

Some Problems in the Numerical Analysis of Elastic Waves

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There are a plethora of high-order methods available for solving wave problems - fundamental differences are related to the meshes used and whether or not dissipative discretizations are preferred. The approach we are pursuing includes:

Hybrid structured-unstructured grids - leverage the geometric flexibility of unstructured grid methods near complex geometric features and the efficiency of structured grid methods in large volumes.

Energy-stable discretizations - we typically use methods which are dissipative as we feel they are more robust in the presence of rapidly changing grids, changes in discretization across grid types, interpolation between grids, nonlinearity. In particular we are using upwind discontinuous Galerkin (DG) methods on unstructured grids and either Hermite methods or upwind Galerkin difference methods on the structured grids. However all the DG methods have energy-conserving versions for those who have a dislike for artificial dissipation.

Radiation boundary conditions with error control - for isotropic problems we have developed optimal local radiation boundary condition sequences, **Complete Radiation Boundary Conditions**. For more complex systems we are working on optimized damping/stretching “super-grid” layers - we’d welcome other ideas!

For acoustics and electromagnetism all of our methods, both for volume discretizations and for radiation boundary conditions, work very well.

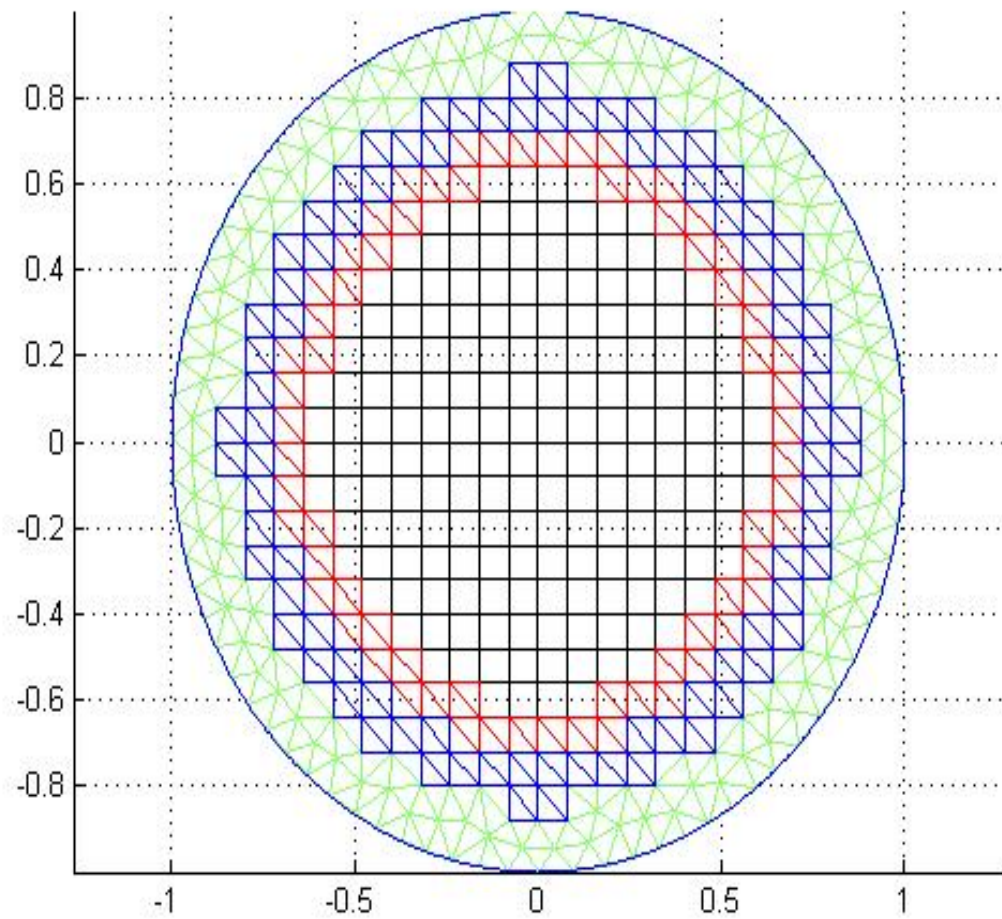
However for elastic waves there are new challenges which cause difficulties and which in some cases remain unresolved. They are associated with:

Multiple wave families with different dispersion relations

Interface/boundary waves (Rayleigh, Stoneley, ...)

Complex wave dispersion relations in anisotropic media and even for isotropic media in waveguides

A numerical analysts apology: here I will focus on some of these problem areas even if some are not relevant for seismic problems.



In general our DG methods are formulated for problems of the form:

$$\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j} \frac{\partial G}{\partial u_{i;j}} - \frac{\partial G}{\partial u_i}, \quad u(x, 0) = u_0(x), \quad \frac{\partial u}{\partial t}(x, 0) = v_0(x), \quad Bu(x, t) = 0, \quad x \in \partial\Omega,$$

$$G(Du, u) > 0 \rightarrow \frac{d}{dt} \int_{\Omega} \frac{1}{2} \left| \frac{\partial u}{\partial t} \right|^2 + G = \text{Boundary Terms.}$$

Example: standard scalar wave equation $G = \frac{c^2}{2} |\nabla u|^2$.

For all $\phi_v \in \Pi^q(\Omega_j)$, $\phi_u \in \Pi^{q+1}(\Omega_j)$

$$\begin{aligned} \int_{\Omega_j} \nabla^2 \phi_u \left(\frac{\partial u^h}{\partial t} - v^h \right) &= \int_{\partial\Omega_j} \nabla \phi_u \cdot \mathbf{n} \left(\frac{\partial u^h}{\partial t} - v^* \right), \\ \int_{\Omega_j} \phi_v \frac{\partial v^h}{\partial t} + c^2 \nabla \phi_v \cdot \nabla u^h - \phi_v f &= c^2 \int_{\partial\Omega_j} \phi_v \mathbf{w}^* \cdot \mathbf{n}, \\ \int_{\Omega_j} \left(\frac{\partial u^h}{\partial t} - v^h \right) &= 0. \end{aligned}$$

To define an **upwind flux** we choose (v^*, \mathbf{w}^*) based on the outward Sommerfeld fluxes, $v^h - c(\nabla u^h) \cdot \mathbf{n}$. Following the standard convention let the superscripts “ \pm ” refer to traces of data from outside and inside the element respectively. Then we impose the following equations whose solution defines the fluxes:

$$\begin{aligned} v^* - c\mathbf{w}^* \cdot \mathbf{n}^- &= v^- - c\nabla u^- \cdot \mathbf{n}^-, \\ v^* - c\mathbf{w}^* \cdot \mathbf{n}^+ &= v^+ - c\nabla u^+ \cdot \mathbf{n}^+, \end{aligned}$$

Energy estimate (note $v^h \neq \frac{\partial u^h}{\partial t}$):

$$E^h(t) = \frac{1}{2} \sum_j \int_{\Omega_j} (v^h)^2 + c^2 |\nabla u^h|^2,$$

satisfies

$$\frac{dE^h}{dt} - \int_{\Omega} v^h f = - \sum_k \int_{B_k} \alpha \beta c \left((v^-)^2 + c^2 (\nabla u^- \cdot \mathbf{n}^-)^2 \right) - \mathcal{D},$$

where $\mathcal{D} = 0$ for the central and alternating fluxes and for the upwind flux

$$\mathcal{D} = \frac{c}{2} \sum_k \int_{F_k} |[[v^h]]|^2 + c^2 [[\nabla u^h]]^2 + c \sum_k \int_{B_k} (\alpha v^- + \beta c \nabla u^- \cdot \mathbf{n}^-)^2.$$

Using the energy estimate and standard arguments adapted from the first-order case we can prove for general grids

$$\|e_v(\cdot, T)\|_{L^2(\Omega)}^2 + \|\nabla e_u(\cdot, T)\|_{L^2(\Omega)}^2 \leq (C_0 + C_1 T) h^{2\sigma} \max_{t \leq T} \left(|u(\cdot, t)|_{H^{q+2}(\Omega)}^2 + |v(\cdot, t)|_{H^{q+1}(\Omega)}^2 \right),$$

where

$$\sigma = \begin{cases} q, & \text{Central/alternating flux,} \\ q + \frac{1}{2}, & \text{Upwind flux.} \end{cases}$$

In one space dimension (and probably on Cartesian grids) we can use the upwind projection technique to improve this to $q + 1$ for both the upwind and alternating flux. **In our experiments so far we observe L^2 -convergence at order $q + 2$ for both the central and alternating flux, but we have no proof.** Note that this is a superconvergence phenomenon in that the equation for $\frac{\partial u^h}{\partial t}$ involves v^h which is of degree q .

Elastic wave equation (isotropic medium - not necessary!)

$$G = \frac{1}{\rho} (\lambda \theta^2 + \mu (e_{11}^2 + e_{22}^2 + e_{33}^2 + 2e_{12}^2 + 2e_{23}^2 + 2e_{13}^2))$$

where

$$\theta = \nabla \cdot u, \quad e_{ij} = \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}.$$

Now we need not only additional equations corresponding to constant states (translational symmetries) but also to rotations since now there are nonconstant fields for which $G = 0$.

$$\int_{\Omega_j} \left(\frac{\partial^2 u_1}{\partial x_2 \partial t} - \frac{\partial^2 u_1}{\partial x_1 \partial t} \right) - \left(\frac{\partial v_1}{\partial x_2} - \frac{\partial v_2}{\partial x_1} \right) = 0$$

Here again we have a general stability and marginally suboptimal convergence analysis.

For codes implementing a full set of benchmark problems see: bitbucket.org/appelo/dg_dath_elastic_v1.0.

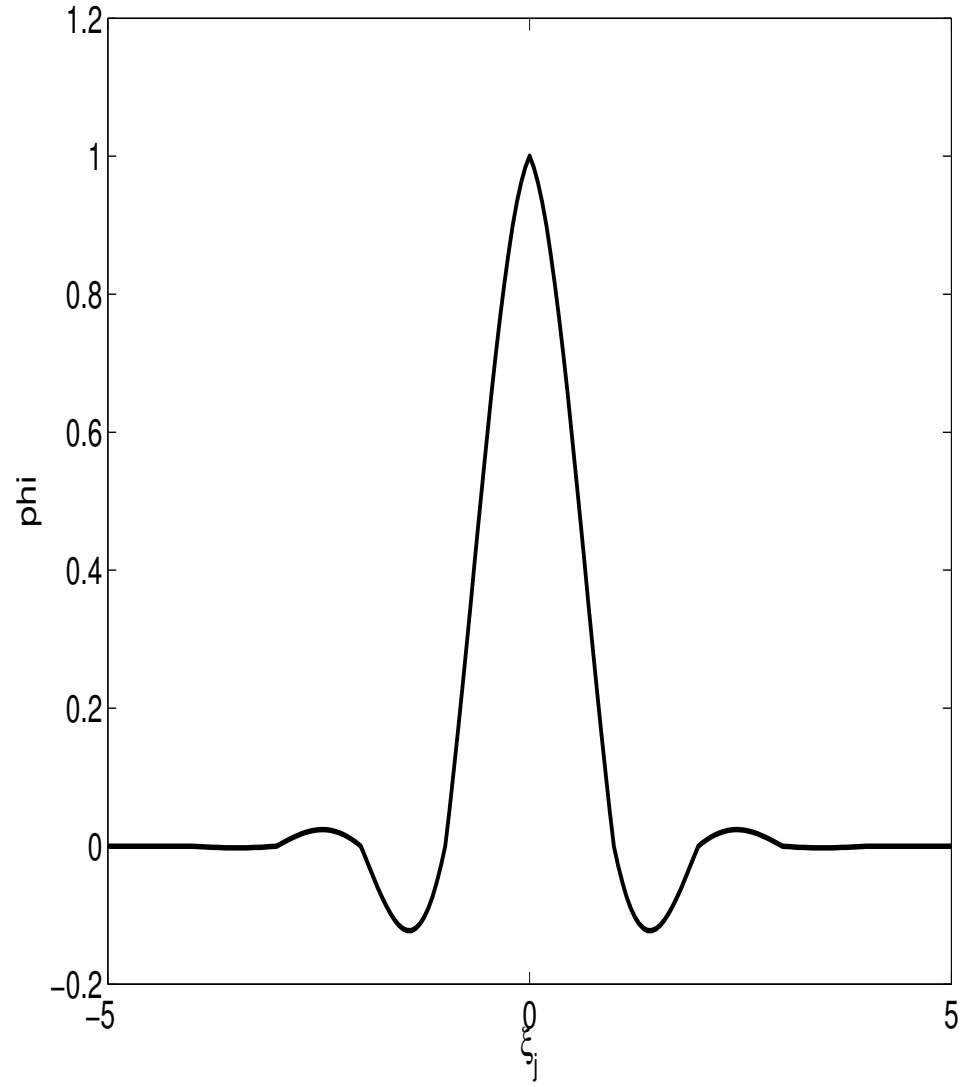
The standard energy-based high order difference methods are the so-called summation-by-parts (SBP) methods - boundary closures of high-order central (or upwind) difference formulas which allow an integration-by-parts formula relative to a quadrature scheme with positive weights. Some results have been obtained by Wilcox and Kozdon on stably coupling SBP methods with DG schemes - not straightforward.

We are pursuing a different approach to the construction of difference methods with energy-stable boundary closures - “global” discontinuous Galerkin method with finite-difference type bases which we call GD (Galerkin finite differences.)

- Basis elements extend across multiple elements to avoid the problems caused by differentiating polynomials near element boundaries. For example a typical Lagrange function would be a continuous piecewise polynomial supported on q cells to the right and to the left - see the upcoming picture.
- Boundary closures are obtained either by extrapolation or by allowing basis elements associated with “ghost” nodes to remain in the basis.

The construction produces compact difference schemes as the mass matrix is not diagonal, however they possess a superconvergence for the dispersion relation. As they are simply a different basis their stable coupling with unstructured grids is automatic.

interior basis function (p=7)



A happy mystery about these methods is that, for Friedrichs systems, **the norm of the derivative matrix is independent of order up through at least thirty-something despite the fact that the boundary basis functions themselves are badly behaved due to the Runge phenomenon** - some magic cancellation is happening due to the bad basis functions appearing in both mass and stiffness matrices. We have yet to analyze this - we have no analytic bounds on the spectrum.

p	3	5	7	9	11	13	15	17
$\Delta x \rho((M^{(p,G)})^{-1} K^{(1,p,G)})$	2.02	2.17	3.41	3.18	3.67	3.81	3.57	3.84
$\Delta x \rho((M^{(p,X)})^{-1} K^{(1,p,X)})$	2.02	2.17	2.27	2.33	2.39	2.43	2.46	2.49

Problems - approximation of Rayleigh or Stoneley waves with nearly incompressible isotropic materials and low order difference methods. (H.-O. Kreiss and Petersson SINUM 2012; K. Virta and G. Kreiss JCP 2015.)

Simple analysis - let

$$\begin{aligned}\epsilon &= \frac{c_S}{c_L} \ll 1 \\ \beta &= \frac{c_R}{c_S} < 1\end{aligned}$$

Then β is given by roots of:

$$\det \begin{pmatrix} (2 - \beta^2) \epsilon^2 & -2i\epsilon^2 \sqrt{1 - \beta^2} \\ 2i\sqrt{1 - \epsilon^2 \beta^2} & 2 - \beta^2 \end{pmatrix} \equiv \det R$$

Nothing exciting happens as $\epsilon \rightarrow 0$: $\beta \rightarrow .833\dots$ However, suppose we introduce discretization errors in applying the free surface boundary conditions:

$$\det(R + O(h^q)) = 0.$$

To avoid a large change in β we expect we need $h \ll \epsilon^{2/q}$

This is seen in numerical experiments - e.g. in the Kreiss-Petterson paper it is observed that for $\epsilon = 0.1$, a wave propagated 20 wavelengths, and second order differences **100PPW are needed to achieve a 5% error!**

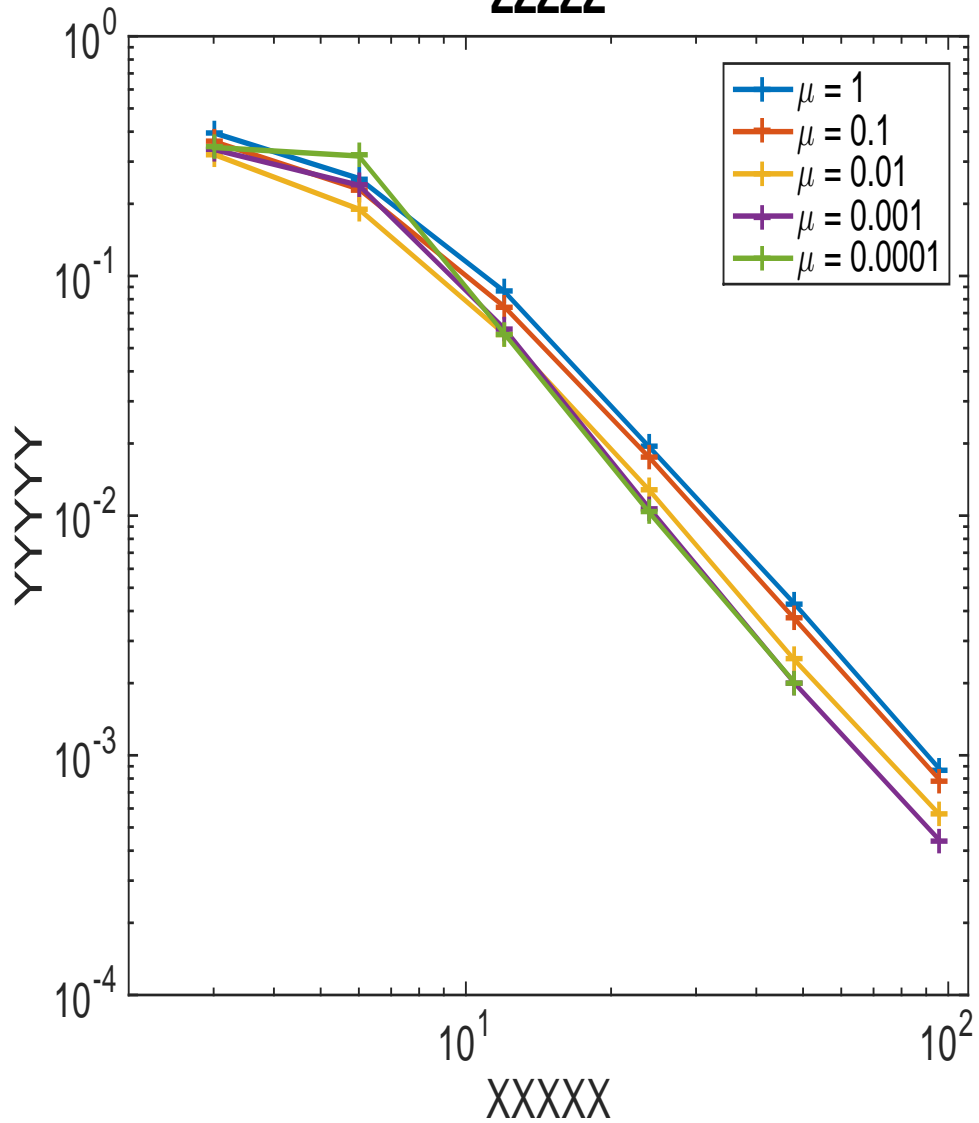
For our Galerkin methods we do not observe this effect. In part this may be explained by the fact that we use higher order, but it appears that more is going on.

Conjecture: the good performance is due to the superconvergence of dispersion errors for Galerkin methods - but we do not yet have a convincing mathematical analysis.

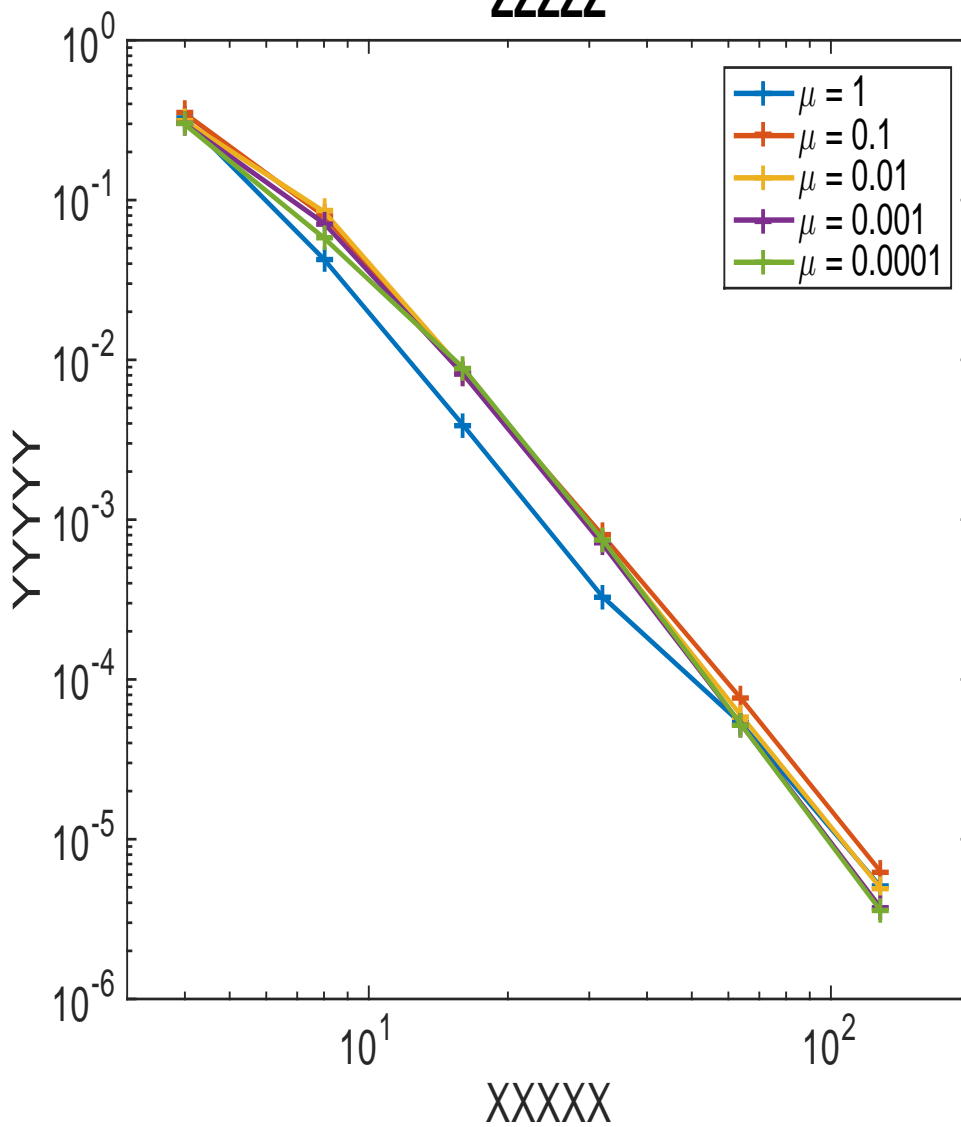
In the following numerical examples we use the new DG formulation with ϵ ranging from 1 to 10^{-2} , $q = 3, 4, 6$, and a propagation distance of 20 wavelengths. (The axes are PPW versus error.)

For the GD schemes we show results for $\epsilon = 1, 0.1$ and q ranging from 2 to 18 and a propagation of about 10 wavelengths. Here we observe superconvergence at double the design accuracy.

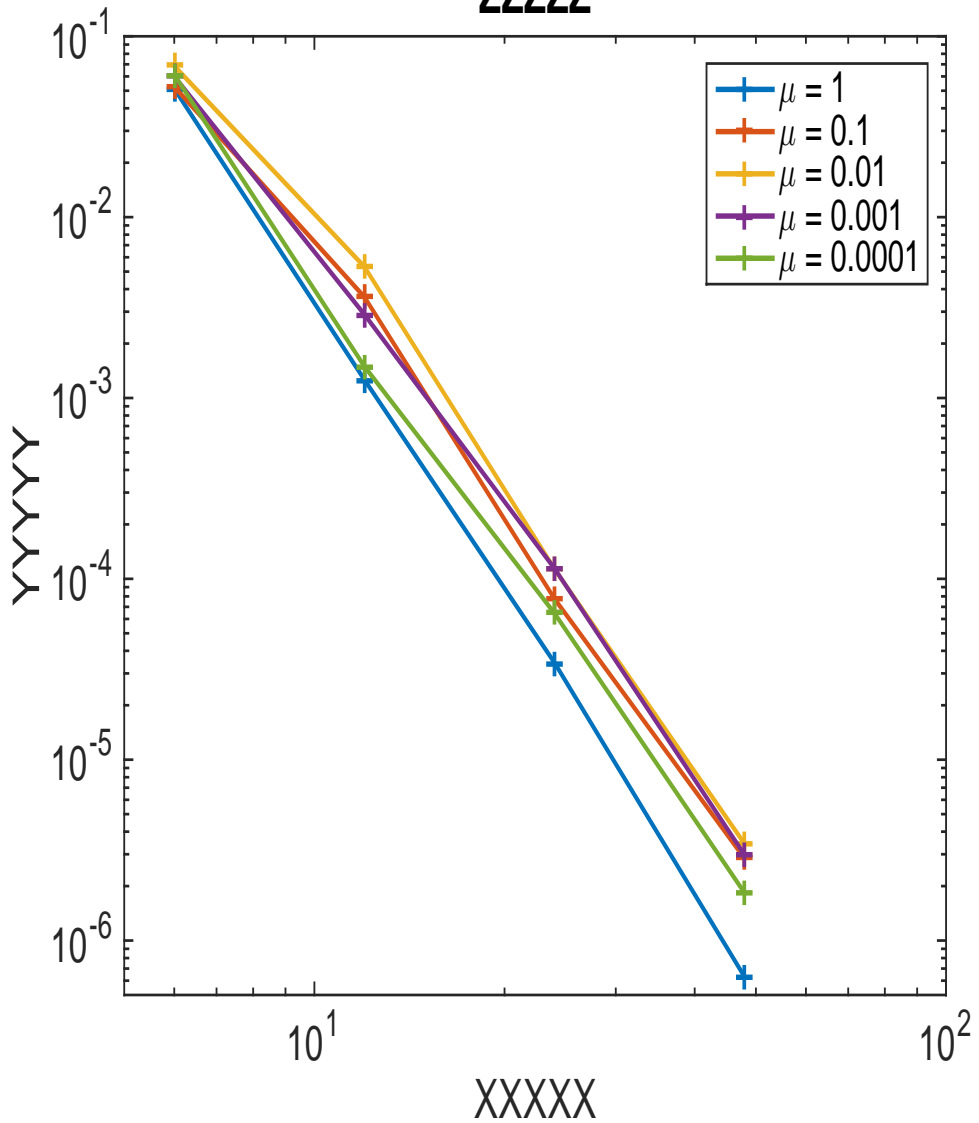
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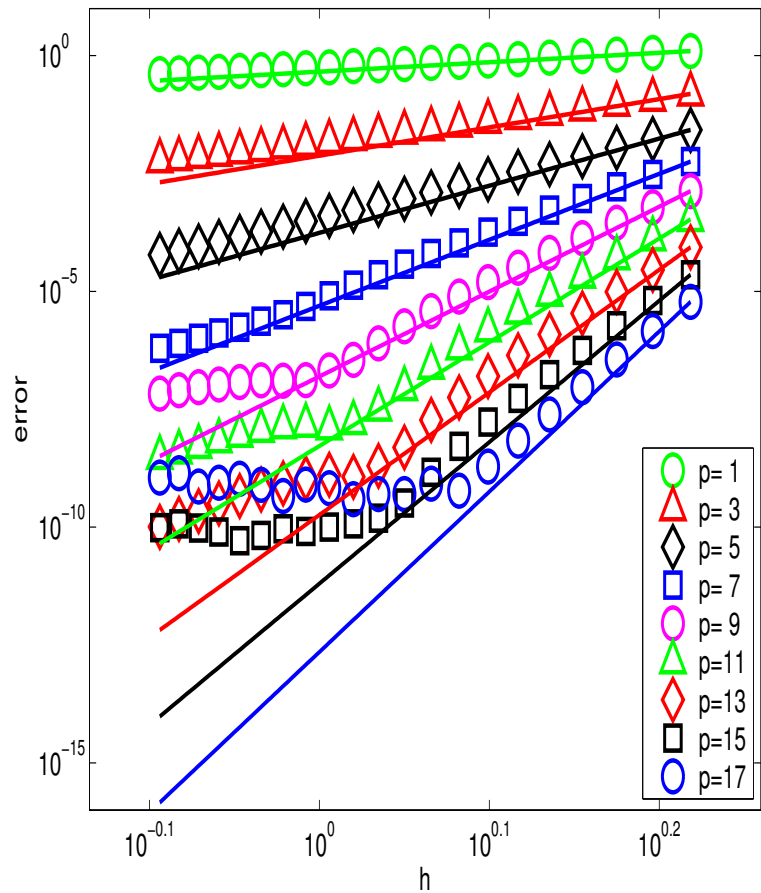
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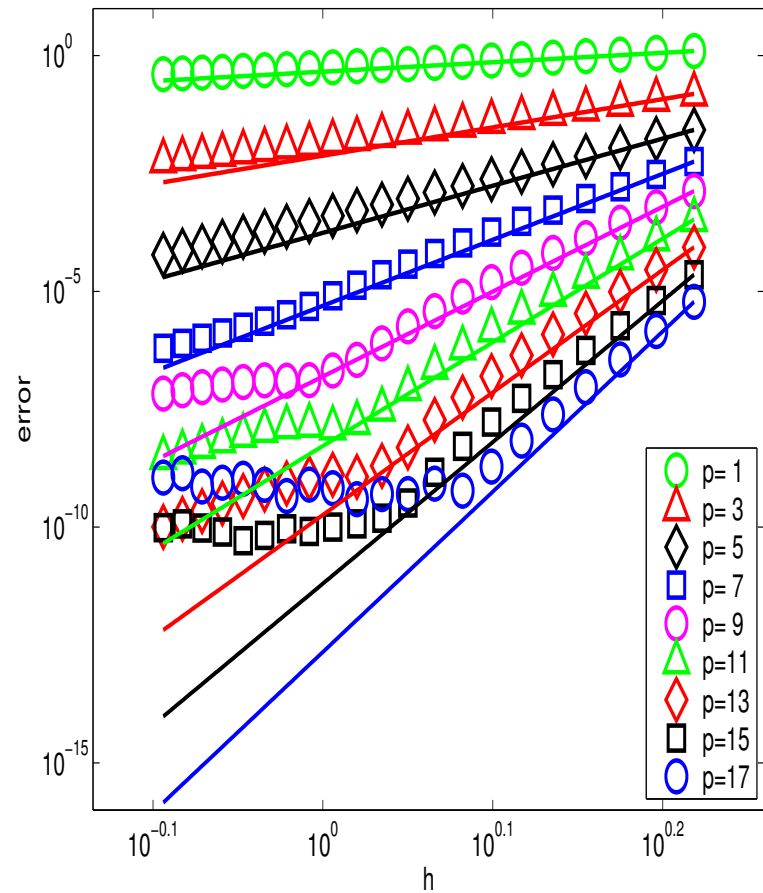
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max norm error in u



max norm error in u



Radiation Boundary Conditions

Since radiation of energy to the far field is a typical feature of wave propagation problems, accurate radiation boundary conditions are a necessary feature of any general-purpose wave solver. Our goal is to produce methods which are:

- Spectrally convergent almost uniformly in time. That is, if P is the number of degrees-of-freedom per boundary point used to apply the approximate radiation condition, ϵ is the error tolerance, T is the simulation time, and δ is a length scale - e.g. the separation of the artificial boundary from scatterers and sources - then

$$P \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{cT}{\delta}.$$

- Geometrically flexible - applicable on a general box.
- Amenable to implementations using standard schemes.
- Automatic - no extensive experimentation needed to determine bc parameters.

We claim that CRBCs are an optimal solution for the wave equation and the Maxwell system. They are similar to the optimal PMLs of Druskin et al (SIAM Rev. 2016) which include optimizations for both propagating and evanescent waves - the difference is that we use T in our optimizations while they use wave speed ranges and evanescent decay ranges. Our implementation is similar to Guddati's optimal midpoint rule rather than Druskin's optimal difference grid, but our derivation is based on differential recursions.

Optimization means for us determining parameters in some assumed form for a rational approximation to the DTN map which minimize some norm of the reflection coefficient for all $\Re s = T^{-1}$, $k \in \mathbb{R}^{n-1}$:

$$\min_{R \in \mathcal{R}} \|\rho(s, k; R)\|_{(T^{-1-i\infty}, T^{-1+i\infty}) \times \mathbb{R}^{n-1}}$$

For acoustics and electromagnetism we can easily characterize the optimal conditions using the Chebyshev equioscillation criterion - we call these Complete Radiation Boundary Conditions (CRBC - H. and Warburton SINUM 2009, H. and Lagrone JCP 2016). Here the form of R is implicitly determined by the recursions, $j = 1, \dots, P$:

$$\begin{aligned} u_0^+ &= u^+ \\ a_j \frac{\partial u_{j-1}}{\partial t} + \frac{\partial u_{j-1}}{\partial x} + \sigma_j u_{j-1} &= \bar{a}_j \frac{\partial u_j}{\partial t} - \frac{\partial u_j}{\partial x} + \bar{\sigma}_j u_j \\ u_p^- &= 0. \end{aligned}$$

In particular we can prove (adapting Newman's argument, Mich. Math. J. 1964) that parameters can be chosen so that to **guarantee an error less than ϵ**

$$P \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{cT}{\delta}.$$

nodes are needed.

The parameters are rapidly computed using the Remez algorithm. A library with various implementations will be available at **www.rbcpack.org** - already contains implementations for second order differences with DG and high order difference implementations coming soon.

For applications to elasticity, using optimal parameters for the scalar wave equation, we can still prove logarithmic error estimates for volume waves, though the parameters may no longer be optimal. (See Baffet, Bielak, Givoli, TH CMAME 2012; Bielak, Givoli, Rabinovich, TH J. Comput. Acoust. 2013; Baffet, Givoli, TH SISC 2014; Rabinovich, Givoli, Bielak, TH AMSES 2015.) For Rayleigh waves, on the other hand, we have no analysis. However the following experiments using optimal parameters for a wave equation with $c = c_S$ show good results.

We expect for more general wave families (Rayleigh, Stoneley, ...) it would be better not to use optimizations tuned to the scalar wave equation but rather those used by Druskin et al (SIAM Rev. 2016) which are tuned to basic parameters such as normal wave speed and evanescent decay rate - we can easily include these in our software but haven't done it yet.

Details of the experiments:

$$\lambda = \rho = 1, \mu = 1, .01.$$

Domain $(-1, 1) \times (0, 5)$.

Boundary forcing: $\sigma_{yy} = 2e^{-40x^2} e^{-(t-14)^4/1000} \sin 2\pi t$ at $y = 5$.

DG discretization with $q = 6$, solve to $T = 50$.

CRBCs at $x = \pm 1$ and Lysmer-Kuhlmeyer (characteristic) bcs at $y = 0$ - we will switch to CRBC on the bottom but didn't implement it yet.

Maximum errors as the boundary condition order increases.

μ	$P = 5$	$P = 9$	$P = 13$
1	2.2(-3)	1.0(-4)	1.1(-5)
.01	4.1(-3)	3.3(-4)	7.8(-5)

However for other problems a phenomenon occurs which causes CRBC and PML difficulties - in particular problems with group velocities and phase velocities mismatched relative to the boundary lead to unstable PMLs and nonconvergent CRBCs.

In elasticity these occur for certain anisotropic media (see, e.g., Bécache, Fauqueux, Joly JCP 2003) and for isotropic waveguides with traction-free conditions (Sketon, Adams, Craster Wave Motion 2007).

There are some ways to get around these problems in special cases - for a single dispersion relation as in dispersive electromagnetic materials one can add convolutions to the CRBC recursions which tune the method to group velocity rather than phase velocity.

For elastic cases under-resolving or thinning PMLs can lead to discrete stability (Duru and G. Kreiss CACP 2012, SISC 2014, Wave Motion 2014), though it is not obvious to me that these are convergent.

Damping layers as approximate radiation boundary conditions - generally one doesn't want to or in some cases one cannot resolve the solution in the layer. Notice that semidiscrete versions take a very similar form to our recursions:

- Fourier-Laplace transform in the tangential direction and time;
- Semidiscretize the layer in the normal direction;

$$L(s, k)[\hat{u}_0, \dots, \hat{u}_N]^T = \hat{u}^+$$

- Solve the resulting algebraic problem to express the relationship between incoming and outgoing variables:

$$\hat{u}_0^- = \hat{u}^- = R(s, k)\hat{u}^+$$

- Optimize the parameters (damping profiles, stretching profiles) by minimizing a norm of the reflection coefficient.

First steps at optimizing a spectral stretching and damping layer - degree N DG discretization of a layer similar to the one proposed by Appelö and Colonius (JCP 2009):

$$H \frac{\partial u}{\partial t} + \eta(z) A \frac{\partial u}{\partial z} + \sum_d B_d \frac{\partial u}{\partial y_d} + (-1)^r \gamma \eta(z) \frac{\partial^r}{\partial z^r} \sigma(z) \frac{\partial^r u}{\partial z^r} = 0$$

$$\eta = 1 - \sigma, \quad \sigma = 1 - (1 - \epsilon) \left(1 - \left(\frac{1 - z}{2} \right)^p \right)^q,$$

with $z \in [-1, 1]$.

Here we choose ϵ small enough that reflections from the end of the layer could not reach the computational domain. We have started a brute force optimization of the parameters p , q , r , γ assuming a bandlimit of 1 (i.e. length scale given by the shortest wavelength of interest, time scale by the highest frequency of interest). The results are a bit disappointing - they present better results using 6th order difference methods with 6th order damping including elastic waveguides.

Results for Bécache et al Medium III (with reverse modes), $\delta = 1$ (minimum wavelengths), $T = 10^3$ (minimum periods), optimization of the average relative energy reflection on a grid in the bandlimited frequency space. The result:

$$p = 3, \quad q = 1 \quad r = 4 \quad \sigma = 10^{-2} \cdot N^{-8}.$$

N	$\bar{\rho}$	ρ_{\max}
0	1.09(-1)	6.48(-1)
16	5.40(-2)	1.64(-1)
20	1.73(-2)	1.34(-1)
24	1.29(-2)	1.15(-1)
28	6.97(-3)	1.07(-1)
32	5.48(-3)	9.92(-1)
36	4.07(-3)	9.43(-1)
40	3.38(-3)	8.92(-2)
44	2.85(-3)	8.49(-2)
48	2.47(-3)	8.10(-2)
52	2.18(-3)	7.72(-2)
56	1.94(-3)	7.37(-2)
60	1.75(-3)	7.03(-2)
64	1.58(-3)	6.70(-2)

Good news: for a difficult case we could guarantee decent accuracy with a fairly thin layer

Bad news: convergence was slow (around second order) and the layer is expensive in comparison with acoustics and electromagnetism.

Other ideas:

Matrix Recursions: Replace the scalar operators in the CRBC recursion with matrices - currently being studied by Lagrone.

Alternative Discretizations of Supergrid: : For example difference methods, Hermite methods

Other Forms of Damping Layers: Unstable PML with stretching as in Duru and Kreiss.

Hardy Space Methods: Halla et al (Num. Math. 2015) show how Hardy space methods in the frequency domain can deal with reverse modes - it is an open question if these methods can be made to work in the time domain.

Direct approximation to R : In the discrete setting one might be able to use automatic rational approximation methods (e.g. rational Krylov methods - see **rktoolbox** by Güttel, guettel.com/rktoolbox).

Nonlocal approximations: For elasticity see, e.g., work by Sofronov et al for VTI models (JCAM 2010).