Towards Efficient Volume-Based Time-Domain Solvers for Scattering Problems

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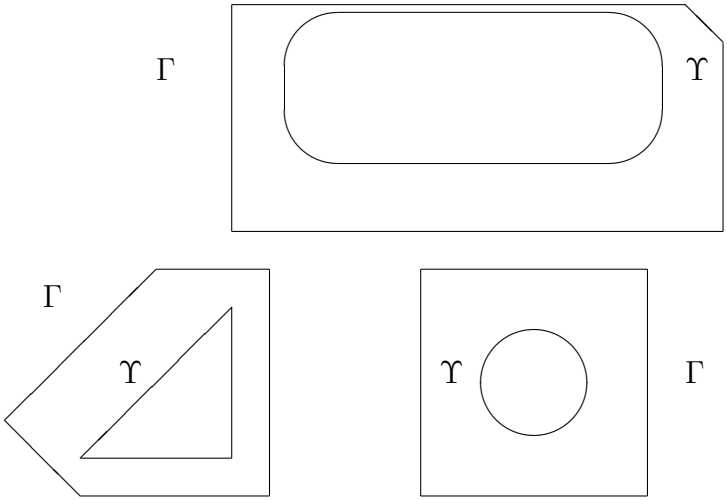


Domains for a multiple scattering problem: Υ is the computational domain, Γ is the artificial boundary.

Components of an efficient solver:

Radiation boundary conditions which provide arbitrary accuracy at small cost (spectral convergence, weak dependence on the simulation time and wavelength)

Algorithms for using the information at or near the boundary to directly propagate the solution to remote locations.

Reliable high-resolution volume discretizations applicable in complex geometry (i.e. on grids that can be generated efficiently).

I will focus on the first two issues, but will also say a little about the third. The key ingredient in treating the boundary condition - propagation problem is the development of efficient, approximate finite representations of time-domain wave fields. These can be used to compute necessary boundary data using the solution (i.e. derive relationships between outgoing and incoming characteristic data) and possibly extend the solution beyond the computational domain. I will review some of the existing accurate radiation boundary condition techniques from this perspective.

Why volume discretizations? Integral equation approaches have the advantage of automatically solving the first two problems and avoiding the third. However:

i. Volume based approaches maintain locality of the time evolution operator. For convex (or not-too-nonconvex) scatterers they should require less work and storage than integral equation approaches.

ii. Numerical methodologies are generally better established.

iii. Somewhat more general (scatterers with nonlinear response).

Is an arbitrarily accurate local radiation boundary condition possible? Yes! Theoretical justification (but not yet a practical method) is given by the following theorem (which I state in less generality than the author). Practically we have developed "almost-local" approaches - i.e. local methods whose stencil may grow logarithmically with tolerance and time.

Theorem [Warchall, Commun. in Part. Diff. Eq., 1991]
Let $\Omega \subset \mathbb{R}^3$ be an open convex set. Let $f(x,t)$,$u_0(x)$,$v_0(x)$ be sufficiently smooth and compactly supported in $\Omega' \subset \Omega$. Finally, let u satisfy $\Box u = f$, $u(x,0) = u_0(x)$, $\frac{\partial u}{\partial t}(x,0) = v_0(x)$. Suppose $\bar{x} \in \partial\Omega$ and Δt is such that $c\Delta t < \text{dist}(\bar{x}, \Omega')$. Then if $u(x,t)$ and $\frac{\partial u}{\partial t}(x,t)$ vanish for all $x \in \Omega$ satisfying $|x - \bar{x}| \leq c\Delta t$, we may conclude that $u(\bar{x}, t + \Delta t) = 0$.

Roughly this says that all the data we need is locally available. S. Lau has developed some interesting exact solution formulas which almost realize the update, but which still use some data outside the set described above.

A brief review of existing accurate methods for the domain truncation problem and the associated wave representation.

i. Expansions in spherical harmonics or (spatial) Fourier series:
These lead to nonlocal boundary conditions but they admit fast, low-memory compressions of the temporal kernels. (Alpert, Greengard, H. (SINUM 2000, JCP 2002), Lubich and Schädle, (SISC 2002), Hiptmair and Schädle, (Computing 2003))

- (Almost) uniform accuracy in time and wave number -

$$\text{Work} \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{R}{\lambda} \cdot N_\Gamma \cdot N_T.$$

- Straightforward implementation (but spatial transforms required),
- No geometric flexibility - expansion valid exterior to spheres.
- Extension to the far field is inefficient (unless you need the solution on a sphere!) Has been done by Grote and Kirsch (JCP 2007) for uncompressed formulations.

ii. Propagating plane waves:

- Local boundary condition sequences - Lindman, Engquist-Majda (70's) Higdon (80's), Givoli and Neta (00's)
- Perfectly matched layer (PML) - Bérenger (90's)
- Geometric flexibility - polygonal artificial boundaries (Collino, Vacus, H. and Warburton, Guddati and Lim for BCs)
- Nonuniform accuracy in time - the representation is generally incomplete unless incoming waves are used! The complexity of the boundary condition depends on the simulation time:

$$\begin{aligned} \text{Work}_{\text{EM}} &\propto \ln\frac{1}{\epsilon}\cdot\frac{cT}{\lambda}\cdot N_\Gamma\cdot N_T, \\ \text{Work}_{\text{PML}} &\propto \ln\frac{1}{\epsilon}\cdot\sqrt{\frac{cT}{\lambda}}\cdot N_\Gamma\cdot N_T. \end{aligned}$$

(PML can be improved (made optimal?) by not resolving the solution in the layer - requires a discrete analysis)

ii. Propagating plane waves - continued:

Propagating plane waves are the basis of Michielssen's plane wave fast time domain method (PWFTD) for integral equations (JCP 1998, IEEE Trans. Ant. Prop. 2003-2004). Michielssen et al make use of a result of Heyman (J. Math. Phys. 1996) which says that such a representation can be made exact with a careful use of time decomposition and source-receiver separation rules.

iii. Equivalent source representations:

Difference potential method of Ryaben'kii and Tsynkov (JCP 2001) - construct an auxiliary function satisfying a forced wave equation in free space which agrees with the solution of the original problem at the artificial boundary. The auxiliary function can be computed efficiently using Fourier methods exploiting the strong Huyghens principle. Fast algorithms with a different method for cosntructing the sources have been developed by Bruno and Hoch. I don't know what sort of asympototic complexity estimates apply to these techniques. Propagation to the far field is straightforward for the Bruno-Hoch algorithm.

iv. Multipole expansions:

Theoretical development by Heyman and Devaney (J. Math. Phys. 1996). Localized construction for boundary conditions on the sphere derived by H. and Hariharan (Appl. Num. Math. 1998), field extension algorithms and multiple scattering applications recently developed by Grote.

$$\text{Work} \propto \ln \frac{1}{\epsilon} \cdot N_\Gamma^{3/2} \cdot N_T.$$

Same restrictions as the conditions based on spherical harmonic expansions and worse asymptotic complexity. However, effectively as efficient in many cases (no spherical harmonic transform) and the extension algorithm is more efficient in that one can limit the angular range.

v. Curvelets:

Theory for curvelet representations of solutions of hyperbolic systems is developed by Candés and Demanet (CPAM 2005). Curvelets are anisotropic vector wavelets with width $\propto$ length^2 corresponding to characteristics propagating in the "thin" direction. According to the theory the action of the solution operator is represented by an approximately sparse, "well-organized" matrix in the curvelet space. Applicable to inhomogeneous media. As yet I don't know of their application to the problems mentioned here or what the complexity of such methods would be. I believe they could be used for the problems described here.

I want to focus on what I will call a complete plane wave representation, one involving both propagating and evanescent modes.

Here is a quick and elementary derivation of the complete plane wave representation for the scalar wave equation. (See also Heyman J. Math. Phys. 37 1996 for a less elementary approach. Analogous frequency domain expansions are used in the Helmholtz FMM.)

Suppose the plane $z = 0$ separates the region containing all sources, inhomogeneities, scatterers etc ($z < -\delta$) and free space ($z > 0$). We can think of this plane as containing one of the boundary faces in the earlier picture. Solve the Dirichlet problem in $z > 0$ by Fourier-Laplace transform in the tangential and time variables:

$$\hat{u}(z, s, k) = e^{-(s^2+|k|^2)^{1/2}z}\hat{u}(0, s, k)$$

Inverting the transform (taking the Laplace inversion contour to be the imaginary axis $s = i\omega$) we separate the integrals into two pieces according the sign of $-\omega^2 + |k|^2$.

The integral in the region $-\omega^2 + |k|^2 = -\cos^2\theta \cdot \omega^2 < 0$ leads to a propagating plane wave field:

$$\int_0^{\pi/2} P(t - z\cos\theta, x, y, \theta)d\theta,$$

and the integral in the region $-\omega^2 + |k|^2 = \sigma^2 > 0$ leads to an evanescent plane wave field:

$$\int_0^{\infty} e^{-\sigma z} E(t, x, y, \sigma)d\sigma$$

The sum of these contributions is an exact representation of the wave field in the half space. We note that each term individually is non-causal so we don't ascribe any direct physical interpretations of the individual terms. (Note that the choice of a different inversion contour leads to multidimensional representation integrals.)

Numerical algorithms follow from finite representations of the wave field which are constructed by approximating the integrals using appropriate quadrature rules. Using Gauss-type rules we expect spectral convergence as the finite representations are refined.

Finite representation:

$$u(x,y,z,t) \approx \sum_{j=0}^{n_p-1} P_j(t - z\cos\theta_j, x, y) + \sum_{j=1}^{n_e} e^{-\sigma_j z} E_j(t,x,y).$$

The quadrature nodes determine the propagation angles, θ_j, as well as the decay rates of the evanescent modes, σ_j. Currently we use:

$$\theta_j = \frac{\pi(c_j+1)}{4}, \quad j = 0,\ldots,n_p-1,$$

where c_j are the left endpoint Gauss-Radau nodes on $[-1,1]$ and

$$\sigma_j = \eta d_j, \quad j = 1,\ldots,n_e,$$

where d_j are the Yarvin-Rokhlin quadrature nodes (Yarvin and Rokhlin, (SIAM J. Sci. Comput. 1999) - available at netlib.) and η is a free parameter to be optimized. (Units of inverse length - dependent on the simulation time, T, and the separation, δ, of the plane $z = 0$ and any inhomogeneities.) Recently we have constructed methods with smaller complex reflection coefficients based on geometric spacings for the nodes in line with known optimal rational approximations to the square root due to Newman, Zolotarev, and more recent work by Ingerman, Druskin and Knizherman (CPAM 2000).

How do we find the amplitudes? To define radiation boundary conditions or PMLs which are exact on the finite representation we don't have to. Precisely, local boundary conditions with $n_p + n_e$ auxiliary functions can be constructed which are exact on this approximate representation independent of the functions P_j and E_j. Our formulation is a generalization of Higdon's from the 80's which allows arbitrary-order implementations using well-behaved auxiliary functions.

For $j = 0, \ldots, n_p - 1$ recursively define:

$$\left(\cos\theta_j \frac{\partial}{\partial t} + \frac{\partial}{\partial z}\right)\psi_j = \left(\cos\theta_j \frac{\partial}{\partial t} - \frac{\partial}{\partial z}\right)\psi_{j+1}$$

with $\psi_0 = u$ and similarly define:

$$\left(\sigma_j + \frac{\partial}{\partial z}\right)\psi_{n_p+j} = \left(\sigma_j - \frac{\partial}{\partial z}\right)\psi_{n_p+j+1}$$

for $j = 1, \ldots, n_e$. (Precisely we define the functions by integrating the equations backwards from $z = +\infty$.)
Note that if we assume the finite representation each subsequent term in the recursion admits a similar finite representation with one fewer term. We thus conclude:

$$\psi_{n_p+n_e+1} = 0,$$

which we use to define our radiation boundary conditions.

We note that the recursive system is formally equivalent to a box scheme discretization of a nonstandard PML with grid spacings $\Delta z = \frac{2}{s\cos\theta_j}$ and $\Delta z = \frac{2}{\sigma_j}$. (See Asvadurov, Druskin, Guddati, Knizherman (SINUM 41 2003) and Guddati and Lim (IJNME 66 2006) for direct derivations of these nonstandard PMLs without the evanescent mode corrections.)

To implement the conditions we like to eliminate the z derivatives in favor of tangential derivatives. These are converted to equations for the auxiliary variables **on the boundary** by using the governing equations to eliminate the normal derivatives in favor of tangential derivatives.

Structure of the auxiliary equations for first order systems:

$$u_t + Au_z + Bu_y = 0,$$

For $0 \le j \le n_p$:

$$(\cos\theta_j A - I)\frac{\partial \psi_j}{\partial t} - B\frac{\partial \psi_j}{\partial y} = (\cos\theta_j A + I)\frac{\partial \psi_{j+1}}{\partial t} + B\frac{\partial \psi_{j+1}}{\partial y},$$

and for $1 \le j \le n_e$:

$$-\frac{\partial \psi_{n_p+j}}{\partial t} - B\frac{\partial \psi_{n_p+j}}{\partial y} + \sigma_j A\psi_{n_p+j} = \frac{\partial \psi_{n_p+j+1}}{\partial t} + B\frac{\partial \psi_{j+1}}{\partial y} + \sigma_j A\psi_{n_p+j+1}.$$

Truncate by:

$$\psi^{\text{in}}_{n_p+n_e+1} = 0,$$

with $\frac{\partial \psi^{\text{out}}_0}{\partial t}$ computed from the interior.

I believe this formulation is near-optimal in terms of computational complexity - in particular I conjecture:

$$\text{Work} \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{cT}{\delta} \cdot N_\Gamma \cdot N_T.$$

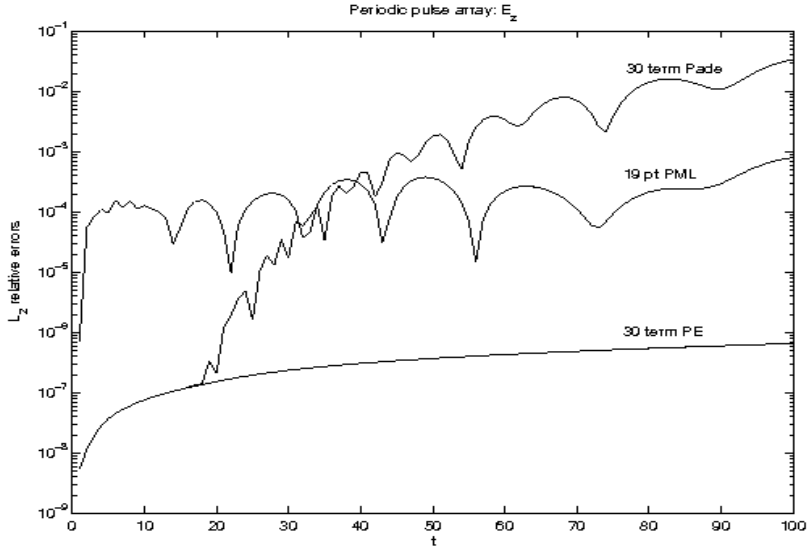
(Note that we want $\delta \sim \lambda$.)

The estimate should be provable using estimates of the complex reflection coefficient following from the theory of rational approximants to the square root (suggested by Druskin) combined with Parseval's relation. Roughly, we need to approximate the square root function on intervals:

$$\left[\frac{\delta^2}{c^2T^2}, 1\right], \quad \left[0, \frac{L^2}{\delta^2 \ln^2 \frac{1}{\epsilon}}\right].$$

For the former we use the fact that Zolotarev's p-term approximation has an error $O\left(\exp\left(\frac{-\pi^2 p}{2 \ln \frac{cT}{\delta}}\right)\right)$ and for the latter we have an approximation with an error $O\left(\frac{L \exp\left(-\pi\sqrt{p}\right)}{\delta \ln \frac{1}{\epsilon}}\right)$.

Here is a numerical example illustrating the improvement in accuracy obtained when the evanescent modes are included. We solve the TM Maxwell system with fields determined by a transversely periodic array of pulses. The solution is well-resolved in space and time (8th order spatial differencing with a graded mesh to stabilize one-sided differencing at the boundary and standard 4th order RK for Maxwell.) Here we use $n_p = n_e = 15$ and compare with 30-term Padé approximants (60th order Engquist-Majda) and a 19-point standard PML with optimized grid stretching. (Errors are computed using an accurate evaluation of an integral representation of the exact solution.)


Periodic pulse array: E_z
30 term Pade
19 pt PML
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To use the new method in exterior domains which we bound by polygons we need **corner compatibility conditions** to connect the auxiliary variables on adjacent edges/faces. Such conditions have been studied for the Padé-based local boundary conditions by Collino and Vacus but their constructions are complex and of somewhat limited scope.

Here we exploit the connection with PML and simply treat the corners as a standard corner PML - i.e. apply the complex/real grid stretching in each dimension. (First done by Guddati and Lim for complex grid stretching.) For a first order system this yields the following equations. (For systems such as Maxwell where the boundary normals will be characteristic some modifications are required.)

$$\begin{aligned}
&\frac{\partial \psi_{k+1,j+1}}{\partial t} + \frac{\partial \psi_{k,j}}{\partial t} + \frac{\partial \psi_{k+1,j}}{\partial t} + \frac{\partial \psi_{k,j+1}}{\partial t} \\
&+S_j A \left(\psi_{k+1,j+1} - \psi_{k+1,j} + \psi_{k,j+1} - \psi_{k,j}\right) \\
&+S_k B \left(\psi_{k+1,j+1} - \psi_{k,j+1} + \psi_{k+1,j} - \psi_{k,j}\right) \quad = 0,
\end{aligned}$$

where

$$S_j w \equiv \begin{cases} \cos\theta_j \frac{\partial w}{\partial t}, & j \le n_p, \\ \sigma_{j-n_p} w, & j > n_p. \end{cases}$$

Truncate by:

$$\psi^{\text{in}}_{k,n_p+n_e+1} = \psi^{\text{in}}_{n_p+n_e+1,j} = 0,$$

with $\frac{\partial \psi^{\text{out}}_{k,0}}{\partial t}$, $\frac{\partial \psi^{\text{out}}_{0,j}}{\partial t}$ computed from the edges. (Here the meanings of in and out are based on the local characteristics in the normal directions. The truncations are combined for $k = j = n_p + n_e + 1$.)

As yet we have no analysis of this corner problem. The hope is that there are no (or very weak) singularities - we have encountered no evidence of any singular behavior in the numerical experiments so far.

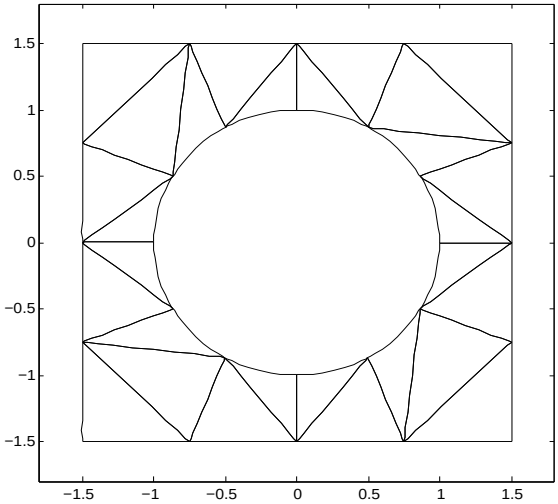
Numerical experiments using a DG code. Point source scattering from the unit cylinder.

Source location: $(2.25, 0)$.

Signal: $\sin^6 t$.

Comparison with an exact solution computed by numerical inversion of the Bessel series in the Laplace domain. Error shown at a point in the shadow region.

Degree 10 polynomials.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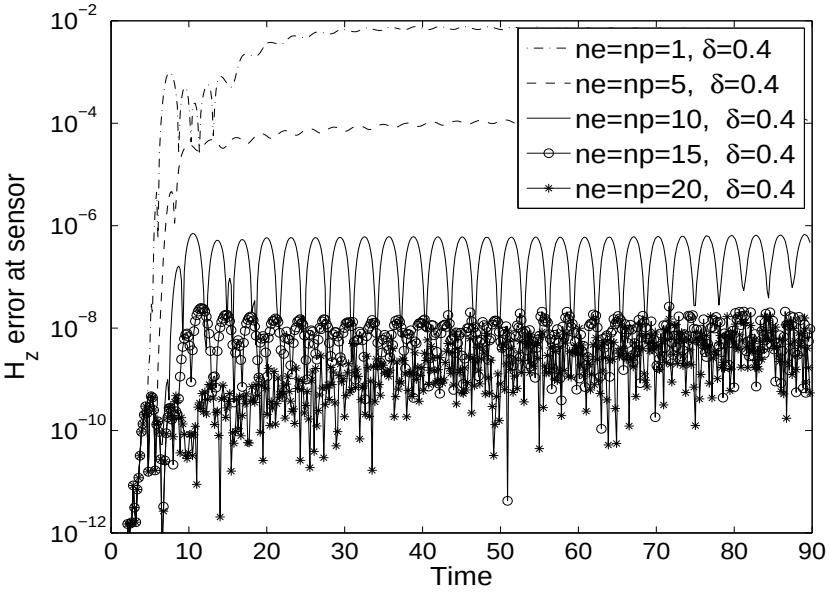
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H_z error at sensor
Time
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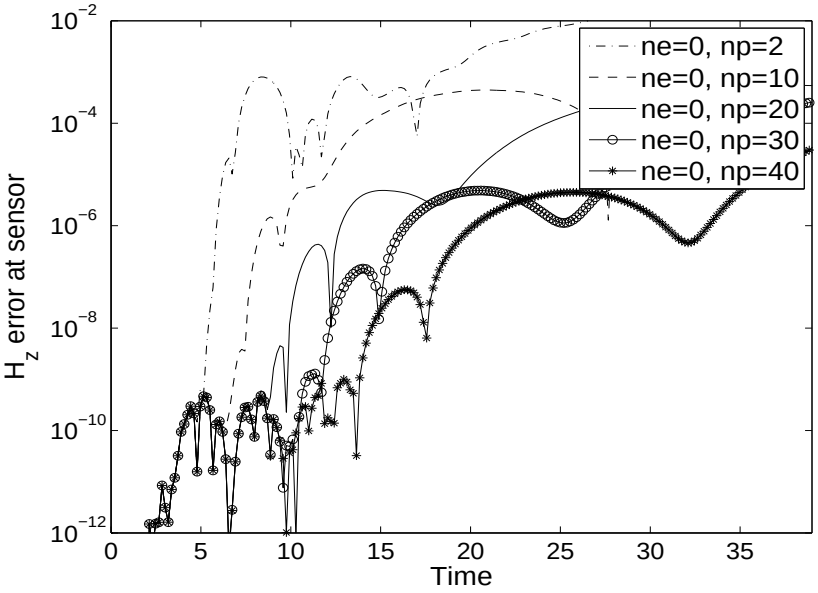
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ne=0, np=40
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
H_z error at sensor
0
5
10
15
20
25
30
35
Time

Some generalizations we have completed:

Second order systems:

We develop a coupled system of second order wave equations on the boundary in analogy with the first order systems shown above.

Stratified media:

For compatible choices of the parameters one can establish a relationship between the auxiliary functions in adjacent media.

Lattice systems:

These have potential applications to multiscale coupling of molecular dynamics and continuum simulations.

However there are some difficult issues associated with dispersive systems.

Anisotropic systems: for anisotropic systems the group velocity, which determines the physical directions of wave propagation which must be respected by stable algorithms, can be mismatched with the direction of the phase velocity, which is fundamental to our representation. Directly, outgoing radiation can appear ingoing and vice versa. For example, our plane wave expansion for the linearized Euler equations takes the form:

$$\int_0^{\pi/2} P((1-U^2)t + z(U-\cos\theta), y - Vt, \theta)d\theta$$
$$+ \int_0^{\infty} e^{-\sigma z} E((1-U^2)t + Uz, y - Vt, \sigma)d\sigma$$

Despite the appearance of waves with the wrong direction of phase velocity we have carried out some preliminary experiments (without corners or evanescent modes) which were stable. The essential point is that such a mismatch is not allowed on the righthand side of the recursions, but these can be chosen freely. The more difficult case of anisotropic elastic waves has yet to be considered. The development of a representation directly incorporating the group velocities is desirable.

High-order/resolution volume discretization methods in complex geometry - strategies for gridding:

i. Composite, overlapping structured grids (e.g. Overture project at LLNL) - on such grids one can use flexible and efficient high-order difference methods. How efficiently can the grids be generated for very complex 3d geometries?

ii. Unstructured grids - high-order/high-resolution discontinuous Galerkin discretizations (e.g. Sledge++ project). Not as efficient as structured grid methods, particularly in terms of time-step stability constraints which grow quadratically with the degree. (Warburton and H. have shown how this can be fixed if one differentiates on the dual grid, but such an approach is complicated for unstructured grids in higher dimensions.) Is there a simpler way to improve efficiency?

iii. Cartesian grids with embedded boundaries. Here the problem is to maintain high accuracy at the boundaries and avoid instabilities associated with small cells. A number of methods have been proposed in recent years: Li and Greengard (JCP 2004), Wandzura (JCP 2004), Zhao and Wei (JCP 2004, ...) There has been little or no theory developed for these!

The latter methods are essentially algebraic - either widening the stencil (Wandzura) or using multiple approximations to the boundary condition (Zhao et al). I will close with a brief description of the method of Li and Greengard which involves an interesting combination of volume and integral equation approaches.

Two ingredients:

1. Two-step integral time-stepping formula for the wave equation leading to explicit, high-order formulas which are stable for fixed time steps and arbitrarily small cells.

2. High-order boundary approximations by using the boundary integral equation to correct the solution updated by the volume solver. This requires the repeated solution of the integral equation with null initial data over a single time step - local problem!

The small cell volume solver follows from the following exact integral formula for solutions of the wave equation (Alpert, Greengard, and H. (JCP 2000)):

$$u(x,t+dt) - 2u(x,t) + u(x,t-dt) = \int_{|x-y|\le dt} G_n(|x-y|,dt)\nabla^2 u(y,t)dy,$$

where

$$G_1(r,dt) = dt - r,$$

$$G_2(r,dt) = (\ln(dt + \sqrt{dt^2 - r^2}) - \ln r)/\pi,$$

$$G_3(r,dt) = 1/(2\pi r).$$

Methods follow from approximating the Laplacian and applying a quadrature rule. The domain of dependence is explicitly respected which allows the circumvension of the small cell problem. (Also applicable to local time-stepping near refinements?)

In conclusion I believe we are in the process of developing satisfactory methods for solving scattering problems in the time domain using volume discretizations.

- I expect they will be somewhat more efficient than integral equation solvers in most cases, primarily due to the fact that they maintain locality in space-time.
- It is useful to think about the methods in terms of the underlying representations of the time-dependent wave fields; there are many options but it is not clear if any are clearly to be preferred.
- The mathematical analysis of apparently useful methods is still incomplete.