Interfaces in the Helmholtz Equation with High Order Accuracy

S. Tsynkov[†,*] **and E. Turkel**[‡,◇]

[†]North Carolina State University, Raleigh, NC, USA
[*]Email: tsynkov@math.ncsu.edu
[‡]Tel Aviv University, Tel Aviv, Israel
[◇]Email: turkel@post.tau.ac.il

Abstract

We consider problems that involve the propagation of waves over large regions of space with smooth, but not necessarily constant, material characteristics, separated by interfaces of arbitrary shape. The external boundaries can also be arbitrarily shaped. We present a numerical methodology for solving such problems that provides high order accuracy. It is based on Calderon's operators and the method of difference potentials and overcomes the difficulties inherent in more traditional approaches.

Introduction

We consider the numerical solution of the Helmholtz equation for the domains where the boundaries and interfaces may not necessarily conform to the mesh. Examples include scattering about complex shapes and bodies with multiple layers or several media. The general formulation involves a geometrically large region of space separated by several arbitrarily shaped interfaces and truncated with an arbitrarily shaped external boundary. The material properties are assumed smooth between the interfaces, whereas at the interfaces they may undergo jumps. Such problems occur frequently in practice in both two and three space dimensions. Due to dispersion and pollution, it is strongly desirable that higher order methods be used to reduce the errors, especially for high frequencies. However, the existence of interfaces usually degrades the accuracy of the scheme. Note that smooth, but not constant, material characteristics lead to variable coefficient extensions to the Helmholtz equation either in the wave number or else within the Laplacian type portion. These correspond to various effects of non-homogeneous media.

We first briefly review the existing methods. Finite differences lead to highly efficient algorithms for smooth solutions on regular grids. It is possible to construct a fourth order accurate approximation to the generalized Helmholtz equation with variable coefficients using a compact 3×3 stencil in two dimension and only the nearest 27 points in three dimensions. This implies that we have a stencil with the same domain of influence as the differential equation, and no special difficulties occur near boundaries that match the coordinate system. One can treat a variety of boundary conditions including those of the Dirichlet, Neumann and Robin type while maintaining the higher order accuracy. Furthermore, the expressions for the matrix entries are relatively simple, leading to a very efficient code. The main difficulties occur for curved shapes and low regularity of solutions.

Another volumetric approach is the finite element method (FEM) and its various extensions (e.g., DEM, DG) which may include wave-like solutions within the basis. This approach is designed to address low regularity and complex geometries. In this family of schemes high order accuracy requires extra degrees of freedom which entails additional computational costs. These extra degrees include internal points within the local cell and also a larger stencil depending on the details of the FEM.

For both finite difference and finite element methods a serious difficulty is the pollution error which requires a mesh density that grows faster than linear as the frequency increases so that the points-per-wavelength does not remain constant. This is partially alleviated by including wave-like elements within the technique, and also by increasing the order of accuracy of the scheme. In doing so, finite differences have the advantage that the stencil size does not increase for a compact fourth order accurate method even in the presence of variable coefficients.

Moreover, in all volumetric approaches for external domains one needs to approximate the Sommerfeld radiation condition in order to maintain a well-posed and accurate solution. Of course, the accuracy of the numerical approximation to the Sommerfeld condition needs to match the accuracy of the interior scheme.

The second approach for linear boundary value problems is to reduce them to integral equations with respect to equivalent boundary sources. In this case there is no limitations on the shape of the boundary. Furthermore, the correct far field behavior is automatically accounted for by the correct choice of the Green's function. One disadvantage of this approach is its relatively narrow range of allowable boundary conditions. It also introduces singular integral kernels, which can be a serious issue in

practice. These two disadvantages are hard to overcome. In general, the approach is limited to constant coefficients (i.e., to homogeneous media). For variable coefficients one needs to numerically construct the Green's function appropriate to the specific equation being solved, which is very expensive. Finally, the integral approach requires the inversion of a dense matrix over the boundary, which can be alleviated though by fast multipole methods.

In our new approach we use Calderon's operators that combine the strong points of both volumetric and boundary methods yet are free from their shortcomings. The general philosophy applies to wave propagation, heat transfer, linear elasticity, electro- and magnetostatics, Stokes flows, etc. In the current study, we shall concentrate on acoustic waves in the frequency domain.

Objectives of the current work

Our main goal is to construct a high order method for problems with solutions that are predominantly smooth but contain interfaces of a general, yet also smooth, shape. The method should match the geometric flexibility of boundary integral methods, but without singular integrals, and while not being limited to constant coefficients.

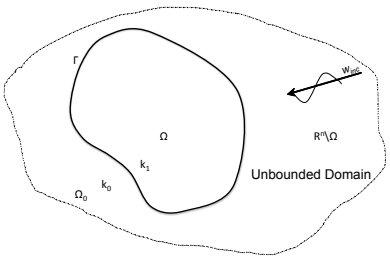

Figure 1: Schematic.

The new technique will use only simple structured grids, e.g., Cartesian or polar. In the regions of smoothness, we employ high order compact schemes [1, 2] on such grids. These schemes are very economical and avoid the redundancy of high order FEM and discontinuous enrichment methods (which automatically allow for irregularities anywhere). The boundaries and interfaces that are not aligned with the grid will be treated by Calderon's operators and the method of difference potentials [3]. This involves no loss of accuracy for arbitrarily shaped boundaries. Unlike finite elements, the approximating space is very narrow, yielding highly efficient methods.

The use of Calderon's operators provides maximum generality for treating the boundary conditions. The boundary representations inherit the accuracy of the core scheme, and high order accuracy is readily achievable for non-conforming boundaries. Hence, no adverse effects due to staircasing occur on regular structured grids with curved boundaries. Variable coefficients present no difficulties. There is no need to consider integral equations of the first or second kind, and no numerical approximation of singular integrals is required. Perhaps most important, the procedure is automatic. The discrete equations are fully characterized in algorithmic terms. It also possible to prove that the equivalent boundary problem that involves the Calderon projection is always well-posed. The extension from internal domains to problems on unbounded domains can be handled in a natural way.

Continuous formulation

We first describe the method for the continuous problem and then extend it to the discrete formulation.

Consider a homogeneous second order PDE $\boldsymbol{L}u = 0$ (e.g., the Helmholtz equation) on the domain $\Omega \subset \mathbb{R}^n$, $\Gamma = \partial\Omega$, with G being the fundamental solution. A generalized Calderon's potential on Ω with vector density $\boldsymbol{\xi}_\Gamma \equiv (\xi_0, \xi_1)|_\Gamma$ is given by [3–5]

$$\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma(\boldsymbol{x}) = \int_\Gamma \left(\xi_0(\boldsymbol{y}) \frac{\partial G}{\partial \boldsymbol{n}}(\boldsymbol{x}-\boldsymbol{y}) - \xi_1(\boldsymbol{y}) G(\boldsymbol{x}-\boldsymbol{y}) \right) ds_{\boldsymbol{y}}.$$

If $\boldsymbol{\xi}_\Gamma = \boldsymbol{Tr}\, u \equiv \left(u,\ \frac{\partial u}{\partial \boldsymbol{n}}\right)\Big|_\Gamma$, this expression reduces to the classical Green's formula for $\boldsymbol{x} \in \Omega$.

The Calderon projection is defined as the trace of the potential at the boundary: $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma = \boldsymbol{Tr}\, \boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma$. Its key property is that $\boldsymbol{\xi}_\Gamma$ satisfies the boundary equation with projection (BEP): $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma = \boldsymbol{\xi}_\Gamma$ iff $\exists u$ in Ω, $\boldsymbol{L}u = 0$ and $\boldsymbol{Tr}u = \boldsymbol{\xi}_\Gamma$.

Let $w(\boldsymbol{x})$ be an auxiliary smooth function such that $\boldsymbol{Tr}w = \boldsymbol{\xi}_\Gamma$, then for $\boldsymbol{x} \in \Omega$ we have:

$$w(\boldsymbol{x}) = \int_\Omega G \boldsymbol{L} w d\boldsymbol{y} + \int_\Gamma \left(w \frac{\partial G}{\partial \boldsymbol{n}} - \frac{\partial w}{\partial \boldsymbol{n}} G \right) ds_{\boldsymbol{y}}.$$

Consequently, $\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma(\boldsymbol{x}) = w(\boldsymbol{x}) - \int_\Omega G \boldsymbol{L} w d\boldsymbol{y},\ \boldsymbol{x} \in \Omega$. Note that this equivalent definition of $\boldsymbol{P}_\Omega$ no longer contains surface integrals. In addition, the potential appears insensitive to the choice of w.

For variable coefficients, we extend this by the following argument. Let $g = \begin{cases} \boldsymbol{L}w, & \boldsymbol{x} \in \Omega, \\ 0, & \boldsymbol{x} \notin \Omega. \end{cases}$ Then, $\int_\Omega G \boldsymbol{L} w d\boldsymbol{y} = \int G g d\boldsymbol{y} \equiv \boldsymbol{G} g$ is a solution to $\boldsymbol{L}v = g$, where $\boldsymbol{G}$ denotes Green's operator. Hence,

$$\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma = w - \boldsymbol{G} g \equiv w - \boldsymbol{G}\left(\boldsymbol{L}w\big|_\Omega\right), \quad \boldsymbol{x} \in \Omega.$$

When $\boldsymbol{L}$ is a more general operator assume there is a unique solution in $\Omega_0 \supset \Omega$ (subject to some BC at $\partial\Omega_0$):

$v = \boldsymbol{G}g$. Then Calderon's potential is given by $\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma = w - \boldsymbol{G}g$, and the projection is $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma = \boldsymbol{Tr}\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma$. It has the same key property: $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma = \boldsymbol{\xi}_\Gamma$ iff $\exists u:\ \boldsymbol{\xi}_\Gamma = \boldsymbol{Tr}u$ and $\boldsymbol{L}u = 0$ in Ω.

Solving equation $\boldsymbol{L}v = g$ on Ω_0 is referred to as the auxiliary problem (AP). There is flexibility in choosing the AP, which implies flexibility in computing $\boldsymbol{P}_\Gamma$ (e.g., there may be no convolutions at all). Note that regardless of the specific AP, the range $\mathrm{Im}\boldsymbol{P}_\Gamma$ stays the same. In other words, changing the AP means changing the projection "angle" onto the same manifold.

For the inhomogeneous equation $\boldsymbol{L}u = f$ in Ω, the BEP also becomes inhomogeneous: $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma + \boldsymbol{Tr}\boldsymbol{G}f = \boldsymbol{\xi}_\Gamma$. If a given $\boldsymbol{\xi}_\Gamma$ satisfies the BEP, then the corresponding solution is given by the generalized Green's formula: $u = \boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma + \boldsymbol{G}f$. We emphasize that all these constructs, and foremost, the equivalence of a PDE in Ω and the BEP on Γ, holds without specifying the boundary conditions.

Given a boundary condition on Γ: $\boldsymbol{l}_\Gamma u = \phi$, it is recast as $\boldsymbol{l}_\Gamma\left(\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma + \boldsymbol{G}f\right) = \phi$, and this equation is solved along with the corresponding BEP only on Γ. This provides a universal approach to accounting for general boundary conditions (rather than only the simplest Dirichlet/Neumann/Robin boundary conditions). So we can be handle equally well other types e.g. slant derivative, mixed, radiation, non-local, etc.

Moreover, interface (e.g., transmission) problems are addressed similarly. Let $\boldsymbol{L}_1 u = \phi_1$ hold on $\mathbb{R}^n \backslash \Omega$, and let the corresponding BEP be

$$\boldsymbol{Q}_\Gamma \boldsymbol{\xi}_\Gamma^{(1)} + \boldsymbol{Tr}\boldsymbol{G}_1 f_1 + \boldsymbol{Tr}u^{(\mathrm{imp})} = \boldsymbol{\xi}_\Gamma^{(1)},$$

where $u^{(\mathrm{imp})}$ is the impinging field (additional excitation). The two BEPs, interior and exterior, are solved along with the given interface condition:

$$\boldsymbol{A}\boldsymbol{\xi}_\Gamma - \boldsymbol{B}\boldsymbol{\xi}_\Gamma^{(1)} = \boldsymbol{\varphi}$$

that can be most general — any $\boldsymbol{A}$, $\boldsymbol{B}$, or $\boldsymbol{\varphi}$.

A very important consideration is that for either constant or variable coefficients, if the original problem on Ω is well-posed, then the reduced boundary problem on Γ is also well-posed. There is no need to consider Fredholm equations of the first or second kind.

Assume the problem: $\boldsymbol{L}u = 0$, $\boldsymbol{l}_\Gamma u = \phi$, is well-posed on Ω: $\|u\| \leqslant c\|\phi\|$, where $c = \mathrm{const}$. The equivalent boundary problem is $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma - \boldsymbol{\xi}_\Gamma = \boldsymbol{0}$, $\boldsymbol{l}_\Gamma(\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma) = \phi$. Then, $\|\boldsymbol{\xi}_\Gamma\| \leqslant c_1\|\phi\|$ because $\boldsymbol{\xi}_\Gamma = \boldsymbol{Tr}u$. Let $\boldsymbol{\psi}_\Gamma$ be a perturbation so that we solve $\boldsymbol{P}_\Gamma \boldsymbol{\xi}_\Gamma - \boldsymbol{\xi}_\Gamma = \boldsymbol{\psi}_\Gamma$, $\boldsymbol{l}_\Gamma(\boldsymbol{P}_\Omega \boldsymbol{\xi}_\Gamma) = \phi$. Then, the following estimate holds for the perturbed problem: $\|\boldsymbol{\xi}_\Gamma\| \leqslant C(\|\phi\| + \|\boldsymbol{\psi}_\Gamma\|)$, where C depends on $\|\boldsymbol{P}_\Omega\|$ and $\|\boldsymbol{P}_\Gamma\|$, but not on ϕ or $\boldsymbol{\psi}_\Gamma$. The proof exploits the split of the entire space of traces $\boldsymbol{\xi}_\Gamma$ into incoming and outgoing waves: $\mathrm{Im}\boldsymbol{P}_\Gamma \oplus \mathrm{Ker}\boldsymbol{P}_\Gamma$ [3, 6].

Discrete formulation

We next consider the extension to the discrete case for Calderon's potentials and projections. Let $\mathbb{N}_0$ and $\mathbb{M}_0$ be two regular grids on the domain Ω_0, on which we approximate u and f, respectively, of the equation $\boldsymbol{L}u = f$. Let $\boldsymbol{L}^{(h)}$ be the discrete operator on the stencil $\mathbb{N}_m$ centered at $m \in \mathbb{M}_0$. We emphasize that the boundary Γ does not have to conform to $\mathbb{N}_0$. Introduce the grid subsets:

$$\mathbb{M}^+ = \mathbb{M}_0 \cap \Omega, \quad \mathbb{M}^- = \mathbb{M}_0 \backslash \mathbb{M}^+ = \mathbb{M} \cap (\Omega_0 \setminus \Omega),$$
$$\mathbb{N}^+ = \bigcup_{m \in \mathbb{M}^+} \mathbb{N}_m, \quad \mathbb{N}^- = \bigcup_{m \in \mathbb{M}^-} \mathbb{N}_m, \quad \gamma = \mathbb{N}^+ \cap \mathbb{N}^-.$$

The grid boundary γ is a set of nodes that straddles Γ.

Let ξ_γ denote the discrete density on γ; and let w be an auxiliary function on $\mathbb{N}_0$, $w|_\gamma = \xi_\gamma \Leftrightarrow \boldsymbol{Tr}_\gamma^{(h)} w = \xi_\gamma$. The difference potential is defined as

$$\boldsymbol{P}_{\mathbb{N}^+}\xi_\gamma = w - \boldsymbol{G}^{(h)}\left(\boldsymbol{L}^{(h)} w\big|_{\mathbb{M}^+}\right), \quad n \in \mathbb{N}^+,$$

where $\boldsymbol{G}^{(h)}$ is the inverse of $\boldsymbol{L}^{(h)}$ obtained by solving the discrete AP on $\mathbb{N}_0$. The difference boundary projection is the trace of the potential: $\boldsymbol{P}_\gamma \xi_\gamma = \boldsymbol{Tr}_\gamma^{(h)} \boldsymbol{P}_{\mathbb{N}^+}\xi_\gamma$, and the corresponding discrete BEP

$$\boldsymbol{P}_\gamma \xi_\gamma + \boldsymbol{Tr}_\gamma^{(h)} \boldsymbol{G}^{(h)} \tilde{f} = \xi_\gamma$$

holds iff $\exists u$ on $\mathbb{N}^+$ such that $\boldsymbol{L}^{(h)}u = \tilde{f}$ on $\mathbb{M}^+$ and $\boldsymbol{Tr}^{(h)}u = \xi_\gamma$, where $\tilde{f}$ may be different from f for a compact scheme [1, 2].

For the exterior domain $\Omega_0 \backslash \Omega$, we similarly have:

$$\boldsymbol{Q}_{\hat{\gamma}}\xi_{\hat{\gamma}} + \boldsymbol{Tr}_{\hat{\gamma}}^{(h)} \boldsymbol{G}_1^{(h)} \tilde{f} + \boldsymbol{Tr}_{\hat{\gamma}}^{(h)} u^{(\mathrm{imp})} = \xi_{\hat{\gamma}},$$

where all the constructs can be different: the grid(s), the scheme, the grid boundary $\hat{\gamma}$, etc. We introduce extension operators from Γ to γ and $\hat{\gamma}$ that empoly Taylor's formula with equation-based derivatives:

$$\xi_\gamma = \boldsymbol{S}\boldsymbol{\xi}_\Gamma, \qquad \xi_{\hat{\gamma}} = \boldsymbol{S}_1 \boldsymbol{\xi}_\Gamma^{(1)}.$$

Then, the two discrete BEPs, interior and exterior, with the foregoing extensions substituted, are solved along with the given interface condition with respect to the unknown boundary functions $\boldsymbol{\xi}_\Gamma$ and $\boldsymbol{\xi}_\Gamma^{(1)}$.

If the domain Ω_0 is unbounded, $\Omega_0 = \mathbb{R}^n$, then the exterior AP needed for computing the projection $\boldsymbol{Q}_{\hat{\gamma}}$ shall be constructed so that to take into account the desired/correct

behavior at infinity. We can assume that in the far field the coefficients are constant. Then, the solution at infinity will satisfy the Sommerfeld condition.

The first approach is to formulate the AP on a regular auxiliary domain (that would contain Ω) such as a circle or a sphere, and truncate is with the appropriate artificial boundary conditions (ABCs). Local ABCs (e.g., by Bayliss and Turkel) are more intuitive, but less accurate. Non-local ABCs obtained in Fourier space after the separation of variables are very accurate and fit naturally into the FFT solver since the auxiliary domain is regular.

The second approach is to formulate the AP on an unbounded Cartesian grid and solve it by convolution with the discrete fundamental solution. The discrete fundamental solution is a non-singular grid function that coincides with the continuous fundamental solution away from the origin and differs from it near the origin. It automatically takes into account the correct behavior of the solution at infinity. The corresponding discrete convolution on the lattice can be computed with log-linear complexity by the fast multipole method.

To solve the resulting discrete equations with respect to the unknown densities on Γ, we need to discretize $\boldsymbol{\xi}_\Gamma$ and $\boldsymbol{\xi}_\Gamma^{(1)}$ themselves. This can be done by choosing various bases on Γ: Fourier, Chebyshev, local bases, etc. A very important consideration is that as long as the solution on Ω and on $\Omega_0\backslash\Omega$ is smooth, and Γ is smooth, the densities $\boldsymbol{\xi}_\Gamma$ and $\boldsymbol{\xi}_\Gamma^{(1)}$ can be efficiently approximated using a small number of terms, and this number will not depend on the size(s) of the grid(s), on which the APs are solved.

The AP needs to be solved repeatedly, for each of the basis functions used for approximating $\boldsymbol{\xi}_\Gamma$ or $\boldsymbol{\xi}_\Gamma^{(1)}$. This can be done efficiently with both direct and iterative solvers, as only the right-hand side of the AP changes between different solves. The choice of the specific solver depends on the formulation. For a bounded auxiliary domain and constant coefficients one can employ FFT or sparse LU. For an unbounded domain and constant coefficients, one can use either FFT/ABCs or convolution with the discrete fundamental solution. For variable coefficients on a bounded domain one can use either a preconditioned Krylov solver or, again, sparse LU. In doing so, the sparse LU will probably be feasible only in 2D.

Once the projection for each basis function has been computed, the coefficients that represent $\boldsymbol{\xi}_\Gamma$ and $\boldsymbol{\xi}_\Gamma^{(1)}$ in the chosen basis are evaluated in the sense of the least squares (by means of QR). Finally, the solution on the domain (either Ω or $\Omega_0\backslash\Omega$) requires one additional solve of the AP (for yet another right-hand side).

Results of computations

Our preliminary numerical results include the solution of a Dirichlet problem for the circle of unit radius using a non-conforming Cartesian grid. The governing equation is a Helmholtz equation with a variable wavelength $k = k(r,\theta) = k_0 e^{-10r^6(r-r_0)^6\cos\theta}$ for $r \leqslant r_0$ and $k = k_0$ for $r > r_0$, where $k_0 = 5$ and $r_0 = 1.6$. The test solution is taken in the form $u = e^{ikx} = e^{ikr\cos\theta}$, which makes the governing equation inhomogeneous: $\Delta u + k^2 u = f$.

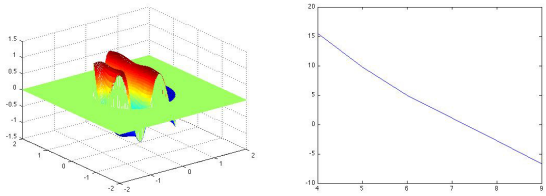

Figure 2: Numerical results.

In Figure 2(left) we show the real part of the solution, and in Figure 2(right) we show the grid convergence on a logarithmic scale. The latter clearly demonstrates fourth order accuracy and thus confirms the theoretical design properties of the method. Future research will include an exterior scattering problem.

References

[1] D. S. Britt, S. Tsynkov, and E. Turkel. A compact fourth order scheme for the Helmholtz equation in polar coordinates. *J. Sci. Comput.*, 45:26–47, 2010.

[2] D. S. Britt, S. Tsynkov, and E. Turkel. Numerical simulation of time-harmonic waves in inhomogeneous media using compact high order schemes. *Commun. Comput. Physics*, 9:520–541, 2011.

[3] V. S. Ryaben'kii. *Method of Difference Potentials and Its Applications*, vol. 30 *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, 2002.

[4] V. S. Ryaben'kii. Boundary equations with projections. *Russian Math. Surveys*, 40:147–183, 1985.

[5] S. V. Tsynkov. On the definition of surface potentials for finite-difference operators. *J. Sci. Comput.*, 18:155–189, 2003.

[6] J. Lončarić, V. S. Ryaben'kii, and S. V. Tsynkov. Active shielding and control of noise. *SIAM J. Applied Math.*, 62:563–596, 2001.