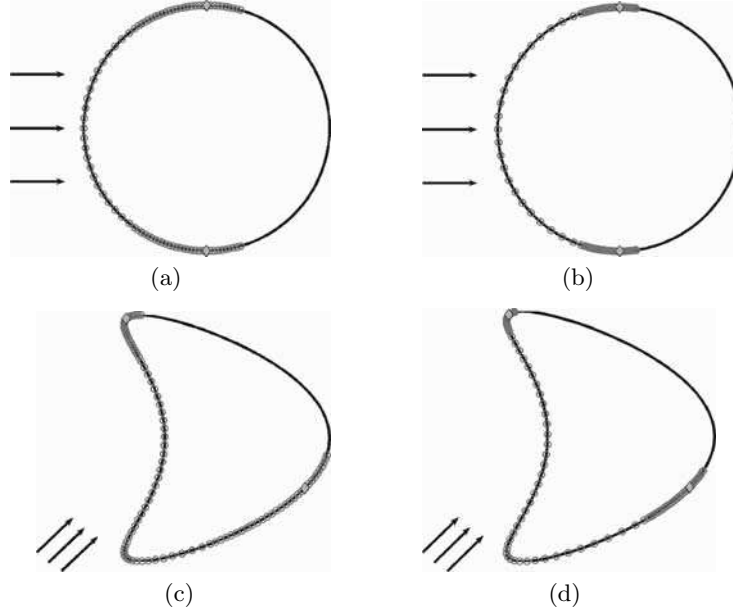


Fig. 5.8. Non-uniform grids, with refinements near the shadowing transitions. Figures (b) and (d) correspond to an eight-fold increase in wavenumber with respect to (a) and (c), respectively, which results in a decrease by half in the size of the boundary layers

where the kernel $G^{\text{slow}}(x, y)$ is slowly oscillatory and the phase function $\psi(x, y)$ can be *explicitly* derived from the (asymptotic behavior of the) Green's function (5.5),

$$\psi(x, y) = |x - y| + \alpha \cdot (y - x). \quad (5.22)$$

The form of the integrals in (5.21), in turn, suggests a mechanism for its evaluation, namely one based on the classical “stationary phase method” [10]. As we have shown [14], although the straightforward application of this asymptotic approach would lead to a non-convergent scheme, the principles on which it is based can still be used to design a convergent algorithm.

More precisely, our numerical procedure relies on the observation that, as suggested by the method of stationary phase, for each fixed target point x , the integral in (5.19) (or, equivalently, that in (5.21)) can be *localized* to a neighborhood of the corresponding *critical points*. These points include all singularities (e.g. $y = x$, the target point itself) and all points where the total phase $\psi(x, \cdot)$ in (5.22) is stationary; note that the evaluation of these points entails a simple geometrical construction (see Fig. 5.9). In more detail, the specific intervals of localization around critical points can be determined from the following result.

Lemma 5.1 ([14]). *Let $p > 1$, $A > 0$, $0 < \varepsilon < A$ and $0 < c < 1$ be given, and let $S(t, t_0, t_1)$ denote a smooth cutoff function that is equal to 1 for $t \leq t_0$ and vanishes for $t > t_1$. Define*

$$f_A(t) = S(t, cA, A) (1 - S(t, -A, -cA))$$

and

$$f_\varepsilon(t) = f_A\left(\frac{At}{\varepsilon}\right)$$

(see Fig. 5.10); then we have

$$\int_{-A}^A f_A(t) e^{ikt^p} dt = \int_{-\varepsilon}^{\varepsilon} f_\varepsilon(t) e^{ikt^p} dt + O\left((k\varepsilon^p)^{-n}\right) \quad \text{for all } n \geq 1.$$

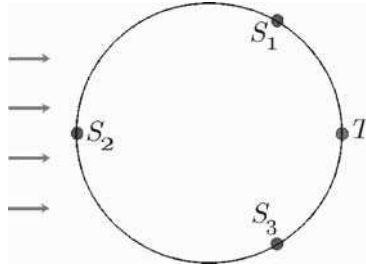


Fig. 5.9. Stationary points S_j corresponding to a fixed target point T for plane wave incidence on a circular cylinder

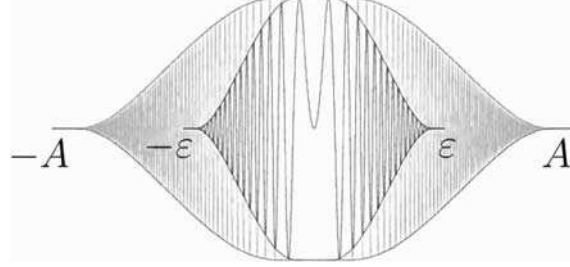


Fig. 5.10. Localized integration: the integral from $-A$ to A can be replaced by that on $[-\varepsilon, \varepsilon]$

That is, under certain conditions on the product $k\varepsilon^p$, the integral between $-\varepsilon$ and ε of $f_\varepsilon(t)e^{ikt^p}$ is a good approximation of the integral of $f_A(t)e^{ikt^p}$ between $-A$ and A .

From Lemma 5.1 it follows that the integrals in (5.19) can be approximated *uniformly in k* by localizing to:

1. A neighborhood of the target point x of radius proportional to the wavelength λ ($p = 1$); and
2. Neighborhoods of each stationary point $y = S_j$ of radius proportional to $\lambda^{1/2}$ ($p = 2$) or $\lambda^{1/3}$ ($p = 3$, at the shadow boundaries).

Indeed, a key element of these choices is the fact that each of these integration neighborhoods contain a *fixed* number of oscillations and, thus, the corresponding integrals can be computed, to any prescribed accuracy, with a fixed number of points, independently of k (the *density* of integration nodes around the critical points does, of course, consequently increase). Figure 5.11 shows a schematic of this procedure for the case of scattering by a circular cylinder of radius a : the top panel displays the integrand in (5.19) corresponding to $ka = 1,000$ together with cutoff functions around the target and stationary points where the integration is confined (note that the support of these cutoff functions may overlap); the bottom panel, in turn, shows the same data but for $ka = 4,000$. Note that, in accordance with the prescriptions above, the size of the support of the cutoff function around the target point is four times smaller than than chosen for $ka = 1,000$, while those of the cutoffs around the stationary points are halved as the frequency is multiplied by four.

5.3.2 Multiple-Scattering Configurations

The discussion in the previous section provides a numerical approach to the evaluation of the solution of the integral equation (5.11) within any given accuracy in times that are independent of the wavenumber, provided the configuration does not result in multiple-scattering at infinite frequencies. This

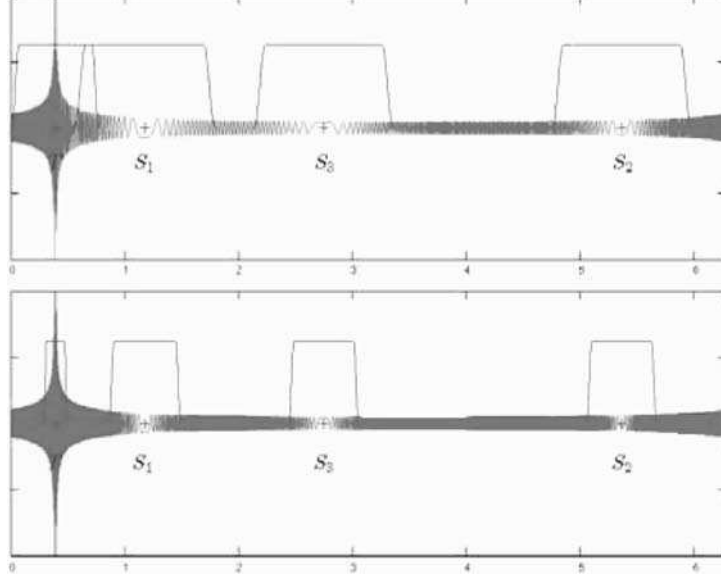


Fig. 5.11. Localized integration: the overall integral can be replaced by that localized near critical points, with decreasing support as k increases. *Top:* $ka = 1,000$; *bottom:* $ka = 4,000$

latter requirement is necessary to validate the ansatz in (5.17) (or, more precisely, the representation in (5.15)) which characterizes the phase of the solution and thus enables its representation with a reduced number of degrees of freedom. Clearly then, a central demand in an approach to extend the ideas to multiple-scattering scenarios relates to the identification of analogous representations that explicitly factor fast oscillations in this latter case. At first glance, the answer is rather straightforward as the phase of *any* solution is governed by the eikonal equation (5.13). An obvious problem arises however in trying to incorporate this information into a numerical scheme since multiple-scattering precisely implies that the eikonal solution is *multi-valued*; see Fig. 5.2.

Fortunately, as we have shown [5, 15, 29], the possible multiple values of the phase can be incorporated *iteratively* into a solution strategy for the integral equation (5.11) at high frequencies. Moreover, this can be done in a manner so that each iteration corresponds to a geometrical reflection. To see this, let us consider a decomposition of the scatterer K into a disjoint union of sub-scatterers K_σ , $\sigma \in \mathcal{I}$, so that the phase of the field scattered by K_σ on a given reflection (i.e. the solution to (5.13)) is single valued on K_τ for $\tau \neq \sigma$ (e.g. K_σ are convex); see Fig. 5.12.

Then, the integral equation (5.11) can be written as

$$(I - R)\eta = f, \quad (5.23)$$

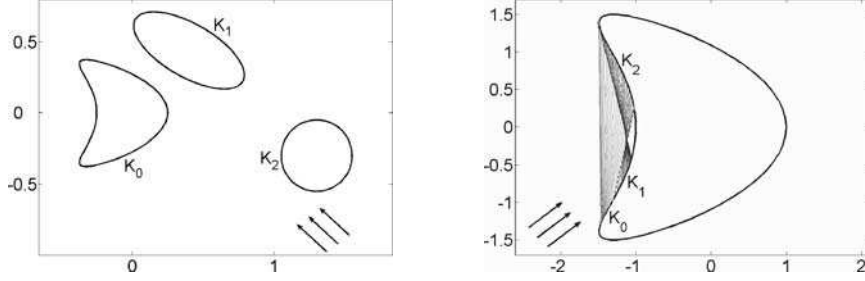


Fig. 5.12. Decomposition of scattering surfaces for evaluation of multiple scattering effects

where $\eta(x) = (\eta_{\sigma_1}(x), \dots, \eta_{\sigma_{|\mathcal{I}|}}(x))^t$ and $f(x) = (f_{\sigma_1}(x), \dots, f_{\sigma_{|\mathcal{I}|}}(x))^t$ with η_σ and f_σ defined on ∂K_σ ,

$$f_\sigma(x) = 2ike^{ik\alpha \cdot x} \alpha \cdot \nu_\sigma(x) \quad \sigma \in \mathcal{I},$$

and the operator R is defined as

$$(R_{\sigma\tau}\eta_\tau)(x) = \int_{\partial K_\tau} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} \eta_\tau(y) ds(y) \quad \text{for } x \in \partial K_\sigma. \quad (5.24)$$

Inverting the diagonal part of (5.23) yields the equivalent relation

$$(I - T)\eta = g \quad (5.25)$$

with

$$g_\sigma = (I - R_{\sigma\sigma})^{-1} f_\sigma, \quad \sigma \in \mathcal{I} \quad (5.26)$$

and

$$T_{\sigma\tau} = \begin{cases} (I - R_{\sigma\sigma})^{-1} R_{\sigma\tau} & \text{if } \sigma \neq \tau, \\ 0 & \text{otherwise.} \end{cases} \quad (5.27)$$

The formulation (5.25) provides a convenient mechanism to account for multiple scattering since the m th term in its Neumann series solution

$$\eta = \sum_{m=0}^{\infty} \eta^m = \sum_{m=0}^{\infty} T^m g \quad (5.28)$$

corresponds exactly to contributions arising as a result of waves that (in the high-frequency regime) have undergone m geometrical reflections. More precisely, we have

$$\eta^m|_{\partial K_\sigma} = \sum_{\substack{\tau_0, \dots, \tau_{m-1} \in \mathcal{I} \\ \sigma \neq \tau_{m-1}, \tau_j \neq \tau_{j-1}}} \eta_{\tau_0, \dots, \tau_{m-1}, \sigma} = \sum_{\substack{\tau_0, \dots, \tau_{m-1} \in \mathcal{I} \\ \sigma \neq \tau_{m-1}, \tau_j \neq \tau_{j-1}}} T_{\sigma\tau_{m-1}} T_{\tau_{m-1}\tau_{m-2}} \cdots T_{\tau_1\tau_0} g_{\tau_0}, \quad (5.29)$$

where each application of a $T_{\sigma\tau}$ entails an evaluation on ∂K_σ of a field generated by a current on ∂K_τ (cf. (5.24)), and its use as an incidence for a

subsequent solution of a (single-)scattering problem on ∂K_σ (corresponding to the inversion of $I - R_{\sigma\sigma}$ in (5.27)). In particular, we have

$$\begin{aligned} \eta_{\tau_0, \dots, \tau_{m-1}, \sigma}(x) &= \int_{\partial K_\sigma} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} \eta_{\tau_0, \dots, \tau_{m-1}, \sigma}(y) \, ds(y) \\ &= \int_{\partial K_{\tau_{m-1}}} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} \eta_{\tau_0, \dots, \tau_{m-1}}(y) \, ds(y) \quad \text{for } x \in \partial K_\sigma, \end{aligned} \quad (5.30)$$

and the nature of the decomposition guarantees that the geometrical phase on each path $(\tau_0, \dots, \tau_{m-1}, \tau_m)$ is *uniquely* defined. In fact, the phase can be explicitly written in the form

$$\varphi(x) = \varphi_{\tau_0, \dots, \tau_{m-1}, \tau_m}(x) = \begin{cases} \alpha \cdot x & \text{if } m = 0 \\ \alpha \cdot x_0^m(x) + \sum_{j=0}^{m-1} |x_{j+1}^m(x) - x_j^m(x)| & \text{if } m \geq 1 \end{cases} \quad (5.31)$$

for $x \in \partial K_{\tau_m}$, where the points

$$(x_0^m(x), \dots, x_m^m(x)) \in \partial K_{\tau_0} \times \dots \times \partial K_{\tau_m} \quad (5.32)$$

satisfy

$$\begin{cases} x_m^m(x) = x \\ \alpha \cdot \nu(x_0^m(x)) < 0 \\ (x_{j+1}^m(x) - x_j^m(x)) \cdot \nu(x_j^m(x)) > 0, \quad j = 1, \dots, m-1 \\ \frac{x_1^m(x) - x_0^m(x)}{|x_1^m(x) - x_0^m(x)|} = \alpha - 2\alpha \cdot \nu(x_0^m(x)) \nu(x_0^m(x)) \\ \frac{x_{j+1}^m(x) - x_j^m(x)}{|x_{j+1}^m(x) - x_j^m(x)|} = \frac{x_j^m(x) - x_{j-1}^m(x)}{|x_j^m(x) - x_{j-1}^m(x)|} \\ -2 \frac{x_j^m(x) - x_{j-1}^m(x)}{|x_j^m(x) - x_{j-1}^m(x)|} \cdot \nu(x_j^m(x)) \nu(x_j^m(x)), \quad j = 1, \dots, m-1 \end{cases} \quad (5.33)$$

and $\nu(x_j^m(x)) = \nu_{\tau_j}(x_j^m(x))$. With this definition then we can set

$$\eta_{\tau_0, \dots, \tau_{m-1}, \tau_m} = \eta_{\tau_0, \dots, \tau_{m-1}, \tau_m}^{\text{slow}}(x) e^{ik\varphi_{\tau_0, \dots, \tau_{m-1}, \tau_m}(x)} \quad (5.34)$$

and (5.30) can be reformulated as

$$\begin{aligned} \eta_{\tau_0, \dots, \tau_{m-1}, \sigma}^{\text{slow}}(x) &= \int_{\partial K_\sigma} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} e^{ik(\varphi_{\tau_0, \dots, \tau_{m-1}, \sigma}(y) - \varphi_{\tau_0, \dots, \tau_{m-1}, \sigma}(x))} \\ &\quad \times \eta_{\tau_0, \dots, \tau_{m-1}, \sigma}^{\text{slow}}(y) \, ds(y) = \rho^{\text{slow}}(x) \quad \text{for } x \in \partial K_\sigma, \end{aligned} \quad (5.35)$$

where

$$\begin{aligned} \rho^{\text{slow}}(x) &= e^{-ik\varphi_{\tau_0, \dots, \tau_{m-1}, \sigma}(x)} \\ &\quad \times \int_{\partial K_{\tau_{m-1}}} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} \eta_{\tau_0, \dots, \tau_{m-1}}^{\text{slow}}(y) e^{ik\varphi_{\tau_0, \dots, \tau_{m-1}}(y)} \, ds(y) \quad \text{for } x \in \partial K_\sigma. \end{aligned} \quad (5.36)$$

Finally, we note that (5.35) possesses the same characteristics as (5.19) in that the integrands are decomposed into an unknown slowly varying envelope ($\eta_{\tau_0, \dots, \tau_{m-1}}^{\text{slow}}$) and a known highly oscillatory function (the product of the Green function and the exponential with phase $\varphi_{\tau_0, \dots, \tau_{m-1}, \sigma}$). Thus the single-scattering method described in Sect. 5.3.1 (based on refined grids near shadowing transitions and localized integration) is directly applicable to the solution of (5.35).

The considerations above guarantee that each successive reflection can be accounted for to any desired accuracy in times that do not increase with increasing wavenumber, but they do not elucidate the relative size of these contributions or their dependence on the geometrical configuration. Recent work [5, 29], however, has shed light on this issue. Indeed, it is shown there that the series (5.28) can be rearranged into a sum of *periodic orbits* (of increasing period), each corresponding to contributions arising from waves that reflect off a fixed subset of (sub)scatterers when these are transversed sequentially in a periodic manner. These orbits thus constitute a fundamental building block for the multiple-scattering effects and, interestingly, they are also amenable to a detailed analysis in the high-frequency regime.

To review this analysis, let us consider a p -periodic sequence $\{\tau_m\}_{m \geq 0} \in \mathcal{I}^\infty$, that is, a sequence such that $\tau_{m+1} \neq \tau_m$ for all $m \geq 0$, and $\tau_{m+qp} = \tau_m$ for $0 \leq m \leq p-1$ and $q \geq 0$. Then a careful asymptotic analysis of the currents successively generated on K_{τ_m} can be pursued to reveal their rate of decay. For two-dimensional, cylindrical configurations we thus find [29] that there exist uniquely determined constants

$$\Phi_p \in \mathbb{R}_+ \quad \text{and} \quad \{\mathcal{L}_r : r = 0, \dots, p-1\} \subset (1, \infty)$$

with the property that, for $x \in \partial K_{\tau_m}$,

$$\left| \frac{\eta_{\tau_0, \dots, \tau_m, \dots, \tau_{m+p}}(x)}{\eta_{\tau_0, \dots, \tau_m}(x)} - \mathcal{R}_\infty(k) \right| \leq \mathcal{O}(k^{-1}\delta^p) + \mathcal{O}(k\delta^{m+p}) + \mathcal{O}(k^0\delta^{m-p}) \quad (5.37)$$

where $\delta < 1$ is a constant and

$$\mathcal{R}_\infty(k) = (-1)^p e^{ik\Phi_p} \prod_{r=0}^{p-1} \frac{1}{\sqrt{\mathcal{L}_r}}. \quad (5.38)$$

The phase Φ_p can be easily characterized (in terms of distance minimizing p -periodic rays) and the numbers $\mathcal{L}_r$ can be obtained recursively starting from $\mathcal{L}_0$ which satisfies a simple quadratic equation; see [29]. For the case $p = 2$, for instance, we have

$$\Phi_2 = 2d = 2|a_0 - a_1| \quad (5.39)$$

where $a_j \in K_{\tau_j}$ are the points that minimize the distance,

$$\sqrt{\mathcal{L}_0 \mathcal{L}_1} = \sqrt{(1 + d\kappa_0)(1 + d\kappa_1)} \left(1 + \sqrt{1 - \frac{1}{(1 + d\kappa_0)(1 + d\kappa_1)}} \right) \quad (5.40)$$

and κ_j denotes the curvature at a_j .

A result analogous to (5.37) holds for three-dimensional configurations [5]. In this case, however, the formula for the rate $\mathcal{R}_\infty(k)$ is significantly more complex, as it is given by

$$\mathcal{R}_\infty(k) = (-1)^p e^{ik\Phi_p} \prod_{r=0}^{p-1} \frac{1}{\sqrt{\det \mathcal{N}_r}} \prod_{r=0}^{p-1} \frac{a_{r+1} - a_r}{|a_{r+1} - a_r|} \cdot \nu_{\tau_r}(a_r), \quad (5.41)$$

where the points $a_j \in K_{\tau_j}$ are the minimizers of the p -periodic distance and the matrices $\mathcal{N}_r$ can be explicitly obtained. For $p = 2$ we have

$$\begin{aligned} \sqrt{\det(\mathcal{N}_0 \mathcal{N}_1)} &= \sqrt{\det((I + d\kappa_0)(I + d\kappa_1))} \\ &\quad \times \det \left(I + \sqrt{I - (I + d\kappa_1)^{-1} U (I + d\kappa_0)^{-1} U^T} \right), \end{aligned} \quad (5.42)$$

where κ_j are the matrices of principal curvatures at the points a_j , and U is a unitary matrix that depends on the rotation between the principal axis at these points.

5.4 Some Numerical Results

In this section we present some numerical results derived from implementations of the ideas described in Sect. 5.3. First, in Sect. 5.4.1 we display examples of application to two-dimensional (cylindrical) geometries; fully three-dimensional results are then presented in Sect. 5.4.2.

5.4.1 Two-Dimensional Simulations

Our first example, in Table 5.1, relates to single-scattering calculations for a circular cylinder of radius a . The tables display results corresponding to (1) the use of localized integration domains around target points of size $\varepsilon_{\text{ref}} = 600(ka)^{-1}$, that is, the size is approximately 95.5 wavelengths; and

Table 5.1. Solution of the scattering problem for a circular cylinder of radius a ; from [14]

25 unknowns, $\varepsilon_{\text{ref}} = 600(ka)^{-1}$				100 Unknowns, $\varepsilon_{\text{ref}} = 3,000(ka)^{-1}$			
ka	# iter.	Rel. Error	CPU time (s)	ka	# iter.	Rel. error	CPU time
1	9	1.0e-12	<1	1	9	1.0e-12	<1 s
10	11	1.6e-4	<1	10	17	3.0e-11	5 s
100	13	9.3e-4	3	100	22	1.5e-5	11 s
1,000	13	8.3e-3	5	1,000	25	3.1e-5	2 m30 s
10,000	15	1.0e-2	6	10,000	27	8.4e-5	3 m12 s
1,00,000	14	1.1e-2	6	1,00,000	30	8.8e-5	3 m43 s

(2) integration domains that are five times larger, or about 477.5 wavelengths (around stationary points the domains are, of course, of corresponding size $\varepsilon_{\text{ref}}^{1/2}$).

As the first part of the table demonstrates, the former parameters lead to a (mean-squared) error of about 1% throughout the frequency spectrum, in total computational times of no more than 6 seconds. The second part, in turn, shows that two additional digits of accuracy can be gained by suitably enlarging the integration regions, while keeping the computational times to under 4 min.

Similar considerations apply to the next example relating to the configuration in Fig. 5.13. The “exact solution” η to (5.11) (that is, a highly resolved numerical solution based on a standard spectral Nystrom approach) is depicted in Fig. 5.14. Figures 5.13a,b display grids that correspond to prescribed errors of 10^{-3} and 10^{-4} for $k = 600$ ($\lambda \approx \text{Perimeter}/900$) respectively; note that the latter requires a deeper incursion into the shadowed zone (as well as wider localized integration intervals). The corresponding slow envelopes and relative errors as computed from the present high-frequency integral-equation

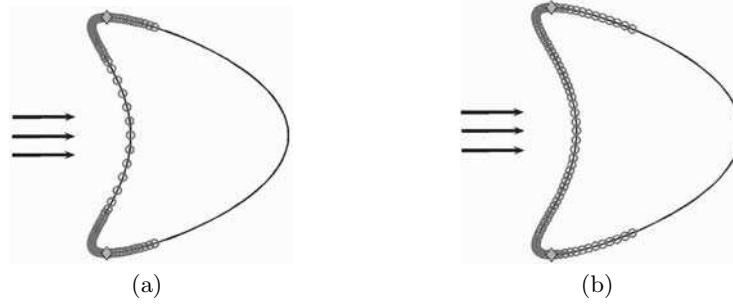


Fig. 5.13. A two-dimensional single-scattering configuration and computational grids for a wavelength $\lambda \approx \text{perimeter}/900$. (a) Grid for a maximum error tolerance of 10^{-3} ; and (b) corresponding grid for a maximum error of 10^{-4} (see Figs. 5.15 and 5.16)

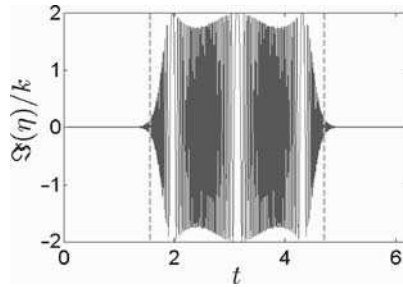


Fig. 5.14. Imaginary part of the surface density η (cf. (5.11)) for the configuration of Fig. 5.13; the *dashed lines* depict the location of the shadow boundaries

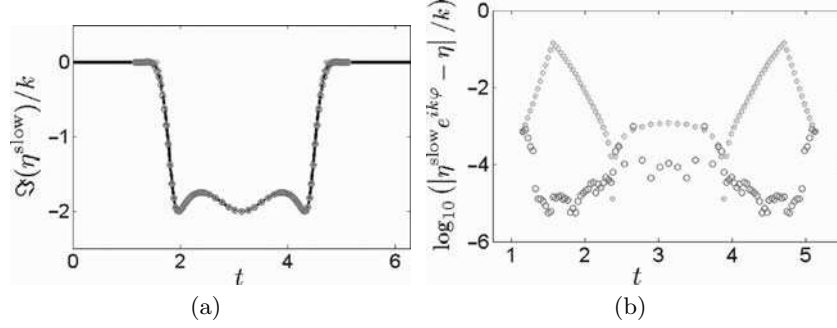


Fig. 5.15. Solution of the scattering problem for the configuration of Fig. 5.13a: (a) imaginary part of the slow density η^{slow} (cf. (5.19)) as computed from the “exact solution” (*black*), the numerical solution (*red*) and the PO approximation (*green*); and (b) errors for the numerical solution (*red*) and those for the PO approximation (*green*)

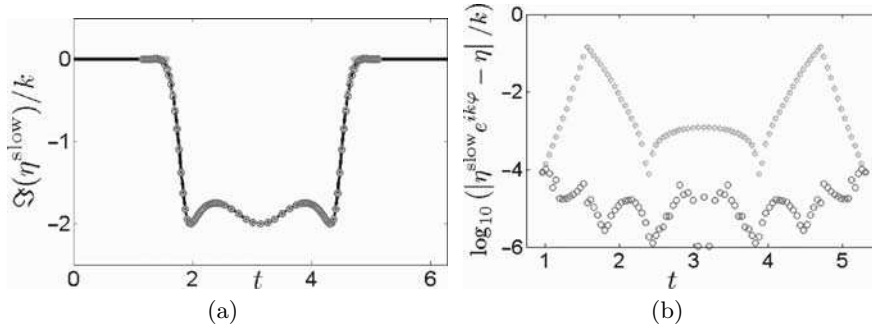


Fig. 5.16. Solution of the scattering problem for the configuration of Fig. 5.13b: (a) imaginary part of the slow density η^{slow} (cf. (5.19)) as computed from the “exact solution” (*black*), the numerical solution (*red*) and the PO approximation (*green*); and (b) errors for the numerical solution (*red*) and those for the PO approximation (*green*)

method are contrasted with those derived from the physical optics (PO) approximation in Figs. 5.15 and 5.16.

The final examples in this section relate to multiple-scattering configurations. First, we present results for the non-convex, disconnected geometry of Fig. 5.17. Figure 5.18 displays the iterated currents $\eta_{\tau_0, \dots, \tau_{m-1}, \tau_m}$ from (5.30), the slow envelopes $\eta_{\tau_0, \dots, \tau_{m-1}, \tau_m}^{\text{slow}}$ defined as in (5.34) and the phases $\varphi_{\tau_0, \dots, \tau_{m-1}, \tau_m}$ in (5.31) evaluated on K_0 and corresponding to $m = 0$, $m = 5$ and $m = 20$ reflections. The plots confirm the slow character of the phase-extracted currents, and they clearly depict the corresponding boundary layers. As described in Sect. 5.3.2 these iterated slowly varying envelopes can be evaluated in frequency-independent computational times using the methodology

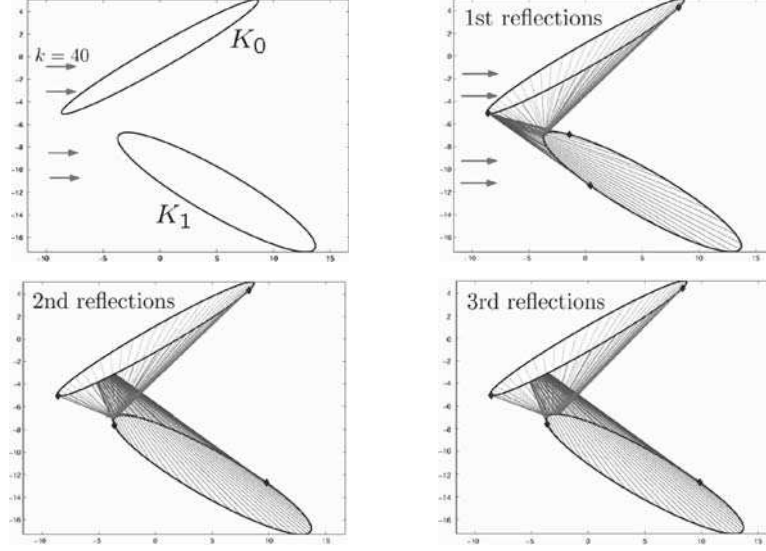


Fig. 5.17. A multiple scattering configuration, and first few geometrical optics reflections

described in Sect. 5.3.1. The approximations to the true current on K_0 that result from partial sums of the iterates (cf. (5.28)) and the corresponding (maximum) errors are displayed in Fig. 5.19.

Still relating to the configuration of Fig. 5.17, in Fig. 5.20 we display results corresponding to the rate of convergence of multiple scattering iterations for this particular case. The figure shows plots of the error

$$\text{Error} = \max_{x \in K_{\tau_m}} \left| \frac{\eta_{\tau_0, \dots, \tau_{2m-2}, \tau_{2m-1}, \tau_{2m}}(x)}{\eta_{\tau_0, \dots, \tau_{2m-2}}(x)} - \mathcal{R}_\infty(k) \right| \quad (5.43)$$

as a function of the reflection number m and the wavenumber k . Here $\Phi_2 \approx 3.396231$ and

$$\frac{1}{\sqrt{\mathcal{L}_1 \mathcal{L}_2}} \approx 0.207786$$

so that, from (5.38), we have

$$\mathcal{R}_\infty(k) = 0.207786 e^{3.396231 i k}.$$

Note that the exponential and linear convergence in m and k respectively are in precise agreement with the estimate in (5.37).

The last two-dimensional example is concerned with a connected, non-convex obstacle under an incidence that generates multiple scattering; see Figure 5.21. The figure displays a grid for a computation at wavenumber $k = 1,200$ ($\lambda \approx \text{Perimeter}/1,800$) and a relative error of less than 1%, and the

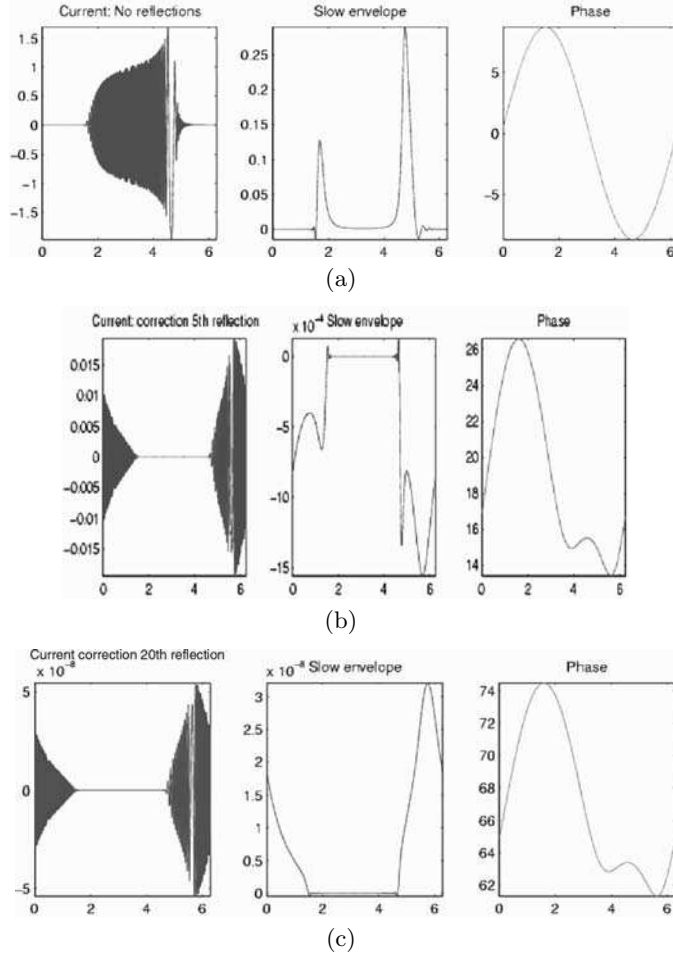


Fig. 5.18. Iterated currents $\eta_{\tau_0, \dots, \tau_{m-1}, \tau_m}$ (left column, cf. (5.30)), slow envelopes $\eta_{\tau_0, \dots, \tau_{m-1}, \tau_m}^{\text{slow}}$ (middle column, cf. (5.34)) and phases $\varphi_{\tau_0, \dots, \tau_{m-1}, \tau_m}$ (right column, cf. (5.31)) on K_0 for the configuration of Fig. 5.17. Top, middle and bottom rows correspond to $m = 0$, $m = 5$ and $m = 20$, respectively

rays and shadow boundaries for the first reflection. Note that the nature of the shadow boundaries SB_j^1 at the first reflection is largely similar to that of SB_j^0 at the zeroth reflection, since they both correspond to grazing rays on a curved surface. The characteristics of the shadow boundary point P , however, are rather distinct as this point arises as a consequence of a “folding” of the illuminating rays. Indeed, as can be verified, a particular consequence of this different behavior relates to the length-scale of the shadowing transition which, in this case, scales like $\lambda^{1/2}$ (rather than $\lambda^{1/3}$, cf. Sect. 5.3.1 and Fig. 5.7).

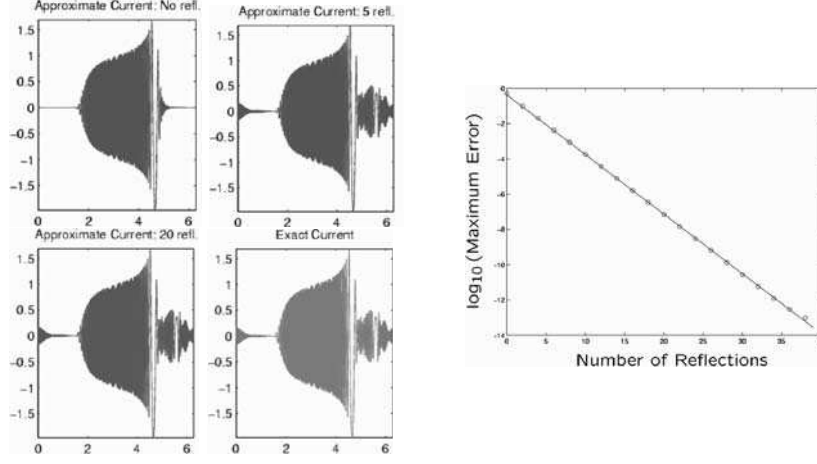


Fig. 5.19. Approximate currents at $m = 0, 5$ and 20 reflections, and maximum errors for the example in Figs. 5.17 and 5.18

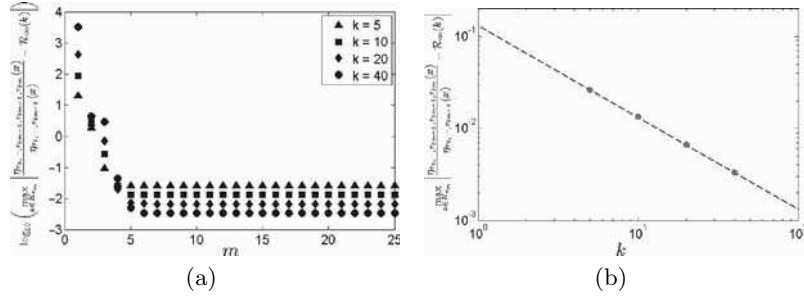


Fig. 5.20. Error (5.43) as a function of m and k for the configuration of Fig. 5.17. The *dashed line* in figure (b) has precisely unit slope

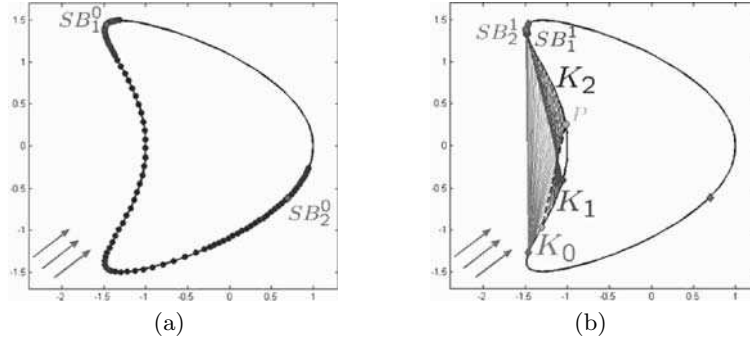


Fig. 5.21. A connected non-convex obstacle under oblique illumination. (a) Grid for solution of the integral equation for $k = 1,200$; the *diamonds* indicate the location of the shadow boundaries SB_j^0 for the zeroth reflection (i.e. corresponding to the plane-wave incidence). (b) Rays and shadow boundaries corresponding to the first reflection; rays emanating from the domains K_0 and K_1 jointly illuminate K_2

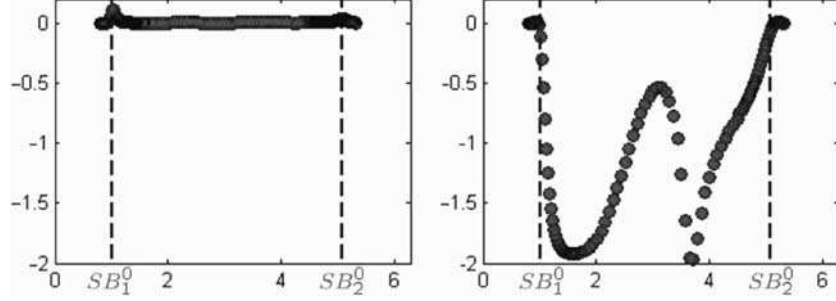


Fig. 5.22. Real (*left*) and imaginary (*right*) parts of the the zeroth order approximation to the (slow envelope of the) induced current, generated in response to the incident radiation for the configuration of Fig. 5.21a with $k = 1200$

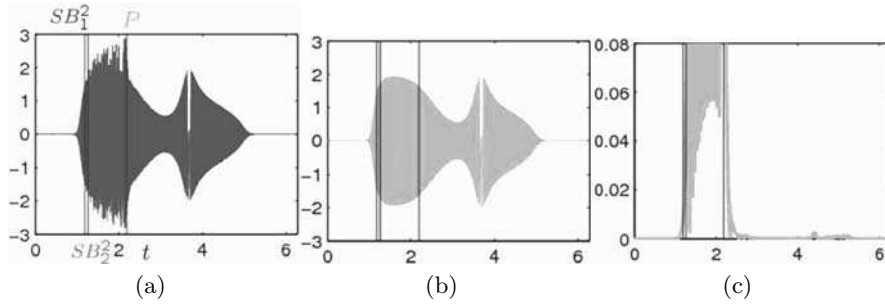


Fig. 5.23. (a) “Exact” (i.e. fully resolved) surface current corresponding to the configuration of Fig. 5.21. (b) Approximation to the current using the slow envelope for the zeroth reflection, cf. Fig. 5.22. (c) Relative error between the functions depicted in (a) and (b), showing that the approximation is accurate precisely outside of the domains affected by multiple-scattering effects

In Fig. 5.22 we show the results of the evaluation, on the grid depicted in Fig. 5.21a, of the zeroth order approximation to the (slow envelope of the) induced current that is generated in response to the incident radiation. Note that the possibility of isolating this contribution to the current is largely due to the localized integration strategy described in Sect. 5.3.1, as this allows us to integrate *only* in the vicinity of critical points of the phase (5.22). Figure 5.23, in turn, shows a comparison of the “exact” (i.e. fully resolved) density with that resulting from the slow envelope in Fig. 5.22. The accuracy of the approximation is evidenced here by the clear resolution of shadowing layers (see e.g. Fig. 5.22a) and, more generally, by the smallness of the errors throughout the areas that do not receive geometrical ray reflections; see Figure 5.23c. This latter figure also clearly demonstrates the need to incorporate multiple scattering effects in the domain K_2 (cf. Fig. 5.21b) wherein reflected rays do arrive.

In order to evaluate these effects, and following the strategy delineated in Sect. 5.3.2, we need to first compute the (normal derivative of) the incident fields in the right-hand side of (5.35). More precisely, we evaluate

$$\rho_0^{\text{slow}} = e^{-ik\varphi_1^0(x)} \int_{K_0} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_0^{\text{slow}}(y) e^{ik\varphi_0(y)} ds(y) \quad (5.44)$$

and

$$\rho_1^{\text{slow}} = e^{-ik\varphi_1^1(x)} \int_{K_1} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_0^{\text{slow}}(y) e^{ik\varphi_0(y)} ds(y) \quad (5.45)$$

where $\varphi_0(y) = \alpha \cdot y$ is the phase of the incident radiation, $\eta_0^{\text{slow}}(y)$ is the current generated at the zeroth reflection (cf. Fig. 5.22), and $\varphi_1^j(x)$ denote the (first reflection) phases on K_2 that result from rays emanating from K_j for $j = 0, 1$ (see Fig. 5.21b); plots of ρ_j^{slow} are presented in Fig. 5.24.

Finally the solution of the problems (5.35) corresponding to each of these incidences can be derived in frequency-independent computational times with the methods presented in Sect. 5.3.1. The resulting slow envelopes $\eta_1^{\text{slow},j}$ for $j = 0, 1$ are displayed in Fig. 5.25a,b. Figure 5.26b, in turn, displays the full (oscillatory) current derived from the sum of contributions from the zeroth and first reflections, and Fig. 5.26c shows the error incurred by the approximation

$$\eta(x) \approx \eta_0^{\text{slow}}(x) e^{ik\varphi_0(x)} + \eta_1^{\text{slow},0}(x) e^{ik\varphi_1^0(x)} + \eta_1^{\text{slow},1}(x) e^{ik\varphi_1^1(x)}.$$

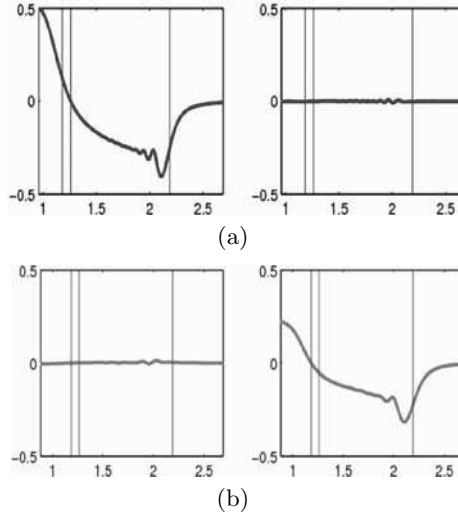


Fig. 5.24. Real (*left*) and imaginary (*right*) parts of the incident fields (5.44), (5.45) generated by the zeroth reflection which constitute the source of illumination for the first reflection. **(a)** and **(b)** correspond to the incident fields generated by the current in the domains K_0 and K_1 , respectively

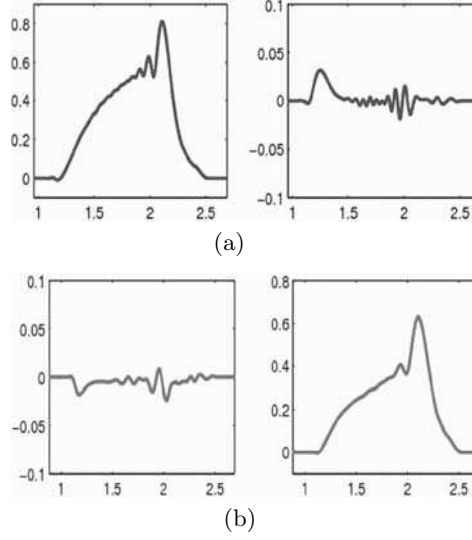


Fig. 5.25. Real (*left*) and imaginary (*right*) parts of the (slow envelopes of the) currents generated at the first reflection by the incidence in Fig. 5.24. (a) and (b) correspond to the densities in K_2 generated by incidences emanating from K_0 and K_1 , respectively

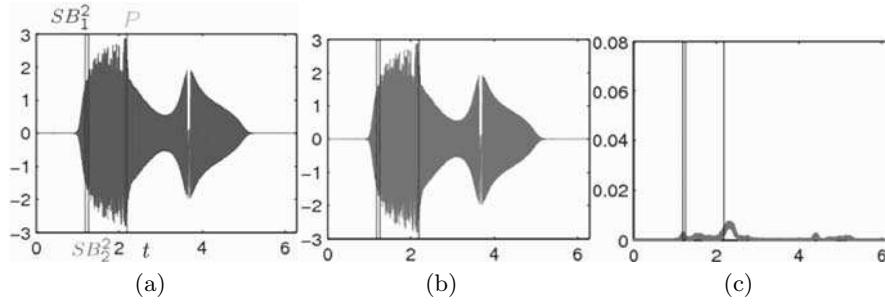


Fig. 5.26. (a) “Exact” (i.e. fully resolved) surface current corresponding to the configuration of Fig. 5.21. (b) Approximation to the current using the sum of contributions from the zeroth and first reflections. (c) Relative error between the functions depicted in (a) and (b), showing that the approximation is accurate throughout the surface of the scatterer

5.4.2 Three-Dimensional Simulations

The first three-dimensional example illustrates our high-frequency integral-equation approach in the case where an infinite (periodic) rough surface is illuminated in its entirety. As discussed in Sect. 5.3.1, in this case an explicit recurrence for the terms η_n^{slow} in (5.20) can be derived from the integral equation through asymptotic evaluations that rely on the fact that, in such instances,

the only critical point y for any fixed target point x is $y = x$ itself [18, 44, 45]. The results we present here [45] correspond to the profile

$$x_3 = f(x_1, x_2) = 3.4 \times 10^{-3} \times \left(\cos(2\pi x_1) + \frac{1}{4} \cos(4\pi x_1) + \frac{1}{6} \sin(6\pi x_1) \right) \\ \times \left(\cos(2\pi x_2) + \cos(4\pi x_2) \right) \quad (5.46)$$

(see Fig. 5.27) and to a solution of the full Maxwell equations. Table 5.2 displays the relative errors incurred by our approximations, up to order ten, in the some illustrative efficiencies $e_{(r,s)}$, along with the corresponding energy defects

$$\varepsilon = \left| 1 - \sum_{(r,s) \text{ is propagating}} e_{(r,s)} \right|.$$

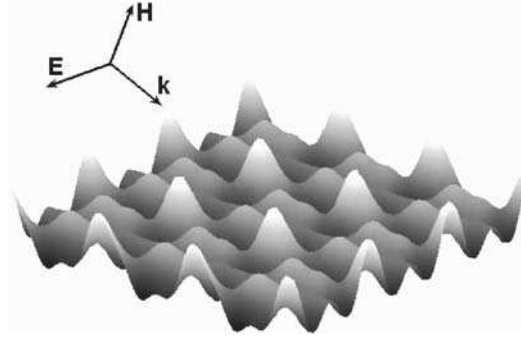


Fig. 5.27. The infinite rough surface (5.46) under H-polarized, high-frequency illumination; cf. Table 5.2

Table 5.2. Efficiencies and relative errors as computed through the recursive evaluation of the series in (5.20)

Efficiency	Scattered energy	Order 0	Order 1	Order 3	Order 5	Order 10
(0,0)	0.2168524774056718e-00	3.67e-04	5.21e-06	1.27e-07	3.13e-09	1.51e-11
(1,0)	0.2163867201690774e-01	2.89e-04	8.52e-06	1.71e-07	9.98e-10	1.11e-11
(1,1)	0.3014199854789860e-01	1.59e-03	1.99e-05	7.13e-08	3.72e-09	4.35e-12
(1,2)	0.2763092444554548e-01	3.44e-04	1.22e-05	2.78e-07	8.41e-09	9.16e-12
(2,2)	0.4699008279945933e-03	3.81e-03	2.35e-04	3.31e-06	1.75e-08	5.59e-11
(2,4)	0.2901776163762193e-03	9.75e-05	1.40e-04	2.50e-06	1.06e-08	7.54e-11
ε	2.05e-15	1.23e-06	4.62e-09	3.33e-12	9.44e-15	6.96e-15

Results for a full electromagnetic calculation (H polarization, incident wavelength $\lambda = 2.1 \times 10^{-2}$ and incidence angles $\Psi = 30^\circ$, $\Phi = 10^\circ$) for the scattering surface in (5.46) (cf. Fig. 5.27); from [45]

The “exact” results were computed with an alternative scheme, the “Method of Variation of Boundaries” [17], that is known to be highly accurate in the “resonance regime” $h \approx \lambda$. The results illustrate the rapid convergence of the overall scheme and the significant improvements over the classical Kirchhoff approximation (corresponding to “Order 0” in the table) that can thus be attained at a very modest additional computational cost.

For the case of a bounded three-dimensional obstacle wherein shadowing cannot be avoided, we present results corresponding to the spherical configuration of Fig. 5.28. Table 5.3 gives the error on the computation of the integral in the high-frequency boundary integral formulation (5.19) for a target point in the shadow region, close to the shadow boundary; see Fig. 5.28a. As shown in Fig. 5.28b, this is a challenging case wherein the associated cutoff functions for localized integration overlap in non-trivial ways. The left part of the table summarizes the results with a windowing function size of $\varepsilon_{\text{ref}} = 500 (ka)^{-1}$, with coarse Cartesian grids of 32×16 points in each of two parameterization patches covering the sphere. Accuracies of about 1% are obtained from $ka = 1,000$ to $ka = 16,000$, in computing times of less than one second on a single 1.5 GHz AMD Athlon processor; note that both the accuracies and the

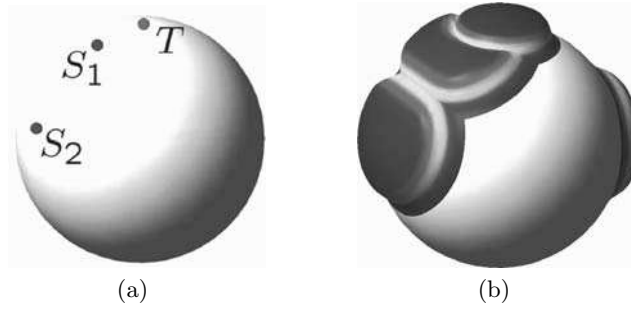


Fig. 5.28. (a) Stationary points S_j corresponding to a fixed target point T for plane wave incidence on a sphere; and (b) corresponding windowing functions for localized integration

Table 5.3. Integration of the exact solution on a sphere of radius a centered at the origin, with the target point T in the shadow region ($\alpha = (1, 0, 0)$, $T \approx a(-0.9, -0.27, -0.36)$); from [13]

$16 \times 32 \times 2$ points, $\varepsilon_{\text{ref}} = 500 (ka)^{-1}$			$32 \times 64 \times 2$ points, $\varepsilon_{\text{ref}} = 1000 (ka)^{-1}$		
ka	Rel. error	CPU time (s)	ka	Rel. error	CPU time (s)
1,000	7.123e-03	0.8	1,000	8.888e-03	2.1
2,000	1.213e-02	0.8	2,000	2.589e-03	1.8
4,000	2.501e-02	0.8	4,000	2.984e-03	1.8
8,000	1.372e-02	0.8	8,000	1.268e-03	1.8
16,000	1.969e-02	0.8	16,000	2.211e-03	1.8

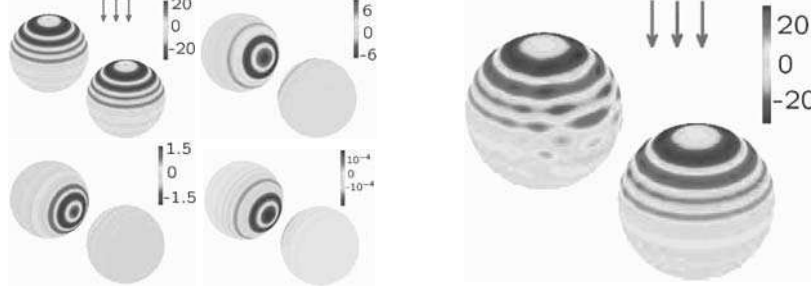


Fig. 5.29. A three-dimensional multiple-scattering configuration composed of two unit spheres separated by a unit distance, illuminated by a plane wave incidence with $k = 16$. *Left:* iterated surface currents $\eta_{\tau_0, \dots, \tau_m}$ for $m = 0, 1, 2, 10$. *Right:* full approximation obtained from the sum of the contributions from the first ten reflections

computational times are independent of frequency. The right part of Table 5.3 shows the results obtained for the same integration problem, but with the size of the reference windowing functions doubled, and with coarse Cartesian grids of 64×32 points; accuracies of about 10^{-3} are obtained throughout the frequency spectrum, in computing times of less than 2 s. Preliminary results from the full implementation of the high-frequency scattering solver for an acoustically soft sphere with $ka = 1,600$ (≈ 500 wavelengths) lead to a relative error on the unknown surface density of 2% in less than 3 h on a 1.5 GHz personal computer [13].

Finally, we present multiple scattering results relating to configurations composed of spheres and ellipsoids. First, for two unit spheres separated by a unit distance, in Fig. 5.29 we display the iterated currents $\eta_{\tau_0, \dots, \tau_m}$ for $m = 0, 1, 2, 10$ as well as the full approximation obtained from the sum of the first ten iterates for a case of plane wave incidence with $k = 16$. In particular, the figure shows that, once stabilized, the induced current for successive reflections can be well approximated by a simple scaling of that corresponding to previous iterations, the factor being given by the rate $\mathcal{R}_\infty(k)$ in (5.41). A further numerical verification of this rate is provided in Table 5.4, where the values of

$$\max |\eta_{\tau_0, \dots, \tau_{2m}}| / \max |\eta_{\tau_0, \dots, \tau_{2m-2}}| \quad \text{on } K_0 \quad (5.47)$$

are displayed for the configurations of Fig. 5.30, for increasing m and k . The tables evidence, again, the stabilization of the currents as m increases for each fixed wavenumber, which implies in particular that the ratios in (5.47) should converge to $|\mathcal{R}_\infty(k)|$ as $k \rightarrow \infty$. As it follows from (5.41) the latter values are independent of k and, in this case, they are

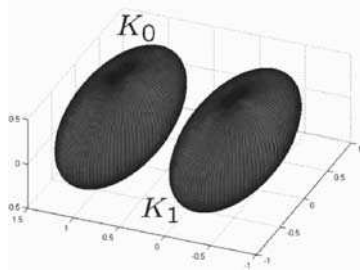
$$|\mathcal{R}_\infty(k)| = 0.2329 \text{ for the parallel ellipsoids and} \quad (5.48)$$

$$|\mathcal{R}_\infty(k)| = 0.2208 \text{ when they are perpendicular} \quad (5.49)$$

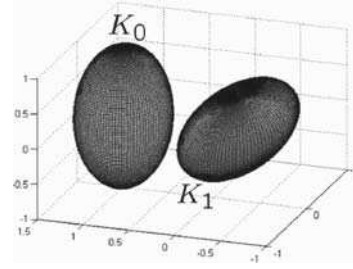
which clearly display the effect of the rotation matrix U in (5.42).

Table 5.4. Values of $\max |\eta_{\tau_0, \dots, \tau_{2m}}| / \max |\eta_{\tau_0, \dots, \tau_{2m-2}}|$ on K_0 for increasing reflection number m and wavenumber k for the configurations of Fig. 5.30. The asymptotic rates $\mathcal{R}_\infty(k)$ have magnitudes 0.2329 for the parallel ellipsoids and 0.2208 when they are perpendicular; from [5]

(a) Parallel ellipsoids						(b) Perpendicular ellipsoids					
m	$k = 4$	$k = 8$	$k = 16$	$k = 32$	$k = 64$	m	$k = 4$	$k = 8$	$k = 16$	$k = 32$	$k = 64$
1	0.4251	0.3393	0.2922	0.2665	0.2542	1	0.2945	0.2570	0.2287	0.2087	0.1970
2	0.2918	0.2665	0.2548	0.2502	0.2488	2	0.2777	0.2533	0.2417	0.2378	0.2357
3	0.2691	0.2499	0.2403	0.2366	0.2357	3	0.2536	0.2357	0.2270	0.2232	0.2221
4	0.2661	0.2475	0.2381	0.2346	0.2337	4	0.2519	0.2341	0.2253	0.2222	0.2211
5	0.2657	0.2472	0.2378	0.2343	0.2335	5	0.2518	0.2340	0.2252	0.2221	0.2210
6	0.2657	0.2471	0.2377	0.2343	0.2335	6	0.2518	0.2340	0.2252	0.2220	0.2210
7	0.2657	0.2471	0.2377	0.2343	0.2335	7	0.2518	0.2340	0.2252	0.2220	0.2210
8	0.2657	0.2471	0.2377	0.2343	0.2335	8	0.2518	0.2340	0.2252	0.2220	0.2210



(a)



(b)

Fig. 5.30. Geometric configurations for the multiple scattering experiments in Table 5.4

5.5 Conclusions

In this chapter we have reviewed the basic ideas behind a novel approach to the solution of high-frequency scattering problems that enables the evaluation of scattering returns within any prescribed accuracy in times that do not depend upon the frequency of radiation. The approach is based on the rigorous solution of integral-equation formulations of the problem which are accelerated through the incorporation of asymptotic high-frequency information and suitably localized integration procedures. Through an array of numerical examples from two- and three-dimensional (scalar and vector) implementations of the resulting schemes we have shown that the ideas reviewed here lead to simulations that entail computational times that are comparable to those associated with the solution of asymptotic models (e.g. geometrical optics) while retaining the rigor and error-controllability of full-wave evaluations.

References

- [1] Abboud, T., Nédélec, J.-C., Zhou, B.: Méthode des équations intégrales pour les hautes fréquences, C. R. Acad. Sci. Paris **318** (1994), 165–170.
- [2] Aberegg, K.R., Peterson, A.F.: Application of the integral equation asymptotic phase method to two-dimensional scattering. IEEE Trans. Antennas Propagat. **43** (1995), 534–537.
- [3] Abgrall, R., Benamou, J.-D.: Big ray tracing and eikonal solver on unstructured grids: Application to the computation of a multivalued traveltime field in the Marmousi model, Geophysics **64** (1999), 230–239.
- [4] Amini, S., Profit, A.: Multi-level fast multipole solution of the scattering problem. Engineering Analysis with Boundary Elements, **27** (2003), 547–564.
- [5] Anand, A., Boubendir, Y., Ecevit, F., Reitich, F.: Analysis of multiple scattering iterations for high-frequency scattering problems. II: The three-dimensional scalar case, Max Planck Institute for Mathematics in the Sciences, Preprint 147 (2006), 1–27.
- [6] Anand, A., Bruno, O.P., Reitich, F.: A spectral geometrical optics solver based on inverse ray tracing, in preparation.
- [7] Andersh, D., Moore, J., Kosanovich, S., Kapp, D., Bhalla, R., Kipp, R., Courtney, T., Nolan, A., German, F., Cook, J., Hughes, J.: Xpatch 4: The next generation in high frequency electromagnetic modeling and simulation software, IEEE National Radar Conference – Proceedings (2000), 844–849.
- [8] Banjail, L., Hackbusch, W.: H - and H^2 -matrices for low and high frequency Helmholtz equation, Max Planck Institute für Mathematik in den Naturwissenschaften Preprint **17** (2005), 1–22.
- [9] Benamou, J.-D., Direct computation of multivalued phase space solutions for Hamilton-Jacobi equations, Comm. Pure Appl. Math. **52** (1999), 1443–1475.
- [10] Bleistein, N., Handelsman, R.A., *Asymptotic Expansions of Integrals* (Dover, New York, 1986).
- [11] Bleszynski, E., Bleszynski, M., Jaroszewicz, T.: AIM: Adaptive integral method for solving large-scale electromagnetic scattering and radiation problems, Radio Sci. **31** (1996), 1225–1251.
- [12] Bouche, D., Molinet, F., Mittra, R.: *Asymptotic Methods in Electromagnetics* (Springer-Verlag, 1997).
- [13] Bruno, O.P., Geuzaine, C.A.: An integration scheme for three-dimensional surface scattering problems, J. Comput. Appl. Math., to appear.
- [14] Bruno, O.P., Geuzaine, C.A., Monro, J.A., Reitich F.: Prescribed error tolerances within fixed computational times for scattering problems of arbitrarily high frequency: the convex case, Phil. Trans. Roy. Soc. London **362** (2004), 629–645.

- [15] Bruno, O.P., Geuzaine, C.A., Reitich, F.: On the $\mathcal{O}(1)$ solution of multiple-scattering problems, *IEEE Trans. Magn.* **41** (2005), 1488–1491.
- [16] Bruno, O.P., Kunyansky, L.A.: A fast, high-order algorithm for the solution of surface scattering problems: basic implementation, tests and applications, *J. Comp. Phys.* **169** (2001), 80–110.
- [17] Bruno, O.P., Reitich, F.: Numerical solution of diffraction problems: a method of variation of boundaries. III. Doubly periodic gratings, *Journal Opt. Soc. Am. A* **10** (1993), 2551–2562.
- [18] Bruno, O.P., Sei, A., Caponi, M.: High-order high-frequency solutions of rough surface scattering problems, *Radio Sci.* **37** (2002), 2/1–2/13.
- [19] Charnotskii, M.I., Tatarskii, V.I.: Tilt-invariant theory of rough-surface scattering: I, *Waves Random Media* **5** (1995), 361–380.
- [20] Chen, M.-H., Cockburn, B., Reitich, F.: High-order RKDG methods for computational electromagnetics, *J. Sci. Comput.* **22** (2005), 205–226.
- [21] Cockburn, B., Kao, C.-Y., Reitich, F.: Scattering and adaptivity within a spectral-discontinuous Galerkin method for Eulerian geometrical optics simulations, in preparation.
- [22] Cockburn, B., Qian, J., Reitich, F., Wang, J.: An accurate spectral/discontinuous finite-element formulation of a phase-space-based level set approach to geometrical optics, *J. Comput. Phys.* **208** (2005), 175–195.
- [23] Cockburn, B., Shu, C.-W.: The Runge-Kutta discontinuous Galerkin finite element method for conservation laws V: Multidimensional systems, *J. Comput. Phys.* **141** (1998), 199–224.
- [24] Cockburn, B., Shu, C.-W.: Runge-Kutta discontinuous Galerkin methods for convection-dominated problems, *J. Sci. Comput.* **16** (2001), 173–261.
- [25] Chew, W.C., Song, J.M., Cui, T.J., Velamparambil, S., Hastriter, M.L., Hu, B.: Review of large scale computing in electromagnetics with fast integral equation solvers, *CMES Comput. Model. Eng. Sci.* **5** (2004), 361–372.
- [26] Colton, D., Kress, R.: *Inverse Acoustic and Electromagnetic Scattering Theory* (Springer-Verlag, Berlin, 1992).
- [27] Crandall, M.G., Lions, P.-L.: Viscosity solutions of Hamilton-Jacobi equations, *Trans. Amer. Math. Soc.* **277** (1983), 1–42.
- [28] Cullen, J.A.: Surface currents induced by short-wavelength radiation, *Phys. Rev. B* **109** (1958), 1863–1867.
- [29] Ecevit, F., Reitich, F.: Analysis of multiple scattering iterations for high-frequency scattering problems. I: The two-dimensional case, *Max Planck Institute for Mathematics in the Sciences*, Preprint 137 (2006), 1–37.
- [30] Engquist, B., Runborg, O.: Computational high frequency wave propagation, *Acta Numerica* (2003), 181–266.
- [31] Fock, V.: *Electromagnetic diffraction and propagation problems* (Pergamon Press, London, 1965).

- [32] Fatemi, E., Engquist, B., Osher, S.J.: Numerical solution of the high frequency asymptotic expansion for the scalar wave equation, *J. Comput. Phys.* **120** (1995), 145–155.
- [33] Gottlieb, S., Shu, C.-W., Tadmor, E.: Strong stability preserving high order time discretization methods, *SIAM Rev.* **43** (2000), 89–112.
- [34] Hassan, O., Morgan, K., Jones, J., Larwood, B., Weatherill, N.P.: Parallel 3D time domain electromagnetic scattering simulations on unstructured meshes, *CMES Comput. Model. Eng. Sci.* **5** (2004), 383–394.
- [35] Hesthaven, J.S., T. Warburton, T.: High-order accurate methods for time-domain electromagnetics, *CMES Comput. Model. Eng. Sci.* **5** (2004), 395–408.
- [36] James, R.M.: A contribution to scattering calculation for small wavelengths - the high frequency panel method. *IEEE Trans. Antennas and Propagat.* **38** (1990), 1625–1630.
- [37] Keller, J., Lewis, R.: *Asymptotic methods for partial differential equations: The reduced wave equation and Maxwell's equations*, *Surv. Appl. Math.* **1** (1995), 1–82.
- [38] Lynch, P.J.: Curvature corrections to rough-surface scattering at high frequencies , *J. Acoust. Soc. Am.* **47** (1970), 804–815.
- [39] Melrose, R.B., Taylor, M.E.: Near peak scattering and the corrected Kirchhoff approximation for a convex obstacle. *Adv. in Math.* **55** (1985), 242–315.
- [40] Namburu, R.R., Mark, E.R., Clarke, J.A.: Scalable electromagnetic simulation environment, *CMES Comput. Model. Eng. Sci.* **5** (2004), 443–453.
- [41] Osher, S., Cheng, L.-T., Kang, M., Shim, H., Tsai, Y.-H.: Geometric optics in a phase-space-based level set and Eulerian framework, *J. Comput. Phys.* **179** (2002), 622–648.
- [42] Perrey-Debain, E., Trevelyan, J., Bettess, P.: Use of wave boundary elements for acoustic computations, *J. Comput. Acoust.* **11** (2003), 305–321.
- [43] Reitich, F., Tamma, K.K.: State-of-the-art, trends and directions in Computational Electromagnetics, *CMES Comput. Model. Eng. Sci.* **5** (2004), 287–294.
- [44] Reitich, F., Turc C.: High-order solutions of three-dimensional rough-surface scattering problems at high-frequencies. I: the scalar case, *Waves Random and Complex Media* **15** (2005), 1–16.
- [45] Reitich, F., Turc C.: High-order solutions of three-dimensional rough-surface scattering problems at high-frequencies. II: the vector electromagnetic case, *Waves Random and Complex Media* **15** (2005), 323–337.
- [46] Rieben, R.N., Rodrigue, G.H., White, D.A.: A high order mixed vector finite element method for solving the time dependent Maxwell equations on unstructured grids, *J. Comput. Phys.* **204** (2005), 490–519.
- [47] Rodriguez, E.: Beyond the Kirchhoff approximation *Radio Sci.* **24** (1989), 681–693.

- [48] Saad, Y., Schultz, M.H.: GMRES: a generalized minimal residual algorithm for solving nonsymmetric linear systems, *SIAM J. Sci. Stat. Comput.* **7** (1986) 857–869.
- [49] Sherer, S.E., Visbal, M.R.: Time-domain scattering simulations using a high-order overset-grid approach, in *Proc. 2005 IEEE Workshop on Computational Electromagnetics in the Time-Domain*, 44–47.
- [50] Symes, W.W., Qian, J.: A slowness matching Eulerian method for multi-valued solutions of eikonal equations, *J. Sci. Comp.* **19** (2003), 501–526.
- [51] van Trier, J., Symes, W.W.: Upwind finite-difference calculation of traveltimes, *Geophysics* **56** (1991), 812–821.
- [52] Vidale, J.: Finite-difference calculation of traveltimes, *Bull. Seism. Soc. Amer.* **78** (1988), 2062–2076.
- [53] Voronovich, A.G.: *Wave Scattering from Rough Surfaces* (Springer-Verlag, New York, 1994).

Recent Studies on Inverse Medium Scattering Problems

G. Bao, S. Hou, and P. Li

6.1 Introduction

Consider the Helmholtz equation in two dimensions,

$$\Delta\varphi(\mathbf{x}) + \kappa^2(1 + q(\mathbf{x}))\varphi(\mathbf{x}) = 0, \quad \mathbf{x} \in \mathbb{R}^2, \quad (6.1)$$

where φ is the total field, κ is a positive real number, known as the wavenumber, and the scatterer q is a function with $q(\mathbf{x}) > -1$ for all $\mathbf{x} \in \mathbb{R}^2$. The function q is assumed to be supported in a bounded domain $\Omega \subset \mathbb{R}^2$, as shown in Fig. 6.1.

Denote the wave vector $\mathbf{k} = (\eta, k(\eta))$, where η is the transverse part of the wave vector and

$$k(\eta) = \begin{cases} \sqrt{\kappa^2 - \eta^2} & \text{for } \kappa > |\eta|, \\ i\sqrt{\eta^2 - \kappa^2} & \text{for } \kappa < |\eta|. \end{cases}$$

The number $|\eta|$ is known as the spatial frequency.

The scatterer is illuminated by a one-parameter family of plane waves

$$\varphi_0(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}}. \quad (6.2)$$

The modes for which $|\eta| \leq \kappa$ correspond to propagating plane waves while the modes with $|\eta| > \kappa$ correspond to evanescent plane waves. For propagating waves, we explicitly have by letting $\eta = \kappa \cos \alpha$ and $k(\eta) = \kappa \sin \alpha$ that

$$\varphi_0(\mathbf{x}) = e^{i\kappa \mathbf{d} \cdot \mathbf{x}}. \quad (6.3)$$

Here $\mathbf{d} = (\cos \alpha, \sin \alpha)$ denotes the propagation direction. For evanescent waves, we explicitly have

$$\varphi_0(\mathbf{x}) = e^{i\eta x_1 - \sqrt{\eta^2 - \kappa^2} x_2}. \quad (6.4)$$

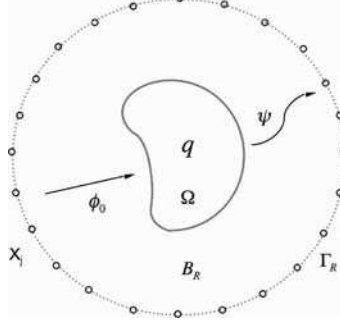


Fig. 6.1. The problem geometry. For a plane wave φ_0 incident on the scatterer q , the scattered wave ψ is measured at $\mathbf{x}_j, j = 1, \dots, m$

These waves are oscillatory parallel to the x_1 axis and decay exponentially along the x_2 axis. The higher the spatial frequency of the evanescent plane waves used to probe the scatterer is, the more rapidly the field decays as a function of depth into the scatterer. It is well known that the high spatial frequency evanescent plane waves may be generated at the interface of two media by total internal reflection [11, 16], which has been in practical use for decades, especially in near-field optics [24]. A recent review on the near-field optics and near-field microscopy may be found in [20]. Evidently, such incident waves satisfy the homogeneous equation

$$\Delta\varphi_0 + \kappa^2\varphi_0 = 0. \quad (6.5)$$

The total field φ takes the form

$$\varphi = \varphi_0 + \psi. \quad (6.6)$$

Here $\psi : \mathbb{R}^2 \mapsto \mathbb{C}$ is the scattered field which satisfies from (6.1), (6.5), and (6.6) that

$$\Delta\psi(\mathbf{x}) + \kappa^2(1 + q(\mathbf{x}))\psi(\mathbf{x}) = -\kappa^2q(\mathbf{x})\varphi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2, \quad (6.7)$$

and the Sommerfeld radiation condition

$$\lim_{r \rightarrow \infty} \sqrt{r} \left(\frac{\partial \psi}{\partial r} - i\kappa\psi \right) = 0, \quad r = |\mathbf{x}|, \quad (6.8)$$

uniformly along all directions $\mathbf{x}/|\mathbf{x}|$.

In this context, the *direct scattering problem* is to determine the scattered field ψ , given the incident field φ_0 and the scatterer q , which has been studied extensively over the last few decades [18, 32, 35]. To serve our general purpose, we restrict to the finite element method for solving the direct problem numerically. A crucial step is to truncate the infinite physical domain to a

bounded domain around the scatterer by introducing suitable artificial boundary conditions for the truncated domain. Based on the Dirichlet-to-Neumann map, a nonlocal transparent boundary condition is adopted for the finite element method. Using the Lax-Milgram lemma and the Fredholm alternative, the direct problem is shown in this survey to have a unique solution for all but possibly a discrete set of wavenumbers. Energy estimates for the scattered field are established, which provide criteria for the weak scattering. For the regularity of the scattered field, the reader is referred to [3]. The *inverse scattering problem* is to reconstruct the scatterer q from the measurements of the scattered field ψ at $\mathbf{x}_j, j = 1, \dots, m$, given the incident field φ_0 . The inverse problem arises naturally in diverse applications such as radar and sonar, geophysical exploration, medical imaging, and nondestructive testing [19, 33]. However, numerical solution of the inverse problem remains challenging for the following two principle reasons. The inverse problem is inherently nonlinear. From the point of view of numerical computations, the problem is also severely ill-posed. In particular, small variations in the measured data can lead to large errors in the reconstruction.

The goal of this chapter is to report our progress on regularized recursive linearization methods for solving the inverse problems for the Helmholtz equation with multiple and single frequency scattering data. The reader is referred to [5–7, 14, 15] for solving the inverse problems in the two-dimensional Helmholtz equation and the three-dimensional Maxwell equations in the case of full aperture data. In the limited aperture case, the reader is referred to [8] and [9] for homogeneous and more recently inhomogeneous background medium. Finally, due to the space limitation, no attempt has been made to cover other relevant approaches. We refer the reader to [21, 26, 34, 39] for related results on the inverse medium scattering problem. See [17, 19] for an account of recent scattering progress on the general inverse scattering problem.

The outline of this chapter is as follows. In Sect. 6.2, the variational problem for direct scattering is analyzed and energy estimates on the scattered field are given. Initial guesses of the reconstruction from the Born approximation or from a direct imaging algorithm are derived in Sect. 6.3. Regularized recursive linearization methods are presented in Sect. 6.4. Section 6.5 is devoted to the numerical study of the proposed methods. The survey is concluded with some general remarks and directions for future research in Sect. 6.6.

6.2 Analysis of the Direct Scattering

In this section, the variational formulation for the direct problem is discussed. The analysis provides some criteria for the weak scattering, which plays an important role in the inversion method.

Let the support of the scatterer Ω be contained in the interior of the ball $B_R = \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < R\}$ with boundary $\Gamma_R = \partial B_R$, as seen in Fig. 6.1. In

the domain $\mathbb{R}^2 \setminus \bar{B}_R$, the solution of (6.7), (6.8) can be written under the polar coordinates as follows:

$$\psi(r, \vartheta) = \sum_{n \in \mathbb{Z}} \frac{H_n^{(1)}(\kappa r)}{H_n^{(1)}(\kappa R)} \hat{\psi}_n e^{in\vartheta}, \quad (6.9)$$

where

$$\hat{\psi}_n = \frac{1}{2\pi} \int_0^{2\pi} \psi(R, \vartheta) e^{-in\vartheta} d\vartheta,$$

and $H_n^{(1)}$ is the Hankel function of the first kind with order n . To proceed, we introduce the following notation. For any function u defined on the circle Γ_R having the Fourier expansion:

$$u = \sum_{n \in \mathbb{Z}} \hat{u}_n e^{in\vartheta}, \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u e^{-in\vartheta} d\vartheta,$$

we define

$$\begin{aligned} \|u\|_{H^{1/2}(\Gamma_R)}^2 &= 2\pi \sum_{n \in \mathbb{Z}} (1+n^2)^{1/2} |\hat{u}_n|^2, \\ \|u\|_{H^{-1/2}(\Gamma_R)}^2 &= 2\pi \sum_{n \in \mathbb{Z}} (1+n^2)^{-1/2} |\hat{u}_n|^2. \end{aligned}$$

Let $\mathcal{T} : H^{1/2}(\Gamma_R) \rightarrow H^{-1/2}(\Gamma_R)$ be the Dirichlet-to-Neumann operator defined as follows: for any $u \in H^{1/2}(\Gamma_R)$,

$$\mathcal{T}u = \frac{1}{R} \sum h_n(\kappa R) \hat{u}_n e^{in\vartheta}, \quad (6.10)$$

where

$$h_n(z) = z \frac{H_n^{(1)'}(z)}{H_n^{(1)}(z)} \quad \text{and} \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u e^{-in\vartheta} d\vartheta.$$

The solution written as in (6.9) satisfies

$$\frac{\partial \psi}{\partial \mathbf{n}} = \mathcal{T}\psi \quad \text{on } \Gamma_R, \quad (6.11)$$

where $\mathbf{n}$ is the unit outward normal to Γ_R .

Following [1], we have

$$z \frac{H_n^{(1)'}(z)}{H_n^{(1)}(z)} = -\frac{f_n(z)}{g_n(z)} + i \frac{z}{g_n(z)}, \quad (6.12)$$

where

$$\begin{aligned} f_n(z) &= c_n^0 + 2c_n^1 \frac{1}{z^2} + \cdots + (n+1)c_n^n \frac{1}{z^{2n}}, \\ g_n(z) &= c_n^0 + c_n^1 \frac{1}{z^2} + \cdots + c_n^n \frac{1}{z^{2n}}, \end{aligned}$$

and

$$c_n^m = \frac{(m+n)!(2m)!}{4^m(m!)^2(n-m)!}.$$

Evidently, we have

$$1 \leq -\operatorname{Re} h_n(z) \leq n+1 \quad \text{and} \quad 0 \leq \operatorname{Im} h_n(z) \leq z. \quad (6.13)$$

To state the boundary value problem, we introduce the bilinear form $a : H^1(B_R) \times H^1(B_R) \rightarrow \mathbb{C}$

$$a(u, v) = (\nabla u, \nabla v) - \kappa^2 ((1+q)u, v) - \langle \mathcal{T}u, v \rangle, \quad (6.14)$$

and the linear functional on $H^1(B_R)$

$$b(v) = \kappa^2 (q\varphi_0, v). \quad (6.15)$$

Here we have used the standard inner products

$$(u, v) = \int_{B_R} u \cdot \bar{v} d\mathbf{x} \quad \text{and} \quad \langle u, v \rangle = \int_{\Gamma_R} u \cdot \bar{v} ds,$$

where the overline denotes the complex conjugate. The direct problem (6.7), (6.8) is equivalent to the following weak formulation: to find $\psi \in H^1(B_R)$ such that

$$a(\psi, \xi) = b(\xi), \quad \forall \xi \in H^1(B_R). \quad (6.16)$$

Throughout this chapter, C stands for a positive generic constant whose value may change step by step, but should always be clear from the context.

Lemma 6.1 *There exists a constant C such that for any $u \in H^{1/2}(\Gamma_R)$ the following inequality holds:*

$$\|\mathcal{T}u\|_{H^{-1/2}(\Gamma_R)} \leq C\|u\|_{H^{1/2}(\Gamma_R)}.$$

Furthermore,

$$-\operatorname{Re} \langle \mathcal{T}u, u \rangle \geq C\|u\|_{L^2(\Gamma_R)}^2 \quad \text{and} \quad \operatorname{Im} \langle \mathcal{T}u, u \rangle \geq 0.$$

Proof. For any function $u \in H^{1/2}(\Gamma_R)$, we have the Fourier series expansion:

$$u = \sum_{n \in \mathbb{Z}} \hat{u}_n e^{in\vartheta}, \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u e^{-in\vartheta} d\vartheta.$$

It follows from the norms for $H^{-1/2}(\Gamma_R)$ and $H^{1/2}(\Gamma_R)$ and (6.13) that

$$\|\mathcal{T}u\|_{H^{-1/2}(\Gamma_R)}^2 = \frac{2\pi}{R^2} \sum_{n \in \mathbb{Z}} \frac{|h_n(\kappa R)|^2}{(1+n^2)^{1/2}} |\hat{u}_n|^2 \leq C \sum_{n \in \mathbb{Z}} (1+n^2)^{1/2} |\hat{u}_n|^2 = C \|u\|_{H^{1/2}(\Gamma_R)}^2.$$

Using the inner product and the Fourier expansion, we arrive at

$$\langle \mathcal{T}u, u \rangle = \frac{2\pi}{R} \sum_{n \in \mathbb{Z}} h_n(\kappa R) |\hat{u}_n|^2.$$

It follows from (6.13) that

$$\begin{aligned} \operatorname{Re} \langle \mathcal{T}u, u \rangle &= \frac{2\pi}{R} \sum_{n \in \mathbb{Z}} \operatorname{Re}(h_n(\kappa R)) |\hat{u}_n|^2 \leq -\frac{2\pi}{R} \sum_{n \in \mathbb{Z}} |\hat{u}_n|^2 = -C \|u\|_{L^2(\Gamma_R)}^2, \\ \operatorname{Im} \langle \mathcal{T}u, u \rangle &= \frac{2\pi}{R} \sum_{n \in \mathbb{Z}} \operatorname{Im}(h_n(\kappa R)) |\hat{u}_n|^2 > 0. \quad \square \end{aligned}$$

Theorem 6.1 *If the wavenumber κ is sufficiently small, the variational problem (6.16) admits a unique weak solution in $H^1(B_R)$. Further, there is a positive constant C which depends only on R , such that*

$$\|\psi\|_{H^1(B_R)} \leq C \kappa^2 \|q\|_{L^\infty(B_R)} \|\varphi_0\|_{L^2(B_R)}. \quad (6.17)$$

Proof. Decompose the bilinear form a into $a = a_1 - \kappa^2 a_2$, where

$$a_1(\psi, \xi) = (\nabla \psi, \nabla \xi) - \langle \mathcal{T} \psi, \xi \rangle \quad \text{and} \quad a_2(\psi, \xi) = ((1+q)\psi, \xi).$$

We conclude that a_1 is coercive from Lemma 6.1

$$|a_1(\psi, \psi)| \geq C \|\psi\|_{H^1(B_R)}^2,$$

Next we prove the compactness of a_2 . Define an operator $\mathcal{A} : L^2(B_R) \rightarrow H^1(B_R)$ by

$$a_1(\mathcal{A}\psi, \xi) = a_2(\psi, \xi), \quad \forall \xi \in H^1(B_R),$$

which gives

$$(\nabla \mathcal{A}\psi, \nabla \xi) - \langle \mathcal{T} \mathcal{A}\psi, \xi \rangle = ((1+q)\psi, \xi).$$

Using the Lax–Milgram lemma and Lemma 6.1, we obtain

$$\|\mathcal{A}\psi\|_{H^1(B_R)} \leq C \|\psi\|_{L^2(B_R)}. \quad (6.18)$$

Thus, $\mathcal{A}$ is bounded from $L^2(B_R)$ to $H^1(B_R)$ and $H^1(B_R)$ is compactly embedded into $L^2(B_R)$. Hence, $\mathcal{A}$ is a compact operator.

Define a function $u \in L^2(B_R)$ by requiring $u \in H^1(B_R)$ and satisfying

$$a_1(u, \xi) = b(\xi), \quad \forall \xi \in H^1(B_R).$$

It follows from the Lax–Milgram lemma again that

$$\|u\|_{H^1(B_R)} \leq C\kappa^2 \|q\|_{L^\infty(B_R)} \|\varphi_0\|_{L^2(B_R)}. \quad (6.19)$$

Using the operator $\mathcal{A}$, we can see that the problem (6.16) is equivalent to find $\psi \in L^2(B_R)$ such that

$$(\mathcal{I} - \kappa^2 \mathcal{A}) \psi = u. \quad (6.20)$$

When the wavenumber κ is small enough, the operator $\mathcal{I} - \kappa^2 \mathcal{A}$ has a uniformly bounded inverse. We then have the estimate

$$\|\psi\|_{L^2(B_R)} \leq C \|u\|_{L^2(B_R)}, \quad (6.21)$$

where the constant C is independent of κ . Rearranging (6.19), we have $\psi = u - \kappa^2 \mathcal{A}\psi$, so $\psi \in H^1(B_R)$ and, by the estimate (6.18) for the operator $\mathcal{A}$, we have

$$\|\psi\|_{H^1(B_R)} \leq \|u\|_{H^1(B_R)} + C\kappa^2 \|\psi\|_{L^2(B_R)}.$$

The proof is complete by combining the above estimate and (6.19). $\square$

Note 1. For the propagating plane wave, the estimated (6.17) can be written as

$$\|\psi\|_{H^1(B_R)} \leq C\kappa^2 |\Omega|^{1/2} \|q\|_{L^\infty(B_R)}. \quad (6.22)$$

The energy estimate of the scattered field (6.22) provide a criterion for weak scattering. From this estimate, it is easily seen that, fixing any two of the three quantities, i.e., the wavenumber, the compact support of the scatterer Ω , and the $L^\infty(B_R)$ norm of the scatterer, the scattering is weak when the third one is small. Especially for the given scatterer q , i.e., the norm and the compact support are fixed, the scattering is weak when the wavenumber is small.

Note 2. For a general wavenumber, from (6.20) the uniqueness and existence follow from the Fredholm alternative, i.e., if κ is not the eigenvalue for the Helmholtz equation in the domain B_R , then the operator $\mathcal{I} - \kappa^2 \mathcal{A}$ has a bounded inverse. However, the bound depends on the wavenumber. Therefore, the constant C in the estimate (6.17) depends on the wavenumber.

Theorem 6.2 *Given the scatterer $q \in L^\infty(B_R)$, for all but possibly a discrete set of wavenumbers, the variational problem (6.16) admits a unique weak solution in $H^1(B_R)$. Further, there is a positive constant C which depends on R and κ , such that*

$$\|\psi\|_{H^1(B_R)} \leq C \|q\|_{L^\infty(B_R)} \|\varphi_0\|_{L^2(B_R)}. \quad (6.23)$$

Note 3. For the evanescent plane wave with $|\eta| > \kappa$, the estimate (6.22) can be written as

$$\|\psi\|_{H^1(B_R)} \leq C (\eta^2 - \kappa^2)^{-1/4} \|q\|_{L^\infty(B_R)}, \quad (6.24)$$

where the constant C depends on κ and R . The above energy estimate also provides a criterion for the weak scattering. For a fixed wavenumber κ and a scatterer q , the scattered field is weak if the spatial frequency of the incident wave $|\eta|$ is large.

6.3 Initial Guess

In this section, we discuss how to generate an initial guess for the proposed recursive linearization method based on either the linearized Lippmann–Schwinger integral equation when the weak scattering is valid, or the multiple signal classification algorithm when the weak scattering may not be valid.

6.3.1 Born Approximation

Rewrite (6.7) as

$$\Delta\psi + \kappa^2\psi = -\kappa^2q(\varphi_0 + \psi). \quad (6.25)$$

From the energy estimates (6.22) and (6.24), the scattered field is weak when the wavenumber κ is small or when the spatial frequency $|\eta|$ is large. By dropping the scattered field at the right-hand side of (6.25) under the weak scattering, we obtain

$$\Delta\psi + \kappa^2\psi = -\kappa^2q\varphi_0, \quad (6.26)$$

which is the well-known Born approximation.

Consider an auxiliary function $\psi_0(\mathbf{x}) = e^{i\kappa\mathbf{p}\cdot\mathbf{x}}$, $\mathbf{p} = (\cos\beta, \sin\beta)$, $\beta \in [0, 2\pi]$. This auxiliary function represents propagating plane waves and hence satisfies (6.5). Multiplying (6.26) by ψ_0 and integrating over B_R on both sides, we have

$$\int_{B_R} \psi_0 \Delta\psi d\mathbf{x} + \kappa^2 \int_{B_R} \psi_0 \psi d\mathbf{x} = -\kappa^2 \int_{B_R} q\varphi_0 \psi_0 d\mathbf{x}. \quad (6.27)$$

Integration by parts yields

$$\int_{B_R} \psi \Delta\psi_0 d\mathbf{x} + \int_{\Gamma_R} \left(\psi_0 \frac{\partial\psi}{\partial\mathbf{n}} - \psi \frac{\partial\psi_0}{\partial\mathbf{n}} \right) ds + \kappa^2 \int_{B_R} \psi_0 \psi d\mathbf{x} = -\kappa^2 \int_{B_R} q\varphi_0 \psi_0 d\mathbf{x}. \quad (6.28)$$

We have by noting (6.5) and the boundary condition (6.11) that

$$\int_{B_R} q\varphi_0 \psi_0 d\mathbf{x} = \frac{1}{\kappa^2} \int_{\Gamma_R} \left(\psi \frac{\partial\psi_0}{\partial\mathbf{n}} - \psi_0 \mathcal{T}\psi \right) ds. \quad (6.29)$$

Using the special form of the incident wave and the auxiliary function, we then get

$$\int_{B_R} qe^{i(\mathbf{k}+\kappa\mathbf{p})\cdot\mathbf{x}} d\mathbf{x} = \frac{1}{\kappa^2} \int_{\Gamma_R} \left(\psi \frac{\partial\psi_0}{\partial\mathbf{n}} - \psi_0 \mathcal{T}\psi \right) ds. \quad (6.30)$$

When the incident waves are propagating waves, i.e., $\mathbf{k} = \kappa \mathbf{d}$, the linear integral equation (6.30) becomes

$$\int_{B_R} q e^{i\kappa(\mathbf{d}+\mathbf{p})\cdot\mathbf{x}} d\mathbf{x} = \frac{1}{\kappa^2} \int_{\Gamma_R} \left(\psi \frac{\partial \psi_0}{\partial \mathbf{n}} - \psi_0 \mathcal{T} \psi \right) ds. \quad (6.31)$$

Since the scatterer q has a compact support, we use the notation

$$\hat{q}(\xi) = \int_{B_R} q(\mathbf{x}) e^{i\kappa(\mathbf{p}+\mathbf{n})\cdot\mathbf{x}},$$

where $\hat{q}(\xi)$ is the Fourier transform of $q(\mathbf{x})$ with $\xi = \kappa(\mathbf{p}+\mathbf{d})$. It is obvious that the domain $[0, 2\pi] \times [0, 2\pi]$ of (α, β) corresponds to the ball $\{\xi \in \mathbb{R}^2 : |\xi| \leq 2\kappa\}$. Thus, the Fourier modes of $q(\mathbf{x})$ in the ball $\{\xi : |\xi| \leq 2\kappa\}$ can be determined. The scattering data with higher wavenumber must be used in order to recover more modes of the true scatterer.

Define the data

$$D(\xi) = \begin{cases} \frac{1}{\kappa^2} \int_{\Gamma_R} \left(\psi \frac{\partial \psi_0}{\partial \mathbf{n}} - \psi_0 \mathcal{T} \psi \right) ds & \text{for } |\xi| \leq 2\kappa, \\ 0 & \text{for } |\xi| > 2\kappa. \end{cases}$$

Equation (6.31) can be formally reformulated as

$$\hat{q}(\xi) = D(\xi). \quad (6.32)$$

Taking the inverse Fourier transform of (6.32) leads to an initial approximation

$$q(\mathbf{x}) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} e^{-i\mathbf{x}\cdot\xi} D(\xi) d\xi, \quad (6.33)$$

which may be implemented by using the fast Fourier transform.

When the incident waves are evanescent, i.e., $\mathbf{k} = (\eta, i\sqrt{\eta^2 - \kappa^2})$, the linear integral equation (6.30) becomes

$$\int_{B_R} q(\mathbf{x}) e^{i(\kappa \cos \beta + \eta)x_1} e^{(i\kappa \sin \beta - \sqrt{\eta^2 - \kappa^2})x_2} d\mathbf{x} = \frac{1}{\kappa^2} \int_{\Gamma_R} \left(\psi \frac{\partial \psi_0}{\partial \mathbf{n}} - \psi_0 \mathcal{T} \psi \right) ds. \quad (6.34)$$

Since the scatterer $q(\mathbf{x})$ has a compact support, (6.34) can be rewritten as

$$\int_{-\infty}^{\infty} \hat{q}(\xi, x_2) e^{(i\kappa \sin \beta - \sqrt{\eta^2 - \kappa^2})x_2} dx_2 = D(\xi, \eta), \quad (6.35)$$

where $\xi = \kappa \cos \beta + \eta$ and $\hat{q}(\xi, x_2)$ is the Fourier transform of $q(\mathbf{x})$ with respect to x_1 . When the spatial frequency $|\eta|$ is large, the incident wave penetrates a thin layer of the scatterer. Thus, the Born approximation allows a reconstruction containing information of the true scatterer in that thin layer. For propagating plane incident waves, the inversion involves data related to the scatterer through the Fourier transform in the case of weak scattering.

For evanescent plane wave, the inversion involves data related to the scatterer through a Fourier (with respect to x_1)–Laplace (with respect to x_2) transform in the case of the weak scattering.

Introduce the integral kernel

$$\mathcal{K}(\xi, \eta; x_2) = e^{(i\kappa \sin \beta - \sqrt{\eta^2 - \kappa^2})x_2}.$$

The integral equation (6.35) can be formally written as

$$\mathcal{K}(\xi)\hat{q}(\xi) = D(\xi). \quad (6.36)$$

In practice, (6.36) is implemented by using the method of least squares with Tikhonov regularization

$$\hat{q}(\xi) = (\lambda \mathcal{I} + \mathcal{K}^* \mathcal{K})^{-1} \mathcal{K}^* D(\xi), \quad (6.37)$$

where λ is a small positive number, $\mathcal{I}$ is the identity operator, and $\mathcal{K}^*$ is the adjoint operator of $\mathcal{K}$. Once $\hat{q}(\xi, x_2)$ is available, an approximation of $q(\mathbf{x})$ may be obtained from the inverse Fourier transform.

6.3.2 MUSIC Algorithm

The MUSIC (MUltiple Signal Classification) algorithm for extended scatterers proposed in [27] is used to generate an image for the shape of the scatterer. The MUSIC algorithm for point scatterers may be found in [25]. The image may be further converted into a level set representation for the scatterer through image processing. See also [2] for an up-to-date discussion on various types of mathematical imaging methods.

The MUSIC Algorithm for Extended Scatterers

Consider plane incident waves illuminating from m evenly spaced angles with a certain wavenumber. The scattered fields are recorded on $\partial\Omega$ with the same m evenly spaced angles. The data collected forms an m -by- m matrix, denoted by P , which is known as the response matrix. For simplicity of discussion, here we have the incident plane wave directions coincide with the recorded scattered field directions. However, the MUSIC algorithm and our continuation method to be discussed later can both handle the general case where the number of incident plane wave directions is different from the number of recorded scattered field directions and the directions do not coincide.

Let $P = U\Sigma V^H$ be the singular value decomposition of the response matrix. Define the illumination vector

$$\mathbf{g}(\mathbf{x}) = [e^{ik\mathbf{x}\cdot\mathbf{d}_1}, \dots, e^{ik\mathbf{x}\cdot\mathbf{d}_m}]^T,$$

where $\mathbf{d}_j$ are the propagation directions of incident waves and $\mathbf{x}$ is any point in the space. The MUSIC imaging function may be introduced:

$$I(\mathbf{x}) = \frac{1}{\|\mathbf{g}(\mathbf{x})\|_2^2 - \sum_{\ell=1}^s |\mathbf{g}(\mathbf{x})^H \mathbf{u}_\ell|^2}, \quad (6.38)$$

where $\mathbf{u}_\ell$ is the ℓ th column of the matrix U and the number of singular vectors s that spans the signal space is determined by the resolution analysis based thresholding algorithm in [27].

The imaging function (6.38) provides an image for the boundary of the scatterer, which may be further converted into a level set representation for the scatterer.

Image Processing and the Level Set Function

In this section, we briefly describe an image processing to convert the image for the boundary of the scatterer into a level set representation, which leads to an initial guess. Additional discussions and results are available in [4].

There are many edge detector algorithms in the literature [12, 13, 31]. Here, we employ a relatively simple approach. Starting with a large domain enclosing the scatterer, we minimize the cost functional

$$C(\partial\Omega) = \int_{\partial\Omega} f(\mathbf{x}) ds, \quad (6.39)$$

where $f(\mathbf{x}) = 1$ if the imaging function $I(\mathbf{x})$ is larger than some threshold and $f(\mathbf{x}) = 100$ otherwise. In other words, on the boundary of the scatterer, f is small. It makes the curve shrink to the boundary of the scatterer by minimizing the functional (6.39). In fact, the function f acts as the weight for the curvature-based force in the curve evolution.

Let $\varphi(\mathbf{x})$ be a level set function that characterizes the curve $\partial\Omega$, i.e., $\varphi(\mathbf{x}) = 0$ on $\partial\Omega$, $\varphi(\mathbf{x}) > 0$ outside Ω ; $\varphi(\mathbf{x}) < 0$ inside Ω . The cost functional can be formulated as [40]

$$C(\partial\Omega) = W(\varphi) = \int_{\mathbb{R}^2} f(\mathbf{x}) \delta(\varphi) |\nabla\varphi| d\mathbf{x}, \quad (6.40)$$

where δ is the Dirac delta function. Taking the derivative with respect to the evolution time t , we have

$$\frac{dW}{dt} = \int_{\mathbb{R}^2} \left(\delta'(\varphi) |\nabla\varphi| \varphi_t + \delta(\varphi) \frac{\nabla\varphi}{|\nabla\varphi|} \cdot \nabla(\varphi_t) \right) f(\mathbf{x}) d\mathbf{x}. \quad (6.41)$$

The level set formulation for shape evolution with the normal velocity $v(\mathbf{x})$ is [36]

$$\varphi_t = -v(\mathbf{x}) |\nabla\varphi|. \quad (6.42)$$

By substituting (6.42) into (6.41) and using $\delta'(\varphi)\nabla\varphi = \nabla(\delta(\varphi))$, we obtain

$$\frac{dW}{dt} = - \int_{\mathbb{R}^2} \left(v(\mathbf{x}) \nabla(\delta(\varphi)) \cdot \nabla\varphi + \delta(\varphi) \frac{\nabla\varphi}{|\nabla\varphi|} \cdot \nabla(v(\mathbf{x}) |\nabla\varphi|) \right) f(\mathbf{x}) d\mathbf{x}. \quad (6.43)$$

Although the evolution velocity is only defined on the moving curve initially, it can be extended by a constant normal extension away from the curve. Since $\nabla\varphi$ is in the normal direction, we have $\nabla v \cdot \nabla\varphi = 0$. Therefore, (6.43) can be rewritten as

$$\frac{dW}{dt} = - \int_{\mathbb{R}^2} \left(\nabla(\delta(\varphi)) \cdot \nabla\varphi + \delta(\varphi) \frac{\nabla\varphi}{|\nabla\varphi|} \cdot \nabla(|\nabla\varphi|) \right) v(\mathbf{x}) f(\mathbf{x}) d\mathbf{x}. \quad (6.44)$$

It follows from the divergence theorem on the first term of the right-hand side of (6.44) that

$$\frac{dW}{dt} = \int_{\mathbb{R}^2} \delta(\varphi) \left(\nabla \cdot (v(\mathbf{x}) f(\mathbf{x}) \nabla\varphi) - \frac{\nabla\varphi}{|\nabla\varphi|} \cdot \nabla(|\nabla\varphi|) v(\mathbf{x}) f(\mathbf{x}) \right) d\mathbf{x}. \quad (6.45)$$

Simple calculations from the product rule yield

$$\frac{dW}{dt} = \int_{\mathbb{R}^2} \delta(\varphi) |\nabla\varphi| v(\mathbf{x}) \nabla \cdot \left(f(\mathbf{x}) \frac{\nabla\varphi}{|\nabla\varphi|} \right) d\mathbf{x}, \quad (6.46)$$

which can be written as a curve integral

$$\frac{dW}{dt} = \int_{\partial\Omega} v(\mathbf{x}) \nabla \cdot \left(f(\mathbf{x}) \frac{\nabla\varphi}{|\nabla\varphi|} \right) ds. \quad (6.47)$$

Let $v(\mathbf{x}) = -\nabla \cdot (f(\mathbf{x}) \frac{\nabla\varphi}{|\nabla\varphi|})$. By substituting it into (6.42), we arrive at the gradient flow for the level set function

$$\varphi_t = |\nabla\varphi| \nabla \cdot \left(f(\mathbf{x}) \frac{\nabla\varphi}{|\nabla\varphi|} \right). \quad (6.48)$$

By using such a normal velocity, we always have $dW/dt < 0$, i.e., the cost functional decreases monotonically in the shape evolution. In practice, a local level set method [37] with reinitialization using a time marching scheme [38] is employed for solving (6.48).

Starting with a box containing all scatterers, the evolution will stop at the convex envelope of the shapes for scatterers in the MUSIC imaging result. The level set function representing the shape of the envelope may be selected as an initial guess.

6.4 Recursive Linearization

In this section, two regularized recursive linearization methods for solving the inverse medium scattering problem with multiple frequency and single frequency are proposed, respectively.

One of the recursive linearization methods, obtained by continuation on the wavenumber κ , requires multiple frequency scattering data. At each

wavenumber κ , the algorithm determines a forward model which produces the prescribed scattering data. At low wavenumber κ , the scattered field is weak. Consequently, the nonlinear equation become essentially a linear one. The algorithm first solves this nearly linear equation at the lowest κ to obtain low-frequency modes of the true scatterer. The approximation is then used to linearize the nonlinear equation at the next higher κ to produce a better approximation which contains more modes of the true scatterer. This process is continued until a sufficiently high wavenumber κ where the dominant modes of the scatterer are essentially recovered.

Another recursive linearization method, obtained by continuation method on the spatial frequency of a one-parameter family of incident plane waves, requires only single frequency scattering data. At each transverse part of the incident wave, the algorithm determines a forward model which produces the prescribed scattering data. Since the incident wave at a high spatial frequency can only penetrate a thin layer of the scatterer, the scattered field is weak. Consequently, the nonlinear equation becomes essentially linear, known as the Born approximation. The algorithm first solves this nearly linear equation at the largest $|\eta|$ to obtain an approximation of the scatterer. This approximation is then used to linearize the nonlinear equation at the next smaller spatial frequency of the incident wave, which can penetrate a thicker layer of the scatterer, to produce a better approximation. When the spatial frequency, $|\eta|$, is smaller than the fixed wavenumber κ , the incident wave becomes usual propagating plane wave, and the whole scatterer is illuminated. This process is continued until the spatial frequency is zero, where the approximation of the scatterer is considered as the final reconstruction.

Multiple Frequency

As discussed in the previous section, when the wavenumber κ is small, the Born approximation allows a reconstruction of those low Fourier modes for the function q . We now describe a procedure that recursively determines better approximations q_κ at $\kappa = \kappa_l$ for $l = 1, 2, \dots$ with the increasing wavenumbers. Suppose now that an approximation of the scatterer, $q_{\tilde{\kappa}}$, has been recovered at some wavenumber $\tilde{\kappa}$, and that the wavenumber κ is slightly larger than $\tilde{\kappa}$. We wish to determine q_κ , or equivalently, to determine the perturbation

$$\delta q = q_\kappa - q_{\tilde{\kappa}}.$$

For the reconstructed scatterer $q_{\tilde{\kappa}}$, we solve at the wavenumber κ the forward scattering problem

$$\Delta \tilde{\psi}_i + \kappa^2(1 + q_{\tilde{\kappa}})\tilde{\psi}_i = -\kappa^2 q_{\tilde{\kappa}} \varphi_0^{(i)} \quad \text{in } B_R, \quad (6.49)$$

$$\frac{\partial \tilde{\psi}_i}{\partial \mathbf{n}} = \mathcal{T} \tilde{\psi}_i \quad \text{on } \Gamma_R, \quad (6.50)$$

where $\varphi_0^{(i)}$ is the incident with incident angle $\alpha_i, i = 1, \dots, n$.

For the scatterer q_κ , we have

$$\Delta\psi_i + \kappa^2(1 + q_\kappa)\psi_i = -\kappa^2 q_\kappa \varphi_0^{(i)} \quad \text{in } B_R, \quad (6.51)$$

$$\frac{\partial\psi_i}{\partial\mathbf{n}} = \mathcal{T}\psi_i \quad \text{on } \Gamma_R. \quad (6.52)$$

Subtracting (6.49) from (6.51) and omitting the second-order smallness in δq and in $\delta\psi_i = \psi_i - \tilde{\psi}_i$, we obtain

$$\Delta\delta\psi_i + \kappa^2(1 + q_{\tilde{\kappa}})\delta u_i^s = -\kappa^2\delta q(\varphi_0^{(i)} + \tilde{\psi}_i) \quad \text{in } B_R, \quad (6.53)$$

$$\frac{\partial\delta\psi_i}{\partial\mathbf{n}} = \mathcal{T}\delta\psi_i \quad \text{on } \Gamma_R. \quad (6.54)$$

Given a solution ψ_i of (6.51), we define the measurements

$$M\psi_i(\mathbf{x}) = [\psi_i(\mathbf{x}_1), \dots, \psi_i(\mathbf{x}_m)]^T. \quad (6.55)$$

The measurement operator M is well defined and maps the scattered field to a vector of complex numbers in $\mathbb{C}^m$, which consists of point measurements of the scattered field at $\mathbf{x}_j, j = 1, \dots, m$.

For the scatterer q_κ and the transmitted field $\varphi_0^{(i)}$, we define the forward scattering operator

$$S(q_\kappa, \varphi_0^{(i)}) = M\psi_i. \quad (6.56)$$

It is easily seen that the forward scattering operator $S(q_\kappa, \varphi_0^{(i)})$ is linear with respect to $\varphi_0^{(i)}$ but nonlinear with respect to q_κ . For simplicity, we denote $S(q_\kappa, \varphi_0^{(i)})$ by $S_i(q_\kappa)$. Let $S'_i(q_{\tilde{\kappa}})$ be the Fréchet derivative of $S_i(q_\kappa)$ and denote the residual operator

$$R_i(q_{\tilde{\kappa}}) = M(\delta\psi_i). \quad (6.57)$$

It follows from the linearization of the nonlinear equation (6.56) that

$$S'_i(q_{\tilde{\kappa}})\delta q = R_i(q_{\tilde{\kappa}}). \quad (6.58)$$

Applying the Landweber iteration [22] to the linearized equation (6.58) yields

$$\delta q = \tau S'_i(q_{\tilde{\kappa}})^* R_i(q_{\tilde{\kappa}}), \quad (6.59)$$

where τ is a positive relaxation parameter and $S'_i(q_{\tilde{\kappa}})^*$ is the adjoint operator of $S'_i(q_{\tilde{\kappa}})$.

In order to compute the correction δq , we need some efficient way to compute $S'_i(q_{\tilde{\kappa}})^* R_i(q_{\tilde{\kappa}})$. Let $R_i(q_{\tilde{\kappa}}) = [\zeta_{i1}, \dots, \zeta_{im}]^T \in \mathbb{C}^m$. Consider the adjoint problem

$$\Delta w_i + \kappa^2(1 + q_{\tilde{\kappa}})w_i = -\kappa^2 \sum_{j=1}^m \zeta_{ij} \delta(\mathbf{x} - \mathbf{x}_j) \quad \text{in } B_R, \quad (6.60)$$

$$\frac{\partial w_i}{\partial\mathbf{n}} = \mathcal{T}^* w_i \quad \text{on } \Gamma_R, \quad (6.61)$$

where the operator $\mathcal{T}^*$ is defined as

$$\mathcal{T}^*u = \kappa \sum_{n \in \mathbb{Z}} \overline{\left(\frac{H_n^{(1)'}(\kappa R)}{H_n^{(1)}(\kappa R)} \right)} \hat{u}_n e^{in\vartheta}, \quad \hat{u}_n = \frac{1}{2\pi} \int_0^{2\pi} u e^{-in\vartheta} d\vartheta.$$

Multiplying (6.53) with the complex conjugate of w_i and integrating over B_R on both sides, we obtain

$$\int_{B_R} \Delta \delta \psi_i \bar{w}_i d\mathbf{x} + \int_{B_R} \kappa^2 (1 + q_{\bar{\kappa}}) \delta \psi_i \bar{w}_i d\mathbf{x} = -\kappa^2 \int_{B_R} \delta q (\varphi_0^{(i)} + \tilde{\psi}_i) \bar{w}_i d\mathbf{x}.$$

Using Green's formula, we have

$$\begin{aligned} \int_{B_R} (\Delta \bar{w}_i + \kappa^2 (1 + q_{\bar{\kappa}}) \bar{w}_i) \delta \psi_i d\mathbf{x} + \int_{\Gamma_R} \left(\frac{\partial \bar{w}_i}{\partial \mathbf{n}} \delta \psi_i - \frac{\partial \delta \psi_i}{\partial \mathbf{n}} \bar{w}_i \right) ds \\ = -\kappa^2 \int_{B_R} \delta q (\varphi_0^{(i)} + \tilde{\psi}_i) \bar{\psi}_i d\mathbf{x}. \end{aligned}$$

It follows from the adjoint equation (6.60) that

$$\sum_{j=1}^m \delta \psi_i(\mathbf{x}_j) \bar{\zeta}_{ij} = \int_{B_R} \delta q (\varphi_0^{(i)} + \tilde{\psi}_i) \bar{w}_i d\mathbf{x}. \quad (6.62)$$

Noting (6.57), (6.58), and the adjoint operator $S'_i(q_{\bar{\kappa}})^*$, the left-hand side of (6.62) may be deduced

$$\begin{aligned} \sum_{j=1}^m \delta u_i^s(\mathbf{x}_j) \bar{\zeta}_{ij} &= \langle M(\delta u_i^s), R_i(q_{\bar{\kappa}}) \rangle_{\mathbb{C}^m} = \langle S'_i(q_{\bar{\kappa}}) \delta q, R_i(q_{\bar{\kappa}}) \rangle_{\mathbb{C}^m} \\ &= \langle \delta q, S'_i(q_{\bar{\kappa}})^* R_i(q_{\bar{\kappa}}) \rangle_{L^2(B_R)} = \int_{B_R} \delta q \overline{S'_i(q_{\bar{\kappa}})^* R_i(q_{\bar{\kappa}})} d\mathbf{x}, \end{aligned} \quad (6.63)$$

where $\langle \cdot, \cdot \rangle_{\mathbb{C}^m}$ and $\langle \cdot, \cdot \rangle_{L^2(B_R)}$ are the standard inner-products defined in the complex vector space $\mathbb{C}^m$ and the square integrable functional space $L^2(B_R)$.

Combining (6.62) and (6.63) yields

$$\int_{B_R} \delta q \overline{S'_i(q_{\bar{\kappa}})^* R_i(q_{\bar{\kappa}})} d\mathbf{x} = \int_{B_R} \delta q (\varphi_0^{(i)} + \tilde{\psi}_i) \bar{w}_i d\mathbf{x},$$

which holds for any δq . It follows that

$$S'_i(q_{\bar{\kappa}})^* R_i(q_{\bar{\kappa}}) = \overline{(\varphi_0^{(i)} + \tilde{\psi}_i)} w_i. \quad (6.64)$$

Using the above result, (6.59) can be written as

$$\delta q = \tau \overline{(\varphi_0^{(i)} + \tilde{\psi}_i)} w_i. \quad (6.65)$$

Thus, for each incident wave, we solve one forward problem (6.49), (6.50) and one adjoint problem (6.60), (6.61). Once δq is determined, $q_{\bar{\kappa}}$ is updated by $q_{\bar{\kappa}} + \delta q$. After completing the p th sweep, we get the reconstructed scatterer $q_{\bar{\kappa}}$ at the wavenumber κ .

Single Frequency

As discussed in the previous section, when the spatial frequency $|\eta|$ is large, the Born approximation allows a reconstruction of the thin layer for the true scatterer. In this section, a regularized recursive linearization method for solving the two-dimensional Helmholtz equation at fixed frequency is proposed.

Choose a large positive number $\eta_{\max}$ and divide the interval $[0, \eta_{\max}]$ into N subdivisions with the endpoints $\{\eta_0, \eta_1, \dots, \eta_N\}$, where $\eta_0 = 0, \eta_N = \eta_{\max}$, and $\eta_{n-1} < \eta_n$ for $1 \leq n \leq N$. We intend to obtain q_η recursively at $\eta = \eta_N, \eta_{N-1}, \dots, \eta_0$.

Suppose now that the scatterer $q_{\tilde{\eta}}$ has been recovered at some $\tilde{\eta} = \eta_{n+1}$ and that $\eta = \eta_n$ is slightly less than $\tilde{\eta}$. We wish to determine q_η , or equivalently, to determine the perturbation

$$\delta q = q_\eta - q_{\tilde{\eta}}.$$

For the reconstructed scatterer $q_{\tilde{\eta}}$, we solve at the spatial frequency η the forward scattering problem

$$\Delta \tilde{\psi}_i + \kappa^2(1 + q_{\tilde{\eta}})\tilde{\psi}_i = -\kappa^2 q_{\tilde{\eta}} \varphi_0^{(i)} \quad \text{in } B_R, \quad (6.66)$$

$$\frac{\partial \tilde{\psi}_i}{\partial \mathbf{n}} = \mathcal{T} \tilde{\psi}_i \quad \text{on } \Gamma_R, \quad (6.67)$$

where the incident wave $\varphi_0^{(i)} = e^{i\eta_i x_1 + i k(\eta_i) x_2}$, $|\eta_i| \geq \eta$.

For the scatterer q_η , we have

$$\Delta \psi_i + \kappa^2(1 + q_\eta)\psi_i = -\kappa^2 q_\eta \varphi_0^{(i)} \quad \text{in } B_R, \quad (6.68)$$

$$\frac{\partial \psi_i}{\partial \mathbf{n}} = \mathcal{T} \psi_i \quad \text{on } \Gamma_R. \quad (6.69)$$

Subtracting (6.66), (6.67) from (6.68), (6.69) and omitting the second-order smallness in δq and in $\delta \psi_i = \psi_i - \tilde{\psi}_i$, we obtain

$$\Delta \delta \psi_i + \kappa^2(1 + q_{\tilde{\eta}})\delta \psi_i = -\kappa^2 \delta q (\varphi_0^{(i)} + \tilde{\psi}_i) \quad \text{in } B_R, \quad (6.70)$$

$$\frac{\partial \delta \psi_i}{\partial \mathbf{n}} = \mathcal{T} \delta \psi_i \quad \text{on } \Gamma_R. \quad (6.71)$$

In order to compute the update δq , we may similarly consider the adjoint equation (6.60) and (6.61). Following from the same procedure as that in the case of multiple frequency, we may have again (6.65).

So for each incident wave with a transverse part η_j , we have to solve one forward problem (6.49), (6.50) along with one adjoint problem (6.60), (6.61). Since the adjoint problem has a similar variational form as the forward problem. Essentially, we need to compute two forward problems at each sweep. Once δq is determined, $q_{\tilde{\eta}}$ is updated by $q_{\tilde{\eta}} + \delta q$. After completing sweeps with $|\eta_j| \geq \eta$, we get the reconstructed scatterer q_η at the spatial frequency η .

6.5 Numerical Experiments

In order to illustrate the performance of our algorithms, we present three numerical examples. The scattering data are obtained by numerical solution of the direct scattering problem, which is implemented by using the finite element method with a perfectly matched layer technique. For stability analysis, some relative random noise is added to the data, i.e., the scattered field takes the form

$$\psi(\mathbf{x}_j) := (1 + \sigma \text{rand})\psi(\mathbf{x}_j), j = 0, \dots, m.$$

Here, rand gives uniformly distributed random numbers in $[-1, 1]$ and σ is a noise level parameter taken to be 0.05 in our numerical experiments. Define the relative error by

$$e_2 = \frac{(\sum_{i,j} |q_{ij} - \tilde{q}_{ij}|^2)^{1/2}}{(\sum_{i,j} |q_{ij}|^2)^{1/2}},$$

where $\tilde{q}$ is the reconstructed scatterer and q is the true scatterer.

Example 1. Reconstruct a scatterer shown in Fig. 6.2a using multiple frequency data. The initial guess is obtained from the Born approximation corresponding to weak scattering at low frequency. See Fig. 6.3 for the relative error of reconstructions using different maximum wavenumber. It is clearly illustrated that the reconstruction is better using a large wavenumber than

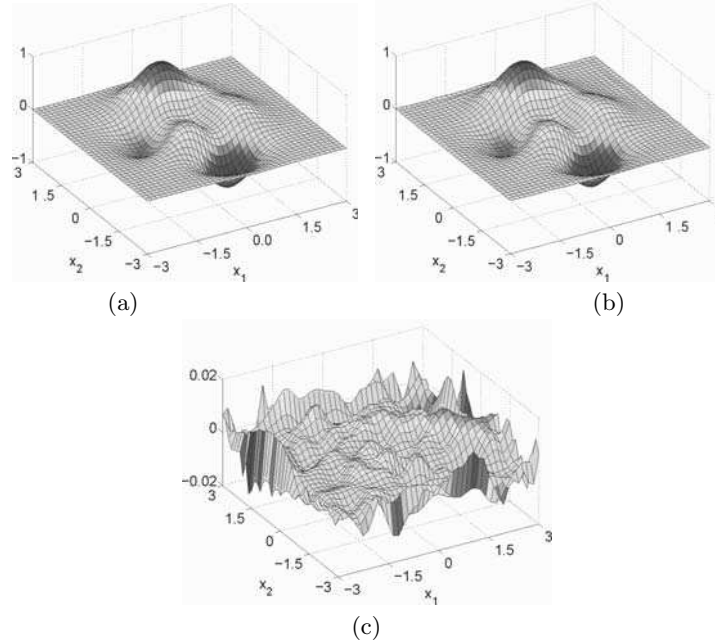


Fig. 6.2. Example 1. (a) the true scatterer; (b) the reconstructed scatterer; (c) the difference between the true scatterer and the reconstructed one

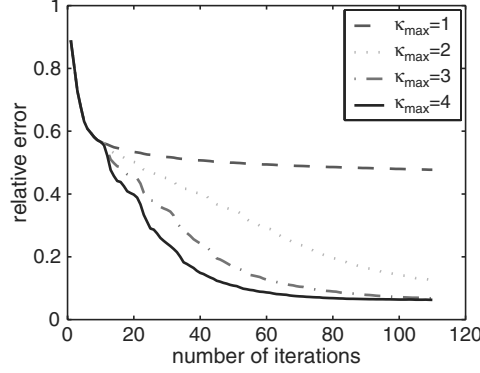


Fig. 6.3. Example 1. The relative error of reconstructions

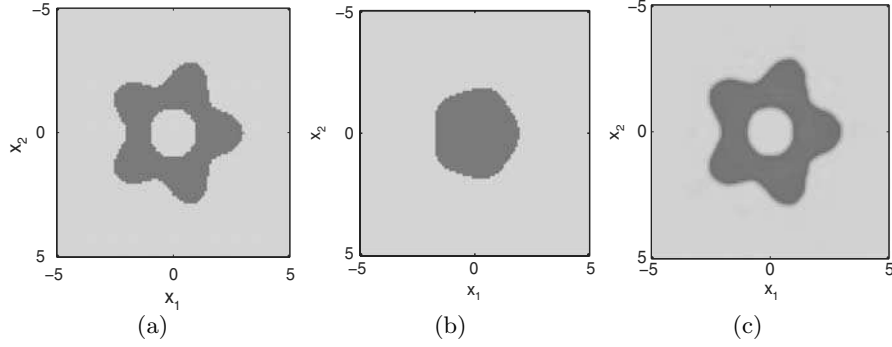


Fig. 6.4. Example 2. (a) the true scatterer; (b) the initial guess; (c) the final reconstruction

that using a smaller one. This result may be explained by Heisenberg's uncertainty principle. Figure 6.2b shows the reconstructed scatterer at wavenumber $\kappa = 4.0$ and Fig. 6.2c plots the difference between the true scatterer and the reconstructed one.

Example 2. Reconstruct a five-leave shape scatterer with a disc of radius 1 removed, see Fig. 6.4a. Figure 6.4b shows the initial guess from the MUSIC algorithm and Fig. 6.4c shows the final reconstruction. The initial guesses are obtained via MUSIC algorithm and a level set representation at the wavenumber $\kappa = 1$. The largest wavenumber used in the recursive linearization algorithm is $\kappa = 6$. The step size for wavenumbers is 0.5, i.e., the number of iteration along wavenumbers is 10. From this example, we observe that the MUSIC algorithm does not provide detailed shape information from the starting low frequency data. However, it is a very fast direct algorithm to provide initial guesses. The final results after recursive linearization is very promising.

Example 3. Reconstruct a scatterer given in Fig. 6.5a using single frequency data with an initial guess from the Born approximation corresponding to weak

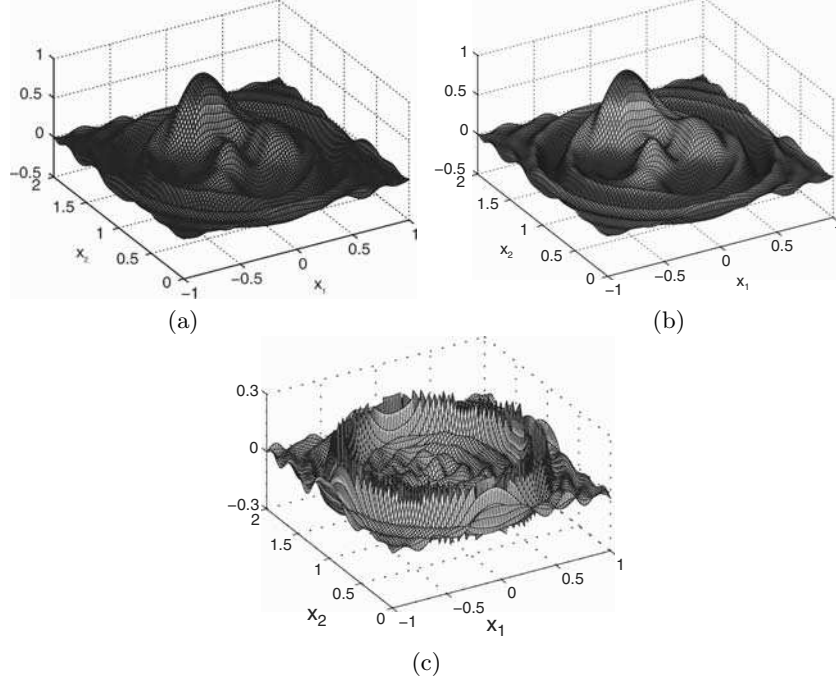


Fig. 6.5. Example 3. (a) the true scatterer; (b) the reconstructed scatterer; (c) the difference between the true scatterer and the reconstructed one

scattering at high spatial frequency. This scatterer is difficult to reconstruct because of the discontinuity across two circles. Figure 6.5b,c respectively shows the reconstructed scatterer and the difference between the true scatterer and the reconstructed using the wavenumber $\kappa = 15$. The plots show that the error of the reconstruction occurs largely around the discontinuity, while the smooth part is recovered more accurately. As expected, the Gibbs phenomenon appears in the reconstructed scatterer near the discontinuity.

6.6 Conclusion

We have presented two regularized recursive linearization methods with respect to the wavenumber and the spatial frequency of a one-parameter family of plane waves. The recursive linearization algorithms are robust and efficient for solving the inverse medium scattering with multiple or single frequency. Finally, we point out some future directions along the line of this work. The first is concerned with the convergence analysis. Although our numerical experiments demonstrate the convergence and stability of the inversion algorithm, no rigorous mathematical analysis of the algorithms is available

at present. Initial attempt has been made recently in [10] to establish convergence results by taking into account of the uncertainty principle. Another direction is to investigate inverse medium problems for Maxwell's equations with limited aperture case. An on-going effort of our group is to extend the approaches in this survey to the more complicated 3D model problems.

References

- [1] H. Ammari and J.-C. Nédélec, *Low-frequency electromagnetic scattering*, SIAM J. Math. Anal., 31 (2000), 836–861.
- [2] H. Ammari and H. Kang, *Reconstruction of Small Inhomogeneities from Boundary Measurements*, Lecture Notes in Mathematics, Vol. 1846, Springer-Verlag, Berlin, 2004.
- [3] G. Bao, Y. Chen, and F. Ma, *Regularity and stability for the scattering map of a linearized inverse medium problem*, J. Math. Anal. Appl., 247 (2000), 255–271.
- [4] G. Bao, S. Hou, and P. Li, *Inverse scattering by a continuation method with initial guesses from a direct imaging algorithm*, preprint.
- [5] G. Bao and P. Li, *Inverse medium scattering for the Helmholtz equation at fixed frequency*, Inverse Problems, 21 (2005), 1621–1641.
- [6] G. Bao and P. Li, *Inverse medium scattering for three-dimensional time harmonic Maxwell equations*, Inverse Problems, 20 (2004), L1–L7.
- [7] G. Bao and P. Li, *Inverse medium scattering problems for electromagnetic waves*, SIAM J. Appl. Math., 65 (2005), 2049–1066.
- [8] G. Bao and J. Liu, *Numerical solution of inverse problems with multi-experimental limited aperture data*, SIAM J. Sci. Comput., 25 (2003), 1102–1117.
- [9] G. Bao and P. Li, *Inverse medium scattering problem in near-field optics*, J. Comput. Math., to appear.
- [10] G. Bao and F. Triki, *Error estimates for the recursive linearization of inverse medium problems*, preprint.
- [11] P. Carney and J. Schotland, *Three-dimensional total internal reflection microscopy*, Opt. Lett., 26 (2001), 1072–1074.
- [12] V. Caselles, F. Catte, T. Coll, and F. Dibos, *A geometric model for active contours in image processing*, Numer. Math, 66 (1993), 1–31.
- [13] V. Caselles, R. Kimmel, and G. Sapiro, *On geodesic active contours*, Int. J. Comput. Vis., 22 (1997), 61–79.
- [14] Y. Chen, *Inverse scattering via Heisenberg uncertainty principle*, Inverse Problems, 13 (1997), 253–282.
- [15] Y. Chen, *Inverse scattering via skin effect*, Inverse Problems, 13 (1997), 649–667.
- [16] D. Courjon and C. Bainier, *Near field microscopy and near field optics*, Rep. Prog. Phys., 57 (1994), 989–1028.

- [17] D. Colton, J. Coyle, and P. Monk, *Recent development in inverse acoustic scattering theory*, SIAM Review, 42 (2000), 369–414.
- [18] D. Colton and R. Kress, *Integral Equation Methods in Scattering Theory*, Wiley, New York, 1983.
- [19] D. Colton and R. Kress, *Inverse Acoustic and Electromagnetic Scattering Theory*, Springer-Verlag, Berlin, 1998.
- [20] D. Courjon, *Near-field Microscopy and Near-field Optics*, Imperial College Press, 2003.
- [21] O. Dorn, E. Miller, and C. Rappaport, *A shape reconstruction method for electromagnetic tomography using adjoint fields and level sets*, Inverse Problems, 16 (2000), 1119–1156.
- [22] H. Engl, M. Hanke, and A. Neubauer, *Regularization of Inverse Problems*, Dordrecht: Kluwer, 1996.
- [23] D. Gilbarg and N. Trudinger, *Elliptic Partial Differential Equations of Second Order*, Springer-Verlag, New York, 1983.
- [24] C. Girard and A. Dereux, *Near-field optics theories*, Rep. Prog. Phys., 59 (1996), 657–699.
- [25] F. K. Gruber, E. A. Marengo, and A. J. Devaney, *Time-reversal imaging with multiple signal classification considering multiple scattering between the targets*, J. Acoust. Soc. Am., 115 (2004), 3042–3047.
- [26] T. Hohage, *On the numerical solution of a three-dimensional inverse medium scattering problem*, Inverse Problems, 17 (2001), 891–906.
- [27] S. Hou, K. Solna, and H. Zhao, *A direct imaging algorithm for extended targets*, Inverse Problems, 22 (2006), 1151–1178.
- [28] K. Ito, K. Kunisch, and Z. Li, *Level-set function approach to an inverse interface problem*, Inverse Problems, 17 (2001), 1225–1242.
- [29] D. Jerison and C. Kenig, *Unique continuation and absence of positive eigenvalues for Schrödinger operators*, Ann. Math., 121 (1985), 463–488.
- [30] J. Jin, *The Finite Element Methods in Electromagnetics*, John Wiley & Sons, 2002.
- [31] M. Kass, A. Witkin, and D. Terzopoulos, *Snakes: Active contour models*, Int. J. Comput. Vis., 1 (1988), 321–331.
- [32] P. Monk, *Finite Element Methods for Maxwell's Equations*, Oxford University Press, Oxford, 2003.
- [33] F. Natterer, *The Mathematics of Computerized Tomography*, Stuttgart: Teubner, 1986.
- [34] F. Natterer and F. Wübbeling, *A propagation-backpropagation method for ultrasound tomography*, Inverse Problems, 11 (1995), 1225–1232.
- [35] J. Nédélec, *Acoustic and Electromagnetic Equations: Integral Representations for Harmonic Problems*, Springer, New York, 2000.
- [36] S. Osher and J. Sethian, *Fronts propagating with curvature-dependent speed: algorithms based on Hamilton-Jacobi formulations*, J. Comput. Phys., 79 (1988), 12–49.
- [37] D. Peng, B. Merriman, S. Osher, H. Zhao, and M. Kang, *A PDE-based fast local level set method*, J. Comput. Phys., 155(2) (1999), 410–438.

- [38] M. Sussman, P. Smereka, and S. Osher, *A level set approach for computing solutions to incompressible two-phase flows*, J. Comput. Phys., 119 (1994), 146–159.
- [39] M. Vögeler, *Reconstruction of the three-dimensional refractive index in electromagnetic scattering by using a propagating-backpropagation method*, Inverse Problems, 19 (2003), 739–753.
- [40] H. Zhao, T. Chan, B. Merriman, and S. Osher, *A variational level set approach to multiphase motion*, J. Comput. Phys., 127 (1996), 179–195.

Time Reversal of Electromagnetic Waves

J. de Rosny, G. Lerosey, A. Tourin, and M. Fink

7.1 Introduction

In a nondissipative medium, the wave equation is time-symmetric. Therefore, for every wave diverging from a pulsed source, there exists in theory a wave, the time-reversed wave, that precisely retraces all its original paths in a reverse order and converges in synchrony at the original source as if time were going backwards. This time-symmetry exists even in a strongly heterogeneous medium where the waves are strongly reflected, refracted, or scattered. In 1989, an original method has been proposed for generating such a time-reversed wave from a surface. This time-reversal technique has led to numerous applications in ultrasound and underwater acoustics such as brain therapy, lithotripsy, nondestructive testing, or underwater telecommunications [7].

In acoustics, an ideal time-reversed procedure begins with the emission of a short pulse by a point-like source, placed at position $\mathbf{r}_0$. The time-dependence of both the pressure, p , and the normal velocity displacements, v_n , of the wave is measured at any point on a surface $\delta\Gamma$ surrounding the source. To time-reverse the wave field inside the volume Γ delimited by the closed surface, both p and v_n have to be time-reversed and emitted from $\delta\Gamma$. The time-reversal operation corresponds to the transformations $p(\mathbf{r}, t) \rightarrow p(\mathbf{r}, T_0 - t)$ and $v_n(\mathbf{r}, t) \rightarrow -v_n(\mathbf{r}, T_0 - t)$. Strictly speaking, the time T_0 is needed to ensure causality. However, by changing the origin of time during the back propagation, T_0 can be set to 0 without loss of generality. These time-reversed signals are then emitted by monopolar and dipolar sources that cover the surface. When the initial short pulse is a Dirac distribution, it has been shown [2] that the time-reversed pressure field, p_{TR} , is given by

$$p_{\text{TR}}(\mathbf{r}, t) \propto G(\mathbf{r}_0, \mathbf{r}, -t) - G(\mathbf{r}_0, \mathbf{r}, +t) , \quad (7.1)$$

where $G(\mathbf{r}_0, \mathbf{r}, t)$ is the causal Green's function ($G(\mathbf{r}_0, \mathbf{r}, t) = 0$ for $t < 0$).¹ $G(\mathbf{r}_0, \mathbf{r}, -t)$ is the anticausal Green's function, i.e., a converging wave. Due to

¹ The Green's function $G(\mathbf{r}_0, \mathbf{r}, t)$ is the field at time t and position $\mathbf{r}$ for a point-like source localized at $\mathbf{r}_0$ that emits a Dirac pulse at time $t = 0$.

energy conservation at the focus position $\mathbf{r}_0$, a diverging wave appears for $t > 0$ ($-G(\mathbf{r}_0, \mathbf{r}, +t)$ term). For a band-limited initial excitation, the interference of the converging and diverging waves gives rise to a focal spot. For a burst of central angular frequency ω , it can be shown that the pressure field distribution around $\mathbf{r}_0$ at time $t = 0$ is given by the Fourier transform of $p_{\text{TR}}(\mathbf{r}, t)$. Equation (7.1) leads to

$$p_{\text{TR}}(\mathbf{r}, \omega) \propto G(\mathbf{r}_0, \mathbf{r}, \omega)^* - G(\mathbf{r}_0, \mathbf{r}, \omega) \quad (7.2)$$

$$\propto \text{Im}G(\mathbf{r}_0, \mathbf{r}, \omega) . \quad (7.3)$$

Therefore, the time-reversed focal spot is governed by the imaginary part of the Green's function. The simplest propagation medium is the isotropic 3D-homogeneous propagation medium. In such a case, it is well known that the Green's function is given by

$$G(\mathbf{r}_0, \mathbf{r}, \omega) = \frac{e^{-ik\|\mathbf{r}-\mathbf{r}_0\|}}{4\pi\|\mathbf{r}-\mathbf{r}_0\|} , \quad (7.4)$$

where k is the wavenumber. Contrary to the real part of G that shows a singularity at $\mathbf{r} = \mathbf{r}_0$, the imaginary part is continuous and proportional to $\sin(k\|\mathbf{r}-\mathbf{r}_0\|)/\|\mathbf{r}-\mathbf{r}_0\|$. So is it for the focal spot. Consequently, the focal spot size equals a half-wavelength in agreement with the diffraction limit.

In this chapter, our goal is to present the very fundamentals of electromagnetic time-reversal as it was previously done for scalar waves (in acoustics). We begin with some generalities about time-symmetry for electromagnetic fields. Then, the link between time-reversal and phase-conjugation is established and an integral relation between a field and its phase conjugated is written. To handle concise expressions, we next introduce a vector that gathers the electric and the magnetic fields and generalizes the Green's function formalism. Finally, we write the so-called integral relation of time-reversal that involves the imaginary part of the Green's function. The full development is reported in the appendices. A close look is given to the final equation predicting the form of the time-reversed field. As an example, the case of the homogeneous medium is investigated. A simplified expression is established under the far-field approximation. We show that under this approximation, small electrical dipoles are sufficient to perform time-reversal. To conclude this chapter, one numerical and one experimental illustration are provided.

7.2 Time-Reversed Electromagnetic Fields

A propagation medium is said “reversible” if a field and its time-symmetric can both propagate in it. In other words, the field and its time-symmetric (i.e., $\psi(\mathbf{r}, t)$ and $\psi(\mathbf{r}, -t)$) are both solutions of the same propagation equation. An electromagnetic wave is described by four vectorial fields, the electric field $\mathbf{E}$, the magnetic field $\mathbf{H}$, the electric displacement $\mathbf{D}$, and the magnetic induction

B. Due to the intrinsic definition of these fields, $\mathbf{E}$ and $\mathbf{D}$ are even under a time-reversal transformation while $\mathbf{H}$ and $\mathbf{B}$ are odd [9]. Introducing the time-reversal operator T , this property can be concisely written as follows

$$\begin{aligned} T\mathbf{E}(\mathbf{r}; t) &= \mathbf{E}(\mathbf{r}; -t) , & T\mathbf{D}(\mathbf{r}; t) &= \mathbf{D}(\mathbf{r}; -t) , \\ T\mathbf{H}(\mathbf{r}; t) &= -\mathbf{H}(\mathbf{r}; -t) , & T\mathbf{B}(\mathbf{r}; t) &= -\mathbf{B}(\mathbf{r}; -t) . \end{aligned} \quad (7.5)$$

The four Maxwell's equations are time-symmetric. Thus the propagation medium is reversible under the assumption that the permittivity and the permeability tensors are themselves time-symmetric.

When wave propagation is linear, the general relation between $\mathbf{D}$ and $\mathbf{E}$ writes $\mathbf{D}(\mathbf{r}; t) = \varepsilon(\mathbf{r}; t) \otimes \mathbf{E}(\mathbf{r}; t)$, where the permeability $\varepsilon(\mathbf{r}, t)$ is a tensor of rank 2 and $\otimes$ is the time convolution product. For the time symmetric fields, this relation becomes $\mathbf{D}(\mathbf{r}; -t) = \varepsilon(\mathbf{r}; -t) \otimes \mathbf{E}(\mathbf{r}; -t)$. But when the propagation medium is reversible, we also have $\mathbf{D}(\mathbf{r}; -t) = \varepsilon(\mathbf{r}; t) \otimes \mathbf{E}(\mathbf{r}; -t)$ because these fields are also solution of the propagation equations. From the two last equations, we deduce that $\varepsilon(\mathbf{r}; t) = \varepsilon(\mathbf{r}; -t)$. Moreover the permeability tensor is causal, i.e., $\varepsilon(\mathbf{r}; t) = 0$ for $t < 0$. Consequently in causal and reversible propagation media, the permittivity tensor writes as to $\varepsilon(\mathbf{r})\delta(t)$. Exactly the same arguments hold for the permeability μ , defined by $\mathbf{B}(\mathbf{r}; t) = \mu(\mathbf{r}; t) \otimes \mathbf{H}(\mathbf{r}; t)$. Hence, the permeability is given by $\mu(\mathbf{r})\delta(t)$. These results are consistent with the Kramers–Kronig relations: the response of a lossless propagation medium is instantaneous [9].

7.3 Time-Reversed and Phase-Conjugated Fields

Let us introduce the Fourier transform $\psi(\mathbf{r}; \omega)$ of a field $\psi(\mathbf{r}; t)$ such as $\psi(\mathbf{r}; \omega) = \int \psi(\mathbf{r}; t) \exp(i\omega t) dt$. The operator T applied to $\psi(\mathbf{r}; \omega)$ is defined by

$$T\psi(\mathbf{r}; \omega) = \int T\psi(\mathbf{r}; t) \exp(i\omega t) dt.$$

Using the definition of T ($T\psi(\mathbf{r}; t) = \psi(\mathbf{r}; -t)$) and doing the change of variable $t \rightarrow -t'$, it comes

$$T\psi(\mathbf{r}; \omega) = \int \psi(\mathbf{r}; t') \exp(-i\omega t') dt'.$$

Since the field $\psi(\mathbf{r}; t')$ is real-valued, the previous expression leads to $\psi(\mathbf{r}; \omega)$

$$T\psi(\mathbf{r}; \omega) = \psi^*(\mathbf{r}; \omega). \quad (7.6)$$

Hence time-reversing a field is formally equivalent to phase-conjugate its Fourier transform. The benefit to work in the frequency domain is to replace time convolutions by simple products. From now on, we work in the frequency domain and omit the explicit frequency dependence of the fields.

7.4 Integral Relation Between two Fields and Their Conjugates

Let us consider two sets of electromagnetic fields $\mathbf{E}_1, \mathbf{H}_1$ and $\mathbf{E}_2, \mathbf{H}_2$ generated, respectively, by the current densities and the magnetization current densities $\mathbf{j}_1, \mathbf{m}_1$ and $\mathbf{j}_2, \mathbf{m}_2$. When ε and μ are hermitian, the following expression can be deduced from the Maxwell's equations (see (7.38) in Appendix A)

$$\nabla \cdot (\mathbf{H}_1^* \times \mathbf{E}_2 + \mathbf{H}_2 \times \mathbf{E}_1^*) = \mathbf{H}_2 \mathbf{m}_1^* + \mathbf{H}_1^* \mathbf{m}_2 + \mathbf{E}_2 \mathbf{j}_1^* + \mathbf{E}_1^* \mathbf{j}_2. \quad (7.7)$$

This expression is a generalization of the energy flux conservation principle. Indeed, when $\mathbf{m}_1 = \mathbf{m}_2, \mathbf{j}_1 = \mathbf{j}_2, \mathbf{H}_1 = \mathbf{H}_2$, and $\mathbf{E}_1 = \mathbf{E}_2$, the integration of (7.7) over a volume V defined by a closed surface δV gives

$$\oint_{\delta V} \mathbf{P} \, d^3r = -\frac{1}{2} \int_V \operatorname{Re} (\mathbf{H}_1^* \mathbf{m}_1 + \mathbf{E}_1^* \mathbf{j}_1) \, d^3r, \quad (7.8)$$

where $\mathbf{P}$ is the Poynting's vector ($\mathbf{P} = \operatorname{Re} (\mathbf{E}_1 \times \mathbf{H}_1^*) / 2$).

7.5 Electromagnetic and Source Vectors

To handle at the same time the electric field and the magnetic field, it is convenient to introduce an electromagnetic vector ψ :

$$\psi(\mathbf{r}) = \begin{pmatrix} \mathbf{E}(\mathbf{r}) \\ i\mathbf{H}(\mathbf{r}) \end{pmatrix}. \quad (7.9)$$

The dimension of ψ equals 6.

In the same way, a source vector q is introduced. It is defined by

$$q(\mathbf{r}) = \begin{pmatrix} i\mathbf{j}(\mathbf{r}) \\ \mathbf{m}(\mathbf{r}) \end{pmatrix}. \quad (7.10)$$

In terms of antenna theory, $\mathbf{j}$ represents a distribution of infinitely small dipoles and $\mathbf{m}$ a distribution of infinitely small current loops.

The definitions of ψ and q have been chosen in order to get even time-reversal transformation of these fields, i.e., $T\psi = \psi^*$ and $Tq = q^*$. With this definition, a special scalar product, represented by a dot, can be introduced:

$$\begin{pmatrix} \mathbf{A}_1 \\ \mathbf{B}_1 \end{pmatrix} \cdot \begin{pmatrix} \mathbf{A}_2 \\ \mathbf{B}_2 \end{pmatrix} = \mathbf{A}_1 \mathbf{B}_1 - \mathbf{A}_2 \mathbf{B}_2. \quad (7.11)$$

Thanks to this definition, the expression of the reciprocity theorem [1] which is usually written as follows:

$$\int \mathbf{E}_2(\mathbf{r}) \mathbf{j}_1(\mathbf{r}) - \mathbf{H}_2(\mathbf{r}) \mathbf{m}_1(\mathbf{r}) \, d^3r = \int \mathbf{E}_1(\mathbf{r}) \mathbf{j}_2(\mathbf{r}) - \mathbf{H}_1(\mathbf{r}) \mathbf{m}_2(\mathbf{r}) \, d^3r, \quad (7.12)$$

becomes

$$\int \psi_1(\mathbf{r}) \cdot q_2(\mathbf{r}) \, d^3r = \int \psi_2(\mathbf{r}) \cdot q_1(\mathbf{r}) \, d^3r. \quad (7.13)$$

7.6 Green's Functions

The Green's function $\bar{G}$ is an operator that linearly relates the field vector distribution to the source vector distribution, namely

$$\psi(\mathbf{r}) = \int \bar{G}(\mathbf{r}', \mathbf{r}) q(\mathbf{r}') d^3 r' . \quad (7.14)$$

For the sake of simplicity, when no confusion can arise, the volume of integration in (7.14) is kept implicit and the integral is written as follows:

$$\int \bar{G}(\mathbf{r}', \mathbf{r}) q(\mathbf{r}') d^3 r' = [\bar{G}(\mathbf{r}) q] . \quad (7.15)$$

The dimension of the Green's function $\bar{G}$ is 6 by 6.

7.7 The Time-Reversal Relation

From (7.7), an integral relation [(7.44) in Appendix A] can be derived using the Green's function formalism previously introduced. Moreover, in Appendix B, it is shown that using the reciprocity theorem the following integral equation can be obtained:

$$\underbrace{\oint_{\delta\Gamma} \bar{G}(\mathbf{r}, \mathbf{r}') (\mathbf{n}(\mathbf{r}') \times [\bar{G}^*(\mathbf{r}') q_1^*]) d^2 r'}_{\psi_S(\mathbf{r})} = -2 \underbrace{\int_{\Gamma} \text{Im} \bar{G}(\mathbf{r}', \mathbf{r}) q_1(\mathbf{r})^* d^3 r'}_{\psi_V(\mathbf{r})}, \quad (7.16)$$

where $\mathbf{n}(\mathbf{r}')$ is the normal vector to the surface $\delta\Gamma$ at position $\mathbf{r}'$. In order to obtain this relation, it has been assumed that the tensors $\varepsilon(\mathbf{r})$ and $\mu(\mathbf{r})$ are both hermitian and symmetric. Obviously, these two properties imply that ε and μ are real. This is consistent with the time-symmetry assumption stated in Sect. 7.2.

In the next two sections, we discuss the physical meaning of the left and right hand sides of (7.16).

7.7.1 Left-Hand Side of (7.16)

The field on the left-hand side, ψ_s , can be interpreted as follows: in a first step, the source q_1 generates the field ψ_1 ($\psi_1(\mathbf{r}) = \bar{G}(\mathbf{r}) q_1$). The electric and magnetic components of $\psi_1(\mathbf{r}')$ are recorded on a closed surface $\delta\Gamma$. The wave field is time-reversed, i.e., $\psi_1(\mathbf{r}')$ is phase-conjugated. From this phase-conjugated field, a new distribution q_{TR} of dipolar/loop current sources on the closed surface is deduced

$$q_{\text{TR}}(\mathbf{r}') = \mathbf{n}(\mathbf{r}') \times \psi_1^*(\mathbf{r}') . \quad (7.17)$$

This expression of q_{TR} can be simplified when the initial sources represented by q_1 are far from the cavity boundaries. In such a case, the electromagnetic wave is locally plane near the closed surface $\delta\Gamma$. Hence the electric and magnetic fields are orthogonal, that is $\mathbf{H} \approx \mathbf{k} \times \mathbf{E}/\eta \|\mathbf{k}\|$, where $\mathbf{k}$ is the wave vector and η is the characteristic impedance of vacuum ($\eta = \sqrt{\mu/\varepsilon}$). Assuming a spherical closed cavity, the local wave vector is normal to the surface ($\mathbf{n} = \mathbf{k}/\|\mathbf{k}\|$), i.e., $\mathbf{H} \approx \mathbf{n} \times \mathbf{E}/\eta$ and the time-reversed source distribution expression can be simplified. It reads

$$q_{\text{TR}}(\mathbf{r}') = -i \begin{pmatrix} \mathbf{E}^*(\mathbf{r}')/\eta \\ -i\eta\mathbf{H}^*(\mathbf{r}') \end{pmatrix}. \quad (7.18)$$

Hence, in the far-field approximation, time-reversing an electromagnetic field simply consists in recording the currents induced in small wires and loop antennas, and time-reversing them.

7.7.2 Right-Hand Side of (7.16)

The sources at the surface generate the field ψ_v inside the volume Γ . This field is directly related to the imaginary part of the Green's function. It can be rewritten using the implicit integration notation

$$\psi_v(\mathbf{r}) = \overline{G}^*(\mathbf{r})q_1^* - \overline{G}(\mathbf{r})q_1^*. \quad (7.19)$$

The first term is equal to ψ_1^* , that is the time-reversal version of ψ_1 . Thus as expected, time-reversing the field from a closed surface $\delta\Gamma$ leads to create the time-reversed field (a converging wave) in the whole volume Γ . However, this field is not created alone; the $-\overline{G}(\mathbf{r})q_1^*$ term is added, which is a “diverging” field. As we discuss in the next section, the interference between the converging and the diverging wave has an impact on the size of the focal spot. But before, it must be pointed out that this extra term “breaks” the time-reversal process. As shown in [18], to recover the converging time-reversed wave $T\psi$ only, one has to time-reverse not only the field on the closed surface but also to time-reverse the initial source itself. The time-reversed source is a source with an excitation term Tq_1 . In such a case, the diverging wave $\overline{G}(\mathbf{r})q_1^*$ is added to the time-reversed wave $\psi_v(\mathbf{r})$. The time-reversed source and the active surface thus generate two diverging waves that are opposite in sign. The destructive interference between these two waves finally leads to only get the converging time-reversed field $T\psi$.

7.8 Focal Spot in a Homogeneous Medium

In acoustics, it has been shown that the interference between the two waves inside a homogeneous medium produces a half-wavelength sized focal spot. Here we show that the same effect occurs for electromagnetic waves. For the sake

of simplicity, we introduce the electric–electric, electric–magnetic, magnetic–electric, and magnetic–magnetic Green’s functions. This set of four Green’s functions form the Green’s function $\bar{G}$

$$\bar{G}(\mathbf{r}, \mathbf{r}_0) = \begin{pmatrix} G_{EE}(\mathbf{r}, \mathbf{r}_0) & G_{EH}(\mathbf{r}, \mathbf{r}_0) \\ G_{HE}(\mathbf{r}, \mathbf{r}_0) & G_{HH}(\mathbf{r}, \mathbf{r}_0) \end{pmatrix}. \quad (7.20)$$

In a homogeneous medium, the propagation is invariant under translation, and consequently the Green’s functions only depend on $\mathbf{R} = \mathbf{r} - \mathbf{r}_0$. The expressions of the electric–electric and magnetic–electric Green’s functions in a homogeneous medium are given by [16]

$$G_{EE}(\mathbf{R})\mathbf{n} = \eta G_s(\mathbf{R}) \left[\left(i + \frac{1}{kR} \right) \left(\frac{\mathbf{n} - 3\hat{\mathbf{R}}(\hat{\mathbf{R}}\mathbf{n})}{R} \right) + k(\mathbf{n} \times \hat{\mathbf{R}}) \times \hat{\mathbf{R}} \right] \quad (7.21)$$

$$G_{EH}(\mathbf{R})\mathbf{n} = \left(ik + \frac{1}{R} \right) G_s(\mathbf{R})(\hat{\mathbf{R}} \times \mathbf{n}), \quad (7.22)$$

where $G_s(\mathbf{R})$ is the scalar Green’s function ($G_s(\mathbf{R}) = \exp(-ikR)/4\pi$) and $\hat{\mathbf{R}} = \mathbf{R}/R$.

Due to the symmetry between electric and magnetic fields, it comes

$$G_{HH}(\mathbf{R}) = \eta^2 G_{EE}(\mathbf{R}), \quad (7.23)$$

$$G_{HE}(\mathbf{R}) = -G_{EH}(\mathbf{R}). \quad (7.24)$$

Singularities of the Green’s function at position $\mathbf{R} = 0$ can only come from the $\frac{e^{-ikR}}{kR}$ and $(i + \frac{1}{kR})\frac{e^{-ikR}}{(kR)^2}$ terms. These terms near $\mathbf{R} = 0$ are well approximated by

$$\frac{e^{-ikR}}{kR} = \frac{1}{kR} - i + o(kR) \quad (7.25)$$

and

$$\left(i + \frac{1}{kR} \right) \frac{e^{-ikR}}{(kR)^2} = \frac{1}{(kR)^3} + \frac{1}{2kR} - \frac{i}{3} + o(kR). \quad (7.26)$$

Hence, only the real part of $\bar{G}(\mathbf{R})$ shows a strong singularity. The fluctuations of the imaginary part of the Green’s are due to the $o(kR)$ terms. In other words, the typical size of the focal spot is of the order of the wavelength.

7.9 Far-Field Time-Reversal by Dipoles

Here we show that in the far-field approximation, it is not necessary to use both the electric dipoles and the magnetic loops to time-reverse a wave; the electric field can be time-reversed using only electric dipoles. This is an important issue in terms of applications where it is difficult to measure/generate at the same time the electric and magnetic fields.

When the electric field is time-reversed by only electric small dipoles, the field ψ_S generated by the close surface is given by

$$\psi_S(\mathbf{r}) = \oint_{\delta\Gamma} \bar{G}(\mathbf{r}, \mathbf{r}') q_{\text{TR}}^d(\mathbf{r}') d^2r', \quad (7.27)$$

where

$$q_{\text{TR}}^d(\mathbf{r}') = -i \begin{pmatrix} \mathbf{E}^*(\mathbf{r}')/\eta \\ 0 \end{pmatrix}. \quad (7.28)$$

The source distribution q_{TR}^d can be expressed as the sum of two source terms with opposite magnetization currents

$$q_{\text{TR}}^d(\mathbf{r}') = -\frac{i}{2} \underbrace{\begin{pmatrix} \mathbf{E}^*(\mathbf{r}')/\eta \\ -i\eta\mathbf{H}^*(\mathbf{r}') \end{pmatrix}}_{q_{\text{TR}}^{\text{in}}(\mathbf{r}')} - \frac{i}{2} \underbrace{\begin{pmatrix} \mathbf{E}^*(\mathbf{r}')/\eta \\ i\eta\mathbf{H}^*(\mathbf{r}') \end{pmatrix}}_{q_{\text{TR}}^{\text{out}}(\mathbf{r}')} . \quad (7.29)$$

The first source term $q_{\text{TR}}^{\text{in}}$ is equal to half the source distribution q_{TR} [see (7.18)]. We have seen in Sect. 7.7 that this term produces the time-reversed wave inside the volume Γ . As for the $q_{\text{TR}}^{\text{out}}(\mathbf{r}')$ term, it generates a local plane wave at position $\mathbf{r}'$ that is opposite in direction to the one due to $q_{\text{TR}}^{\text{in}}(\mathbf{r}')$ because the magnetic currents are opposite in sign. Thus the second source term produces a wave toward the outside of the closed volume that does not interfere with the time-reversed wave inside the volume. Note that unless a very special geometry for the surface $\delta\Gamma$ is used, such as two infinite parallel planes, the wave produced by $q_{\text{TR}}^{\text{out}}$ source does not exhibit particular focusing properties.

7.10 Numerical Simulation

We used the simulation software called *Numerical Electromagnetics Code* (NEC) [14]. It is based on a moment method. This software that computes the complex fields at one frequency is well suited for analyzing the radiation of wire antennas. The numerical computation has been performed with 124 time-reversal dipoles uniformly distributed over a six-wavelength radius sphere. The initial dipole is at the center O of the sphere and its polarization is parallel to the unit vector $\hat{\mathbf{z}}$.

At first, amplitude, phase, and direction of the electric field radiated by this dipole are recorded at the 124 time-reversal elements. Then, the 124 fields are phase conjugated, and re-emitted by the dipoles on the sphere. In Fig. 7.1 is plotted the z -component of the electric field along the x -axis with respect to the distance to O . To compare with, the imaginary part of the z - z component of the electric-electric Green's function has been computed along the x axis. From (7.21), it follows that

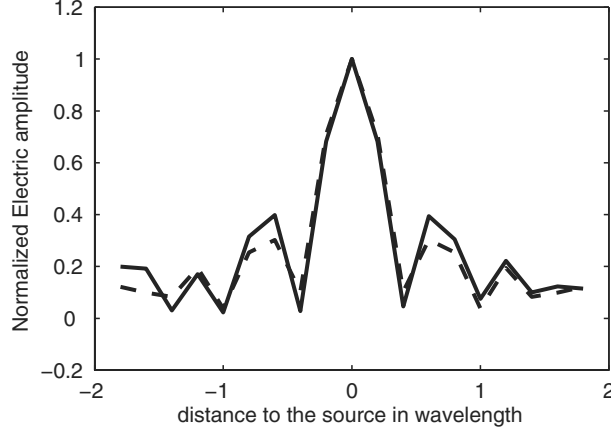


Fig. 7.1. Normalized amplitude of the z -component of the electric field with respect to the distance to the initial emitting dipole along the x -axis. Continuous (resp. *dash-dotted*) line corresponds to the time-reversed field, i.e, the focal spot (resp. the imaginary part of the Green's function)

$$\hat{\mathbf{z}}G_{\text{EE}}(R\hat{\mathbf{x}})\hat{\mathbf{z}} = \frac{\eta}{4\pi} [\cos(kR) - i\sin(kR)] \left[\left(i + \frac{1}{kR} \right) \frac{1}{R^2} - k \right]. \quad (7.30)$$

From this expression, the imaginary part can be easily deduced

$$\text{Im} \hat{\mathbf{z}}G_{\text{EE}}(R\hat{\mathbf{x}})\hat{\mathbf{z}} = \frac{\eta}{4\pi} \left[\frac{\cos(kR)}{R^2} - \sin(kR) \left(\frac{1}{kR^3} - k \right) \right]. \quad (7.31)$$

The function $\text{Im} \hat{\mathbf{z}}G_{\text{EE}}(R\hat{\mathbf{x}})\hat{\mathbf{z}}$ is plotted in Fig. 7.1. The agreement with the simulation result is excellent which confirms our theoretical approach.

7.11 Experimental Results

Several time-reversal experiments have already been reported [8, 10, 12]. To implement time-reversal for microwaves, we have built the experimental setup presented in Fig. 7.2. The electronic part consists of a waveform generator and a scope working around 2.45 GHz with a 250 MHz bandwidth. This setup stands for a single channel Time Reversal Mirror (TRM). A pair of 8-channel switches is used, the first one to emulate a eight-channel TRM, the other one to emulate a 8-channel receiver. As we are limited to 8 antennas for the TRM, the experiments have been conducted in a reverberation chamber consisting of a $1 - m^3$ aluminum cavity. Indeed, thanks to the image theorem, the reflections off the cavity boundaries create many virtual images of the time-reversal antennas and the back-propagated field is close to the one obtained if the reverberating surfaces were replaced by time-reversal antennas completely surrounding the source [4, 6].

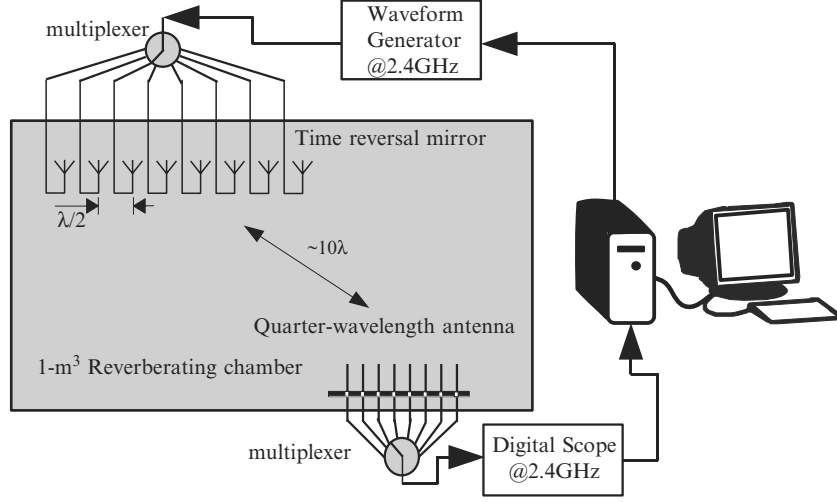


Fig. 7.2. Experimental setup

We used two kinds of antennas: commercial monodirectional WIFI antennas are used on the TRM side whereas on the receiving part the field is scanned with a homemade antenna array. This array consists of eight quarter-wavelength thin wires on a ground plane which avoids cable parasitic radiations. The spacing between antennas is 1.56 cm, i.e., $\lambda/8$. Using such an “ideal” array allows one to estimate the spatial focusing.

In an usual time-reversal experiment, the initial source emits a short pulse and the impulse responses are recorded at each antenna of the TRM. In practice, we use a slightly different procedure to record the set of impulse responses between the antenna at position O where one intends to refocus back and the time-reversal mirror made of eight antennas. Here each antenna of the TRM emits successively a 10-ns long pulse and the corresponding impulse responses are recorded at the antenna O and digitized by the scope. Due to reciprocity of the medium, these two sets of impulse responses are strictly identical. Figure 7.3a shows a typical impulse response between two antennas within the cavity. We see that the reverberation time of the cavity is about $\tau_R = 250$ ns which means a spreading of the initial pulse by a factor 25. This actually depends on the chosen antenna pair. Thus we estimate the spread time among the set of 64 possible responses recorded between the eight elements of the emitting array (TRM), and the eight elements of the receiving array. An average value of 16 is finally found.

The eight responses are then time-reversed, normalized by their maximum amplitude, and successively transmitted by each antenna of the TRM. In Fig. 7.3b is plotted the resulting time compression obtained in summing the contributions produced by each antenna of the TRM. A pulse of 10 ns is recovered which is the time-reversed replica of the initial 10-ns long pulse.

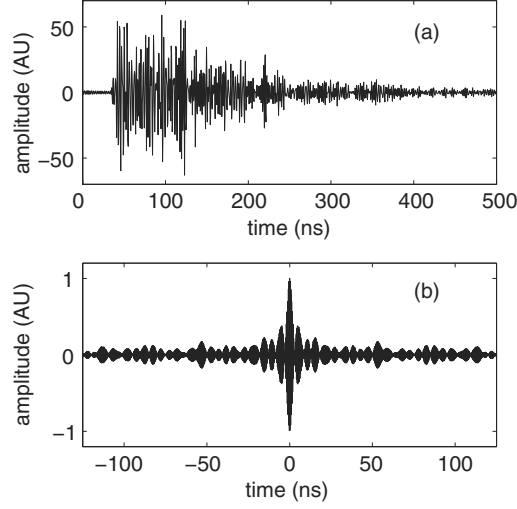


Fig. 7.3. (a) One impulse response between one antenna of the TRM and one antenna of the quarter wavelength antenna array. (b) Temporal focusing after time-reversal

This pulse is surrounded by sidelobes. In the reverberating cavity, the Green's function is not exactly equal to the free space one. It adds to the direct wavefront, the echoes due to the multiple reflections off the boundaries. The temporal side lobes are due to these echoes.

We now study the spatial focusing. Time-reversal focusing in disordered media has been studied both experimentally and theoretically for ultrasound in [3, 5, 6], theoretically for electromagnetic fields in random media in [15], and used in communications in [8, 11]. Experimental characterization of the TR focal spot for wide-band electromagnetic waves is really interesting both for applied and theoretical physics. The quarter-wavelength antenna array has been used in order to scan the TR focal spot with minimum corruption. The field could be scanned by moving an antenna in the plane around the focusing point but this procedure would affect the measurement since a radiator is also a scatterer and hence modifies an electromagnetic field. In Fig. 7.4 is plotted the maximum of the TR wave with respect to the distance from the antenna onto which the wave is refocused back. Our antennas being vertically polarized, we are sensitive to the z component of the field and the direction of scanning, x , is perpendicular to this direction. The expression of the z component of the time-reversed electric field is given by (7.31).

However, from an experimental point of view, we do not record E_z , but the current that this field induces. The full development of the model is out of the scope of this chapter and will be presented elsewhere. Especially, we have shown that the measured current also depends on the mutual coupling

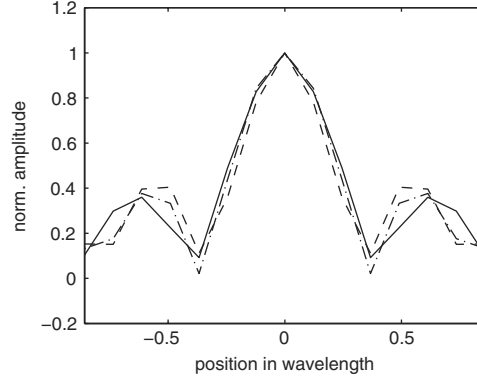


Fig. 7.4. Three time-reversal focal spots: experimental data (*dashed line*), imaginary part of the Green's function (*continuous line*), and theory (*dash-dotted line*)

between antennas [17]. We see that the experimental focal spot obtained with the 8-channel TRM is in good agreement with the theoretical prediction.

7.12 Conclusion

In this chapter, we have introduced an integral formulation for time-reversal of electromagnetic waves. It is valid when the medium is at the same time reciprocal and time-symmetric. As in acoustics, the focal spot is governed by the imaginary part of the Green's function. Under the far-field approximation, the electric field has only to be time-reversed from small electric dipoles to generate the time-reversed wave. Numerical and experimental results confirm our approach.

The theory presented in this chapter is very general; (7.16) enables one to predict the focal spot in any kind of medium (homogeneous or heterogeneous), and for example when the initial source is surrounded by a dense clutter of small metallic wires placed in the near-field [13]. In such a case, we have experimentally demonstrated that the time-reversed wave focuses on a sub-wavelength spot. That experimental result tells us that in such a cluttered medium the imaginary part of the Green's function oscillates much faster than the vacuum wavelength. One way to interpret this result is to use the evanescent wave formalism. Indeed, the evanescent waves are usually lost in a homogeneous medium and thus do not participate to the focal spot : the focal spot size cannot be smaller than half-a-wavelength. But thanks to the metallic wires, they can be converted into propagating waves. Thus when the propagating waves are time-reversed, these propagating waves are converted back into evanescent components and may give rise to a sub-wavelength spot.

A Proof of Equation (7.7)

Let us consider two sets of electromagnetic fields $\mathbf{E}_1, \mathbf{H}_1$ and $\mathbf{E}_2, \mathbf{H}_2$ that are respectively generated by the current densities and the magnetization current densities $\mathbf{j}_1, \mathbf{m}_1$ and $\mathbf{j}_2, \mathbf{m}_2$. These fields are solution of the Maxwell's generalization of the Ampère's law

$$\nabla \times \mathbf{H}_1^* = \mathbf{j}_1^* - i\omega \mathbf{D}_1^* \quad (7.32)$$

$$\nabla \times \mathbf{H}_2 = \mathbf{j}_2 + i\omega \mathbf{D}_2, \quad (7.33)$$

and solution of the Faraday's law

$$-\nabla \times \mathbf{E}_1^* = \mathbf{m}_1^* - i\omega \mathbf{B}_1^* \quad (7.34)$$

$$-\nabla \times \mathbf{E}_2 = \mathbf{m}_2 + i\omega \mathbf{B}_2, \quad (7.35)$$

In most propagation media, the electric flux density linearly depends on the electric field density, i.e., $\mathbf{D} = \varepsilon \mathbf{E}$ where ε is the permittivity tensor. In the same way $\mathbf{B} = \mu \mathbf{H}$ where μ is the permeability tensor. Both tensors μ and ε can depend on position.

Using these properties, $\mathbf{E}_1^*$ times (7.33) plus $\mathbf{E}_2$ times (7.32) leads to

$$\mathbf{E}_2 \nabla \times \mathbf{H}_1^* + \mathbf{E}_1^* \nabla \times \mathbf{H}_2 = \mathbf{E}_2 \mathbf{j}_1^* + \mathbf{E}_1^* \mathbf{j}_2 + i\omega (\mathbf{D}_2 \mathbf{E}_1^* - \mathbf{E}_2 \mathbf{D}_1^*), \quad (7.36)$$

and $\mathbf{H}_2$ times (7.34) plus $\mathbf{H}_1^*$ times (7.35) writes

$$-\mathbf{H}_1^* \nabla \times \mathbf{E}_2 - \mathbf{H}_2 \nabla \times \mathbf{E}_1^* = \mathbf{H}_2 \mathbf{m}_1^* + \mathbf{H}_1^* \mathbf{m}_2 + i\omega (\mathbf{B}_2 \mathbf{H}_1^* - \mathbf{H}_2 \mathbf{B}_1^*). \quad (7.37)$$

Adding (7.36) and (7.37) leads to the following differential equation

$$\nabla (\mathbf{H}_1^* \times \mathbf{E}_2 + \mathbf{H}_2 \times \mathbf{E}_1^*) = \mathbf{H}_2 \mathbf{m}_1^* + \mathbf{H}_1^* \mathbf{m}_2 + \mathbf{E}_2 \mathbf{j}_1^* + \mathbf{E}_1^* \mathbf{j}_2. \quad (7.38)$$

This expression has been obtained, thanks to the vectorial identity

$$\nabla \mathbf{A} \times \mathbf{B} = \mathbf{B} (\nabla \times \mathbf{A}) - \mathbf{A} (\nabla \times \mathbf{B}). \quad (7.39)$$

Moreover, it has been assumed that $\mathbf{D}_2 \mathbf{E}_1^* = \mathbf{E}_2 \mathbf{D}_1^*$ and $\mathbf{B}_2 \mathbf{H}_1^* = \mathbf{H}_2 \mathbf{B}_1^*$. In other words, (7.38) is obtained when the permittivity and permeability tensors are hermitian. Both sides of (7.38) are integrated over a volume V delimited by a closed surface δV . Using the Green's theorem on the left hand side, it comes

$$\begin{aligned} \oint_{\delta V} (\mathbf{H}_1^* \times \mathbf{E}_2 + \mathbf{H}_2 \times \mathbf{E}_1^*) \cdot \mathbf{n} \, d^2 r \\ = \int_V \mathbf{H}_2 \mathbf{m}_1^* + \mathbf{H}_1^* \mathbf{m}_2 + \mathbf{E}_2 \mathbf{j}_1^* + \mathbf{E}_1^* \mathbf{j}_2 \, d^3 r, \end{aligned} \quad (7.40)$$

where $\mathbf{n}$ is the normal to surface $\delta\Gamma$. Using the mixed product properties, the previous expression can be rewritten

$$\begin{aligned} & \oint (\mathbf{n} \times \mathbf{H}_1^*) \mathbf{E}_2 + (\mathbf{E}_1^* \times \mathbf{n}) \mathbf{H}_2 \, d^2r \\ &= \int \mathbf{H}_2 \mathbf{m}_1^* + \mathbf{H}_1^* \mathbf{m}_2 + \mathbf{E}_2 \mathbf{j}_1^* + \mathbf{E}_1^* \mathbf{j}_2 \, d^3r . \end{aligned} \quad (7.41)$$

Replacing the fields by their equivalent six-dimension vectors (see Sect. 7.5), it comes

$$\oint_{\delta\Gamma} \psi_2(\mathbf{r}') \cdot [\mathbf{n}(\mathbf{r}') \times \psi_1^*(\mathbf{r}')] \, d^2r' = \int_{\Gamma} [\psi_1^*(\mathbf{r}') \cdot q_2(\mathbf{r}') - \psi_2(\mathbf{r}') \cdot q_1^*(\mathbf{r}')] \, d^3r' , \quad (7.42)$$

where the $\times$ product operator is defined by

$$\mathbf{n} \times \begin{pmatrix} \mathbf{A} \\ \mathbf{B} \end{pmatrix} = \begin{pmatrix} \mathbf{n} \times \mathbf{B} \\ \mathbf{n} \times \mathbf{A} \end{pmatrix} . \quad (7.43)$$

Finally, using the Green's function formalism introduced in 7.6, it follows that

$$\begin{aligned} & \oint_{\delta\Gamma} [\bar{G}(\mathbf{r}') q_2] \cdot [\mathbf{n}(\mathbf{r}') \times (\bar{G}^*(\mathbf{r}') q_1^*)] \, d^2r' \\ &= \int_{\Gamma} q_2(\mathbf{r}') \cdot [\bar{G}^*(\mathbf{r}') q_1^*] - q_1^*(\mathbf{r}') [\bar{G}(\mathbf{r}') q_2] \, d^3r' . \end{aligned} \quad (7.44)$$

B Reciprocity

The integral form of the reciprocity theorem is given by [1]

$$\int \mathbf{E}_1 \mathbf{j}_2 + \mathbf{H}_2 \mathbf{m}_1 - \mathbf{E}_2 \mathbf{j}_1 - \mathbf{H}_1 \mathbf{m}_2 \, d^3r = 0 . \quad (7.45)$$

By introducing electromagnetic and source vectors, this expression can be rewritten as follows

$$\int \psi_1(\mathbf{r}) \cdot q_2(\mathbf{r}) \, d^3r = \int \psi_2(\mathbf{r}) \cdot q_1(\mathbf{r}) \, d^3r . \quad (7.46)$$

Using the Green's function formalism introduced in (7.6), one obtains

$$\int q_2(\mathbf{r}) \cdot \bar{G}(\mathbf{r}) q_1 \, d^3r = \int q_1(\mathbf{r}) \cdot \bar{G}(\mathbf{r}) q_2 \, d^3r . \quad (7.47)$$

This expression remains valid when q_1 is replaced by q_1^* ,

$$\int q_2(\mathbf{r}) \cdot \bar{G}(\mathbf{r}) q_1^* \, d^3r = \int q_1^*(\mathbf{r}) \cdot \bar{G}(\mathbf{r}) q_2 \, d^3r . \quad (7.48)$$

Thus, as long as the propagation medium is reciprocal, (7.44) can be rewritten as

$$\begin{aligned} & \int_{\Gamma} \oint_{\delta\Gamma} q_2(\mathbf{r}) \cdot \bar{G}(\mathbf{r}', \mathbf{r}) [\mathbf{n}(\mathbf{r}') \times (\bar{G}^*(\mathbf{r}') q_1^*)] d^2 r' d^3 r \\ &= \int_{\Gamma} q_2(\mathbf{r}) \cdot [\bar{G}^*(\mathbf{r}) q_1^*] - q_2(\mathbf{r}) \cdot [\bar{G}(\mathbf{r}) q_1^*] d^3 r, \end{aligned} \quad (7.49)$$

where relation (7.47) has been used twice, once in the left-hand side of (7.44) and another time in the right-hand side. This relation is valid whatever q_2 is, and so q_2 can be omitted.

$$\oint_{\delta\Gamma} \bar{G}(\mathbf{r}', \mathbf{r}) [\mathbf{n}(\mathbf{r}') \times (\bar{G}^*(\mathbf{r}') q_1^*)] d^2 r' = [\bar{G}^*(\mathbf{r}) q_1^*] - [\bar{G}(\mathbf{r}) q_1^*]. \quad (7.50)$$

Identity (7.50) is the starting point of the mathematical justification of properties of electromagnetic time-reversal.

References

- [1] C.A. Balanis, *Antenna Theory Analysis and Design*, Wiley-Interscience, 2005.
- [2] D. Cassereau and M. Fink, Time-reversal of ultrasonic fields. III. Theory of the closedtime-reversal cavity, *IEEE Trans. Ultrasonics, Ferroelectrics and Frequency Control* 39 (1992), 579–592.
- [3] A. Derode, A. Tourin, and M. Fink, Random multiple scattering of ultrasound. II. Is time reversal a self-averaging process?, *Phys. Rev. E* 64 (2001), 036606, doi = 10.1103/PhysRevE.64.036606.
- [4] C. Draeger, J.-C. Aimé, and M. Fink, One-channel time-reversal in chaotic cavities: Experimental results, *J. Acous. Soc. Amer.* 105 (1999), 618–625.
- [5] C. Draeger and M. Fink, One-channel time-reversal in chaotic cavities: Theoretical limits, *J. Acous. Soc. Amer.* 105 (1999), 611–617.
- [6] C. Draeger and M. Fink, One-Channel Time Reversal of Elastic Waves in a Chaotic 2D-Silicon Cavity, *Phys. Rev. Lett.* 79 (1997), 407–410.
- [7] M. Fink, Time Reversed Acoustics, *Physics Today* 50 (1997), 34.
- [8] B.E. Henty and D.D. Stancil, Multipath-Enabled Super-Resolution for rf and Microwave Communication using Phase-Conjugate Arrays, *Phys. Rev. Lett.* 93 (2004), 243904.
- [9] J.D. Jackson, *Classical Electrodynamics*, John Wiley & Sons Inc, 1975.
- [10] G. Lerosey, J. de Rosny, A. Tourin, A. Derode, and M. Fink, Time reversal of wideband microwaves, *Appl. Phys. Lett.* 88 (2006), 154101.
- [11] G. Lerosey, J. de Rosny, A. Tourin, A. Derode, G. Montaldo, and M. Fink, Time reversal of electromagnetic waves and telecommunication, *Radio Sci.* 40 (2005), RS612.

- [12] G. Lerosey, J. de Rosny, A. Tourin, A. Derode, G. Montaldo, and M. Fink, Time Reversal of Electromagnetic Waves, *Phys. Rev. Lett.* 92 (2004), 193904.
- [13] G. Lerosey, J. de Rosny, A. Tourin, and M. Fink, Focusing Beyond the Diffraction Limit with Far-Field Time Reversal, *Science* 315 (2007), 1120.
- [14] T. Marshall, Numerical Electromagnetics Code, <http://www.nec2.org/>.
- [15] C. Oestges, A.D. Kim, G. Papanicolaou, and A.J. Paulraj, Characterization of space-time focusing in time-reversed random fields, *IEEE Trans. Antenn. Prop.* 53 (2005), 283–293.
- [16] S. J. Orfanidis, *Electromagnetic Waves and Antennas*, Electronic book : <http://www.ece.rutgers.edu/~orfanidi/ewa>, 2004.
- [17] J. de Rosny, G. Lerosey and M. Fink, in preparation.
- [18] J. de Rosny and M. Fink, Overcoming the Diffraction Limit in Wave Physics Using a Time-Reversal Mirror and a Novel Acoustic Sink, *Phys. Rev. Lett.* 89 (2002), 124301.

Addition Theorem

B. He and W.C. Chew

8.1 Introduction

The addition theorem, which arises from the conservation of linear momentum, has wide applications in physical problems [7]. In recent years, it has played an increasingly important role in multiple scattering theory [1, 2]. More recently, it is intimately related to fast algorithms in computational electromagnetics [3].

In multiple scattering problems, the translation of multipoles from one coordinate system to another facilitates the formal solutions to these problems. When the wavenumber is zero, these problems reduce to static problems where the fields produced by the sources are Coulombic, or that they are solutions to Laplace equation. In early days, the addition theorem can also be used to formulate solutions to many-body problems in gravitation.

This translation between coordinate systems is described by addition theorem for scalar fields or vector fields. The addition theorem of scalar fields along an arbitrary direction is first derived by Friedman and Russek [4]. It was generalized to vector fields by Stein [5] and Cruzan [6]. It was further generalized to tensor fields by Danos and Maximon [7]. Their formulations can be expressed simply in terms of Wigner $3-j$ and $6-j$ symbols.

These multipoles are angular momentum eigenstates [7]. In Sect. 8.2, we will briefly review angular momenta and the additions of angular momenta. In Sect. 8.3, we will discuss a general translation. A general translation can be viewed as the multiplication of two rotations and a translation along the z axis. In Sects. 8.4 and 8.5, we will discuss the addition theorem for scalar, vector fields, and tensor fields following Danos and Maximon's method. In Sect. 8.6, we will review the diagonal forms of translation operators which are important for fast algorithms.

8.2 Angular Momentum

In this section, we give a brief overview of angular momentum. One can refer to some quantum mechanics books, e.g., [8, 9], for basic concepts of angular momentum. For a more detailed discussion on angular momentum, one can refer to [10–12].

8.2.1 Basic Concepts of Angular Momentum

In classical mechanics the angular momentum of a particle is defined by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}, \quad (8.1)$$

where $\mathbf{r}$ is the position vector of the particle and $\mathbf{p}$ is its linear momentum. In quantum mechanics, $\mathbf{L}$ is an operator whose components, which are also operators, obey the commutation rules

$$[L_x, L_y] = iL_z; [L_y, L_z] = iL_x; [L_z, L_x] = iL_y. \quad (8.2)$$

Here, we set $\hbar = 1$. The square of the angular momentum is defined as

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2. \quad (8.3)$$

Since $[\mathbf{L}^2, L_z] = 0$, one can choose eigenvectors of $\mathbf{L}^2$ and L_z simultaneously. The eigenvectors are expressed by Dirac notation $|lm\rangle$ such that

$$\mathbf{L}^2|lm\rangle = l(l+1)|lm\rangle, \quad (8.4)$$

$$L_z|lm\rangle = m|lm\rangle, \quad (8.5)$$

with the values of l and m

$$l = 0, 1, 2, \dots, \quad (8.6)$$

$$m = -l, -l+1, \dots, l. \quad (8.7)$$

It turns out that the eigenvectors $|lm\rangle$ can be represented as spherical harmonic functions $Y_{lm}(\vartheta, \varphi)$ in coordinate space $\langle\vartheta\varphi|$ as

$$\langle\vartheta\varphi|lm\rangle = Y_{lm}(\vartheta, \varphi). \quad (8.8)$$

Namely, spherical harmonic functions $Y_{lm}(\vartheta, \varphi)$ are the eigenfunctions which diagonalize $\mathbf{L}^2$ and L_z simultaneously.

Generally, the angular momentum denoted by $\mathbf{J}$ in quantum physics can be defined by operators similar to (8.2)

$$[J_x, J_y] = iJ_z; [J_y, J_z] = iJ_x; [J_z, J_x] = iJ_y. \quad (8.9)$$

The eigenvectors of $\mathbf{J}^2$ and J_z are given by

$$\mathbf{J}^2|jm\rangle = j(j+1)|jm\rangle, \quad (8.10)$$

$$J_z|jm\rangle = m|jm\rangle, \quad (8.11)$$

with the values of j and m

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \quad (8.12)$$

$$m = -j, -j+1, \dots, j. \quad (8.13)$$

This definition (8.9) permits the existence of spin operator denoted by $\mathbf{S}$, which arises from quantum mechanics, and has no classical counterpart.

8.2.2 Clebsch–Gordan Coefficients

The coupling of two angular momenta arises when the total angular momentum of a single particle is the sum of two parts (orbital and spin), or two particles. Now consider two angular momenta $\mathbf{J}_1$ and $\mathbf{J}_2$

$$\mathbf{J}_1^2 |j_1 m_1\rangle = j_1(j_1 + 1) |j_1 m_1\rangle, \quad (8.14)$$

$$J_{1z} |j_1 m_1\rangle = m_1 |j_1 m_1\rangle, \quad (8.15)$$

$$\mathbf{J}_2^2 |j_2 m_2\rangle = j_2(j_2 + 1) |j_2 m_2\rangle, \quad (8.16)$$

$$J_{2z} |j_2 m_2\rangle = m_2 |j_2 m_2\rangle. \quad (8.17)$$

In the uncoupled representation, which is a direct product

$$|j_1 m_1\rangle |j_2 m_2\rangle, \quad (8.18)$$

$\mathbf{J}_1^2$, J_{1z} and $\mathbf{J}_2^2$, J_{2z} are diagonal. One lets

$$|j_1 m_1 j_2 m_2\rangle \equiv |j_1 m_1\rangle |j_2 m_2\rangle \quad (8.19)$$

to simplify the notation. The total angular momentum $\mathbf{J}$ is defined by the sum of $\mathbf{J}_1$ and $\mathbf{J}_2$, that is,

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2. \quad (8.20)$$

Since $\mathbf{J}^2$ and J_z commute with $\mathbf{J}_1^2$ and $\mathbf{J}_2^2$, one can seek eigenvectors of $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$, and J_z simultaneously. One denotes these eigenvectors as $|j_1 j_2 j m\rangle$, which are called coupled representation.

The functions $|j_1 m_1 j_2 m_2\rangle$ are a complete set of the two angular momenta,

$$\sum_{m_1 m_2} |j_1 m_1 j_2 m_2\rangle \langle j_1 m_1 j_2 m_2| = \mathcal{I}, \quad (8.21)$$

where $\mathcal{I}$ is an identity operator. The identity operator $\mathcal{I}$ acts on $|j_1 j_2 j m\rangle$ to give

$$|j_1 j_2 j m\rangle = \mathcal{I} |j_1 j_2 j m\rangle = \sum_{m_1 m_2} \langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle |j_1 m_1 j_2 m_2\rangle. \quad (8.22)$$

In the above, $\langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle$ are called the Clebsch–Gordan coefficients. The sequence of possible values of j is

$$|j_1 - j_2|, |j_1 - j_2| + 1, \dots, j_1 + j_2. \quad (8.23)$$

If we apply the conservation of angular momentum $J_z = J_{1z} + J_{2z}$ to (8.22), we obtain

$$m = m_1 + m_2. \quad (8.24)$$

This suggests that the double sum in (8.22) is actually a single sum.

The Clebsch–Gordan coefficients can be expressed in terms of Wigner 3- j symbols as [10–12]

$$\langle j_1 m_1 j_2 m_2 | j_1 j_2 j m \rangle = (-1)^{j_1 - j_2 + m} \sqrt{2j + 1} \times \begin{pmatrix} j_1 & j_2 & j \\ m_1 & m_2 & -m \end{pmatrix}. \quad (8.25)$$

Wigner 3- j symbol has following properties: (1) It is invariant by an even permutation of columns:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_3 & j_1 \\ m_2 & m_3 & m_1 \end{pmatrix} = \begin{pmatrix} j_3 & j_1 & j_2 \\ m_3 & m_1 & m_2 \end{pmatrix}. \quad (8.26)$$

(2) An odd permutation of columns is equivalent to multiplication by $(-1)^{j_1 + j_2 + j_3}$:

$$(-1)^{j_1 + j_2 + j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = \begin{pmatrix} j_2 & j_1 & j_3 \\ m_2 & m_1 & m_3 \end{pmatrix} = \begin{pmatrix} j_1 & j_3 & j_2 \\ m_1 & m_3 & m_2 \end{pmatrix}. \quad (8.27)$$

(3) Symmetry relation:

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix} = (-1)^{j_1 + j_2 + j_3} \begin{pmatrix} j_1 & j_2 & j_3 \\ -m_1 & -m_2 & -m_3 \end{pmatrix}. \quad (8.28)$$

The Addition of Two Orbital Angular Momenta

Consider a two-particle system (Fig. 8.1), whose coordinates are $\mathbf{r}_1 = (r_1, \vartheta_1, \varphi_1)$ and $\mathbf{r}_2 = (r_2, \vartheta_2, \varphi_2)$. Correspondingly, their orbital angular momenta are $\mathbf{L}_1 = \mathbf{r}_1 \times \mathbf{p}_1$ and $\mathbf{L}_2 = \mathbf{r}_2 \times \mathbf{p}_2$. The total angular momentum of this two-particle system is

$$\mathbf{L} = \mathbf{L}_1 + \mathbf{L}_2. \quad (8.29)$$

The quantum states of $\mathbf{L}$, $\mathbf{L}_1$, and $\mathbf{L}_2$ can be denoted by $|l_1 l_2 l m\rangle$, $|l_1 m_1\rangle$, and $|l_2 m_2\rangle$. Applying (8.22) to (8.29), we have

$$|l_1 l_2 l m\rangle = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2 | l_1 l_2 l m \rangle |l_1 m_1\rangle |l_2 m_2\rangle. \quad (8.30)$$

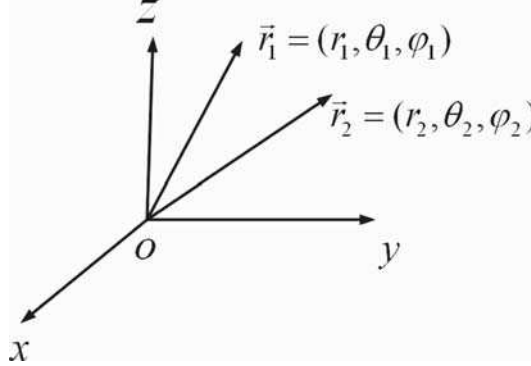


Fig. 8.1. A two-particle system

Now the projection of both sides of (8.30) into the coordinate space $\langle \vartheta_1 \varphi_1 | \langle \vartheta_2 \varphi_2 |$ gives

$$\langle \vartheta_1 \varphi_1 | \langle \vartheta_2 \varphi_2 | l_1 l_2 l m \rangle = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2 | l_1 l_2 l m \rangle Y_{l_1 m_1}(\vartheta_1, \varphi_1) Y_{l_2 m_2}(\vartheta_2, \varphi_2). \quad (8.31)$$

In the above, we can denote $\langle \vartheta_1 \varphi_1 | \langle \vartheta_2 \varphi_2 | l_1 l_2 l m \rangle$ as

$$\langle \vartheta_1 \varphi_1 | \langle \vartheta_2 \varphi_2 | l_1 l_2 l m \rangle = Y_{l_1 l_2 m}^{[l]}(\vartheta_1, \varphi_1, \vartheta_2, \varphi_2). \quad (8.32)$$

Thus, (8.31) can be written as

$$Y_{l_1 l_2 m}^{[l]}(\vartheta_1, \varphi_1, \vartheta_2, \varphi_2) = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2 | l_1 l_2 l m \rangle Y_{l_1 m_1}(\vartheta_1, \varphi_1) Y_{l_2 m_2}(\vartheta_2, \varphi_2). \quad (8.33)$$

Denote $\mathbf{Y}^{[l]}(\vartheta, \varphi)$ the set of the spherical harmonics

$$\mathbf{Y}^{[l]}(\vartheta, \varphi) \equiv \{Y_{lm}(\vartheta, \varphi); m = -l, -l+1, \dots, l\}. \quad (8.34)$$

It follows that (8.33) may be written compactly as

$$Y_{l_1 l_2 m}^{[l]}(\vartheta_1, \varphi_1, \vartheta_2, \varphi_2) = \left[\mathbf{Y}^{[l_1]}(\vartheta_1, \varphi_1) \otimes \mathbf{Y}^{[l_2]}(\vartheta_2, \varphi_2) \right]_m^{[l]}. \quad (8.35)$$

Note that the spherical harmonic functions in the above equation have different ϑ, φ , although particle 1 and 2 are in the same coordinate system (Fig. 8.1).

The Addition of an Orbital Angular Momenta and a Spin

Let $e_s^{[S]}$ be the eigenvectors of the spin $\mathbf{S}$. They are also called unit tensors. For example, for $S = 1$, the unit tensors are $e_{-1}^{[1]}$, $e_0^{[1]}$, and $e_{+1}^{[1]}$, which can be written in terms of the Cartesian unit vectors $\hat{x}$, $\hat{y}$, and $\hat{z}$ as [10]

$$e_{-1}^{[1]} = (\hat{x} - i\hat{y})/\sqrt{2}, \quad (8.36)$$

$$e_0^{[1]} = \hat{z}, \quad (8.37)$$

$$e_{+1}^{[1]} = -(\hat{x} + i\hat{y})/\sqrt{2}. \quad (8.38)$$

Let the total angular momentum $\mathbf{J}$ be the summation of the orbital angular momentum $\mathbf{L}$ and the spin $\mathbf{S}$

$$\mathbf{J} = \mathbf{L} + \mathbf{S}. \quad (8.39)$$

Now a tensor spherical harmonics denoted by $Y_{lSM}^{[J]}(\vartheta, \varphi)$ can be defined by coupling the orbital angular momentum states with the spin [10–12].

$$Y_{lSM}^{[J]}(\vartheta, \varphi) = \sum_{m's'} \langle lm'Ss' | lSJM \rangle Y_{lm'}(\vartheta, \varphi) e_{s'}^{[S]}. \quad (8.40)$$

Denote $\mathbf{e}^{[S]}$ the set of the eigenvectors of spin $\mathbf{S}$

$$\mathbf{e}^{[S]} \equiv \left\{ e_{s'}^{[S]}; s' = -S, -S+1, \dots, S \right\}. \quad (8.41)$$

The tensor spherical harmonics $Y_{lSM}^{[J]}$ can also be written compactly in terms of $\mathbf{Y}^{[l]}$ and $\mathbf{e}^{[S]}$

$$Y_{lSM}^{[J]}(\vartheta, \varphi) = \left[\mathbf{Y}^{[l]}(\vartheta, \varphi) \otimes \mathbf{e}^{[S]} \right]_M^{[J]}. \quad (8.42)$$

8.2.3 Wigner 6- j Symbols

Now consider the addition of three angular momenta

$$\mathbf{J} = \mathbf{J}_1 + \mathbf{J}_2 + \mathbf{J}_3. \quad (8.43)$$

The total angular momentum $\mathbf{J}$ can be obtained by three possible coupling schemes

$$\mathbf{J} = (\mathbf{J}_1 + \mathbf{J}_2) + \mathbf{J}_3, \quad (8.44)$$

$$\mathbf{J} = \mathbf{J}_1 + (\mathbf{J}_2 + \mathbf{J}_3), \quad (8.45)$$

$$\mathbf{J} = (\mathbf{J}_1 + \mathbf{J}_3) + \mathbf{J}_2. \quad (8.46)$$

Let us denote $\mathbf{J}_{12} = \mathbf{J}_1 + \mathbf{J}_2$, $\mathbf{J}_{13} = \mathbf{J}_1 + \mathbf{J}_3$, and $\mathbf{J}_{23} = \mathbf{J}_2 + \mathbf{J}_3$. These three coupling schemes give three different representations, which may be denoted by

$$|(j_1 j_2) J_{12} j_3, JM\rangle, \quad (8.47)$$

$$|j_1(j_2 j_3) J_{23}, JM\rangle, \quad (8.48)$$

$$|(j_1 j_3) J_{13} j_2, JM\rangle. \quad (8.49)$$

Since these three different representations describe the same physical system, they are related by unitary transformations. For example, the transformation between representation (8.47) and (8.48) is

$$|j_1(j_2j_3)J_{23}, JM\rangle = \sum_{J_{12}} R_{J_{12}, J_{23}} |(j_1j_2)J_{12}j_3, JM\rangle, \quad (8.50)$$

where the coefficients $R_{J_{12}, J_{23}}$ can be written in terms of Wigner 6- j symbol, e.g.

$$R_{J_{12}, J_{23}} = (-1)^{j_1+j_2+j_3+J} \sqrt{(2J_{12}+1)(2J_{23}+1)} \times \left\{ \begin{matrix} j_1 & j_2 & J_{12} \\ j_3 & J & J_{23} \end{matrix} \right\}. \quad (8.51)$$

Wigner 6- j symbol has the following properties:

(1) It is invariant by any permutation of columns, e.g.,

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} = \left\{ \begin{matrix} j_2 & j_1 & j_3 \\ j_5 & j_4 & j_6 \end{matrix} \right\}. \quad (8.52)$$

(2) It is invariant by any interchange of the upper and lower elements in each of any two columns, e.g.,

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ j_4 & j_5 & j_6 \end{matrix} \right\} = \left\{ \begin{matrix} j_1 & j_5 & j_6 \\ j_4 & j_2 & j_3 \end{matrix} \right\}. \quad (8.53)$$

(3) If it has a zero element, it has a simple formulation, e.g.,

$$\left\{ \begin{matrix} j_1 & j_2 & j_3 \\ 0 & j_4 & j_5 \end{matrix} \right\} = \frac{\delta_{j_3j_4} \delta_{j_2j_5} (-1)^{j_1+j_2+j_3}}{\sqrt{(2j_2+1)(2j_3+1)}}. \quad (8.54)$$

8.3 Rotation and Translation

We shall discuss two fundamental transformations from one coordinate system into another, rotation, and translation. We limit our discussion on the transformation properties of spherical wave functions. For plane and cylinder wave functions, one can refer to [13].

8.3.1 Rotation

A general rotation in three-dimensional space (Fig. 8.2) can be described by Euler angle (α, β, γ) . The rotation operator R_o can be written in terms of Euler angle (α, β, γ) as [10]

$$R_o(\alpha, \beta, \gamma) = \exp(i\alpha J_z) \cdot \exp(i\beta J_y) \cdot \exp(i\gamma J_z). \quad (8.55)$$

Now consider a physical (scalar) quantity ψ which is a function of (r, ϑ, φ) in coordinate (x, y, z) , and it can be written as $\psi(r, \vartheta, \varphi)$. On the other hand, in coordinate (x', y', z') , it can be also written as $\psi'(r, \vartheta', \varphi')$. It follows that

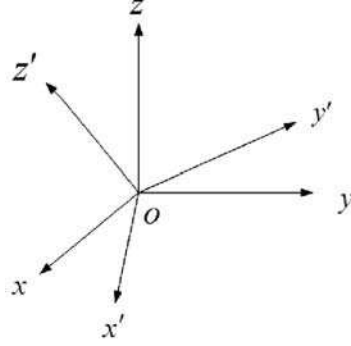


Fig. 8.2. Rotation

$$\psi(r, \vartheta, \varphi) = \psi'(r, \vartheta', \varphi'). \quad (8.56)$$

Thus, the effect of the rotation $R_o(\alpha, \beta, \gamma)$ can be expressed by

$$R_o(\alpha, \beta, \gamma)\psi(r, \vartheta, \varphi) = \psi(r, \vartheta', \varphi'). \quad (8.57)$$

Since $[R_o, L^2] = 0$, that is, the rotation operator R_o does not change l , applying (8.57) to spherical function $Y_{lm'}(\vartheta, \varphi)$ gives

$$Y_{lm}(\vartheta', \varphi') = \sum_{m'} D_{m'm}^l(\alpha, \beta, \gamma) Y_{lm'}(\vartheta, \varphi), \quad (8.58)$$

where $D_{m'm}^l(\alpha, \beta, \gamma)$ is the matrix element of rotation operator, that is,

$$D_{m'm}^l(\alpha, \beta, \gamma) = \langle lm' | R_o(\alpha, \beta, \gamma) | lm \rangle. \quad (8.59)$$

Let $\Psi_{lm}(r, \vartheta, \varphi) = j_l(kr)Y_{lm}(\vartheta, \varphi)$ the solutions of the scalar Helmholtz equation

$$\nabla^2 \psi + k^2 \psi = 0, \quad (8.60)$$

where $j_l(kr)$ is the spherical Bessel function. Using (8.58), we obtain the rotation transformation of $\Psi_{lm'}(r, \vartheta, \varphi)$

$$\Psi_{lm}(r, \vartheta', \varphi') = \sum_{m'} D_{m'm}^l(\alpha, \beta, \gamma) \Psi_{lm'}(r, \vartheta, \varphi). \quad (8.61)$$

8.3.2 Translation

A general translation $T(\mathbf{R})$ in three-dimensional space (Fig. 8.3) can be written as

$$T(\mathbf{R}) = \exp(i\mathbf{R} \cdot \mathbf{P}), \quad (8.62)$$

where $\mathbf{P}$ is the linear momentum. The translation transformation of $\Psi_{lm'}(r', \vartheta', \varphi')$ can be derived by the use of plane wave expansion (also called “Fourier transformation in spherical coordinates”)[1, 7]

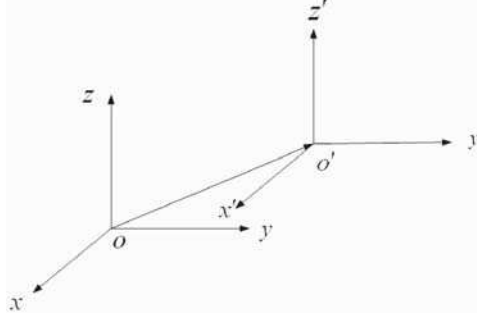
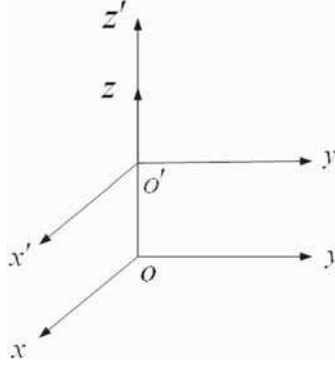


Fig. 8.3. Translation

Fig. 8.4. Translation along z axis

$$\Psi_{lm}(r, \vartheta, \varphi) = \sum_{l'm'} T_{l'm',lm}(R, \Theta, \Phi) \Psi_{l'm'}(r', \vartheta', \varphi'), \quad (8.63)$$

where $T_{l'm',lm}(R, \Theta, \Phi)$ are the matrix element of translation operator $T(\mathbf{R})$. Notice that both the right-hand side and the left-hand side are the solutions to Helmholtz equation, and from the completeness of the eigensolutions of Helmholtz equation, the above is viable. The matrix element $T_{l'm',lm}(R, \Theta, \Phi)$ can be evaluated by

$$T_{l'm',lm}(R, \Theta, \Phi) = \sum_{l''m''} i^{l'+l''-l} (-1)^m [4\pi(2l'+1)(2l+1)(2l''+1)]^{1/2} \\ \times \begin{pmatrix} l' & l & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & l & l'' \\ m' & -m & m'' \end{pmatrix} \Psi_{l''m''}(R, \Theta, \Phi).$$

Let us denote a special translation along the z axis (Fig. 8.4) by $T(R\hat{z})$. Under the translation $T(R\hat{z})$, the angle φ does not change. Thus, m remains unchanged in the translation (8.63). The summation of (8.63) becomes a single summation with respect to l' . Then (8.63) can be simplified to

$$\Psi_{lm}(r, \vartheta, \varphi) = \sum_{l'} T_{l'm, lm}(R, 0, 0) \Psi_{l'm}(r', \vartheta', \varphi). \quad (8.64)$$

Meanwhile, the matrix elements of $T(R\hat{z})$ is simplified to

$$T_{l'm', lm}(R, 0, 0) = \sum_{l''} i^{l'+l''-l} (-1)^m [(2l'+1)(2l+1)(2l''+1)]^{1/2} \\ \times \begin{pmatrix} l' & l & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & l & l'' \\ m & -m & 0 \end{pmatrix} j_{l''}(kR). \quad (8.65)$$

8.3.3 Decomposition of a General Translation

A general translation denoted by $T(\mathbf{R})$ can be performed by

$$T(\mathbf{R}) = D(R_o^{-1}) T(R\hat{z}) D(R_o). \quad (8.66)$$

That is, one first rotates the coordinate system such that the z axis along the direction of the translation, e.g., $D(R_o)$, and then shifts along z axis, e.g., $T(R\hat{z})$, and rotates back, e.g., $D(R_o^{-1})$. Note that each operation on matrix representations of right-hand side of (8.66) can be performed by a single summation (c.f. (8.61) and (8.64)). This property of (8.66) is crucial to reducing the complexities of translation operations [3, 14–17]. For detailed analysis, one can refer to [17].

8.4 Scalar Addition Theorem

The addition theorem for scalar fields along an arbitrary direction is first derived by Friedman and Russek [4]. For an earlier historical survey on addition theorem, one can refer to [7].

8.4.1 Scalar Addition Theorem

The translation (8.63) is also called scalar addition theorem for the regular spherical wave functions $\Psi_{lm}(r, \vartheta, \varphi)$. It can be generalized to singular spherical wave functions [1, 7]. Let $z_l(x)$ be either the spherical Bessel function of the first kind $j_l(x)$, the spherical Bessel function of the second kind $y_l(x)$, the spherical Hankel function of the first kind $h_l^{(1)}(x)$, and the spherical Hankel function of the second kind $h_l^{(2)}(x)$. Denote $\tilde{\Psi}_{lm}$ be

$$\tilde{\Psi}_{lm}(r, \vartheta, \varphi) = z_l(kr) Y_{lm}(\vartheta, \varphi). \quad (8.67)$$

Let $\alpha(lm|l'm'|l''m'')$ be

$$\alpha(lm|l'm'|l''m'') = i^{l'+l''-l} (-1)^m [4\pi(2l'+1)(2l+1)(2l''+1)]^{1/2} \\ \times \begin{pmatrix} l' & l & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & l & l'' \\ m' & -m & m'' \end{pmatrix}. \quad (8.68)$$

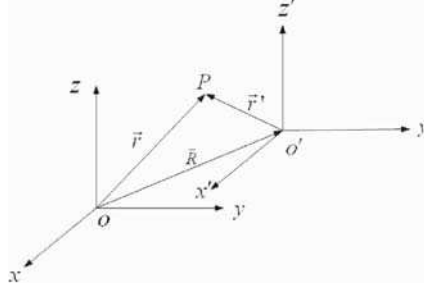


Fig. 8.5. Addition theorem

The matrix element $T_{l'm',lm}(R, \Theta, \Phi)$ can be written compactly as

$$T_{l'm',lm}(R, \Theta, \Phi) = \sum_{l''m''} \alpha(lm|l'm'|l''m'') \Psi_{l''m''}(R, \Theta, \Phi). \quad (8.69)$$

We introduce the matrix element $\tilde{T}_{l'm',lm}(R, \Theta, \Phi)$ be

$$\tilde{T}_{l'm',lm}(R, \Theta, \Phi) = \sum_{l''m''} \alpha(lm|l'm'|l''m'') \tilde{\Psi}_{l''m''}(R, \Theta, \Phi). \quad (8.70)$$

The scalar addition theorem for $\tilde{\Psi}_{lm}$ reads

$$\tilde{\Psi}_{lm}(r, \vartheta, \varphi) = \begin{cases} \sum_{l'm'} T_{l'm',lm}(R, \Theta, \Phi) \tilde{\Psi}_{l'm'}(r', \vartheta', \varphi'), & r' > R, \\ \sum_{l'm'} \tilde{T}_{l'm',lm}(R, \Theta, \Phi) \Psi_{l'm'}(r', \vartheta', \varphi'), & r' < R. \end{cases} \quad (8.71)$$

From the view point of the group theory, the addition theorem just expresses as the multiplication laws of the group elements [18]. Since $\mathbf{r} = \mathbf{R} + \mathbf{r}'$, we have

$$T(\mathbf{r}) = T(\mathbf{R})T(\mathbf{r}'). \quad (8.72)$$

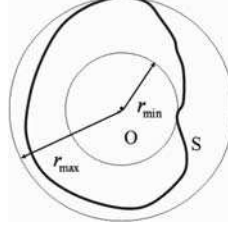
The matrix representation of (8.72) is

$$T_{lm,l'm'}(\mathbf{r}) = \sum_{l''m''} T_{lm,l''m''}(\mathbf{R}) T_{l''m'',l'm'}(\mathbf{r}'). \quad (8.73)$$

The above equation (8.73) is a more general form of addition theorem [18–20]. Letting $l' = 0$ and $m' = 0$ in (8.73) gives the (8.63).

8.4.2 Rotation and Translation Transformations for T-Matrix

The T-matrix method is one of the most powerful techniques for solving electromagnetic, acoustic, and elastodynamic scattering problems [21–28]. Here we use scalar waves to illustrate the basic concepts of T-matrix methods. We expand the incident wave ψ_{in} and scattered wave ψ_{sc} in spherical wave functions as follows:

**Fig. 8.6.** One scatterer bounded by surface S

$$\psi_{\text{in}}(\mathbf{r}) = \sum_{lm} a_{lm} \Psi_{lm}(\mathbf{r}), \quad r < r_{\min}, \quad (8.74)$$

$$\psi_{\text{sc}}(\mathbf{r}) = \sum_{lm} f_{lm} \tilde{\Psi}_{lm}(\mathbf{r}), \quad r > r_{\max}, \quad (8.75)$$

where $r_{\min}$ and $r_{\max}$ are the radii of the inscribed sphere and escribed sphere (cf. Fig. 8.6). Due to the linearity of the Maxwell equations, the scattering system can be viewed as a linear system. Thus, one can introduce the so-called T-matrix $\mathcal{T}$ to connect the coefficient f_{lm} with the coefficient a_{lm} as follows [22]:

$$f_{lm} = \sum_{l'm'} \mathcal{T}_{lm,l'm'} a_{l'm'}. \quad (8.76)$$

We shall discuss the rotation and translation transformations for T-matrix, which are quite useful for solving the scattering problems.

Rotation Transformation for T-Matrix

Let $\mathcal{T}$ be the T-matrix in coordinate system (x, y, z) , and $\mathcal{T}'$ be the T-matrix in coordinate system (x', y', z') (c.f. Fig. 8.2). Since the matrix $\mathcal{T}$ encodes the same physical information as the matrix $\mathcal{T}'$, and the rotation of coordinate systems can be considered as a unitary transformation, we have

$$\mathcal{T} = D(\alpha, \beta, \gamma) \mathcal{T}' D^{-1}(\alpha, \beta, \gamma). \quad (8.77)$$

Since

$$D^{-1}(\alpha, \beta, \gamma) D(\alpha, \beta, \gamma) = I, \quad (8.78)$$

that is,

$$D^{-1}(\alpha, \beta, \gamma) = D(-\gamma, -\beta, -\alpha), \quad (8.79)$$

Equation (8.77) can be written as follows:

$$\mathcal{T} = D(\alpha, \beta, \gamma) \mathcal{T}' D(-\gamma, -\beta, -\alpha). \quad (8.80)$$

Its more explicit form reads

$$\Upsilon_{lm,l'm'} = \sum_{m_1=-l}^{m_1=l} \sum_{m'_1=-l'}^{m'_1=l'} D_{mm_1}^l(\alpha, \beta, \gamma) \Upsilon'_{lm_1,l'm'_1} D_{m'_1m'}(-\gamma, -\beta, -\alpha), \quad (8.81)$$

which is identical to the formulation derived from [25, 26].

Translation Transformation for T-Matrix

Let Υ be the T-matrix in coordinate system (x, y, z) , and Υ' be the T-matrix in coordinate system (x', y', z') (c.f. Fig. 8.3). Similar to the rotation transformation for T-matrix, the translation transformation for T-matrix reads as follows [2]

$$\Upsilon = \overline{\tilde{T}(\mathbf{R})} \Upsilon' \overline{\tilde{T}(-\mathbf{R})}. \quad (8.82)$$

The property (8.82) is crucial to express the T-matrix for multiple obstacles, in which the translation transformation of one coordinate system to another is necessary. In multiple obstacles case, the translation $\tilde{T}(\mathbf{R})$ represents a propagation from one obstacle to another obstacle. One can refer to [2, 23, 29] for more detailed discussion.

8.5 Tensor Addition Theorem

The addition theorem was generalized to vector fields by Stein [5] and Cruzan [6]. One can also refer to [1, 30–34] for the derivation and discussion of vector addition theorem. The addition theorem was further generalized to tensor fields by Danos and Maximon [7].

8.5.1 Tensor Wave Functions

The tensor wave functions are defined by

$$\Psi_{lSM}^{[J]}(r, \vartheta, \varphi) \equiv j_l(kr) Y_{lSM}^{[J]}(\vartheta, \varphi). \quad (8.83)$$

Similarly, the tensor singular wave functions are defined by

$$\tilde{\Psi}_{lSM}^{[J]}(r, \vartheta, \varphi) \equiv z_l(kr) Y_{lSM}^{[J]}(\vartheta, \varphi). \quad (8.84)$$

Note that in the case $S = 0$, the tensor harmonics $Y_{lSM}^{[J]}(\vartheta, \varphi)$ becomes the usual spherical harmonics $Y_{lm}(\vartheta, \varphi)$, and the tensor wave field $\Psi_{lSM}^{[J]}(r, \vartheta, \varphi)$ becomes $\Psi_{lm}(r, \vartheta, \varphi)$, e.g., $\Psi_{l0m}^{[l]}(r, \vartheta, \varphi) = \Psi_{lm}(r, \vartheta, \varphi)$. For $S = 1$, the tensor spherical harmonics becomes usual vector spherical harmonics $Y_{l1M}^{[J]}(\vartheta, \varphi)$ by

setting $S = 1$. According to the addition of angular momenta (c.f. Sect. 2), the value l can be only $J - 1$, J , and $J + 1$. Thus, one can drop subscript 1 in $Y_{l1M}^{[J]}(\vartheta, \varphi)$. It follows that these three vector spherical harmonics can be denoted as

$$Y_{J-1,M}^{[J]}(\vartheta, \varphi), Y_{J,M}^{[J]}(\vartheta, \varphi), Y_{J+1,M}^{[J]}(\vartheta, \varphi). \quad (8.85)$$

The corresponding vector spherical wave functions can be denoted as

$$\Psi_{J-1,M}^{[J]}(r, \vartheta, \varphi), \Psi_{J,M}^{[J]}(r, \vartheta, \varphi), \Psi_{J+1,M}^{[J]}(r, \vartheta, \varphi), \quad (8.86)$$

which are

$$\Psi_{J-1,M}^{[J]}(r, \vartheta, \varphi) = j_{J-1}(kr)Y_{J-1,M}^{[J]}(\vartheta, \varphi), \quad (8.87)$$

$$\Psi_{J,M}^{[J]}(r, \vartheta, \varphi) = j_J(kr)Y_{J,M}^{[J]}(\vartheta, \varphi), \quad (8.88)$$

$$\Psi_{J+1,M}^{[J]}(r, \vartheta, \varphi) = j_{J+1}(kr)Y_{J+1,M}^{[J]}(\vartheta, \varphi). \quad (8.89)$$

Similarly, the vector singular wave functions are defined by

$$\tilde{\Psi}_{J-1,M}^{[J]}(r, \vartheta, \varphi), \tilde{\Psi}_{J,M}^{[J]}(r, \vartheta, \varphi), \tilde{\Psi}_{J+1,M}^{[J]}(r, \vartheta, \varphi), \quad (8.90)$$

which are

$$\tilde{\Psi}_{J-1,M}^{[J]}(r, \vartheta, \varphi) = z_{J-1}(kr)Y_{J-1,M}^{[J]}(\vartheta, \varphi), \quad (8.91)$$

$$\tilde{\Psi}_{J,M}^{[J]}(r, \vartheta, \varphi) = z_J(kr)Y_{J,M}^{[J]}(\vartheta, \varphi), \quad (8.92)$$

$$\tilde{\Psi}_{J+1,M}^{[J]}(r, \vartheta, \varphi) = z_{J+1}(kr)Y_{J+1,M}^{[J]}(\vartheta, \varphi). \quad (8.93)$$

These vector spherical wave functions are the solutions of vector Helmholtz equation

$$\nabla^2 \mathbf{A} + k^2 \mathbf{A} = 0. \quad (8.94)$$

8.5.2 Hansen Multipole Harmonic Fields

Using the vector identity

$$\nabla^2 \mathbf{A} = \nabla \nabla \cdot \mathbf{A} - \nabla \times \nabla \times \mathbf{A}, \quad (8.95)$$

one may write the vector Helmholtz equation as

$$\nabla \nabla \cdot \mathbf{A} - \nabla \times \nabla \times \mathbf{A} + k^2 \mathbf{A} = 0. \quad (8.96)$$

The formulation of (8.96) implies that there are two types of harmonic solutions, which can be denoted by $\mathbf{A}_c$ and $\mathbf{A}_d$. The vectors $\mathbf{A}_c$ and $\mathbf{A}_d$ have the property

$$\nabla \times \mathbf{A}_c \neq 0, \quad \nabla \cdot \mathbf{A}_c = 0, \quad (8.97)$$

$$\nabla \times \mathbf{A}_d = 0, \quad \nabla \cdot \mathbf{A}_d \neq 0. \quad (8.98)$$

According to Helmholtz decomposition, a vector $\mathbf{A}$ can be decomposed into $\mathbf{A}_c$ and $\mathbf{A}_d$, e.g.,

$$\mathbf{A} = \mathbf{A}_c + \mathbf{A}_d. \quad (8.99)$$

Substituting (8.99) into (8.96), and using (8.97) and (8.98), the vector Helmholtz equation can be divided into two equations

$$\nabla \nabla \cdot \mathbf{A}_d + k^2 \mathbf{A}_d = 0, \quad (8.100)$$

$$-\nabla \times \nabla \times \mathbf{A}_c + k^2 \mathbf{A}_c = 0. \quad (8.101)$$

These two types of solutions are often written in terms of Hansen multipole harmonic fields [35] denoted by $\mathbf{M}_{JM}(\mathbf{r})$, $\mathbf{N}_{JM}(\mathbf{r})$, and $\mathbf{L}_{JM}(\mathbf{r})$, which are defined by

$$\mathbf{M}_{JM}(\mathbf{r}) = \nabla \times [\mathbf{r} \tilde{\psi}_{lm}(r, \vartheta, \varphi)], \quad (8.102)$$

$$\mathbf{N}_{JM}(\mathbf{r}) = \frac{1}{k} \nabla \times \nabla \times [\mathbf{r} \tilde{\psi}_{lm}(r, \vartheta, \varphi)], \quad (8.103)$$

$$\mathbf{L}_{JM}(\mathbf{r}) = \frac{1}{k} \nabla [\tilde{\psi}_{lm}(r, \vartheta, \varphi)]. \quad (8.104)$$

Here we add subscripts JM to $\mathbf{M}_{JM}(\mathbf{r})$, $\mathbf{N}_{JM}(\mathbf{r})$, and $\mathbf{L}_{JM}(\mathbf{r})$ to emphasize their dependence on the quantum numbers J and M (c.f. (8.108), (8.109), and (8.110)). It can be shown that the Hansen multipole harmonic fields $\mathbf{M}_{JM}(\mathbf{r})$, $\mathbf{N}_{JM}(\mathbf{r})$, and $\mathbf{L}_{JM}(\mathbf{r})$ have the divergence and curl properties:

$$\nabla \times \mathbf{M}_{JM}(\mathbf{r}) \neq 0, \quad \nabla \cdot \mathbf{M}_{JM}(\mathbf{r}) = 0, \quad (8.105)$$

$$\nabla \times \mathbf{N}_{JM}(\mathbf{r}) \neq 0, \quad \nabla \cdot \mathbf{N}_{JM}(\mathbf{r}) = 0, \quad (8.106)$$

$$\nabla \times \mathbf{L}_{JM}(\mathbf{r}) = 0, \quad \nabla \cdot \mathbf{L}_{JM}(\mathbf{r}) \neq 0. \quad (8.107)$$

That is, the Hansen multipole harmonic fields $\mathbf{M}_{JM}(\mathbf{r})$ and $\mathbf{N}_{JM}(\mathbf{r})$ describe solenoidal fields and $\mathbf{L}_{JM}(\mathbf{r})$ describes longitudinal fields. The relation between the Hansen multipole harmonic fields and vector spherical wave fields may be expressed by [32]

$$\mathbf{M}_{JM}(\mathbf{r}) = \left[-i\sqrt{J(J+1)} \right] \tilde{\Psi}_{J,M}^{[J]}(r, \vartheta, \varphi), \quad (8.108)$$

$$\mathbf{N}_{JM}(\mathbf{r}) = \left[\frac{(J+1)\sqrt{J}}{\sqrt{2J+1}} \right] \tilde{\Psi}_{J-1,M}^{[J]}(r, \vartheta, \varphi) - \left[\frac{J\sqrt{J+1}}{\sqrt{2J+1}} \right] \tilde{\Psi}_{J+1,M}^{[J]}(r, \vartheta, \varphi), \quad (8.109)$$

$$\mathbf{L}_{JM}(\mathbf{r}) = \left[\frac{\sqrt{J}}{\sqrt{2J+1}} \right] \tilde{\Psi}_{J-1,M}^{[J]}(r, \vartheta, \varphi) + \left[\frac{\sqrt{J+1}}{\sqrt{2J+1}} \right] \tilde{\Psi}_{J+1,M}^{[J]}(r, \vartheta, \varphi). \quad (8.110)$$

8.5.3 Addition Theorem for Tensor Multipole Fields

We shall briefly derive the addition theorem for tensor fields following Danos and Maximon's method [7]. The addition theorems for scalar and vector fields, which are the special cases for tensor fields with spin $S = 0$ and $S = 1$, are especially important in practical applications.

A Derivation of Addition Theorem for Tensor Multipole Fields

The addition of three angular momenta facilitates the derivation of the addition theorem for tensor fields. The notations for the angular momenta $\mathbf{L}$, $\mathbf{L}'$, $\mathbf{L}''$, $\mathbf{S}$, $\mathbf{J}$, and $\mathbf{J}'$, and their quantum numbers showed in Table 8.1.

The relations among these angular momenta are

$$\mathbf{J} = \mathbf{L}'' + \mathbf{L}' + \mathbf{S}, \quad (8.111)$$

$$= \mathbf{L} + \mathbf{S}, \quad (8.112)$$

$$\mathbf{L} = \mathbf{L}'' + \mathbf{L}', \quad (8.113)$$

$$\mathbf{J}' = \mathbf{L}' + \mathbf{S}. \quad (8.114)$$

Using (8.25) and (8.35), we rewrite the scalar addition theorem (8.63) as

$$\begin{aligned} \Psi_{lm}(r, \vartheta, \varphi) &= \sum_{l'l''} i^{l'+l''-l} (-1)^{l'-l''} [4\pi(2l'+1)(2l''+1)]^{1/2} \times \begin{pmatrix} l' & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad j_{l''}(kR) j_{l'}(kr') \left[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi') \right]_m^{[l]}. \end{aligned} \quad (8.115)$$

Note that the term $[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi')]_m^{[l]}$ can be viewed as the addition of two angular momenta

$$\mathbf{L} = \mathbf{L}'' + \mathbf{L}'. \quad (8.116)$$

Coupling $\mathbf{e}^{[S]}$ to both sides of (8.115) gives

$$\begin{aligned} \Psi_{lSM}^{[J]}(r, \vartheta, \varphi) &= \sum_{l'l''} i^{l'+l''-l} (-1)^{l'-l''} [4\pi(2l'+1)(2l''+1)]^{1/2} \times \begin{pmatrix} l' & l'' & l \\ 0 & 0 & 0 \end{pmatrix} \\ &\quad j_{l''}(kR) j_{l'}(kr') \left\{ \left[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi') \right]_m^{[l]} \otimes \mathbf{e}^{[S]} \right\}_M^{[J]}. \end{aligned} \quad (8.117)$$

Table 8.1. The angular momenta

Angular momenta	Quantum numbers
$\mathbf{L}$	l, m
$\mathbf{L}'$	l', m'
$\mathbf{L}''$	l'', m''
$\mathbf{S}$	S, s'
$\mathbf{J}$	J, M
$\mathbf{J}'$	J', M'

The term $\left\{ \left[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi') \right]_m^{[l]} \otimes \mathbf{e}^{[S]} \right\}_M^{[J]}$ can be viewed as the addition of three angular momenta

$$\mathbf{J} = (\mathbf{L}'' + \mathbf{L}') + \mathbf{S}. \quad (8.118)$$

Using (8.50), one can express the term $\left\{ \left[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi') \right]_m^{[l]} \otimes \mathbf{e}^{[S]} \right\}_M^{[J]}$ in terms of $\left\{ \mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \left[\mathbf{Y}^{[l']}(\vartheta', \varphi') \otimes \mathbf{e}^{[S]} \right]_{M'}^{[J']} \right\}_M^{[J]}$ as

$$\begin{aligned} & \left\{ \left[\mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \mathbf{Y}^{[l']}(\vartheta', \varphi') \right]_m^{[l]} \otimes \mathbf{e}^{[S]} \right\}_M^{[J]} \\ &= \sum_{J'} (-1)^{l''+l'+S+J} \sqrt{(2J'+1)(2l+1)} \\ & \times \left\{ \begin{matrix} l'' & J' & J \\ S & l & l' \end{matrix} \right\} \times \left\{ \mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \left[\mathbf{Y}^{[l']}(\vartheta', \varphi') \otimes \mathbf{e}^{[S]} \right]_{M'}^{[J']} \right\}_M^{[J]}, \end{aligned} \quad (8.119)$$

where the term $\left\{ \mathbf{Y}^{[l'']}(\Theta, \Phi) \otimes \left[\mathbf{Y}^{[l']}(\vartheta', \varphi') \otimes \mathbf{e}^{[S]} \right]_{M'}^{[J']} \right\}_M^{[J]}$ can be viewed as the addition of three angular momenta

$$\mathbf{J} = \mathbf{L}'' + (\mathbf{L}' + \mathbf{S}). \quad (8.120)$$

Substituting (8.119) into (8.117), we obtain the addition theorem for tensor fields

$$\Psi_{lSM}^{[J]}(r, \vartheta, \varphi) = \sum_{l'J'M'} T_{l'J'M', lJM}^{[S]}(R, \Theta, \Phi) \Psi_{l'SM'}^{[J']}(r', \vartheta', \varphi'). \quad (8.121)$$

The matrix elements $T_{l'J'M', lJM}^{[S]}(R, \Theta, \Phi)$ are calculated by

$$T_{l'J'M', lJM}^{[S]}(R, \Theta, \Phi) = \sum_{l''m''} \alpha^{[S]}(lJM|l'J'M'|l''m'') \Psi_{l''m''}^{[J]}(R, \Theta, \Phi), \quad (8.122)$$

with the coefficient

$$\begin{aligned} \alpha^{[S]}(lJM|l'J'M'|l''m'') &= i^{l'+l''-l} (-1)^{S+M} \\ & \times [4\pi(2l'+1)(2l+1)(2l''+1)(2J'+1)(2J+1)]^{1/2} \\ & \times \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J & J' & l'' \\ -M & M' & m'' \end{pmatrix} \left\{ \begin{matrix} l'' & J' & J \\ S & l & l' \end{matrix} \right\}. \end{aligned} \quad (8.123)$$

Here we have corrected the coefficients given by [7]. There is also a sign error before M in [32].

Scalar Addition Theorem: $S = 0$

For $S = 0$, we can obtain the scalar addition theorem. The symmetry relation (8.28) suggests that $\begin{pmatrix} l' & l'' & l \\ 0 & 0 & 0 \end{pmatrix}$ is nonzero only if $(l' + l'' + l)$ is an even integer. Plugging $S = 0$ into (8.114) and (8.112), we have $J' = l'$, $M' = m'$, $J = l$, and $M = m$. It follows that for $S = 0$, the coefficient $\alpha^{[S]}(lJM|l'J'M'|l''m'')$ becomes

$$\alpha^{[0]}(lJM|l'J'M'|l''m'') = i^{l'+l''-l}(-1)^m \times [4\pi(2l'+1)(2l+1)(2l''+1)]^{1/2} \times \begin{pmatrix} l' & l & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} l' & l & l'' \\ m' & -m & m'' \end{pmatrix}, \quad (8.124)$$

which is the same as the coefficient of the scalar addition theorem (8.68).

Vector Addition Theorem: $S = 1$

For $S = 1$, we can obtain the vector addition theorem

$$\Psi_{l1M}^{[J]}(r, \vartheta, \varphi) = \sum_{l'J'M'} T_{l'J'M',lJM}^{[1]}(R, \Theta, \Phi) \Psi_{l'1M'}^{[J]}(r', \vartheta', \varphi'). \quad (8.125)$$

The matrix elements $T_{l'J'M',lJM}^{[1]}(R, \Theta, \Phi)$ are calculated by

$$T_{l'J'M',lJM}^{[1]}(R, \Theta, \Phi) = \sum_{l''m''} \alpha^{[1]}(lJM|l'J'M'|l''m'') \Psi_{l''m''}(R, \Theta, \Phi), \quad (8.126)$$

with the coefficient

$$\begin{aligned} \alpha^{[1]}(lJM|l'J'M'|l''m'') &= i^{l'+l''-l}(-1)^{1+M} \\ &\times [4\pi(2l'+1)(2l+1)(2l''+1)(2J'+1)(2J+1)]^{1/2} \\ &\times \begin{pmatrix} l & l' & l'' \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} J & J' & l'' \\ -M & M' & m'' \end{pmatrix} \begin{Bmatrix} l'' & J' & J \\ 1 & l & l' \end{Bmatrix}. \end{aligned} \quad (8.127)$$

Introducing $\mathbf{r}_<$ as the smaller and $\mathbf{r}_>$ as the larger of $\mathbf{R}$ and $\mathbf{r}'$, one can generalize the vector addition theorem (8.125) to include singular wave functions as follows [32]

$$\tilde{\Psi}_{l1M}^{[J]}(\mathbf{r}) = \sum_{l'J'M'l''m''} \alpha^{[1]}(lJM|l'J'M'|l''m'') \tilde{\Psi}_{l1M}^{[J]}(\mathbf{r}_>) \Psi_{l''m''}(\mathbf{r}_<). \quad (8.128)$$

Plugging (8.108), (8.109), and (8.110) into (8.128), we can obtain the vector addition theorem in terms of Hansen multipole harmonic fields $\mathbf{M}_{JM}(\mathbf{r})$, $\mathbf{N}_{JM}(\mathbf{r})$, and $\mathbf{L}_{JM}(\mathbf{r})$ from (8.126) [32]. One is often more interested in vector addition theorem of divergence-free vector harmonic fields, e.g., $\mathbf{M}_{JM}(\mathbf{r})$ and $\mathbf{N}_{JM}(\mathbf{r})$ than that of curl-free vector harmonic fields, e.g., $\mathbf{L}_{JM}(\mathbf{r})$ [1, 2, 31, 33, 36–40].

8.6 Diagonal Forms of Translation Matrix

The diagonalization of the translation operators is a crucial step in the fast multipole method [3, 41–44] for solving the integral equations of electrodynamic and elastodynamic problems. The diagonalization of the translation operator has been reported in [45–47]. Following [47], we shall give a brief derivation of the diagonalization of the translation operator by the use of a plane-wave basis and a series of similarity transforms.

The coefficient $\alpha(lm|l'm'|l''m'')$ (c.f. (8.68)) can also be written in terms of the Gaunt coefficient [48] (the solid angle integral of a triple product of spherical harmonics) as [1]

$$\alpha(lm|l'm'|l''m'') = 4\pi i^{l'+l''-l} \int d\Omega_k Y_L(\Omega_k) Y_{L'}^*(\Omega_k) Y_{L''}^*(\Omega_k), \quad (8.129)$$

where the index L denotes (l, m) , and

$$\int d\Omega_k = \int_0^{2\pi} \int_0^\pi \sin(\vartheta_k) d\vartheta_k d\varphi_k. \quad (8.130)$$

In order to emphasize the dependence of the functions $T_{L',L}(\mathbf{R})$ and $\Psi_{L''}(\mathbf{R})$ on the wave number k , we rewrite them as $T_{L',L}(k, \mathbf{R})$ and $\Psi_{L''}(k, \mathbf{R})$. Thus the matrix element $T_{L',L}(k, \mathbf{R})$ (c.f. (8.69)) can be cast in the form as

$$T_{L',L}(k, \mathbf{R}) = \sum_{L''} 4\pi i^{l'+l''-l} \Psi_{L''}(k, \mathbf{R}) \int d\Omega_k Y_L(\Omega_k) Y_{L'}^*(\Omega_k) Y_{L''}^*(\Omega_k), \quad (8.131)$$

and the matrix element $\tilde{T}_{L',L}(k, \mathbf{R})$ (c.f. (8.70)) can be cast in the form as

$$\tilde{T}_{L',L}(k, \mathbf{R}) = \sum_{L''} 4\pi i^{l'+l''-l} \tilde{\Psi}_{L''}(k, \mathbf{R}) \int d\Omega_k Y_L(\Omega_k) Y_{L'}^*(\Omega_k) Y_{L''}^*(\Omega_k). \quad (8.132)$$

In a fast multipole algorithm, one of key steps is to compute [3]

$$\tilde{T}_{L,L'}(k, \mathbf{R}_{ij}) = \sum_{L_1, L'_1} T_{L,L_1}(k, \mathbf{R}_{i\lambda}) \tilde{T}_{L_1, L'_1}(k, \mathbf{R}_{\lambda\lambda'}) T_{L'_1, L'}(k, \mathbf{R}_{\lambda'j}). \quad (8.133)$$

Substituting (8.131) and (8.132) into (8.133), we have

$$\begin{aligned} \tilde{T}_{L,L'}(k, \mathbf{R}_{ij}) &= \sum_{L_1, L'_1} \sum_{L''_1} 4\pi i^{l+l'_1+l''_1-l_1} \Psi_{L''_1}(k, \mathbf{R}_{i\lambda}) \int d\Omega_k Y_{L_1}(\Omega_k) Y_{L'}^*(\Omega_k) Y_{L''_1}^*(\Omega_k) \\ &\quad \times \sum_{L''} 4\pi i^{l_1+l''-l'_1} \tilde{\Psi}_{L''}(k, \mathbf{R}_{\lambda\lambda'}) \int d\Omega'_k Y_{L'_1}(\Omega'_k) Y_{L_1}^*(\Omega'_k) Y_{L''}^*(\Omega'_k) \\ &\quad \times \sum_{L''_2} 4\pi i^{l'_1+l''_2-l'-l''} \Psi_{L''_2}(k, \mathbf{R}_{\lambda'j}) \int d\Omega''_k Y_{L'}(\Omega''_k) Y_{L'_1}^*(\Omega''_k) Y_{L''_2}^*(\Omega''_k). \end{aligned} \quad (8.134)$$

Using the plane-wave expansion [49]

$$e^{i\mathbf{k}\cdot\mathbf{R}} = \sum_{L''} 4\pi i^{L''} Y_{L''}^*(\Omega_k) \Psi_{L''}(k, \mathbf{R}), \quad (8.135)$$

we can write (8.134) as

$$\begin{aligned} \tilde{T}_{L,L'}(k, \mathbf{R}_{ij}) &= \sum_{L_1, L'_1} i^{l-l_1} \int d\Omega_k Y_{L_1}(\Omega_k) Y_{L_1}^*(\Omega_k) e^{i\mathbf{k}\cdot\mathbf{R}_{i\lambda}} \\ &\times \sum_{L''} 4\pi i^{l_1+l''-l'_1} \tilde{\Psi}_{L''}(k, \mathbf{R}_{\lambda\lambda'}) \int d\Omega'_k Y_{L'_1}(\Omega'_k) Y_{L'_1}^*(\Omega'_k) Y_{L''}^*(\Omega'_k) \\ &\times i^{l'_1-l'} \int d\Omega''_k Y_{L'}(\Omega''_k) Y_{L'_1}^*(\Omega''_k) e^{i\mathbf{k}\cdot\mathbf{R}_{\lambda'j}}. \end{aligned} \quad (8.136)$$

Using the completeness relation [50]

$$\delta(\Omega_k - \Omega'_k) = \sum_L Y_L(\Omega_k) Y_L^*(\Omega'_k), \quad (8.137)$$

we simplify (8.136) to be

$$\tilde{T}_{L,L'}(k, \mathbf{R}_{ij}) = \int d\Omega'_k i^l Y_L^*(\Omega'_k) e^{i\mathbf{k}\cdot\mathbf{R}_{i\lambda}} \check{T}_{L,L'}(k, \Omega'_k, \mathbf{R}_{\lambda\lambda'}) i^{-l'} Y_{L'}(\Omega'_k) e^{i\mathbf{k}\cdot\mathbf{R}_{\lambda'j}}, \quad (8.138)$$

where

$$\check{T}_{L,L'}(k, \Omega'_k, \mathbf{R}_{\lambda\lambda'}) = \sum_{L''} 4\pi i^{l''} \tilde{\Psi}_{L''}(k, \mathbf{R}_{\lambda\lambda'}) Y_{L''}^*(\Omega'_k). \quad (8.139)$$

The integration of (8.138) can be approximated by a single finite summation by the use of quadrature rules. This single finite summation clearly shows that the factor $\check{T}_{L,L'}(k, \Omega'_k, \mathbf{R}_{\lambda\lambda'})$ is diagonal so that the calculation of $\tilde{T}_{L,L'}(k, \mathbf{R}_{ij})$ via (8.138) is a lot more efficient than that via (8.133).

8.7 Conclusions

We have discussed two fundamental transformations from one coordinate system into another, that is, rotation and translation. These transformations have wide applications in science and engineering, especially in scattering problems. From the viewpoint of group theory, the angular momenta provide the generators of the rotation. The addition theorem arises from translation transformation. The addition of three angular momenta facilitates the derivation of the addition theorem for tensor fields. We have reviewed the diagonal forms of translation operators, which is critical in some fast multipole methods.

Acknowledgements

The authors would like to thank Prof. Ta-Pei Cheng and Dr. Nail Gumerov for helpful discussions.

References

- [1] W. C. Chew, *Waves and Fields in Inhomogeneous Media*. New York: IEEE Press, 1995 (first printing 1990).
- [2] P. A. Martin, *Multiple Scattering: Interaction of Time-harmonic Waves with N Obstacles*. Cambridge: Cambridge University Press., 2006.
- [3] W. C. Chew, J. M. Jin, E. Michielssen, and J. M. Song, *Fast and Efficient Algorithms in Computational Electromagnets*. Boston: Artech House, 2001.
- [4] B. Friedman and J. Russek, "Addition theorems for spherical waves," *Quarterly Appl. Math.*, vol. 12, pp. 13–23, 1954.
- [5] S. Stein, "Addition theorems for spherical wave functions," *Quarterly Appl. Math.*, vol. 19, pp. 15–24, 1961.
- [6] O. R. Cruzan, "Translational addition theorems for spherical vector functions," *Quarterly Appl. Math.*, vol. 20, pp. 33–40, 1962.
- [7] M. Danos and L. C. Maximon, "Multipole matrix elements of the translation operator," *J. Math. Phys.*, vol. 6, pp. 766–778, 1965.
- [8] R. Shankar, *Principle of Quantum Mechanics*. New York: Plenum Press, 1994.
- [9] J. J. Sakurai, *Modern Quantum Mechanics*. Menlo Park, California: The Benjamin/Cummings Publishing Company, Inc., 1985.
- [10] A. R. Edmonds, *Angular Momentum in Quantum Mechanics*. Princeton: Princeton Univ. Press, 1960.
- [11] E. M. Rose, *Elementary Theory of Angular Momentum*. New York: Wiley, 1957.
- [12] L. C. Biedenharn and J. D. Louck, *Angular Momentum in Quantum Physics*. Reading, Massachusetts: Addison-Wesley Publishing Company, 1981.
- [13] A. Boström, G. Kristensson, and S. Ström, "Transformation properties of plane, spherical and cylindrical scalar and vector wave functions," *Field Representations and Introduction to Scattering* (eds. V. V. Vardan, A. Lakhtakia & V. K. Varadan), Elsevier Science Publishers, 165–210, 1991.
- [14] S. Koc and W. C. Chew, "Calculation of acoustical scattering from a cluster of scatterers," *J. Acoust. Soc. Am.*, vol. 103, pp. 721–734, 1998.
- [15] L. F. Greengard and J. Huang, "A new version of the fast multipole method for screened coulomb interactions in the three dimensions," *J. Comput. Phys.*, vol. 180, pp. 642–658, 2002.

- [16] H. Cheng, W. Y. Grutchfield, Z. Gimbutas, L. F. Greengard, J. F. Ethridge, J. Huang, V. Rokhlin, N. Yarvin, and J. Zhao, "A wideband fast multipole method for the Helmholtz equation in three dimensions," *J. Comput. Phys.*, vol. 216, pp. 300–325, 2006.
- [17] N. A. Gumerov and R. Duraiswami, "Recursions for the computation of multipole translation and rotation coefficients for the 3-d Helmholtz equations," *SIAM J. Sci. Comput.*, vol. 25, no. 4, pp. 1344–1381, 2003.
- [18] J. D. Talman, *Special Functions: A Group Theoretic Approach*. New York: W. A. Benjamin, Inc., 1968.
- [19] W. Miller, "Some applications of the representation theory of the Euclidean group in three-space," *Commun. Pure Appl. Math.*, vol. 17, pp. 527–540, 1964.
- [20] W. Miller, *Lie Theory and Special Functions*. New York: Academic Press, 1968.
- [21] P. C. Waterman, "Matrix formulation of electromagnetic scattering," *Proc. IEEE*, vol. 53, pp. 805–812, 1965.
- [22] —, "Symmetry, unitarity, and geometry in electromagnetic scattering," *Phys. Rev. D*, vol. 3, pp. 825–839, 1971.
- [23] B. Peterson and S. Strom, "T matrix for electromagnetic scattering from an arbitrary number of scatters and representations of $E(3)$," *Phys. Rev. D*, vol. 8, no. 10, pp. 3661–3678, 1973.
- [24] M. I. Mishchenko, G. Videen, V. A. Babenko, N. G. Khlebtsov, and T. Wriedt, "T-matrix theory of electromagnetic scattering by particles and its applications: a comprehensive reference database," *J. Quant. Spectrosc. Radiat. Transfer*, vol. 88, pp. 357–406, 2004.
- [25] L. Tsang, J. A. Kong, and R. T. Shin, *Theory of Microwave Remote Sensing*. New York: John Wiley & Sons, 1985.
- [26] M. I. Mishchenko, L. D. Travis, and A. A. Lacis, *Scattering, Absorption, and Emission of Light by Small Particles*. Cambridge: Cambridge University Press, 2002.
- [27] L. Gürel and W. C. Chew, "Scattering solution of three-dimensional array of patches using the recursive T-matrix algorithms," *IEEE Microwave and Guided Wave Letters*, vol. 2, no. 5, pp. 182–184, May 1992.
- [28] —, "Recursive T-matrix algorithms for the solution of electromagnetic scattering from strip to patch geometries," *IEEE Trans. Antennas Propagat.*, vol. 41, no. 1, pp. 91–99, January 1993.
- [29] B. Peterson and S. Strom, "Matrix formulation of acoustic scattering from an arbitrary number of scatters," *J. Acoust. Soc. Am.*, vol. 56, no. 3, pp. 771–780, September 1974.
- [30] G. T. F. Borghese, P. Denti and O. I. Sindoni, "An addition theorem for vector Helmholtz harmonics," *J. Math. Phys.*, vol. 21, pp. 2754–2755, 1980.
- [31] W. C. Chew, "A derivation of the vector addition theorems," *Microwave Opt. Tech. Lett.*, vol. 3, no. 7, pp. 256–260, July 1990.

- [32] B. U. Felderhof and R. B. Jones, "Addition theorems for spherical wave solutions of the vector Helmholtz equation," *J. Math. Phys.*, vol. 28, pp. 836–839, 1987.
- [33] R. C. Wittmann, "Spherical wave operators and the translation formulas," *IEEE Trans. Antennas Propagat.*, vol. 36, no. 8, pp. 1078–1087, August 1988.
- [34] R. J. A. Tough, "The transformation properties of vector multipole fields under a translation of coordinate origin," *J. Phys. A: Math. Gen.*, vol. 10, no. 7, pp. 1079–1087, 1977.
- [35] W. W. Hansen, "A new type of expansion in radiation problems," *Phys. Rev.*, vol. 47, pp. 139–143, 1935.
- [36] L. Tsang and J. A. Kong, "Effective propagation constant for coherent electromagnetic waves in media embedded with dielectric scatterers," *J. Appl. Phys.*, vol. 53, no. 11, pp. 7162–73, 1982.
- [37] J. H. Bruning and Y. T. Lo, "Multiple scattering of EM waves by spheres, part I and II," *IEEE Trans. Antennas Propagat.*, vol. 19, no. 3, pp. 378–400, 1971.
- [38] K. T. Kim, "The translation formular for vector multipole fields and the recurrence relations of the translation coefficients of the scalar and vector multipole fields," *IEEE Trans. Antennas Propagat.*, vol. 44, no. 11, pp. 1482–1487, November 1996.
- [39] W. C. Chew, "Recurrence relations for three-dimensional scalar addition theorem," *J. Electromag. Waves. Appl.*, vol. 6, no. 2, pp. 133–142, 1992.
- [40] W. C. Chew and Y. M. Wang, "Efficient ways to compute the vector addition theorems," *J. Electromag. Waves. Appl.*, vol. 7, no. 5, pp. 651–665, 1993.
- [41] V. Rokhlin, "Rapid solution of integral equations of scattering theory in two dimensions," *J. Comput. Phys.*, vol. 86, no. 2, pp. 414–439, 1990.
- [42] R. Coifman, V. Rokhlin, and S. Wandzura, "The fast multipole method for the wave equation: A pedestrian prescription," *IEEE Ant. Propag. Mag.*, vol. 35, no. 3, pp. 7–12, 1993.
- [43] N. Nishimura, "Fast multipole accelerated boundary integral equation methods," *Appl. Mech. Rev.*, vol. 55, no. 4, pp. 299–324, July 2002.
- [44] N. A. Gumerov and R. Duraiswami, *Fast Multipole Methods for the Helmholtz Equation in Three Dimensions*. Amsterdam: Elsevier, 2004.
- [45] V. Rokhlin, "Diagonal forms of translation operators for the Helmholtz equation in three dimensions," *Appl. Comp. Harmon. Anal.*, vol. 1, pp. 82–93, 1993.
- [46] M. Epton and B. Dembart, "Multipole translation theory for three-dimensional Laplace and Helmholtz equations," *SIAM J. Sci. Comput.*, vol. 16, no. 4, pp. 865–897, 1995.
- [47] W. C. Chew, S. Koc, J. M. Song, C. C. Lu, and E. Michielssen, "A succinct way to diagonalize the translation matrix in three dimensions," *Microwave Opt. Technol. Lett.*, vol. 15, no. 3, pp. 144–147, June 1997.

- [48] J. A. Gaunt, “The triplets of helium,” *Philos. Trans. Roy. Soc. Ser. A*, vol. 228, pp. 151–196, 1929.
- [49] J. A. Stratton, *Electromagnetic Theory*. New York: McGraw-Hill, 1941.
- [50] J. D. Jackson, *Classical Electrodynamics*. New York: John Wiley & Sons, 1998.

Index

- a posteriori error estimate, 39, 44, 55
- acoustic scattering, 41, 56
- adaptive algorithm, 49
- addition theorem, 203, 212
- adjoint equation, 179
- Ampère’s law, 199
- angular momentum, 203, 204
- ansatz, 13, 143
- artificial boundary, 106
- artificial boundary condition, 167
- asymptotic high-frequency theories, 129

- Beck–Hiptmair–Hoppe–Wohlmuth
interpolant, 43
- Biot–Savart Law, 52
- Born approximation, 172, 173, 177
- boundary element method, 2
- boundary integral equations, 129

- Calderón projector, 3, 15
- Clebsch–Gordan coefficients, 205
- combined field integral equation, 132
- computational complexity, 65
- continuation method, 177
- Crank–Nicolson scheme, 121

- dielectric coefficient, 41
- diffraction limit, 188
- direct scattering problem, 166
- Dirichlet-to-Neumann map, 2, 15, 19, 57, 167, 168
- discrete inf-sup estimate, 30
- discretization error, 115, 119

- eddy current problem, 51
- edge element, 26
- eikonal equation, 130, 133, 143
- electric conductivity, 51
- electric field, 51, 108
- electric-field integral equation, 69
- electromagnetic vector, 190
- evanescent wave, 165
- evanescent waves, 198
- exact nonreflecting boundary condition, 106, 111, 118
- extended scatterer, 174

- far-field, 192
- Faraday’s law, 199
- fast Fourier transform, 67, 173
- fast multipole method, 67, 133
- finite difference approximation, 119
- finite element approximation, 42
- finite elements, 129
- finite-difference time-domain method, 119
- flux conservation, 190
- focal spot, 188, 192, 195, 197
- Fredholm alternative, 3, 10, 171

- Gårding inequality, 11, 14, 15, 21
- Galerkin discretization, 25, 27
- geometrical optics, 129, 133, 136
- Gibbs phenomenon, 183
- Green’s formula, 6, 15, 179
- Green’s function, 67, 68, 132, 141, 187

- Hankel function, 46, 47, 168
- Hansen multipole harmonic field, 217

- Heisenberg's uncertainty principle, 182
- Helmholtz decomposition, 217
- Helmholtz equation, 56, 130, 131, 165, 210
- Helmholtz-type decomposition, 4, 13, 27, 54
- high-frequency integral-equation approach, 149, 155, 157
- high-frequency scattering, 137
- Hodge-type decomposition, 4, 13
- image theorem, 195
- impedance boundary condition, 66
- inf-sup estimate, 32
- inverse Fourier transform, 173
- inverse Laplace transform, 57
- inverse scattering problem, 167
- kinetic formulation, 134
- Kirchhoff's approximation, 157
- Kirchhoff's equation, 87
- Kramers–Kronig relations, 189
- Lagrange interpolant, 82
- Lagrangian finite element, 39
- Landweber iteration, 178
- Laplace transform, 116
- Laplace–Beltrami operator, 45, 109
- Lax–Milgram lemma, 171
- layer potential, 8
- level set function, 175
- Liouville formulation, 135
- Lippmann–Schwinger integral equation, 172
- Lipschitz polyhedron, 5
- Lipschitz screen, 42
- local boundary condition, 115
- Luneberg–Kline expansion, 133
- Macdonald formula, 47, 60
- magnetic field, 51, 108
- magnetic permeability, 41, 51
- magnetic-field integral equation, 69
- Maxwell singularity, 44
- Maxwell's equations, 108, 190
- multiconductor transmission line, 87
- multilevel fast multipole method, 68
- multiple scattering, 136, 137, 142, 203
- multipole moment, 73
- MUSIC algorithm, 172, 174
- Nédélec edge element, 39, 48, 54
- near-field optics, 166
- non-convex obstacle, 39, 150
- nonlocal boundary condition, 110
- nonlocal transparent boundary condition, 167
- parallelization, 79
- penetrable scatterer, 1
- plane wave, 165
- plane wave time-domain algorithm, 66
- PML absorbing layer, 40, 46
- Poynting's vector, 190
- propagating wave, 165
- quasi-optimality property, 41
- quasi-static Maxwell's equations, 51
- Rao–Wilton–Glisson function, 70
- rate of convergence, 150
- reciprocity theorem, 190
- recursive linearization, 167, 172, 176, 177
- Rellich's embedding theorem, 5
- Rellich's lemma, 2
- response matrix, 174
- reverberation chamber, 195
- reversible medium, 188
- Ritz–Galerkin discretization, 2
- Robin-type boundary condition, 17
- scattering data, 173
- Scott–Zhang interpolant, 43
- shadow boundary, 136, 151, 152
- shape evolution, 175
- Silver–Müller radiation condition, 119
- Silver–Müller radiation condition, 7
- singular value decomposition, 174
- Sobolev spaces, 4
- Sommerfeld radiation condition, 56, 131, 166
- source vector, 190
- spectral Nystrom approach, 148
- spherical harmonics, 108
- split-field PML method, 58
- stability analysis, 181

- Stratton–Chu representation formula, 4
- sub-wavelength spot, 198
- tetrahedral triangulation, 42
- Tikhonov regularization, 174
- time dependent electromagnetic scattering, 106
- time reversal, 187
- time reversal mirror, 195
- time reversal relation, 191
- time reversed dipoles, 193
- time symmetry, 188
- time-domain adaptive integral method, 66, 71
- time-domain integral equation, 69
- time-harmonic electromagnetic scattering, 45
- Toeplitz structure, 75
- transport equation, 133
- unique continuation, 2
- unsplit-field PML method, 58
- variational formulation, 167
- vector spherical harmonics, 45, 109, 116
- wave equation, 106, 111
- weak scattering, 172
- weakly singular kernel, 132

Editorial Policy

1. Volumes in the following three categories will be published in LNCSE:

- i) Research monographs
- ii) Lecture and seminar notes
- iii) Conference proceedings

Those considering a book which might be suitable for the series are strongly advised to contact the publisher or the series editors at an early stage.

2. Categories i) and ii). These categories will be emphasized by Lecture Notes in Computational Science and Engineering. **Submissions by interdisciplinary teams of authors are encouraged.** The goal is to report new developments – quickly, informally, and in a way that will make them accessible to non-specialists. In the evaluation of submissions timeliness of the work is an important criterion. Texts should be well-rounded, well-written and reasonably self-contained. In most cases the work will contain results of others as well as those of the author(s). In each case the author(s) should provide sufficient motivation, examples, and applications. In this respect, Ph.D. theses will usually be deemed unsuitable for the Lecture Notes series. Proposals for volumes in these categories should be submitted either to one of the series editors or to Springer-Verlag, Heidelberg, and will be refereed. A provisional judgment on the acceptability of a project can be based on partial information about the work: a detailed outline describing the contents of each chapter, the estimated length, a bibliography, and one or two sample chapters – or a first draft. A final decision whether to accept will rest on an evaluation of the completed work which should include

- at least 100 pages of text;
- a table of contents;
- an informative introduction perhaps with some historical remarks which should be accessible to readers unfamiliar with the topic treated;
- a subject index.

3. Category iii). Conference proceedings will be considered for publication provided that they are both of exceptional interest and devoted to a single topic. One (or more) expert participants will act as the scientific editor(s) of the volume. They select the papers which are suitable for inclusion and have them individually refereed as for a journal. Papers not closely related to the central topic are to be excluded. Organizers should contact Lecture Notes in Computational Science and Engineering at the planning stage.

In exceptional cases some other multi-author-volumes may be considered in this category.

4. Format. Only works in English are considered. They should be submitted in camera-ready form according to Springer-Verlag's specifications.

Electronic material can be included if appropriate. Please contact the publisher.

Technical instructions and/or LaTeX macros are available via <http://www.springer.com/east/home/math/math+authors?SGWID=5-40017-6-71391-0>. The macros can also be sent on request.

General Remarks

Lecture Notes are printed by photo-offset from the master-copy delivered in camera-ready form by the authors. For this purpose Springer-Verlag provides technical instructions for the preparation of manuscripts. See also *Editorial Policy*.

Careful preparation of manuscripts will help keep production time short and ensure a satisfactory appearance of the finished book.

The following terms and conditions hold:

Categories i), ii), and iii):

Authors receive 50 free copies of their book. No royalty is paid. Commitment to publish is made by letter of intent rather than by signing a formal contract. Springer-Verlag secures the copyright for each volume.

For conference proceedings, editors receive a total of 50 free copies of their volume for distribution to the contributing authors.

All categories:

Authors are entitled to purchase further copies of their book and other Springer mathematics books for their personal use, at a discount of 33.3% directly from Springer-Verlag.

Addresses:

Timothy J. Barth
NASA Ames Research Center
NAS Division
Moffett Field, CA 94035, USA
e-mail: barth@nas.nasa.gov

Michael Griebel
Institut für Numerische Simulation
der Universität Bonn
Wegelerstr. 6
53115 Bonn, Germany
e-mail: griebel@ins.uni-bonn.de

David E. Keyes
Department of Applied Physics
and Applied Mathematics
Columbia University
200 S. W. Mudd Building
500 W. 120th Street
New York, NY 10027, USA
e-mail: david.keyes@columbia.edu

Risto M. Nieminen
Laboratory of Physics
Helsinki University of Technology
02150 Espoo, Finland
e-mail: rni@fyslab.hut.fi

Dirk Roose
Department of Computer Science
Katholieke Universiteit Leuven
Celestijnenlaan 200A
3001 Leuven-Heverlee, Belgium
e-mail: dirk.roose@cs.kuleuven.ac.be

Tamar Schlick
Department of Chemistry
Courant Institute of Mathematical
Sciences
New York University
and Howard Hughes Medical Institute
251 Mercer Street
New York, NY 10012, USA
e-mail: schlick@nyu.edu

Mathematics Editor at Springer:
Martin Peters
Springer-Verlag
Mathematics Editorial IV
Tiergartenstrasse 17
D-69121 Heidelberg, Germany
Tel.: *49 (6221) 487-8185
Fax: *49 (6221) 487-8355
e-mail: martin.peters@springer.com

Lecture Notes in Computational Science and Engineering

1. D. Funaro, *Spectral Elements for Transport-Dominated Equations*.
2. H. P. Langtangen, *Computational Partial Differential Equations*. Numerical Methods and Diffpack Programming.
3. W. Hackbusch, G. Wittum (eds.), *Multigrid Methods V*.
4. P. Deufhard, J. Hermans, B. Leimkuhler, A. E. Mark, S. Reich, R. D. Skeel (eds.), *Computational Molecular Dynamics: Challenges, Methods, Ideas*.
5. D. Kröner, M. Ohlberger, C. Rohde (eds.), *An Introduction to Recent Developments in Theory and Numerics for Conservation Laws*.
6. S. Turek, *Efficient Solvers for Incompressible Flow Problems*. An Algorithmic and Computational Approach.
7. R. von Schwerin, *Multi Body System SIMulation*. Numerical Methods, Algorithms, and Software.
8. H.-J. Bungartz, F. Durst, C. Zenger (eds.), *High Performance Scientific and Engineering Computing*.
9. T. J. Barth, H. Deconinck (eds.), *High-Order Methods for Computational Physics*.
10. H. P. Langtangen, A. M. Bruaset, E. Quak (eds.), *Advances in Software Tools for Scientific Computing*.
11. B. Cockburn, G. E. Karniadakis, C.-W. Shu (eds.), *Discontinuous Galerkin Methods*. Theory, Computation and Applications.
12. U. van Rienen, *Numerical Methods in Computational Electrodynamics*. Linear Systems in Practical Applications.
13. B. Engquist, L. Johnsson, M. Hammill, F. Short (eds.), *Simulation and Visualization on the Grid*.
14. E. Dick, K. Rienslagh, J. Vierendeels (eds.), *Multigrid Methods VI*.
15. A. Frommer, T. Lippert, B. Medeke, K. Schilling (eds.), *Numerical Challenges in Lattice Quantum Chromodynamics*.
16. J. Lang, *Adaptive Multilevel Solution of Nonlinear Parabolic PDE Systems*. Theory, Algorithm, and Applications.
17. B. I. Wohlmuth, *Discretization Methods and Iterative Solvers Based on Domain Decomposition*.
18. U. van Rienen, M. Günther, D. Hecht (eds.), *Scientific Computing in Electrical Engineering*.
19. I. Babuška, P. G. Ciarlet, T. Miyoshi (eds.), *Mathematical Modeling and Numerical Simulation in Continuum Mechanics*.
20. T. J. Barth, T. Chan, R. Haines (eds.), *Multiscale and Multiresolution Methods*. Theory and Applications.
21. M. Breuer, F. Durst, C. Zenger (eds.), *High Performance Scientific and Engineering Computing*.
22. K. Urban, *Wavelets in Numerical Simulation*. Problem Adapted Construction and Applications.
23. L. F. Pavarino, A. Toselli (eds.), *Recent Developments in Domain Decomposition Methods*.

24. T. Schlick, H. H. Gan (eds.), *Computational Methods for Macromolecules: Challenges and Applications*.
25. T. J. Barth, H. Deconinck (eds.), *Error Estimation and Adaptive Discretization Methods in Computational Fluid Dynamics*.
26. M. Griebel, M. A. Schweitzer (eds.), *Meshfree Methods for Partial Differential Equations*.
27. S. Müller, *Adaptive Multiscale Schemes for Conservation Laws*.
28. C. Carstensen, S. Funken, W. Hackbusch, R. H. W. Hoppe, P. Monk (eds.), *Computational Electromagnetics*.
29. M. A. Schweitzer, *A Parallel Multilevel Partition of Unity Method for Elliptic Partial Differential Equations*.
30. T. Biegler, O. Ghattas, M. Heinkenschloss, B. van Bloemen Waanders (eds.), *Large-Scale PDE-Constrained Optimization*.
31. M. Ainsworth, P. Davies, D. Duncan, P. Martin, B. Rynne (eds.), *Topics in Computational Wave Propagation*. Direct and Inverse Problems.
32. H. Emmerich, B. Nestler, M. Schreckenberg (eds.), *Interface and Transport Dynamics*. Computational Modelling.
33. H. P. Langtangen, A. Tveito (eds.), *Advanced Topics in Computational Partial Differential Equations*. Numerical Methods and Diffpack Programming.
34. V. John, *Large Eddy Simulation of Turbulent Incompressible Flows*. Analytical and Numerical Results for a Class of LES Models.
35. E. Bänsch (ed.), *Challenges in Scientific Computing - CISC 2002*.
36. B. N. Khoromskij, G. Wittum, *Numerical Solution of Elliptic Differential Equations by Reduction to the Interface*.
37. A. Iske, *Multiresolution Methods in Scattered Data Modelling*.
38. S.-I. Niculescu, K. Gu (eds.), *Advances in Time-Delay Systems*.
39. S. Attinger, P. Koumoutsakos (eds.), *Multiscale Modelling and Simulation*.
40. R. Kornhuber, R. Hoppe, J. Périaux, O. Pironneau, O. Wildlund, J. Xu (eds.), *Domain Decomposition Methods in Science and Engineering*.
41. T. Plewa, T. Linde, V. G. Weirs (eds.), *Adaptive Mesh Refinement – Theory and Applications*.
42. A. Schmidt, K. G. Siebert, *Design of Adaptive Finite Element Software*. The Finite Element Toolbox ALBERTA.
43. M. Griebel, M. A. Schweitzer (eds.), *Meshfree Methods for Partial Differential Equations II*.
44. B. Engquist, P. Lötstedt, O. Runborg (eds.), *Multiscale Methods in Science and Engineering*.
45. P. Benner, V. Mehrmann, D. C. Sorensen (eds.), *Dimension Reduction of Large-Scale Systems*.
46. D. Kressner (ed.), *Numerical Methods for General and Structured Eigenvalue Problems*.
47. A. Boriçi, A. Frommer, B. Joó, A. Kennedy, B. Pendleton (eds.), *QCD and Numerical Analysis III*.
48. F. Graziani (ed.), *Computational Methods in Transport*.

49. B. Leimkuhler, C. Chipot, R. Elber, A. Laaksonen, A. Mark, T. Schlick, C. Schütte, R. Skeel (eds.), *New Algorithms for Macromolecular Simulation*.
50. M. Bücker, G. Corliss, P. Hovland, U. Naumann, B. Norris (eds.), *Automatic Differentiation: Applications, Theory, and Implementations*.
51. A.M. Bruaset, A. Tveito (eds.), *Numerical Solution of Partial Differential Equations on Parallel Computers*.
52. K.H. Hoffmann, A. Meyer (eds.), *Parallel Algorithms and Cluster Computing*.
53. H.-J. Bungartz, M. Schäfer (eds.), *Fluid-Structure Interaction*.
54. J. Behrens, *Adaptive Atmospheric Modeling*.
55. O. Widlund, D. Keyes (eds.), *Domain Decomposition Methods in Science and Engineering XVI*.
56. S. Kassinos, C. Langer, G. Iaccarino, P. Moin (eds.), *Complex Effects in Large Eddy Simulations*.
57. M. Griebel, M.A Schweitzer (eds.), *Meshfree Methods for Partial Differential Equations III*.
58. A.N. Gorban, B. Kégl, D.C. Wunsch, A. Zinovyev (eds.), *Principal Manifolds for Data Visualization and Dimension Reduction*.
59. H. Ammari (ed.), *Modeling and Computations in Electromagnetics: A Volume Dedicated to Jean-Claude Nédélec*.

For further information on these books please have a look at our mathematics catalogue at the following URL: www.springer.com/series/3527

Monographs in Computational Science and Engineering

1. J. Sundnes, G.T. Lines, X. Cai, B.F. Nielsen, K.-A. Mardal, A. Tveito, *Computing the Electrical Activity in the Heart*.

For further information on this book, please have a look at our mathematics catalogue at the following URL: www.springer.com/series/7417

Texts in Computational Science and Engineering

1. H. P. Langtangen, *Computational Partial Differential Equations*. Numerical Methods and Diffpack Programming.
2. A. Quarteroni, F. Saleri, *Scientific Computing with MATLAB and Octave*.
3. H. P. Langtangen, *Python Scripting for Computational Science*.
4. H. Gardner, G. Manduchi, *Design Patterns for e-Science*.
5. M. Griebel, S. Knapek, G. Zumbusch, *Numerical Simulation in Molecular Dynamics*.

For further information on these books please have a look at our mathematics catalogue at the following URL: www.springer.com/series/5151