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► **To cite this version:**

Lonny Thompson. A review of finite-element methods for time-harmonic acoustics. Journal of the Acoustical Society of America, 2006, 119 (3), pp.1315-1330. 10.1121/1.2164987 . hal-03680855

HAL Id: hal-03680855

<https://hal.science/hal-03680855>

Submitted on 29 May 2022

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A review of finite-element methods for time-harmonic acoustics

Lonny L. Thompson^{a)}

Department of Mechanical Engineering, Clemson University, Clemson, South Carolina 29634-0921

State-of-the-art finite-element methods for time-harmonic acoustics governed by the Helmholtz equation are reviewed. Four major current challenges in the field are specifically addressed: the effective treatment of acoustic scattering in unbounded domains, including local and nonlocal absorbing boundary conditions, infinite elements, and absorbing layers; numerical dispersion errors that arise in the approximation of short unresolved waves, polluting resolved scales, and requiring a large computational effort; efficient algebraic equation solving methods for the resulting complex-symmetric (non-Hermitian) matrix systems including sparse iterative and domain decomposition methods; and a posteriori error estimates for the Helmholtz operator required for adaptive methods. Mesh resolution to control phase error and bound dispersion or pollution errors measured in global norms for large wave numbers in finite-element methods are described. Stabilized, multiscale, and other wave-based discretization methods developed to reduce this error are reviewed. A review of finite-element methods for acoustic inverse problems and shape optimization is also given.

I. INTRODUCTION

Finite-element methods (FEM) for time-harmonic acoustics governed by the reduced wave equation (Helmholtz equation) have been an active research area for nearly 40 years. Initial applications of finite-element methods for time-harmonic acoustics focused on interior problems with complex geometries including direct and modal coupling of structural acoustic systems for forced vibration analysis, frequency response of acoustic enclosures, and waveguides (Craggs, 1972; Gladwell, 1966; Nefske *et al.*, 1982; Petyt *et al.*, 1976; Young and Crocker, 1975; Zienkiewicz and Newton, 1969). In recent years, tremendous progress in the development of improved finite-element methods for time-harmonic acoustics including exterior problems in unbounded domains, which incorporate knowledge of wave behavior into the algorithm, combined with parallel sparse iterative and domain decomposition solvers, are moving the application of FEM into the higher frequency (wave number) regimes.

The exterior acoustics problem in unbounded domains presents a special challenge for finite-element methods. In order to use the FEM for exterior problems, the unbounded domain is usually truncated by an artificial boundary Γ yielding a bounded computational domain Ω ; see Fig. 1. Reducing the size of the bounded domain reduces the computation cost, but must be balanced by the ability to minimize any spurious wave reflection with a computationally efficient and geometrically flexible truncation boundary treatment. The first complete finite-element approach for modeling acoustic radiation and scattering in unbounded domains appears in the impedance matching technique presented by Hunt *et al.* 1974, 1975. Recent numerical treatments including infinite elements, absorbing layers, local absorbing boundary condi-

tions, and exact nonlocal boundary conditions have proven to be effective in handling acoustic scattering problems in unbounded domains, especially for large-scale problems requiring iterative and parallel solution methods and for modeling inhomogeneities and acoustic-structure interaction. The method of choice depends on the shape and complexity of the scattering object, inhomogeneities, frequency range, and resolution requirements, among other parameters.

A natural way of modeling the acoustic region exterior to a scattering/radiating object is to introduce a boundary element discretization of the surface S based on an integral representation of the exact solution in the exterior (Burton and Miller, 1971; Colton and Kreiss, 1983; Walsh *et al.*, 2004). Using the free-space Green's function (fundamental solution), the boundary element method (BEM) only requires surface discretization on S , reducing the d -dimensional problem to a $(d-1)$ -dimensional one, and automatically satisfies the required Sommerfeld radiation condition at infinity (Sommerfeld, 1912). The BEM naturally incorporates surface impedance conditions but is limited in the ability to model complex, inhomogeneous regions. Application of the classical BEM for acoustic scattering requires solution of large, dense, complex linear systems due to the nonlocal support of the fundamental solution leading to high computational expense and storage requirements.

The finite-element method (FEM) is able to solve problems in nonhomogeneous media and allows for a natural coupling with complex structures. For exterior problems in unbounded domains, special techniques are required to reduce spurious reflection to a level below that of the discretization error. The numerical advantage of the FEM is that they lead to sparse matrices, which by avoiding calculations on zeros, significantly speed up computations and reduce memory requirements. Complexity estimates (Harari and Hughes, 1992) and numerical evidence (Burnett, 1994) have shown that domain-based methods such as the FEM are an

^{a)}Electronic mail: lonny.thompson@ces.clemson.edu

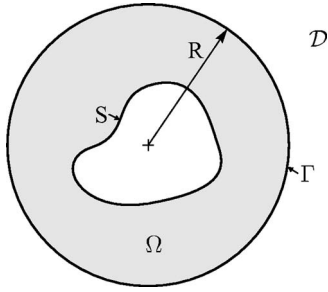


FIG. 1. Artificial truncation boundary Γ defining finite computational domain Ω for the exterior problem.

effective alternative to the BEM for exterior acoustics problems, especially for large systems due to the sparse structure of the resulting system matrices. With the recent developments in fast multipole methods which accelerate the calculation of matrix-vector products in iterative integral methods (Chen and Chen, 2004; Chew *et al.*, 1997, 2004; Darrigrand, 2002; Darve, 2000; Epton and Dembart, 1995; Fischer *et al.*, 2004; Greengard *et al.*, 1998; Gumerov and Duraiswami, 2004; Rockhlin, 1993; Sakuma and Yasuda, 2002; Schneider, 2003), the method with the best efficiency is less clear, yet the FEM retains the advantages of robustness and natural integration with other discrete models in coupled problems. It is also possible to couple the finite method with boundary integral methods (Fischer and Gaul, 2005), and other domain-based methods such as global Trefftz-based wave methods which are effective at high frequencies on moderate geometrical complexity (Van Hal *et al.*, 2003).

A difficulty of the standard Galerkin FEM applied to short-wave problems with wavelengths smaller than the geometrical parameters defining the domain has been the ability to accurately resolve oscillating wave solutions at higher frequencies (wave numbers). The difficulty of simultaneously achieving accuracy and efficiency at high wave numbers has been cited as one of the most challenging problems in scientific computation (Zienkiewicz, 2000). The failure to adequately control numerical dispersion errors not only inaccurately approximates the oscillatory part of the solution, but has a global pollution effect that builds up over the whole computational domain. The pollution effect is related to the loss of stability of the Helmholtz operator at large wave numbers. Due to challenges in accurately resolving short wave solutions at higher frequencies, many alternative and creative finite-element methods have been developed in the last decade including high-order methods, stabilized Galerkin methods, multiscale variational methods, and other wave-based discretization methods. A common theme of many of these improved finite-element methods is that they incorporate knowledge of wave behavior into the solution algorithm. Other recent improvements which are pushing the FEM into larger wave number regimes include the development of efficient iterative solvers with accelerating preconditioners, and domain decomposition parallel solution methods for the resulting sparse complex-symmetric (non-Hermitian) matrix systems arising from discretization of the Helmholtz operator.

In this paper, recent developments in finite-element methods for time-harmonic acoustics, including treatments of unbounded domains are reviewed. Topics include local and nonlocal Dirichlet-to-Neumann (DtN) nonreflecting boundary conditions, infinite elements, and absorbing layers for exterior problems; discretization methods which reduce numerical dispersion error arising in the approximation of short unresolved waves; efficient algebraic equation solving methods including sparse iterative and domain decomposition methods; a posteriori error estimates, adaptive methods; acoustic inverse problems, and shape optimization.

II. THE EXTERIOR PROBLEM IN UNBOUNDED DOMAINS

Let V be the domain of an object with boundary S . The exterior domain is defined by the unbounded region $\mathcal{R} = \mathbb{R}^3 \setminus V$. Time-harmonic acoustics is governed by the Helmholtz differential equation. For exterior problems defined on unbounded domains, solutions are required to satisfy the *Sommerfeld radiation condition* at infinity (Sommerfeld, 1912). The differential form of the boundary-value problem for exterior problems in unbounded domains may be stated for a general impedance surface condition as: Given wave number-dependent boundary data $g(\mathbf{x}; k) \in \mathbb{C}$, $\beta(\mathbf{x}; k) \in \mathbb{C}$; Find the complex-valued scalar field $u(\mathbf{x}; k) \in \mathbb{C}$, such that

$$\nabla^2 u + k^2 u = 0, \quad \text{in } \mathcal{R} = \mathbb{R}^3 \setminus V \quad (1)$$

$$\frac{\partial u}{\partial n} + \beta u = g, \quad \text{on } S \quad (2)$$

$$\lim_{r \rightarrow \infty} r \left(\frac{\partial u}{\partial r} - iku \right) = 0. \quad (3)$$

Here, $u(\mathbf{x})$ represents the spatial part of the acoustic pressure or velocity potential, with wavenumber $k \in \mathbb{C}$, $\text{Im}(k) \geq 0$. The sign convention for the phase is $e^{-i\omega t}$, where $i = \sqrt{-1}$ and ω is the natural frequency. The normal derivative $(\partial u / \partial n) := \nabla u \cdot \mathbf{n}$ defines the gradient in the direction of the unit outward vector normal to S . In the above, $r = \|\mathbf{x}\|$ is a radius centered near the origin of the sound source. The *Sommerfeld radiation condition* (3) allows only outgoing waves proportional to $\exp(ikr)$ at infinity. The radiation condition requires that energy flux at infinity be positive, thus ensuring unique solutions.

Finite-element methods typically introduce an artificial boundary Γ , which divides the original unbounded domain into two regions: a bounded computational domain Ω discretized with the finite-element method and an infinite residual region $\mathcal{D} = \mathcal{R} \setminus \Omega$; see Fig. 1. Reducing the size of the bounded computational domain decreases the computational cost and memory storage. Methods for modeling the exterior complement $\mathcal{D} = \mathcal{R} \setminus \Omega$, i.e., the infinite region exterior to the artificial boundary Γ , can be divided into three main categories: local or nonlocal absorbing (nonreflecting) boundary conditions, infinite elements, and absorbing layers. Infinite element methods represent the exterior complement by assuming a radial approximation with outgoing wave behavior. Matched absorbing layers attempt to decay outgoing waves

in a relatively thin layer exterior to Γ . For the nonreflecting (absorbing) boundary conditions, the outgoing wave solution in \mathcal{D} is represented by a relation of the unknown solution and its derivative on the artificial truncation boundary Γ . Options include matching exact analytical series solutions Hunt *et al.*, 1974, 1975, as used in the nonlocal Dirichlet-to-Neumann (DtN) map (Keller and Givoli, 1989), and various local approximations. The artificial boundary Γ is usually taken to be a surface defined in separable coordinates for efficiency, e.g., a sphere or spheroid. Formulations on nonseparable boundaries have also been developed; in this case the formulations are usually applied directly to the surface of the scatterer, thus completely avoiding discretization in Ω , e.g., Antoine, 2002; Antoine *et al.*, 1999; Shirron and Dey, 2002. Unbounded domain treatments may also be derived for acoustic waveguide problems (Bayliss *et al.*, 1983; Givoli, 1999; Murphy and Ching-Bing, 1989).

For absorbing boundary conditions, the originally unbounded exterior problem is replaced by an equivalent reduced problem defined on the bounded domain Ω : Find $u(\mathbf{x}) \in \mathbb{C}$, such that

$$\nabla^2 u + k^2 u = 0, \quad \text{in } \Omega \quad (4)$$

$$\frac{\partial u}{\partial n} + \mathcal{B}u = g, \quad \text{on } S \quad (5)$$

$$\frac{\partial u}{\partial n} = \mathcal{B}u, \quad \text{on } \Gamma \quad (6)$$

where \mathcal{B} is a linear operator called the *Dirichlet-to-Neumann* (DtN) map relating Dirichlet data to the outward normal derivative of the solution on Γ . The DtN operator \mathcal{B} approximates the Sommerfeld radiation condition at a finite boundary Γ , and must satisfy the condition $\text{Im}(u, \mathcal{B}u)_\Gamma \neq 0$ to ensure unique solutions. The DtN operator \mathcal{B} is usually either a differential (local) or integral (nonlocal) operator, or combination of both. Physically, the DtN operator \mathcal{B} represents radiation admittance relating pressure u (Dirichlet data) to normal velocity v_n which is proportional to the normal derivative $\partial u / \partial n = i\omega \rho v_n$ (Neumann data), on the truncation boundary Γ .

III. LOCAL ABSORBING BOUNDARY CONDITIONS

Absorbing boundary conditions should annihilate any spurious reflections at the artificial boundary (which are incoming). For local absorbing boundary conditions defined on a sphere, the development is based on the idea of annihilating radial terms in the Atkinson-Wilcox radial expansion in powers of $1/kr$ (Atkinson, 1949; Wilcox, 1956)

$$u(r, \theta, \varphi; k) = \frac{e^{ikr}}{ikr} \sum_{l=0}^{\infty} \frac{f_l(\theta, \varphi; k)}{(kr)^l}. \quad (7)$$

This expansion is valid for radius $r\theta > r_0$, where r_0 is the radius of a spherical (or spheroidal) surface circumscribing the target/radiator, labeled S in Fig. 1, and any inhomogeneities of the domain Ω . Outside r_0 , and in particular the radius R of the truncation surface, the exterior domain must be ho-

mogeneous and may not contain any objects/obstacles. Bayliss *et al.* (1982) showed that a sequence of local differential operators can be used to annihilate terms in this expansion. The first two local operators acting on the expansion for u , with their corresponding remainders are

$$G_1 u = \left(\frac{\partial}{\partial r} - \mathcal{B}_1 \right) u = O(1/kr)^3, \quad (8)$$

$$G_2 u = \left(\frac{\partial}{\partial r} + \frac{2}{r} - \mathcal{B}_1 \right) \left(\frac{\partial}{\partial r} - \mathcal{B}_1 \right) u = O(1/kr)^5, \quad (9)$$

where

$$\mathcal{B}_1 = ik - \frac{1}{r}. \quad (10)$$

In the case of the second-order operator G_2 , the second-order radial derivative is replaced by second-order angular derivatives using the Helmholtz equation expressed in spherical coordinates. Setting the remainders to zero results in approximate local radiation boundary conditions which are easily implemented in standard finite-element methods. The corresponding local BGT boundary conditions are defined by relating the radial (normal) derivative to Dirichlet data in the form of the differential map,

$$\frac{\partial u}{\partial r} = \mathcal{B}_j u, \quad (11)$$

where for $j=1$, the first-order operator \mathcal{B}_1 is defined in (10) and for $j=2$, the second-order BGT operator is

$$\mathcal{B}_2 = \mathcal{B}_1 + \frac{1}{2\mathcal{B}_1} \Delta_\Gamma. \quad (12)$$

The second-order angular derivatives appearing in (12) are defined by

$$\Delta_\Gamma u := \nabla_\Gamma \cdot \nabla_\Gamma u = \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2},$$

where

$$\nabla_\Gamma := \frac{1}{r} \frac{\partial}{\partial \theta} \mathbf{e}_\theta + \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi} \mathbf{e}_\varphi.$$

The corresponding weak (variational) form of the boundary value problem with the \mathcal{B}_2 BGT operator is: Find the trial solution u , such that, for all test functions w

$$B(w, u) - B_\Gamma(w, u) = F(w), \quad (13)$$

where

$$B(w, u) := \int_{\Omega} (\nabla w \cdot \nabla u - k^2 w u) dx + \int_S \beta w u ds,$$

$$B_\Gamma(w, u) := \int_{\Gamma} \mathcal{B}_1 w u d\Gamma - \int_{\Gamma} \frac{1}{2\mathcal{B}_1} \nabla_\Gamma w \cdot \nabla_\Gamma u d\Gamma,$$

$$F(w) := \int_S w g ds,$$

with differential surface area $d\Gamma = R^2 \sin \theta d\theta d\varphi$ on a spherical truncation boundary of radius R . The \mathcal{B}_1 and \mathcal{B}_2 operators both satisfy a required uniqueness condition, $\text{Im}[B_\Gamma(u, u)] > 0$ (or < 0), for all u evaluated on Γ , $u \neq 0$ (Grote and Keller, 1995; Harari and Hughes, 1992). The differential operators \mathcal{B}_j , $j=1,2$, are relatively simple to implement and retain the local sparse structure of the finite-element method. The local condition \mathcal{B}_2 is preferred since, for a fixed radius, it is more accurate compared to \mathcal{B}_1 , as can be seen from the orders of the remainders in (9). Direct finite-element implementation of high-order operators \mathcal{B}_j , $j \geq 3$, are problematic in conventional finite-element methods since regularity in angular derivatives higher than standard $C^0(\Gamma)$ are required (Givoli *et al.*, 1997).

Conventional finite-element methods partition the computational domain Ω into nonoverlapping subdomains (elements) Ω_e with continuous piecewise polynomials. In the standard h -version, basis (shape) functions $N_i(\mathbf{x})$, associated with element nodes are C^0 continuous interpolation functions with compact support. The continuous approximation is written as the linear combination,

$$u^h(\mathbf{x}) = \sum_{i=1}^{N_{\text{dof}}} N_i(\mathbf{x}) d_i = \mathbf{N}^T(\mathbf{x}) \mathbf{d}, \quad (14)$$

where $\mathbf{N} \in \mathbb{R}^{N_{\text{dof}}}$ is a column vector of standard C^0 basis functions, and $\mathbf{d} \in \mathbb{C}^{N_{\text{dof}}}$ is a column vector containing the N_{dof} unknown nodal values $d_i = u^h(\mathbf{x}_i)$, where $u^h(\mathbf{x}_i)$ is the approximation of the solution u at node \mathbf{x}_i . Using a standard Galerkin finite-element approximation, test (weighting) functions w^h are expressed as a linear span of the same basis functions. Substitution into (13) leads to the sparse, complex-symmetric (non-Hermitian) linear algebraic system,

$$\mathbf{Z} \mathbf{d} = \mathbf{f}, \quad \mathbf{Z} = (\mathbf{S} - k^2 \mathbf{M} - \mathbf{K}_\Gamma), \quad (15)$$

with matrix coefficients

$$(\mathbf{S})_{ij} = \int_{\Omega} \nabla N_i \cdot \nabla N_j dx + \int_S \beta N_i N_j ds,$$

$$(\mathbf{M})_{ij} = \int_{\Omega} N_i N_j dx,$$

$$(\mathbf{K}_\Gamma)_{ij} = \int_{\Gamma} \mathcal{B}_1 N_i N_j d\Gamma - \int_{\Gamma} \frac{1}{2\mathcal{B}_1} \nabla_\Gamma N_i \cdot \nabla_\Gamma N_j d\Gamma.$$

The excitation vector

$$(\mathbf{f})_i = \int_S N_i g ds, \quad (16)$$

is in general complex-valued, and wave number dependent. The contribution from the local absorbing conditions are found in the k -dependent sparse matrix \mathbf{K}_Γ associated with node points on the boundary Γ . Further details of the finite-element implementation such as element mapping, integration, and assembly of element arrays are found in standard finite-element textbooks, e.g., Hughes, 2000; Petyt, 1990. The local support of the element shape functions gives the advantage of being able to handle complex geometries and producing sparse matrices which are solved efficiently by avoiding storage and computation of zero coefficients. For large three-dimensional problems at high wave numbers k , accurate resolution requires a large number of elements leading to large sparse matrices. In this case, iterative solvers are preferred over direct factorization methods due to the lower memory requirements and parallel computing performance.

Other local absorbing conditions which attempt to annihilate incoming waves include the Enquist and Majda (1977) and Feng (1983) conditions. In a numerical study by Shirron (1998), the accuracy of the BGT conditions are the most accurate, especially for low modes and tight boundaries. The first- and second-order BGT conditions have been widely used Bossut and Decarpigny, 1989; Kechroud *et al.*, 2004; Tezaur *et al.*, 2001 and have been generalized to spheroidal (Grote and Keller, 1995) and arbitrary convex surfaces (Antoine *et al.*, 1999). The use of spheroidal or rectangular coordinates allows the artificial boundary to obtain a tight fit around elongated objects. For spheroidal, and other convex shapes, the conditions tend to lose accuracy for higher wave numbers (Tezaur *et al.*, 2002). Low-order approximate conditions require careful placement when computing the response over a range of frequencies; the size of the computational domain and the mesh density must be carefully selected to achieve a prescribed accuracy. If not placed sufficiently far from the radiating/scattering object, low-order local approximate absorbing boundary conditions may produce large spurious reflections which can pollute the entire numerical solution.

Complexity estimates show that it is usually more efficient to use high-order accurate absorbing conditions which enable smaller computational domains. The development of high-order local boundary conditions for which the order can be easily increased to a desired level are usually based on using auxiliary variables to eliminate higher-order derivatives (Givoli, 2004; Hagstrom, 1999; Hagstrom and Hariharan, 1998; Huan and Thompson, 2000; Thompson *et al.*, 2001; van Joolen *et al.*, 2003). While generally derived for the time-dependent case, time-harmonic counterparts are readily implemented with time derivatives replaced by $i\omega$, $\omega = kc$, where c is wave speed.

IV. THE DTN NONREFLECTING BOUNDARY CONDITION

An alternative to high-order local absorbing conditions are nonlocal DtN nonreflecting boundary conditions. The conceptual foundation and experimental validation for the DtN finite-element method are presented for both acoustic radiation and scattering in the impedance matching technique of Hunt *et al.*, 1974, 1975. In Hunt (1974), the relationship between the pressure (Dirichlet data) and its normal derivative (Neumann data) on a spherical surface Γ is obtained using the surface Helmholtz integral equation with boundary condition $\partial u / \partial n = i\omega\rho v_n$, and then by expanding the analytical solution for the pressure u and normal velocity v_n in terms of spherical harmonics and matching coefficients. In Keller and Givoli (1989) the DtN map on a sphere of radius R is constructed directly and implemented in the standard Galerkin finite-element method by expanding the outgoing acoustic field in a spherical harmonic series,

$$u(r, \theta, \varphi) = \sum_{n=0}^{N-1} \frac{h_n(kr)}{h_n(kR)} \sum_{m=-n}^n u_{nm} Y_{nm}(\theta, \varphi), \quad (17)$$

with coefficients

$$u_{nm} = (u, Y_{nm})_{\mathcal{S}} := \int_0^{2\pi} \int_0^{\pi} u(R, \theta, \varphi) Y_{nm}^* d\mathcal{S}. \quad (18)$$

In the above, $d\mathcal{S} = \sin\theta d\theta d\varphi$ is the differential surface element on the unit sphere \mathcal{S} , parametrized by $0 < \theta < \pi$, $0 < \varphi < 2\pi$, and

$$Y_{nm}(\theta, \varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos\theta) e^{im\varphi}$$

are angular spherical harmonics such that $Y_{n,(-m)} = (-1)^m Y_{nm}^*$; the star denotes complex conjugate; and $h_n(kr)$ are outgoing radial spherical Hankel functions. The DtN map is then obtained by evaluating the normal derivative of (17) on the boundary at $r=R$, and implemented as a “natural” boundary condition with standard finite-element basis functions for u on the surface Γ . Givoli (1999) recognized that the DtN finite-element method could be generalized to other boundary value problems with infinite domains. The operator is nonlocal since the coefficients u_{nm} in (18) require integration over the whole surface. The DtN map exactly represents all harmonics in the solution up to the number of terms included in the truncated series expansion as measured by N . For higher harmonics $n > N-1$, the truncated DtN models the boundary Γ with the homogeneous Neumann condition $\partial u / \partial r = 0$ at $r=R$. As a consequence, nonunique solutions may result when k^2 matches an interior resonance associated with the Laplacian operator. Harari and Hughes (1992) showed that this difficulty can be eliminated by using a sufficient number of harmonics N . However, the restriction may require more terms in the DtN map than may be necessary to achieve a desired accuracy, leading to a potential for excessive computation.

This problem is circumvented if a modified truncated DtN operator (Grote and Keller, 1995) is used, $\mathcal{M}^* = (\mathcal{M}_N - \mathcal{B}_N) + \mathcal{B}$, where \mathcal{B} is any computationally efficient approxi-

mation to the DtN operator with the uniqueness property $\text{Im}(u, \mathcal{B}u)_{\Gamma} \neq 0$, and $(\mathcal{M}_N - \mathcal{B}_N)$ is the truncation of $\mathcal{M} - \mathcal{B}$ to the first N modes. The modified DtN condition provides unique solutions at all wave numbers irrespective of the number of harmonics N included in the series. Suitable operators \mathcal{B} include local absorbing boundary conditions. The boundary condition \mathcal{B}_2 is preferred over \mathcal{B}_1 , since it provides an improved matrix preconditioner for iterative solvers and gives more accurate solutions when the number of harmonics N used in the truncated DtN series is not sufficient to capture important modes $n > N-1$ in the solution. Applying the local \mathcal{B}_2 operator to (17) gives the modified DtN

$$\frac{\partial u}{\partial r} = \mathcal{B}_2 u + \sum_{n=2}^{N-1} \beta_n \sum_{m=-n}^n u_{nm} Y_{nm}(\theta, \varphi), \quad (19)$$

where

$$\beta_n = k \frac{h_n'(kR)}{h_n(kR)} + \frac{n(n+1)}{2\mathcal{B}_1 r^2} - \mathcal{B}_1. \quad (20)$$

The \mathcal{B}_1 modified DtN is a special case obtained by omitting the second term with $n(n+1)$ and starting the summation at $n=1$. Thompson and Pinsky (1996) recognized that these conditions also annihilate up to the first $N=2$ spherical modes corresponding to $n=0$ and $n=1$ in the expansion (17) and thus are equivalent to the first two localized DtN conditions derived in Harari and Hughes (1992).

Nonlocal conditions are very accurate, yet couple all solution unknowns on Γ , thus potentially rendering a full dense matrix with associated solution cost and memory requirements. However, if separable boundaries are utilized such as spheres or spheroids, a special structure in the resulting data structures may be exploited to avoid storage of a full dense matrix. Bayliss *et al.* (1985) appear to be the first to recognize that a global DtN radiation boundary condition formed by a harmonic expansion, and relating Dirichlet-to-Neumann data on a separable boundary can be split as a vector outer product which then can be used to perform matrix-by-vector multiplies in iterative solvers without the need for assembling a dense matrix.

The contribution of the DtN operator to the complex-symmetric (non-Hermitian) system matrix is defined by the admittance matrix,

$$\mathbf{K}_{\text{dtn}} = R^2 \sum_{n=2}^{N-1} \beta_n \sum_{m=-n}^n \mathbf{c}_{nm} \mathbf{c}_{nm}^T, \quad (21)$$

where $\mathbf{c}_{nm} = (\mathbf{N}, Y_{nm})_{\mathcal{S}}$ are vectors of size equal to the number of unknowns on the truncation boundary Γ .

Due to the special structure of the DtN map defined on a separable boundary as a summation of vector outer products, we recognize that the Sherman-Morrison algorithm in conjunction with direct solvers may be used to preserve the sparsity of the finite-element equations with a series of rank-1 vector updates. For Krylov subspace iterative solvers the computationally intensive kernel is the repeated operation of matrix-by-vector products with vector iterates. The special structure of the DtN matrix \mathbf{K}_{dtn} , as a summation of rank-1 vector updates can be exploited to avoid direct evaluation of

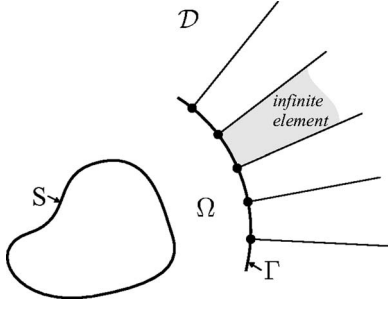


FIG. 2. Infinite element topology.

matrix-vector products with \mathbf{K}_{dtN} with significantly reduced storage and cost (Oberai *et al.*, 1998). The matrix-vector product of the DtN operator can also be carried out at the element level, preserving standard element-based data structures (Malhotra and Pinsky, 1996). Oberai *et al.* 1998, Thompson *et al.* (1999) have shown that the local operator \mathbf{K}_Γ provides a good approximation to the spectral properties of the complete system matrix which includes the DtN matrix \mathbf{K}_{dtN} , and thus can be used as an efficient preconditioner to accelerate convergence. Parallel iterative methods provide a means for dividing the problem into subsystems which when solved in parallel, provide compute time speedup, and for distributed-memory computer systems, the ability to scale up to very large systems. Ianculescu and Thompson (2003) showed that the symmetric outer-product structure of the DtN matrix \mathbf{K}_{dtN} can be exploited to compute in parallel with one collective communication per iteration with a vector size equal to the number of harmonics included in DtN series expansion; the effect on the overall communication is roughly that of a relatively small dot-product interprocessor communication. Numerical studies reported in Ianculescu and Thompson (in press) show that due to the special structure, and ability to tightly fit around scattering objects with minimal spurious reflection, the nonlocal DtN condition can be implemented with significant overall cost savings compared to the local operators \mathcal{B}_1 and \mathcal{B}_2 .

The extension of the \mathcal{B}_2 modified DtN map in spheroidal coordinates suitable for finite-element implementation is given in Thompson *et al.*, 1999. Grote and Keller (1995) derived a related modified DtN condition for spheres and spheroids using the second-order BGT operator in native form involving second-order radial derivatives (instead of angular derivatives), a form which is not suitable for standard finite-element approximation. Further details and discussions of the properties of DtN nonreflecting boundary conditions are given in Givoli (1999) and Thompson and Pinsky (2004).

V. INFINITE ELEMENTS

Infinite elements replace the nonreflecting boundary condition on Γ with a single layer of elements with infinite extent. The infinite elements are constructed with radial wave functions which automatically satisfy the Sommerfeld condition (3) at infinity; see Fig. 2. Test and trial solutions in

the region Ω_X exterior to Γ are usually separated into radial and angular functions; for a spherical boundary Γ with radius R (Astley, 2000),

$$w = \sum_{\mu} \sum_{\nu} c_{\mu\nu} W_{\nu}(r) N_{\mu}(\theta, \varphi), \quad (22)$$

$$u = \sum_{\mu} \sum_{\nu} d_{\mu\nu} U_{\nu}(r) N_{\mu}(\theta, \varphi). \quad (23)$$

In the above, N_{μ} are angular basis functions which match the interior finite-element discretization on the surface Γ . Radial functions are defined to match the outgoing wave character of the radial expansion (7),

$$U_{\nu}(r) = R_{\nu}(\xi) e^{ik(r-R)}.$$

Here, the radial basis functions R_{ν} are polynomial functions in the inverse radius variable $\xi = (R/r)$, where $r := \|\mathbf{x}\| > R$ is the radial position exterior to Γ . Different definitions of the radial polynomial functions lead to changes in the conditioning of the resulting system matrix. Several alternatives for the radial test (weighting) functions have been proposed; the three most common choices are

$$W_{\nu}(r) = \begin{cases} U_{\nu}(r), & \text{Bettess - Burnett unconjugated} \\ U_{\nu}^*(r), & \text{Burnett conjugated} \\ \xi^2 U_{\nu}^*(r), & \text{Astley - Leis conjugated.} \end{cases}$$

Bettess (1977, 1992) pioneered the infinite element concept and selected the test function to be the same as the trial solution basis. Burnett (1994), Burnett and Holford 1998a, b extended the formulation to spheroidal and ellipsoidal coordinates, and was the first work to express the shape functions as separable tensor products of radial and transverse functions, resulting in improved performance and efficiency. A quantitative error analysis of the unconjugated infinite elements is given in Burnett and Holford (1998a). Alternatively, the weighting (test) function is conjugated. In the Astley-Leis infinite element (Astley *et al.*, 1998a) the conjugated weighting function is scaled by a geometric factor. It was later recognized that this formulation fits within the variational framework of Leis (1986). The unconjugated infinite element leads to matrix coefficients involving one-dimensional radial infinite integrals which are oscillatory and well-defined, and can be evaluated using high-order Gauss-Legendre quadrature. For the conjugated elements, the oscillatory plane-wave components cancel so that the radial coefficients may be integrated analytically in closed form, resulting in wave number-independent matrices which are proportional to ik and k^2 , a feature which allows for a direct local time-dependent counterpart (Astley *et al.*, 1998b).

The unconjugated Burnett formulation, regardless of the definition for the radial function R_{ν} , gives the highest accuracy in the near field, yet exhibits instability and ill-conditioning for higher radial orders (Ihlenburg, 2000; Shirron and Babuska, 1998). For the Astley-Leis conjugated schemes, although less accurate in the near field, in the case of a spherical boundary, R_{ν} can be constructed so that the formulation remains stable and convergent in the far field (Astley, 2000; Astley and Hamilton, 2000, Dreyer and von

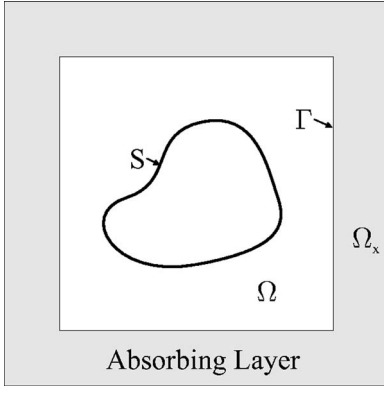


FIG. 3. Absorbing layer topology.

Estorff, 2003; Gerdes, 1998; Shirron and Babuska, 1998). However, the performance of both conjugated and unconjugated formulations deteriorates at larger wavenumbers and highly elongated artificial interfaces (Astley and Coyette, 2001).

VI. ABSORBING BOUNDARY LAYERS

The perfectly matched layer (PML) concept originally introduced by Berenger (1994) for electromagnetic waves is another option for modeling the far field for the exterior acoustics problem. The interface and PML are usually formulated in rectilinear Cartesian coordinates, allowing a tight fit around elongated objects (see Fig. 3), but can also be formulated in spherical and other general curvilinear coordinates. The idea is to introduce an exterior layer of finite thickness at an artificial interface such that outgoing plane waves are absorbed prior to reaching the outer-layer truncation boundary. By splitting the scalar field into nonphysical components satisfying equations which describe decaying waves, and proper selection of PML coefficients, plane-wave reflection for an arbitrary angle of incidence is theoretically eliminated.

In the absorbing layer Ω_x , splitting the field in Cartesian coordinates $\mathbf{x}=(x_1, x_2, x_3)=(x, y, z)$, leads to a modified Helmholtz equation with complex-valued anisotropic material properties suitable for standard finite-element implementation (Harari *et al.*, 2000; Turkel and Yefet, 1998; Wu *et al.*, 1997),

$$\nabla \cdot (\mathbf{D} \nabla u) + k^2 s u = 0, \quad \text{in } \Omega_x. \quad (24)$$

The corresponding weak form in the complete computational region $\Omega \cup \Omega_x$ is

$$\int_{\Omega \cup \Omega_x} (\nabla w \cdot \mathbf{D} \nabla u - k^2 s w \cdot u) dx = F(w). \quad (25)$$

In the above, $s=s_1 s_2 s_3$, and $\mathbf{D}=\text{diag}\{s_2 s_3 / s_1, s_1 s_3 / s_2, s_1 s_2 / s_3\}$ is a diagonal, complex-valued material matrix, with coefficients $s_i(x_i)=1+(i\sigma_i)/k$, defined by a distribution of absorption functions $\sigma_i(x_i)$, $i=1, 2, 3$, usually taken to vary quadratically from a value of zero at the interface of the physical domain to a maximal value at the truncation of the layer. In the physical domain Ω , $s_i=1$, $i=1, 2, 3$. In layers normal to the x_1 direction, $\sigma_2=\sigma_3=0$. Only in cor-

ner regions are all σ_i values nonzero. Optimal placement of the interface, layer thickness, number of elements, and variation of absorption functions and their maximal value, which reduce error due to spurious reflection of decayed waves off the layer truncation boundary to be less than the discretization error, are open questions (Collino and Monk, 1998). The PML layer converges to perfect wave absorption as the thickness of the layer is increased (Tsynkov and Turkel, 2001). However, a compromise between a thin layer which requires a rapid variation of the absorption parameters and a thick layer which requires more elements is required (Turkel and Yefet, 1998).

VII. DISCRETIZATION METHODS FOR THE HELMHOLTZ EQUATION

A. Galerkin finite-element methods

Accuracy of finite-element approximations based on Galerkin's method is characterized by phase (dispersion) errors. In order to control dispersion, the element size must be adapted to the wave number such that the number of elements per wavelength is held below a resolution limit. The resolution is determined by the nondimensional wave number $kh=2\pi h/\lambda$, where λ is the wavelength and h is a measure of the element size. A discrete dispersion analysis can be used to quantify the limiting value on mesh resolution.

For a uniform mesh of finite elements with piecewise linear interpolation in one dimension, and neglecting boundary conditions, the sparse system matrix \mathbf{Z} is tridiagonal; neglecting sources, each interior equation corresponds to a repeated finite difference stencil centered at a typical node point x_j of the form

$$Z_2 u^h(x_{j-1}) + 2Z_1 u^h(x_j) + Z_2 u^h(x_{j+1}) = 0, \quad (26)$$

where $Z_1(kh)=1-(kh)^2/3$ and $Z_2(kh)=-(kh)^2/6-1$ are coefficients obtained by assembly of element matrices. The solution of the difference stencil admits homogeneous plane-wave solutions of the form $u^h(x_j)=u_0 e^{i\tilde{k}x_j}$ where \tilde{k} is an unknown numerical wave number. Substituting this solution into the difference stencil leads to a dispersion relation relating the numerical wave number \tilde{k} to the continuous wave number k of the form, $\cos(\tilde{k}h)=-Z_1(kh)/Z_2(kh)$. For small kh , a Taylor series expansion reveals the dispersion error of order (Thompson and Pinsky, 1994)

$$(\tilde{k}-k)/k = -\frac{1}{24}(kh)^2 + O(kh)^4. \quad (27)$$

The numerical wave number remains real valued corresponding to propagating waves, provided $|Z_1(kh)/Z_2(kh)| < 1$, which requires the continuous wave number k to be bounded by the cutoff value, $kh \leq \sqrt{12}$, corresponding to a minimum resolution of $\lambda/h > 2$, i.e., just under 2 elements per wavelength. Beyond this value, \tilde{k} is complex valued, resulting in rapid amplitude decay (evanescent behavior).

B. Mesh resolution rules for low-order elements

Ihlenburg (1998), Ihlenburg and Babuska (1995) showed that the error measured in the usual L_2 integral norm, which characterizes averaged amplitude differences, is controlled by a wave number-dependent stability constant times the approximation error. For linear finite elements of size h ,

$$\left(\int_{\Omega} |u^h - u|^2 dx \right)^{1/2} \leq (C_1 + C_2 kL)(kh)^2, \quad (28)$$

where L is a characteristic length scale, and C_1, C_2 are constants independent of the wave number and element size. The meaning of (28) is that the integral norm is controlled by a sum of two errors, where the first term $C_1 \cdot (kh)^2$ is proportional to the usual approximation error, and the second term $C_2 \cdot (kL)(kh)^2$ has an additional dependence on kL . The second term has sometimes been referred to as a ‘‘pollution’’ error related to a loss of stability at large wave numbers (Bayliss *et al.*, 1985). The second term increases even though the nondimensional wave number kh is held fixed with a constant number of elements per wavelength ($\lambda/h = \text{constant}$). In general, however, if the number of elements per wavelength λ/h is increased (kh decreased), it follows that the second term also decreases, thus reducing the error in amplitudes. To control local approximation error it is often suggested that one take at least ten ($\lambda/h > 10$) linear elements per wavelength for a phase error of a few percent, i.e., keep the element size below $h < \lambda/10$. However, to control amplitude error, a characteristic length scale of the domain, L , should be accounted for such that $(kL)(kh)^2 < P$, where P is an admissible pollution error determined from computational experience (Ihlenburg, 2003).

A simple way to improve both dispersion and pollution error for low-order elements is to use slightly underintegrated stiffness and mass matrices with special numerical quadrature rules. For 4-node bilinear quadrilateral and 8-node trilinear ‘‘brick’’ elements, use of quadrature evaluation points $\pm\sqrt{2}/3$ in each direction in the parent element with unit weights gives a higher-order accurate dispersion error from $O(kh)^2$ to $O(kh)^4$, (Challa, 1998). This same observation for 4-node quadrilateral elements was later rediscovered in Guddati and Yue (2004), where it was demonstrated numerically that the high-order accuracy is maintained for unstructured meshes. In Thompson and Kuntong (2005) it is shown that for 3-node linear triangle elements, the dispersion error is reduced from $O(kh)^2$ to $O(kh)^4$ by using three-quadrature points for the mass matrix m^e sampled at $(\xi, \eta, 1 - \xi - \eta) = (1/3 + \sqrt{10}/6, 1/3 - \sqrt{10}/12, 1/3 - \sqrt{10}/12)$ in natural coordinates with three symmetric permutations and conventional weights $\sum_{j=1}^3 W_j = 1$, $W_j = 1/3$. For 4-node tetrahedral elements for three-dimensional analysis, using the special quadrature rule $(\xi, \eta, \zeta, 1 - \xi - \eta - \zeta) = (1/4 + \sqrt{21}/8, 1/4 - \sqrt{21}/24, 1/4 - \sqrt{21}/24, 1/4 - \sqrt{21}/24)$, with multiplicity 4, and standard weights $\sum_{j=1}^4 W_j = 1$, $W_j = 1/4$, yields increased phase accuracy compared to standard Galerkin.

C. High-order approximation

Dispersion error can be minimized by using higher-order polynomial approximations, e.g., hp-version of FEM and spectral elements. The number of elements per wavelength to obtain a given discretization error depends strongly on the order of the element basis functions. A dispersion analysis similar to that outlined above for linear elements can be carried out for high-order polynomials of order $p \geq 2$, and after condensation of internal solution unknowns, a dispersion relation in the same form as the linear $p=1$ case is obtained. Thompson and Pinsky (1994) and Ihlenburg (1998) show that the relative phase error is $O(kh)^{2p}$. The cutoff value prior to evanescent behavior grows with the increase of approximation order p ; however, before reaching this value the numerical wave number is complex valued on small ‘‘stopping band’’ intervals (Thompson and Pinsky, 1995). As a result, kh should be kept below the first cutoff value of $kh \leq \sqrt{12}$. Ihlenburg (1998) showed that the error measured in the $H^1(\Omega)$ global norm is order $kL(kh/2p)^{2p}$, and thus for quadratic and higher-order elements $p \geq 2$, and resolved waves such that kh/p is small, the dispersion is relatively small. For high wave numbers $kh \geq 1$, Ainsworth (2004) has shown that dispersion error is virtually eliminated when p is increased to a regime in which the error decays at a super-exponential rate, such that $2p+1 > kh + c(kh)^{1/3}$, where c is a user-defined constant; $c=2$ is suggested. Since higher-order elements generally provide greater computational efficiency, fewer degrees of freedom are generally needed to achieve a given discretization error for oscillatory wave solutions (Deraemaeker *et al.*, 1999; Dey, 2003; Thompson and Pinsky, 1994). For high-order quadrilateral elements with quadratic Lagrange polynomial basis functions of order $p=2$, high-order accuracy is achieved by evaluating the stiffness and mass matrices with special quadrature points $\xi_1 = -\xi_3 = -\sqrt{13}/15$, $\xi_2 = 0$, and corresponding weights $W_1 = W_3 = 5/13$, $W_2 = 16/13$, in each natural coordinate direction (Challa, 1998).

D. Stabilized Galerkin methods

For low-order elements, reduced dispersion error may be achieved using residual-based methods such as Galerkin least-squares (GLS) and related methods. Least-squares stabilization stands out among the numerous approaches that have been proposed for reducing resolution requirements of standard Galerkin finite-element methods for time-harmonic acoustics by combining substantial improvement in accuracy with simple implementation. In the GLS method the Galerkin variational form is modified by appending residuals of the governing Helmholtz equation in a consistent least-squares form (Harari and Hughes, 1992),

$$B(w, u) + \int_{\tilde{\Omega}} \tau \mathcal{L} w \mathcal{L} u dx = F(w). \quad (29)$$

Here, $\mathcal{L} = \nabla^2 + k^2$ is the Helmholtz differential operator, and $\tilde{\Omega}$ denotes integration over element interiors. The element parameter τ is usually determined from discrete dispersion

analysis and selected to minimize or eliminate dispersion error in the numerical solution.

For two-dimensional quadrilateral (Q4) elements, the value of τ is determined by enforcing numerical and continuous wave numbers to coincide $\tilde{k}=k$ (Thompson and Pinsky, 1995)

$$\tau = \frac{1}{k^2} \left[1 - \frac{6}{(kh)^2} \left(\frac{1 - \cos \alpha_x}{2 + \cos \alpha_x} + \frac{1 - \cos \alpha_y}{2 + \cos \alpha_y} \right) \right], \quad (30)$$

where $(\alpha_x, \alpha_y) = kh(\cos \pi, \sin \pi)$. For uniform meshes this value eliminates dispersion error for plane waves in the angular direction π . In general, solutions to the Helmholtz equation can be expanded in terms of plane waves with the predominant direction unknown a priori. By preselecting the angle $\pi_0 = \pi/8$ in (30), the phase error, while not eliminated, is reduced significantly for all other wave angles (Thompson and Pinsky, 1995). For unstructured finite-element meshes the Laplacian operator appearing in (29) is usually neglected and the element size h can be taken as an average over the mesh or $h = \sqrt{A}$, where A is the element area. Numerical evidence shows that the GLS-FEM is relatively insensitive to the precise definition of the measure of element size (Harari and Magoules, 2004; Harari *et al.*, 1996; Thompson and Thangavelu, 2002). The additional cost of computing the GLS contribution is trivial, yet gives substantial improvement in accuracy, even on unstructured meshes. Values for τ on triangle, quadratic, and trilinear brick elements are given in Harari and Nogueira, 2002; Harari *et al.*, 1996; Thompson and Pinsky, 1995. Successful generalization of residual based methods to waves in plate bending elements and acoustic fluid—structure interaction are given in Thompson, 2003, and Thompson and Sankar, 2001.

Many of the generalized Galerkin methods can be derived within the variational multiscale (VMS) framework (Hughes *et al.*, 1998), including the method of residual-free bubbles (Franca *et al.*, 1997), also related to nearly optimal Petrov-Galerkin methods (Barbone and Harari, 2001). For the GLS method defined in (29), the mesh-dependent stability parameter τ may be interpreted as an algebraic approximation of a global integral operator for unresolved fine scales obtained by a separation of coarse finite-element polynomials and enhanced fine scales within the VMS framework. Multiscale considerations also underlie the residual-based method in Oberai and Pinsky, 2000, which includes the Helmholtz residual in least-squares form over element interiors $\tilde{\Omega}$, plus an additional residual defined over interelement boundaries $\tilde{\Gamma}$. In this case, the variational form assuming negligible Laplacian operation is

$$B(w, u) + k^2(\tau w, u)_{\tilde{\Omega}} - (\gamma w, \llbracket u, n \rrbracket)_{\tilde{\Gamma}} - (\gamma \llbracket w, n \rrbracket, u)_{\tilde{\Gamma}} = F(w),$$

where $\llbracket u, n \rrbracket$ is the jump in discontinuous gradients across common element edges. Using this framework, Oberai and Pinsky (2000) find mesh parameters τ and γ for Q4 linear quadrilateral elements which produce a leading order phase error for all plane-wave directions of order $O(kh)^6$; a substantial improvement over standard Galerkin linear Q4 elements. Further discussions relating residual and other stabi-

lized methods within the VMS framework are given in Harari, 2004.

E. Wave-based discretization methods

Wave-based methods exploit known solutions such as plane waves, or other analytical solutions to define or enrich the approximate solution space. Element-free methods (EFM) based on moving least-squares, and partition-of-unity methods (PUM), provide a means to incorporate analytical wave functions within local basis functions. For the Helmholtz equation solutions can be approximated using increasing numbers of basis functions in the form of plane waves (Babuska and Melenk, 1997; Bettess *et al.*, 2003; Laghrouche and Bettess, 2000; Laghrouche *et al.*, 2002; Melenk and Babuska, 1996); in 2D problems, $\mathcal{V} = \{e^{ik(x \cos \theta_m + y \sin \theta_m)}, \theta_m = 2\pi m/n\}$, where $m=0, 1, \dots, n-1$, $n=1, 2, \dots$. Suleau and Bouillard (2000) have shown that dispersion and pollution errors can be reduced by adding a sufficient number of plane-wave basis functions within the element-free moving least-squares method. Plane-wave basis functions have also been multiplied with standard piecewise polynomial shape functions as a partition-of-unity finite element method (Laghrouche and Bettess, 2000; Strouboulis *et al.*, 2000). The general integral that arises in the element matrices can be written as the product of plane waves, and polynomials. Such integrals are highly oscillatory and difficult to evaluate efficiently using standard techniques. Burnett and Soroka (1972) and Pierce *et al.* (2002) offer well-proven techniques for evaluating highly oscillatory integrals. Ortiz and Sanchez (2001) derive special integration techniques which isolate the oscillatory effects to one dimension. Another approach to reducing integration costs is given in Bettess *et al.*, 2003; Laghrouche *et al.*, 2002. While reducing dispersion and pollution error, a drawback of these approaches is the potential for ill-conditioning of the resulting system matrices which may disrupt the practical convergence of the method. Empirical rules relating condition number, number of wave directions, and wave number are given in Laghrouche *et al.*, 2002.

Least-squares methods (Monk and Wang, 1999; Stojek, 1998) minimize the least-squares difference in jumps of the solution and its normal derivative across element edges. The use of discontinuous solution spaces allows for the use of a plane-wave basis. The ultraweak variational formulation (Cessenat and Despres, 2003, 1998; Huttunen *et al.*, 2002) is another approach to using discontinuous local plane-wave solutions of the Helmholtz equation on each element. In this approach integration-by-parts is used to derive a variational formulation that weakly enforces continuity conditions between elements via local transmitting impedance conditions. An advantage of this approach is that integrations are carried out over element boundaries only and can be evaluated in closed form. Other wave-based methods are the weak element method (Goldstein, 1986), and the iterative defect-correction meshless method (Lacroix *et al.*, 2003). A difficulty with wave-based methods is that plane-wave, or other free-wave solutions, used as basis functions, often lead to ill-conditioning of the resulting system matrix as the number

of wave functions per element is increased, or refined element meshes are used. Another approach which may be derived in the framework of multiscale methods is the discontinuous enrichment method (DEM), where standard finite-element polynomial field is enriched within each element by adding plane-wave basis functions, and Lagrange multipliers are introduced at element interfaces to enforce a weak continuity of the solution (Farhat *et al.*, 2003). Using element level condensation, the system matrices are reported to be better conditioned than the PUM.

VIII. A POSTERIORI ERROR ESTIMATES AND ADAPTIVE METHODS

Adaptive methods use *a posteriori* error estimates to control discretization error in the numerical solution (Ainsworth and Oden, 2000). A posteriori error estimates are computed by postprocessing the numerical solution. For standard finite-element methods, a posteriori error estimates are used to control mesh refinement, both element size h , and polynomial order p distribution. The most common a posteriori error estimates are residual (both explicit and implicit), and recovery type. Implicit residual methods involve the solution of local or global problems which usually require very little cost compared to solving the original finite-element solution. Explicit methods relate the residual of the original governing equation localized to each element and do not require solving any auxiliary problems. Since the residual is a measure of numerical error, the error estimate can be used as a refinement indicator for adaptive strategies.

Stewart and Hughes (1996) used explicit residual methods based on the use of adjoint equations and duality arguments to develop adaptive strategies for the finite-element discretization of the Helmholtz equation. The error estimator depends on a stability constant which is approximated by solving global eigenvalue problems, which may be costly to compute. Irimie and Bouillard (2001) use standard explicit residual methods to estimate the error for the Helmholtz equation. Babuska *et al.* (1997) and Bouillard (1999) studied implicit element residual methods to estimate the finite-element error. Bouillard and Ihlenburg (1998, 1999) studied the gradient recovery-based error estimators based on the Zienkiewicz-Zhu patch recovery technique, and found that the estimator converges with mesh refinement for all wave numbers, although the estimate underestimates the error at high wave number. Attempts to estimate the pollution error are studied in Babuska *et al.* (1997). Initial studies of goal-oriented adaptive methods which measure the error in quantities of interest other than global norms are reported in Peraire and Patera, 1999; Sarrate *et al.*, 1999. For finite-element solutions with sufficient resolution and for which the pollution error is under control, i.e., $kL(kh)^2 \ll 1$, the quality of both the residual-based error estimators and recovery-type methods are good. However, since local error estimators do not detect pollution error, the quality deteriorates as the wave number k increases.

IX. ITERATIVE SOLUTION METHODS

The system of equations $\mathbf{Zd}=\mathbf{f}$, $\mathbf{Z} \in \mathbb{C}^{N_{\text{dof}} \times N_{\text{dof}}}$, resulting from the Galerkin FEM applied to the Helmholtz equation is sparse, complex, and symmetric (non-Hermitian and generally not diagonally dominant). Direct solution methods based on Gaussian elimination or factorization become exceedingly expensive both in terms of memory and computation when solving large systems of this class, especially for larger wave numbers. The primary iterative solution method for these types of systems are complex versions of Krylov subspace methods. In order to accelerate convergence a preconditioner is required. Standard preconditioners such as incomplete LU factorization (ILU) are optimal for matrices with diagonal dominance. However, the matrices which arise from the Helmholtz equation can be indefinite without diagonal dominance, making standard ILU not as practical and can exhibit breakdown at high wave numbers.

One possible approach is to recast the complex-symmetric system into Hermitian positive-definite form by multiplying by the Hermitian transpose, resulting in the normal equations $\mathbf{Z}^H \mathbf{Zd}=\mathbf{Z}^H \mathbf{f}$. The above system can be solved with the well-known conjugate gradient iterative method, with incomplete Cholesky factorization or other preconditioners. A difficulty of this approach is that the condition number of $\mathbf{Z}^H \mathbf{Z}$ is the square of \mathbf{Z} , so that convergence may be slow. Another possibility is to replace the complex-symmetric system $(\mathbf{A}+i\mathbf{B})(\mathbf{x}+i\mathbf{y})=\mathbf{a}+i\mathbf{b}$, with a real symmetric system,

$$\begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B} & -\mathbf{A} \end{bmatrix} \begin{bmatrix} \mathbf{x} \\ -\mathbf{y} \end{bmatrix} = \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix},$$

where $\mathbf{A} \in \mathbb{R}^{N_{\text{dof}} \times N_{\text{dof}}}$ and $\mathbf{B} \in \mathbb{R}^{N_{\text{dof}} \times N_{\text{dof}}}$. However, in this form, the system may become even more difficult to precondition.

Specialized preconditioners based on the original complex-symmetric matrix \mathbf{Z} appear to give the best results with significant acceleration, even at high wave numbers. In Made (2001), prior to incomplete factorization, the real part of the preconditioning matrix is made less indefinite, by perturbations to the diagonal entries. This was shown to exhibit significant reduction of iteration counts in the GMRES method (Saad and Schultz, 1986). A similar idea is used in Erlangga *et al.*, 2004 with a shifted-Laplace preconditioner built on the modified Helmholtz equation $\nabla^2 - ik^2$, which is a generalization of the preconditioners introduced in Bayliss *et al.* (1983). In Kechroud *et al.* (2004) incomplete LU factorization with threshold (ILUT), and the Crout form of ILU were used as preconditioners combined with the GMRES iterative solver. It was reported that stagnation issues arise with high fill-in. The authors promise improvements by adding a damping parameter during the factorization process. Multifrontal incomplete factorization methods have also been applied to complex-symmetric indefinite systems with good results (Qu and Fish, 2002).

Suitable iterative solvers for sparse complex symmetric matrix systems other than GMRES include BICG-STAB (Vander Vorst, 1992), QMR (Freund, 1991) and TF-QMR (Freund, 1993) methods. Some numerical comparisons of the alterna-

tive iterative solvers are reported in Mazzia and Pini (2003) and elsewhere. The best combination of iterative solver and preconditioner seems to be problem dependent. From the author's experience, BICG-STAB appears to be robust for complex-symmetric systems at high wave number.

Other preconditioning approaches include analytic factorization methods (Gander and Nataf, 2001) and fictitious domain methods (FDM). The FDM is based on embedding the original domain into a larger one with a simple geometry (Marchuk *et al.*, 1986). In the algebraic FDM (closely related to capacitance matrix methods) the linear system resulting from the finite-element discretization is replaced by an equivalent, but enlarged, system corresponding to a simple-shaped domain containing the original domain. In this enlarged, yet simplified form, efficient iterative preconditioners are constructed based on locally perturbed orthogonal fitted meshes. Applications of the algebraic FDM for acoustic scattering are reported in Elman and O'Leary, 1998; Ernst, 1996; Heikkola *et al.*, 1999, 2003. Other solver techniques for the Helmholtz equation include multigrid methods (Brandt and Livshitz, 1997; Elman *et al.*, 2001; Lee *et al.*, 2000; Vanele *et al.*, 1998).

For acoustic scattering problems, the incident field is often represented by a plane wave, $u^{\text{inc}}(\mathbf{x}) = \exp(ik\mathbf{x} \cdot \boldsymbol{\nu})$, $\boldsymbol{\nu} = (\cos \alpha, \sin \alpha \cos \beta, \sin \alpha \sin \beta)$ with a sweep over different incident directions α and β . This leads to a problem with fixed left-hand-side matrix and multiple right-hand-side forcing vectors. Malhotra *et al.* (1997) show how to efficiently solve the multiple right-hand-side problem with QMR methods.

A. Multifrequency solution methods

Often a large number of frequency (wave number) evaluations are required over a broad band to characterize the system response or when an inverse Fourier transform is needed to construct a corresponding time-domain solution. Since the complex-symmetric matrix $\mathbf{Z} = (\mathbf{S} - k^2\mathbf{M} - \mathbf{K}_r)$ is wave number dependent, the solution generally involves a separate inversion at each wave number k , causing the computation cost to grow linearly with the number of wave number evaluations. Djellouli *et al.* (2001) present an approach based on Padé approximation to compute multifrequency evaluations efficiently by solving a reference scattering problem with multiple excitation vectors and local BGT boundary conditions to characterize frequency derivatives of the scattered field. In Ingel (2000) and Thompson *et al.* (2001), domain decomposition concepts are combined with interpolation of substructure (subdomain) matrices over frequency bands of interest to accelerate multifrequency solutions.

For problems with frequency-independent excitation \mathbf{f} , matrix Padé approximation via the Lanczos (PVL) process can be used to obtain an efficient algorithm which grows sublinearly for the simultaneous solution of the Helmholtz equation over multiple frequencies in a window based on a Krylov projection to a subspace of much smaller dimension than the original system size (Feldmann and Freund, 1995; Freund, 1999; Simoncini and Perotti, 2002). Wagner *et al.* 2003a, b show that the PVL process can be implemented

efficiently with the nonlocal modified DtN by utilizing the special structure of the admittance matrix. Efficient algorithms based on this PVL approach over multiple frequencies have not been demonstrated for the general case of frequency dependent excitation $\mathbf{f}(k)$ which is required for general acoustic scattering and radiation problems.

B. Domain decomposition methods

Domain decomposition methods provide an effective means of problem subdivision for parallel processing. Classical Schur complement-based domain-decomposition methods have difficulties when applied to the Helmholtz equation since the inversion of the matrix $\mathbf{A}_i = (\mathbf{S}_i - k^2\mathbf{M}_i)$ defined on each interior subdomain will be singular when the wave number corresponds to a resonance frequency (eigenvalue) of the pencil $(\mathbf{K}_i, \mathbf{M}_i)$. The first resonance will occur at a resolution of less than two subdomains per wavelength (Thompson *et al.*, 2001).

Kim (1998) uses the Robin-type impedance (transmission) interface conditions presented in Benamou and Despres (1997) and Despres (1993) in a Schwarz-type domain decomposition method to improve convergence; however, the iteration count increases with many subdomains. Cai *et al.* (1998) demonstrated an overlapping Schwarz method with GMRES acceleration and coarse grid corrections to improve convergence. Another additive Schwarz domain decomposition method with the Robin-type subdomain interface transmission conditions has been proposed in Susan-Resiga and Atassi (1998), where the nonlocal DtN nonreflecting boundary condition is computed with an iterative lag to maintain sparsity of the parallel subdomain solves. In Larsson (1999) a preconditioned restarted GMRES iterative method is used for the solving the Helmholtz equation, including nonlocal nonreflecting boundary conditions. Domain decomposition is used with a Schur complement algorithm and fast preconditioners for the subdomains to accelerate convergence.

In Farhat *et al.* (2000) and Tezaur *et al.* (2002), a non-overlapping domain decomposition method called FETI-H, based on two-level Lagrange multipliers and the alternating Robin-type transmission conditions at subdomain interfaces of the continuous operator form $\mathcal{A}^{(s)} = ik$, presented in Benamou and Despres (1997) and Despres (1993), is used to solve the Helmholtz equation with second-order local nonreflecting boundaries. The matrices restricted to each subdomain Ω_s are $\mathbf{Z}^{(s)} = (\mathbf{S}^{(s)} - k^2\mathbf{M}^{(s)} - \mathbf{K}_r^{(s)} + ik\mathbf{A}^{(s)})$. Here, $\mathbf{A}^{(s)}$ are regularization matrices associated with the operator $\mathcal{A}^{(s)} = ik$, and defined by integration over subdomain interfaces,

$$\mathbf{d}^{(s)T} \mathbf{A}^{(s)} \mathbf{d}^{(s)} = \sum_{\substack{t=1 \\ t \neq s}}^p \epsilon^{st} \int_{\partial\Omega_s \cap \partial\Omega_t} u^2.$$

Here, $\mathbf{d}^{(s)}$ is the unknown vector restricted to subdomain Ω_s , and $\epsilon^{st} \in \{0, \pm 1\}$, $\epsilon^{st} = -\epsilon^{ts}$. The use of regularization matrices for the Helmholtz operator provides for a unique solution on each subdomain. Inclusion of the alternating regularization matrix on the interface boundaries cancel upon global assembly, thus reverting to the original problem, and leading to nonsingular and invertible matrices $\mathbf{Z}^{(s)}$. The transmission

conditions can be interpreted as a simple local preconditioner of the linear system condensed on the interface. Improved transmission conditions with tangential derivatives of the form $\mathcal{A}^{(s)} = \alpha^{(s)} + \beta^{(s)} \partial_{\tau^2}^2$, with coefficients $\alpha^{(s)}, \beta^{(s)}$, and unit tangential vector τ , have been derived based on Fourier analysis of the Steklov-Poincaré operators in a half-space (Collino *et al.*, 2000). Optimized coefficients have been chosen to minimize the convergence rate of the Jacobi algorithm in the closely related additive Schwarz method with no overlap (Gander *et al.*, 2002). In Magoules *et al.*, 2004, it is shown that the optimal augmented interface operator $\mathcal{A}^{(s)}$ is the Schur complement of the outer domain. Approximations of this Schur complement with sparse approximate inverse methods and incomplete factorization are investigated.

X. ACOUSTIC INVERSE PROBLEMS AND SHAPE OPTIMIZATION

Acoustic inverse problems which involve determining the shape of a body from an acoustic far-field pattern for the scattering of time-harmonic waves can be interpreted as a nonlinear ill-posed operator equation with the operator mapping the boundary onto the far field. Regularized Newton iterative methods provide accurate and robust solutions to the inverse obstacle scattering equation (Kress, 2003). Gradient-type methods based on regularized Newton or quasi-Newton optimization requires computation of shape derivatives. The derivatives are computed from solutions to the Helmholtz equation with different right-hand sides corresponding to the number of parameters in the boundary representation. Implementation of the regularized Newton method which incorporates exact sensitivities of far-field patterns with iterative finite-element solutions to the direct time-harmonic problem are given in Farhat *et al.* (2002). An alternate Newton-type method calculates the shape derivatives efficiently by solving an associated adjoint problem (Feijoo *et al.*, 2004). The adjoint method for the computation of shape derivatives and smoothing for finding regular solutions is related to the shape optimization problem (Jameson, 1988), where observations of a numerical solution to the Helmholtz equation provides an objective function which is formulated as a multipoint nonlinear optimization problem. Habbal (1998) and Bangtsson *et al.* (2003) consider shape optimization of a sound barrier and acoustic horn, respectively, using the regularized Newton iterations and the finite-element method. The shape optimization problem is solved using a gradient-based search method where the gradient is provided by solving the associated adjoint equations. Developments in coupled FEM-BEM structural-acoustic optimization and sensitivity analysis are reported in Fritze (2005) and Marburg (2002).

XI. CONCLUSION

Solutions to the challenging problem of developing accurate and efficient finite-element methods for time-harmonic acoustic radiation and scattering have a rich history of successes. It is expected that this trend will continue leading to many new and exciting developments in the future.

ACKNOWLEDGMENTS

I thank the anonymous reviewers for valuable comments and suggestions which greatly improved the quality of this article.

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