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Second-Order Transmission Conditions for the Helmholtz Equation

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1 Introduction

Several domain decomposition methods for the solution of elliptic problems have been proposed, analyzed, and successfully implemented during the past decade [BW86, BPS86, GW88, HTJ88, Lio88, Lio90]. In recent years these ideas have been extended to non-elliptic equations such as the Helmholtz equation [Des91, Des93, Des95, Ben95] and the harmonic Maxwell system [DJR92].

It is well-known [Lio88] that iterative methods using the Dirichlet or Neumann transmission conditions may not converge to the exact solution; the use of (first-order) Robin conditions on the inter-domain boundaries assures the convergence of the sequence of iterates. In practice, however, this convergence tends to be very slow. In this paper a set of second-order Robin-type transmission conditions is proposed. The new transmission conditions significantly improve the rate of convergence of the iterates. After a brief overview of the general problem, including a general domain decomposition formulation, the specific model with second-order Robin-type transmission conditions is presented. A numerical example is used to demonstrate the benefits of this method. The discussion in this paper is intended to motivate the new algorithm and illustrate the type of improvements that are possible. A full description of the method with the accompanying theory is under development.

2 General Problem

Many applications in electromagnetics, acoustics, and elasticity require the solution of a wave equation on an unbounded domain. A number of methods have been created for the reduction of the problem to a bounded domain. A common approach is to truncate the exterior domain and impose an appropriate boundary condition on the artificial boundary. The exact "radiation" boundary condition (RBC) is non-local (in both space

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and time); numerous spatially local approximate RBCs have also been developed (see, *e.g.*, [Giv91]). Interest in domain decomposition methods for the solution of these problems arises from the fact that the direct solution of realistic scattering problems require the solution of large, sparse, complex-valued systems of linear equations. Domain decomposition methods are employed to create an iterative method requiring the direct solution of related problems on a small subdomain, typically a single bi-quadratic finite element.

The model problem selected for this investigation is the time-reduced scalar wave equation, *i.e.*, the Helmholtz equation, in the exterior, Ω^+, of a two-dimensional scatterer, Ω:

$$\begin{aligned} -\triangle u - \omega^2 u &= f && \text{in } \Omega^+ && (2.1)\\ u &= g_0 && \text{on } \partial\Omega && (2.2)\\ \left|\tfrac{\partial u}{\partial r} - i\omega u\right| &= o(r^{-1/2}) && \text{as } r \to \infty, \text{ uniformly in } \theta. && (2.3) \end{aligned}$$

Note that the Sommerfeld radiation condition, (2.3), prevents the creation of energy at infinity. Thus, the problem has at most one solution.

The corresponding problem on a bounded domain is obtained by truncating the domain at an artificial boundary, Γ^t, and replacing (2.3) with a RBC with tangential boundary operator, $\mathcal{B}$. That is,

$$\begin{aligned} -\triangle u - \omega^2 u &= f && \text{in } \Omega^t && (2.4)\\ u &= g_0 && \text{on } \Gamma && (2.5)\\ \tfrac{\partial u}{\partial n} + \mathcal{B}u &= g_j && \text{on } \Gamma^t. && (2.6) \end{aligned}$$

Selection of Γ^t and $\mathcal{B}$ should be made so that a solution to (2.4)–(2.6) is both a good approximation to the solution to (2.1)–(2.3) and can be numerically computed in an efficient manner. Balancing these opposing constraints can be difficult and, in practice, often depends on the specific application. For example, a particularly effective combination used in many electromagnetics problems is to place Γ^t about one wavelength from the (convex hull of the) scatterer and to use the Kriegsmann RBC for $\mathcal{B}$ [KTU89, LWMP96]. For a long, thin rectangular scatterer and a reasonable discretization of the resulting domain the linear system involves more than 7,000 unknowns. While this is a considerable savings over the system of more than 35,000 unknowns that results from the use of a circular artificial boundary, the benefits are seen in scattering problems. (The 3-D vector problem presents even more problems.)

3 Domain Decomposition Methods for the Helmholtz Equation

A nonoverlapping domain decomposition method is a natural choice for the iterative solution of (2.4)–(2.6) . Let Ω^t be partitioned into a finite number of nonoverlapping subdomains Ω_j. The interfaces between subdomains are denoted by Σ_{jk}; Γ_j and Γ_j^t denote the intersections of a subdomain with the scatterer and artificial boundary, respectively. That is, $\Omega^t = \bigcup_{j\in J}\Omega_j$, $\Sigma_{jk} := \partial\Omega_j \cap \partial\Omega_k$ for all $j \neq k$, $\Gamma_j := \partial\Omega_j \cap \Gamma$, and $\Gamma_j^t := \partial\Omega_j \cap \Gamma^t$. The outward unit normal vector, relative to Ω_j, is ν_j and $g_j := g|_{\Gamma_j^t}$.

Table 1 Lowest-order radiation boundary conditions, $\mathcal{B}u := \alpha u + \beta \frac{\partial^2 u}{\partial \tau^2}$.

Order	Type	α	β
0	Neumann	0	0
1	Robin	$i\omega$	0
2	Robin	$i\omega$	$\frac{i}{2\omega}$

The iterative domain decomposition algorithm requires an initial solution, u_j^0, often zero, on each subdomain, then computes the sequence u_j^n of functions that satisfies

$$(-\triangle - \omega^2)u_j^{n+1} = f \qquad \text{in } \Omega_j \tag{3.7}$$

$$u_j^{n+1} = g_0 \qquad \text{on } \Gamma_j \tag{3.8}$$

$$(\tfrac{\partial}{\partial \nu_j} + \mathcal{B})u_j^{n+1} = g_j \qquad \text{on } \Gamma_j^t \tag{3.9}$$

$$(\tfrac{\partial}{\partial \nu_j} + \mathcal{T})u_j^{n+1} = (-\tfrac{\partial}{\partial \nu_k} + \mathcal{T})u_k^n \qquad \text{on } \Sigma_{jk} \quad \forall k \tag{3.10}$$

where $\mathcal{T}$ is the tangential differential operator used as the interface condition between adjacent subdomains.

The convergence of this method depends primarily on the choice of the tangential boundary operators $\mathcal{B}$ and $\mathcal{T}$. The Neumann and two lowest-order Robin-type radiation boundary operators are summarized in Table 1. It is well-known [Lio88, Lio90] that the Dirichlet and Neumann transmission conditions do not guarantee convergence of the iterations for all values of the frequency ω. Després [Des91, Des93, Des95] has shown that a convergent iterative method does result from the use of the first-order Robin-type boundary condition for both $\mathcal{B}$ and $\mathcal{T}$. The convergence is in both $H^1(\Omega_j)$ for all j and, under additional smoothness assumptions on the subdomains, in $H^{-\frac{1}{2}-\epsilon}(\Omega^t)$ for all $\epsilon \in (0, \frac{1}{2}]$. [1]

In practice, however, this algorithm exhibits a surprisingly slow rate of convergence [Des93]. A noticeable improvement in the rate of convergence is obtained if an under-relaxed version of the transmission condition is used, *i.e.*, replace (3.10) with

$$(\frac{\partial}{\partial \nu_j} + \mathcal{T})u_j^{n+1} = (1-\delta)(-\frac{\partial}{\partial \nu_k} + \mathcal{T})u_k^n + \delta(\frac{\partial}{\partial \nu_j} + \mathcal{T})u_j^n \qquad \text{on } \Sigma_{jk} \quad \forall k \tag{3.11}$$

for some value of the relaxation parameter $\delta \in [0, 1)$.

A better approximation to the original wave propagation problem on an unbounded domain (2.1)–(2.3) is obtained when the second-order RBC is applied on the artificial boundary. It is conjectured that the use of the second-order transmission condition similarly improves the convergence of the domain decomposition method. The analysis

1 While Després' results are developed for the special case in which there is no scatterer, *i.e.*, $\Gamma = \emptyset$, it is easily seen that the same holds for the more general problem.

of this problem is not substantially different from the analysis of the problem with first-order radiation and transmission conditions. The second-order tangential derivative introduces some additional technicalities into the analysis of this algorithm, but the same general approach can still be applied.

4 Variational Formulation

The simplicity of this method and its similarity to the first-order algorithm (and others of the same type) is clearly demonstrated by the variational formulation of the problem. Introduce the flux on the boundary and each interface as a Lagrange multiplier $\lambda_j := \left.\frac{\partial u}{\partial \nu_j}\right|_{\partial\Omega_j}$ (see, *e.g.*, [Des93]). Let the standard L_2 inner product be denoted by $(\cdot,\cdot)$ and the $H^{-1/2}$ — $H^{1/2}$ duality pairing by $\langle\cdot,\cdot\rangle$. The function space $\mathcal{H}(\Omega_j)$ contains all functions in $H^1(\Omega_j)$ with sufficient (tangential) smoothness on the boundary to assure that

$$\mathcal{B} : \mathcal{H}(\Omega_j) \to H^{-1/2}(\Gamma_j^t) \qquad \text{and} \qquad \mathcal{T} : \mathcal{H}(\Omega_j) \to H^{-1/2}(\Sigma_{jk}) \text{ for all } k.$$

The variational problem corresponding to the under-relaxed version of (3.7)–(3.10) is:

given initial functions u_j^0 on Ω_j and λ_j^0 on $\partial\Omega_j$, find (for all j) the (complex-valued) functions $u_j^{n+1} \in \mathcal{H}(\Omega_j)$ with $u_j^{n+1} = g_0$ on Γ_j and $\lambda_j^{n+1} \in H^{-1/2}(\partial\Omega_j)$ such that

$$\begin{aligned}
\left(\nabla u_j^{n+1}, \nabla v\right)_{\Omega_j} &- \omega^2 \left(u_j^{n+1}, v\right)_{\Omega_j} + \left\langle \mathcal{B} u_j^{n+1}, v\right\rangle_{\Gamma_j^t} + \sum_k \left\langle \mathcal{T} u_j^{n+1}, v\right\rangle_{\Sigma_{jk}} \\
&= \sum_k \left\langle \delta\lambda_j^n - (1-\delta)\lambda_k^n, v\right\rangle_{\Sigma_{jk}} \\
&\quad + \sum_k \left\langle \mathcal{T}\left(\delta u_j^n + (1-\delta) u_k^n\right), v\right\rangle_{\Sigma_{jk}} \\
&\quad + (f, v)_{\Omega_j} + \langle g_j, v\rangle_{\Gamma_j^t} \qquad (4.12)\\
\left\langle \lambda_j^{n+1}, w\right\rangle_{\Gamma_j^t} &= \langle g_j, w\rangle_{\Gamma_j^t} - \left\langle \mathcal{B} u_j^{n+1}, w\right\rangle_{\Gamma_j^t} \qquad (4.13)\\
\left\langle \lambda_j^{n+1}, w\right\rangle_{\Sigma_{jk}} &= -\langle \lambda_k^n, w\rangle_{\Sigma_{jk}} + \left\langle \mathcal{T}(u_k^n - u_j^{n+1}), w\right\rangle_{\Sigma_{jk}} \qquad (4.14)
\end{aligned}$$

for all (real-valued) test functions $v \in \mathcal{H}(\Omega_j)$ that vanish on Γ_j and $w \in H^{1/2}(\partial\Omega_j)$.

Note that, except under special conditions on $\mathcal{B}$ and the smoothness of the domains, these variational problems are not Hermitian.

5 Computational Results

To illustrate the improvements that can be expected from this algorithm, consider the following test problem. Let $\Omega^t := (0,1)\times(0,1)$ and $\Gamma := \emptyset$. Subdivide Ω^t into n

vertical strips, *i.e.*, for $j = 1, 2, \ldots, n$, $\Omega_j = (\frac{j-1}{n}, \frac{j}{n}) \times (0,1)$, $\Sigma_{jk} = \emptyset$ for $k \neq j+1$, and $\Sigma_{j,j+1} = \{(\frac{j}{n}, y) : y \in (0,1)\}$ $(j = 1, 2, \ldots, n-1)$. Let $\mathcal{B}u := \alpha u + \beta \frac{\partial^2 u}{\partial \tau^2}$ with coefficients taken from Table 1. On each subdomain the test and trial functions are chosen to be bi-quadratic.[2] Initialize both the solution, u_j^0, and Lagrange multipliers, λ_j^0, to zero. Computing the next iterate on one subdomain involves the solution of a 9×9 complex-valued linear system to compute u_j^{n+1} and four 3×3 complex-valued linear systems to compute λ_j^{n+1} along each edge.

All that remains is to select the data for the problem: f and g_j. Let U be a bi-quadratic function on Ω^t and choose $f = -\triangle U - \omega^2 U$ and $g_j = -\frac{\partial U}{\partial \nu_j} + \mathcal{B}U$, for each $j = 1, 2, \ldots, n$. Thus, the exact solution to (4.12)–(4.14) is $u = U$. The iterations terminate when the relative error of the solution and Lagrange multiplier on each subdomain, measured in the appropriate L_2-norm, falls below a specified threshold. That is, for a given $\epsilon > 0$, $\max_j \left\{ \left\| u_j^{n+1} - U \right\|_{L_2(\Omega_j)}, \left\| \lambda_j^{n+1} - \frac{\partial U}{\partial \nu_j} \right\|_{L_2(\partial\Omega_j)} \right\} < \epsilon$.A convergence test based on relative error might seem more appropriate, but some of the exact values of the Lagrange multipliers vanish in the examples of interest. In fact, since all relevant norms of the exact solution either vanish or exceed unity, the above absolute error test is actually a slightly more stringent condition.

Note that while this choice of data avoids all issues relating to approximation error, it is not consistent with the original scattering problem — U does not satisfy the Sommerfeld radiation condition. Regardless, this is still a valid test of a solution algorithm for the solution of the boundary value problem (2.4)–(2.6).

The optimal choice of the relaxation parameter is not known. The random selection of $\delta \in [0.7, 1)$ for each iteration is reported, by Després [Des93], to yield unexpectedly good results. In an effort to work with a deterministic algorithm for this project, a single value for δ must be selected; the value $\delta = 0.8$ appears to be close to optimal for a wide range of problems.

The results in Table 4, obtained using $\epsilon = 10^{-3}$, are representative of the performance that can be expected from this algorithm. In each case, the problems utilizing second-order radiation and transmission conditions converge faster than the corresponding problem with first-order conditions; the specific improvement ranges from 10% to 70% and averages a little more than 50%. The benefits of under-relaxation are also evident in all test cases. It is interesting, however, to note that the improvement due to under-relaxation is noticeably greater for the first-order problems.

6 Additional Issues

The experimental results are encouraging, but several issues remain unanswered. Partial answers are summarized where possible. Computational evidence referred to in this section is based on examples closely related to those presented here.

- Note that under-relaxation can be used, independently, on each term in the transmission condition. Is there any advantage to relaxing the two terms

2 Note that while solutions to this problem are complex-valued, it suffices to use real-valued bases for the test and trial spaces.

Table 2 Comparison of iterations to convergence for first- and second-order Robin transmission conditions with and without under-relaxation.

Exact Solution	Grid	# Iterations to Convergence: order 1, $\delta = 0$	order 1, $\delta = 0.8$	order 2, $\delta = 0$	order 2, $\delta = 0.8$
1	2×1	214	13	63	12
1	4×1	285	27	100	22
1	8×1	517	69	177	40
1+x	2×1	239	153	122	58
1+x	4×1	415	258	212	122
(1+x)(1+y)	2×1	256	165	76	63
(1+x)(1+y)	4×1	445	277	151	130

(λ_j^{n+1} and $\mathcal{T}u_j^{n+1}$) by different amounts? Likewise, would other aspects of the problem benefit from the use of under-relaxation, smoothing, or other modification to the standard iteration?

- The results in [Des93] are based on the relative L_2-error of the solution; there is no guarantee that the Lagrange multipliers have converged. In fact, computational tests indicate that the Lagrange multipliers converge much slower than the solution in each subdomain.
- Choosing the initial solution to be zero is easy to implement. It is also somewhat simpler to analyze. Is there a better choice for the initial solution?
- Table 2 appears to indicate that the number of iterations is roughly linear in the number of vertical strips. While this general trend is observed in larger tests, the correlation seems to not be as strong as the results presented in Table 2 might suggest. This implies that the current implementation, with one element per subdomain, is not likely to be optimal for large problems. Is it possible to find an optimal balance between the selection of a decomposition, the efficiency of the subdomain solver, and the transmission of information between subdomains?
- These tests always require that $\mathcal{B} = \mathcal{T}$. Preliminary computational tests in which $\mathcal{B}$ and $\mathcal{T}$ are Robin-type boundary operators of different orders can, when combined with the appropriate use of under-relaxation, be convergent. More specifically, while the local Robin-type boundary operators are optimal (in a certain sense) for use on the truncation boundary, are the same operators the optimal choice for the transmission condition? Related work in this direction (see, *e.g.*, [HTJ88, GCJ95]) recommends the use of non-local transmission conditions.

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