Complete Radiation Boundary Conditions, Optimal Grids, and Hermite Methods

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A tale of two converging research projects devoted to constructing optimal radiation boundary conditions for time-domain wave problems:

Complete radiation boundary conditions: TH and friends ...

**Optimal PML: VD and friends ...**

The goal is to produce methods which are:

- Spectrally convergent: 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, and η is some measure of the difficulty of the problem

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

- Geometrically flexible - applicable on a general box.

- Amenable to implementations using standard schemes.

- Automatic - no extensive experimentation needed to determine bc parameters.

It is still an open question if one can find approximate radiation boundary conditions with all the desired properties for general hyperbolic systems - in particular all known methods fail to converge when applied to typical systems with reverse modes - waves with group velocity and phase velocity oriented differently with respect to the boundary - e.g. waves in crystals, elastic waveguides, ...

$$x = -\delta \qquad x = 0$$
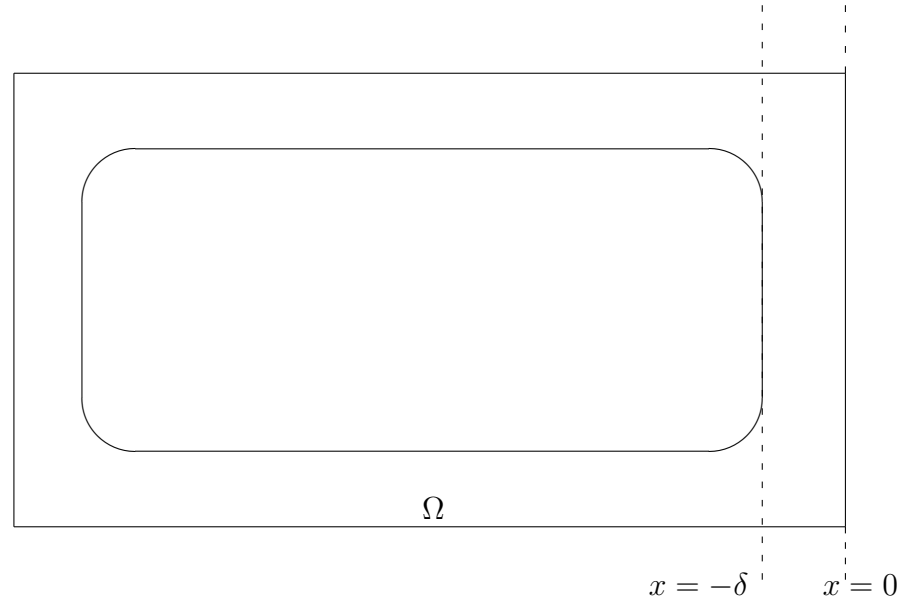
Computational domain, Ω, for a scattering problem with a rectangular artificial boundary.

The simplest case - the scalar wave equation and its first order formulation (in $2 + 1$ dimensions for simplicity):

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$$

or

$$
\begin{aligned}
\frac{\partial u}{\partial t} + c\frac{\partial v}{\partial x} + c\frac{\partial w}{\partial y} &= 0 \\
\frac{\partial v}{\partial t} + c\frac{\partial u}{\partial x} &= 0 \\
\frac{\partial w}{\partial t} + c\frac{\partial u}{\partial y} &= 0
\end{aligned}
$$

Exact boundary condition in a half-space (or waveguide) - use Fourier-Laplace (in $(y - t)$) transformations. Here s is dual to t and k is dual to y. Then we have:

$$\gamma \hat{u} + c\frac{\partial \hat{u}}{\partial x} = 0,$$

$$\gamma = \left(s^2 + k^2\right)^{1/2}.$$

The branch corresponds to outgoing group velocity $(s = i\omega)$ or exponential decay $\Re s > 0$.

We can explicitly invert the transforms to get a representation of the exact condition in integral form:

$$\frac{\partial u}{\partial t} + \mathcal{F}^{-1}\left(k^2(J_1(kt)/t) * (\mathcal{F}u)\right) + c\frac{\partial u}{\partial x} = 0$$

This may look hopelessly expensive due to the space-time integrals, but in fact we (and others) have constructed a fast, low-memory compression of the time integral operator (Alpert, Greengard, H. (SINUM 2000, JCP 2002), Lubich and Schädle, (SISC 2002), Hiptmair and Schädle, (Computing 2003)). Thus the complexity of applying the exact condition is:

$$O\left(\ln\frac{1}{\epsilon} \cdot \ln\frac{cT}{\lambda}\right)$$

The problem is that the construction of the nonlocal conditions breaks down if there are corners - restricted to waveguides and spheres. (For spheres we have the added difficulty of computing spherical harmonic transforms.)

Geometrically flexible approaches are based on approximating the time convolutions by something which can be evaluated using local operators.
This corresponds to rational approximations to γ.

$$\gamma \approx R(s,k)$$

Two problems:

How do we determine optimal (in some sense) rational approximants R and how fast do they converge?

How do we practically implement approximate conditions based on R?

The early 2000's - methods for implementing arbitrary-order approximants R tuned to propagating modes:

$$\gamma = \cos\theta s, \quad 0 \le \theta < \frac{\pi}{2}$$

Then an optimal R would interpolate γ for some angles $a_j = \cos\theta_j$.

H. and Warburton construction (Wave Motion 2003):

$$\prod_{j=1}^{P} \frac{a_{2j-1}s + c\frac{\partial}{\partial x}}{a_{2j}s - c\frac{\partial}{\partial x}} u = 0$$

This produces an interpolant as it is exact for propagating modes with angles corresponding to a_j. Practical implementation involves auxiliary variables:

$$u = u_0$$

$$a_{2j-1}\frac{\partial u_{j-1}}{\partial t} - \frac{\partial v_{j-1}}{\partial t} = a_{2j}\frac{\partial u_j}{\partial t} + \frac{\partial v_j}{\partial t}$$

$$a_{2j-1}\frac{\partial v_{j-1}}{\partial t} - \frac{\partial u_{j-1}}{\partial t} - c\frac{\partial w_{j-1}}{\partial y} = a_{2j}\frac{\partial v_j}{\partial t} + \frac{\partial u_j}{\partial t} + c\frac{\partial w_j}{\partial y}$$

$$\frac{\partial w_j}{\partial t} + c\frac{\partial u_j}{\partial y} = 0.$$

with termination - e.g.

$$u_P - v_P = 0.$$

Asvadurov, Druskin, Guddati, Knizherman (SINUM 2003) - optimal PML:

Based on their theory of optimal grids they note that rational functions written as Stieltjes fractions are the discrete impedance functions of a standard three point difference method with grid spacings $h_j s$, $\hat{h}_j s$.

$$\frac{\partial u_j}{\partial t} + \frac{1}{\hat{h}_j}\left(\frac{\partial v_{j+1/2}}{\partial t} - \frac{\partial v_{j-1/2}}{\partial t}\right) + c\frac{\partial w_j}{\partial y} = 0$$

$$\frac{\partial v_{j+1/2}}{\partial t} + \frac{1}{h_j}\left(\frac{\partial u_{j+1}}{\partial t} - \frac{\partial u_j}{\partial t}\right) = 0$$

$$\frac{\partial w_j}{\partial t} + c\frac{\partial u_j}{\partial y} = 0.$$

with termination

$$u_P = 0.$$

How are these related? Reinterpret HW auxiliary functions as grid functions.

VD and friends : u_j and v_j located on staggered grids with

$$\frac{\partial v_j}{\partial x} \approx \frac{1}{\hat{h}_j} \left(\frac{\partial v_{j+1/2}}{\partial t} - \frac{\partial v_{j-1/2}}{\partial t} \right)$$

$$\frac{\partial u_{j+1/2}}{\partial x} \approx \frac{1}{h_j} \left(\frac{\partial u_{j+1}}{\partial t} - \frac{\partial u_j}{\partial t} \right)$$

TH and friends u_j and v_j collocated and derivatives approximated like a box scheme:

$$\frac{\partial u_{j+1}}{\partial x} + \frac{\partial u_j}{\partial x} \approx a_{2j} \frac{\partial u_{j+1}}{\partial t} - a_{2j-1} \frac{\partial u_j}{\partial t}.$$

If we take $a_{2j-1} = a_j$ we have a grid spacing $h_j = \frac{1}{a_{2j}s}$ - equivalent to the optimal midpoint rule of Guddati and Lin (IJNME 2006)!

What about the parameters? Old approach (70's) would be Padé approximation (Engquist and Majda) - optimized for near-normal incidence. To optimize over a range of angles Druskin et al note that one can use:

For a fixed range of angles $\theta \in [0, \theta_{\max}]$ the maximum reflection coefficient is minimized using Zolotarev approximations - then for $\eta = 1/\cos\theta_{\max}$ we need

$$P \propto \ln\frac{1}{\epsilon} \cdot \ln\eta,$$

as desired.

For an arbitrary range one can use Newman's approximations which lead to

$$P \propto \left(\ln\frac{1}{\epsilon}\right)^2$$

These can be implemented using either method. **Alas, our experiments and analysis showed they didn't always work as hoped particularly for long times, T!**

Analysis: first carried out for Padé approximants - (TH Acta Numerica 1999 in the frequency domain and Diaz-Joly SIAP 2005 for exact time-domain solutions) - show that $P \propto T$ are needed.

Experiments: de Castro's thesis (UNM 2006) - Newman nodes were even a little worse as $T \to \infty$. (See TH, de Castro, Givoli, Tzemach JCA 2006.) We'll see some pictures from the paper (unfortunately I've lost the ps files).

What's wrong? **We can't ignore the evanescent spectrum! - We need new optimal nodes that treat both propagating and evanescent waves.**

The CRBC approach (TH and Warburton SINUM 2009) - develop approximations along the Laplace inversion contour

$$\Re s = \frac{1}{T}$$

where T is a time scale over which we want to guarantee accuracy - for example the simulation time and also introduce a length scale, δ, which is the minimal separation between sources and the radiation boundary.

We first derive a convenient representation for γ via some elementary computations.

$$\gamma = \cos \phi \cdot s + \frac{1}{cT} \cdot \frac{\sin^2 \phi}{\cos \phi}$$

with $|\phi| < \frac{\pi}{2}$ everywhere on the inversion contour!

The angle variable ϕ is **not** a plane wave propagation angle. This formula for the square root gives a **complete representation** of the wave field in a half space. Outgoing plane waves by contrast are an incomplete representation - the contribution of evanescent modes is also needed. (See, e.g., Heyman, J. Math. Phys., 1996.) The poor long time accuracy of standard radiation boundary conditions and PMLs is due to their lack of accuracy for evanescent modes.

We interpolate at an optimal set of nodes, ϕ_j. We will prove that interpolation nodes can be chosen so that to guarantee an error less than ϵ up to time T

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

nodes are needed.

The estimate is proven using estimates of the complex reflection coefficient adapting Newman's famous construction of exponentially convergent rational approximations to $|x|$ (Mich. Math. J. 1964) combined with Parseval's relation.

Directly we show that the claimed estimate holds for approximations of the form:

$$\cos \phi_j = \left(2 \frac{\delta}{cT \ln \frac{1}{\epsilon}} \right)^{j/(2P)}, \quad j = 0, \dots, 2P - 1.$$

Idea: The absolute value of the complex reflection coefficient is given by:

$$|R| = e^{-\frac{2\zeta}{\cos \phi}} \prod_{j=0}^{q} \frac{(\cos \phi - \cos \phi_j)^2}{(\cos \phi + \cos \phi_j)^2},$$

where $\zeta = \frac{\delta}{cT}$. Given a tolerance ϵ we need only choose the interpolation nodes ϕ_j to make the product small for

$$\cos \phi > 2\zeta \cdot \frac{1}{\ln \frac{1}{\epsilon}}.$$

For $\cos \phi_j = a^j$, $\cos \phi \in (a^{r+1}, a^r)$, $a = \left(\frac{2\zeta}{\ln \frac{1}{\epsilon}}\right)^{1/P}$ we have:

$$
\begin{aligned}
|\mathcal{K}| &\leq \prod_{j=0}^{r} \left(\frac{a^j - a^{r+1}}{a^j + a^{r+1}}\right)^2 \cdot \prod_{j=r+1}^{P} \left(\frac{a^j - a^r}{a^j + a^r}\right)^2 \\
&\leq \prod_{j=1}^{P+1} \left(\frac{1 - a^j}{1 + a^j}\right)^2 \leq \prod_{j=1}^{P+1} e^{-4a^j} = e^{-4a\frac{1-a^{P+1}}{1-a}}.
\end{aligned}
$$

The tolerance is met if $a = 1 - O(\ln^{-1} \frac{1}{\epsilon})$ leading to the estimate of P. In practice we can use the Remez algorithm to compute optimal nodes. We emphasize that the reflection coefficient in this case directly leads to an error estimate, in contrast with the reflection coefficient for propagating plane waves which is often shown in the literature.

Convergence of the Complete Radiation Boundary Conditions
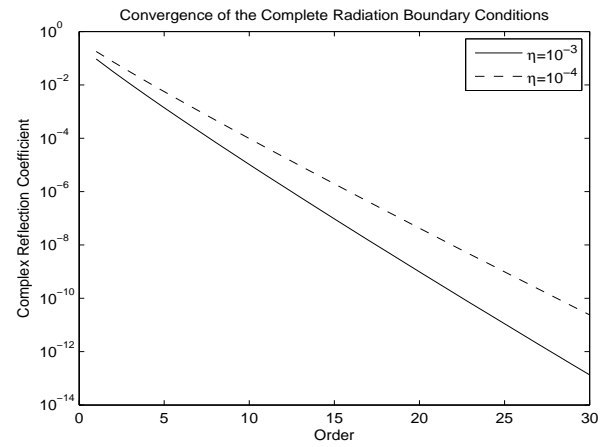
The implementation using our recursions (or equivalently the midpoint rule for the grid interpretation) simply adds lower order terms to the formulas:

$$a_{2j-1}\frac{\partial u_{j-1}}{\partial t} + \sigma_{2j-1}u_{j-1} - \frac{\partial v_{j-1}}{\partial t} =$$

$$a_{2j}\frac{\partial u_j}{\partial t} + \sigma_{2j}u_j + \frac{\partial v_j}{\partial t}$$

$$a_{2j-1}\frac{\partial v_{j-1}}{\partial t} + \sigma_{2j-1}v_{j-1} - \frac{\partial u_{j-1}}{\partial t} - c\frac{\partial w_{j-1}}{\partial y} =$$

$$a_{2j}\frac{\partial v_j}{\partial t} + \sigma_{2j}v_j + \frac{\partial u_j}{\partial t} + c\frac{\partial w_j}{\partial y}$$

$$\frac{\partial w_j}{\partial t} + c\frac{\partial u_j}{\partial y} = 0.$$

Presumably they can also be implemented using VD's formulas but I haven't worked out the details.
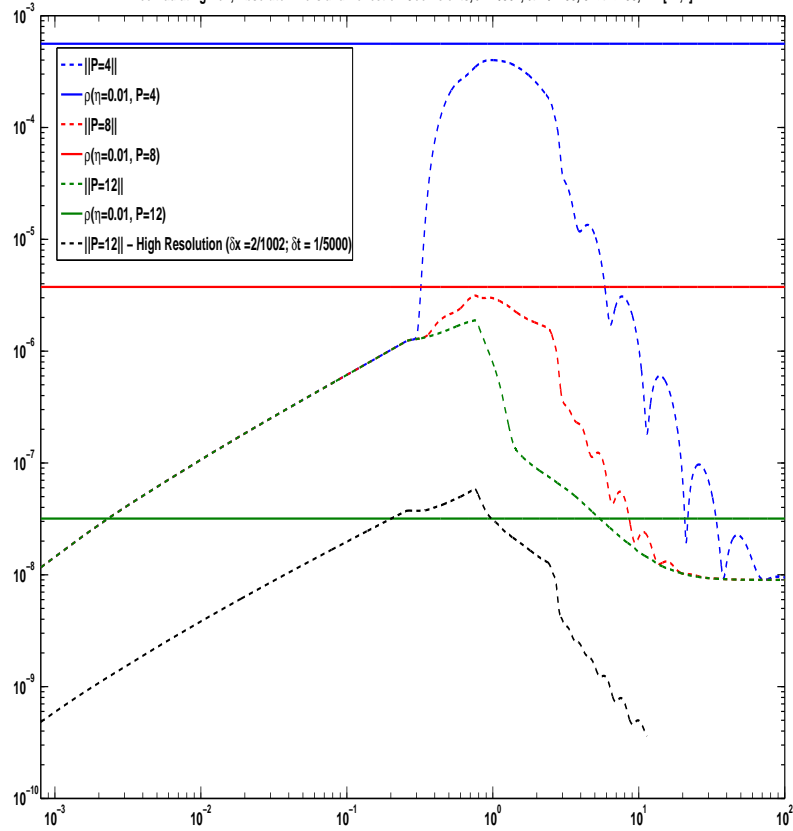
Numerical examples illustrating the accuracy obtained when the new approximations are included:
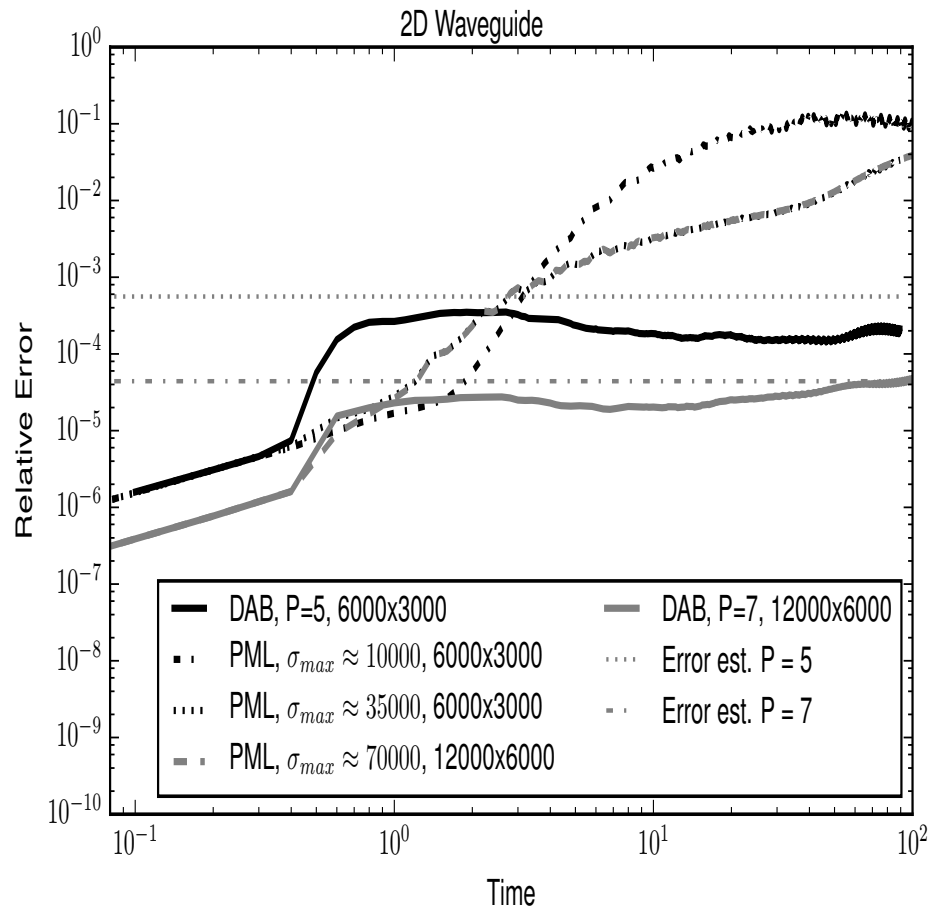
- Acoustics in free space with a Gaussian point source (due to Kurt Stein) - The CRBCs were imposed at $x = \pm 1$, $y = \pm 1$, and $z = \pm 1$. The solution is computed using grid-stabilized 8th order spatial differencing (H. and Hagstrom, JCP 2007, JCP 2012).

- Maxwell's equations with a point source in a waveguide (2d and 3d) using the **rbcpack** implementation of DAB for the Yee scheme (due to John Lagrone, JCP 2016). Here we also see the long time loss of accuracy of PML.
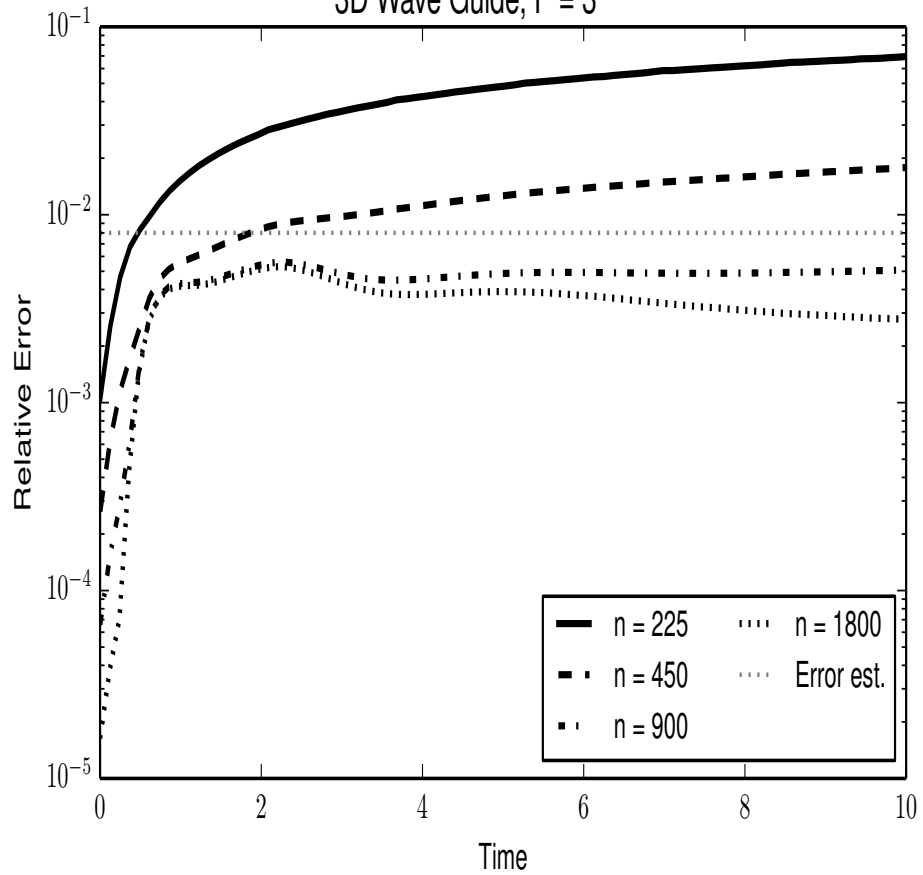
rbcpack will contain implementations for:

- The Yee scheme (a finite difference scheme which is a workhorse in the EM community)

- DG schemes

- Central difference schemes

Free Radiating Box, Absolute Errors and Reflection Coefficients, $\delta x=2/502, \delta t=1/1250, 0 < t < 100, x \in [-1,1]^3$

2D Waveguide

Legend:
- DAB, P=5, 6000x3000
- PML, $\sigma_{max} \approx 10000$, 6000x3000
- PML, $\sigma_{max} \approx 35000$, 6000x3000
- PML, $\sigma_{max} \approx 70000$, 12000x6000
- DAB, P=7, 12000x6000
- Error est. P = 5
- Error est. P = 7

Axis labels: Time (horizontal), Relative Error (vertical)

3D Wave Guide, P = 3

What about optimizations constructed without reference to a time scale? The one almost joint paper of TH, VD and Guddati. One can combine Newman/Zolotarev approximations in the propagating and evanescent regimes. **For the optimal grid approach this simply means that some of the grid spacings are imaginary (proportional to s) and some are real.**

What is proven in the unpublished manuscript is that the optimal estimates still hold in the frequency domain - adding real parameters doesn't mess up the propagating mode reflection coefficients and vice versa.

With Kim (Numer. Math. in review) we have used these Newman approximations for the Helmholtz equation and extended the analysis to include corner conditions.

We also have tried the approach in the time domain although we haven't produced time-domain error estimates we have produced numerical estimates - see TH and Lau CICP J. Comput. Math. 2007.

$$P \propto \ln \frac{1}{\epsilon} \cdot \ln \frac{cT}{\lambda_{\mathrm{min}}}.$$

Leap-frog Hermite methods for the scalar wave equation - use a staggered grid - the approximations $u(x, t_n)$ and $u(x, t_{n+1/2})$ are **piecewise tensor-product Hermite interpolants** on staggered grids. Now the evolution is given by:

$$
\begin{aligned}
u(\mathbf{x}, t_{n+1}) &= \mathcal{IS}u(\mathbf{x}, t_{n+1/2}) - u(\mathbf{x}, t_n) \\
v(\mathbf{x}, t_{n+3/2}) &= \mathcal{IS}u(\mathbf{x}, t_{n+1}) - u(\mathbf{x}, t_{n+1/2})
\end{aligned}
$$

where $\mathcal{S}$ is the **exact** leap-frog evolution operator - in Fourier space

$$
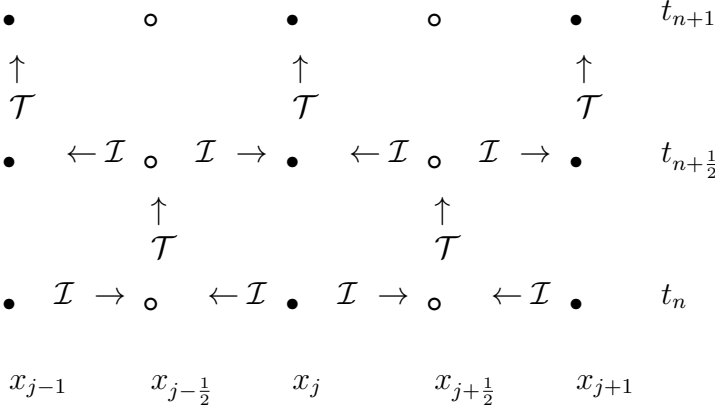\hat{\mathcal{S}} = \hat{\mathcal{S}}_+ + \hat{\mathcal{S}}_- \equiv e^{i|k|\Delta t/2} + e^{-i|k|\Delta t/2}
$$

and $\mathcal{I}$ is the Hermite interpolation operator: **operator which constructs an interpolant of tensor product degree $2m + 1$ using tensor product degree m polynomial data at the cell vertices**.
In 3 dimensions on the cell $[x_1, x_2] \times [y_1, y_2] \times [z_1, z_2]$ construct a tensor product polynomial of degree $2m + 1$ in each coordinate (total degree $6m + 3$) satisfying (now with multi-index notation):

$$
D^\alpha P(x_j, y_k, z_l) = f_{j,k,l,\alpha}, \quad 0 \le \alpha_i \le m.
$$

How can we evaluate $\mathcal{S}$? So long as the physical CFL condition is satisfied - that is so long as waves can't propagate from the cell edges to the cell center in a half time step - $\mathcal{S}v$ **at the cell center** is a polynomial in space-time. Since we only use the nodal data when we compute $\mathcal{IS}v$ that's all we need!

Schematic description of the numerical process for a full time step. Solid circles represent the base mesh and open circles represent the dual mesh. $\mathcal{I}$ is the Hermite interpolation operator and $\mathcal{T}$ is the time evolution operator.

$$
\begin{array}{ccccccccc}
\bullet & & \circ & & \bullet & & \circ & & \bullet & t_{n+1} \\
\uparrow & & & & \uparrow & & & & \uparrow & \\
\mathcal{T} & & & & \mathcal{T} & & & & \mathcal{T} & \\
\bullet & \leftarrow\mathcal{I} \;\; \circ \;\; \mathcal{I}\rightarrow & \bullet & \leftarrow\mathcal{I} \;\; \circ \;\; \mathcal{I}\rightarrow & \bullet & t_{n+\frac{1}{2}} \\
& \uparrow & & & \uparrow & \\
& \mathcal{T} & & & \mathcal{T} & \\
\bullet & \mathcal{I}\rightarrow \;\; \circ \;\; \leftarrow\mathcal{I} & \bullet & \mathcal{I}\rightarrow \;\; \circ \;\; \leftarrow\mathcal{I} & \bullet & t_n \\
\\
x_{j-1} & x_{j-\frac{1}{2}} & x_j & x_{j+\frac{1}{2}} & x_{j+1}
\end{array}
$$

Stability and convergence - we combine energy conservation for the continuous problem with the projection property of Hermite interpolation.

$$\langle f, g \rangle_{m+1} = \int_{x_0}^{x_{N_1}} \int_{y_0}^{y_{N_2}} \int_{z_0}^{z_{N_3}} \frac{\partial^{3m+3} f}{\partial x^{m+1} \partial y^{m+1} \partial z^{m+1}} \frac{\partial^{3m+3} g}{\partial x^{m+1} \partial y^{m+1} \partial z^{m+1}}$$

Proof: integration by parts on each interval/cell.

Theorem: If $\Delta t < h/c$ and the solution of the wave equation is sufficiently smooth then the approximate solution produced by the leap-frog Hermite method converges at order $2m$.

Note: a similar result can be proven for Maxwell's equations and a staggered Hermite discretization:

$$
\begin{aligned}
E(\mathbf{x}, t_{n+1}) &= \mathcal{IM} H(\mathbf{x}, t_{n+1/2}) + E(\mathbf{x}, t_n) \\
H(\mathbf{x}, t_{n+3/2}) &= -\mathcal{IM} E(\mathbf{x}, t_{n+1}) + H(\mathbf{x}, t_{n+1/2})
\end{aligned}
$$

Continuous energy for leap-frog:

Define for u a solution of the scalar wave equation:

$$U_\pm(\mathbf{x}, t) = u(\mathbf{x}, t) - \mathcal{S}_\pm u(\mathbf{x}, t - \Delta t/2)$$

Then

$$U_\pm(\mathbf{x}, t + \Delta t/2) = \mathcal{S}_\mp U_\pm(\mathbf{x}, t)$$

Recalling that $\hat{\mathcal{S}}_\pm = e^{\pm i |k| \Delta t/2}$ we see that all L^2-based Sobolev norms of $U_\pm$ are conserved.

For the approximate solution u we obtain a similar result in the seminorm for which $\mathcal{I}$ is a projection:

$$V_\pm(\mathbf{x}, t_{n+1}) = \mathcal{I} \mathcal{S}_\mp V_\pm(\mathbf{x}, t_{n+1/2}) + (\mathcal{I} - 1) \mathcal{S}_\pm V_\mp(\mathbf{x}, t_{n+1/2})$$

which implies

$$|V_+(\cdot, t_{n+1})|^2_{m+1} + |V_-(\cdot, t_{n+1})|^2_{m+1} = \left| V_+(\cdot, t_{n+1/2}) \right|^2_{m+1} + \left| V_-(\cdot, t_{n+1/2}) \right|^2_{m+1}$$

Proof outline:

1. Use the energy equalities to estimate the seminorm of the errors, $E_\pm = U_\pm - V_\pm$.

$$|E_\pm(\cdot, t)|_{m+1} = O(h^{m+1})$$

2. Use the energy estimate to prove convergence of the conserved quantities in L^2 -

$$\|E_\pm(\cdot, t_{n+1})\| \le \|E_\pm(\cdot, t_{n+1/2})\| + O(h^{m+1}) \cdot \left(\left| E_+(\cdot, t_{n+1/2}) \right|_{m+1} + \left| E_-(\cdot, t_{n+1/2}) \right|_{m+1} \right)$$
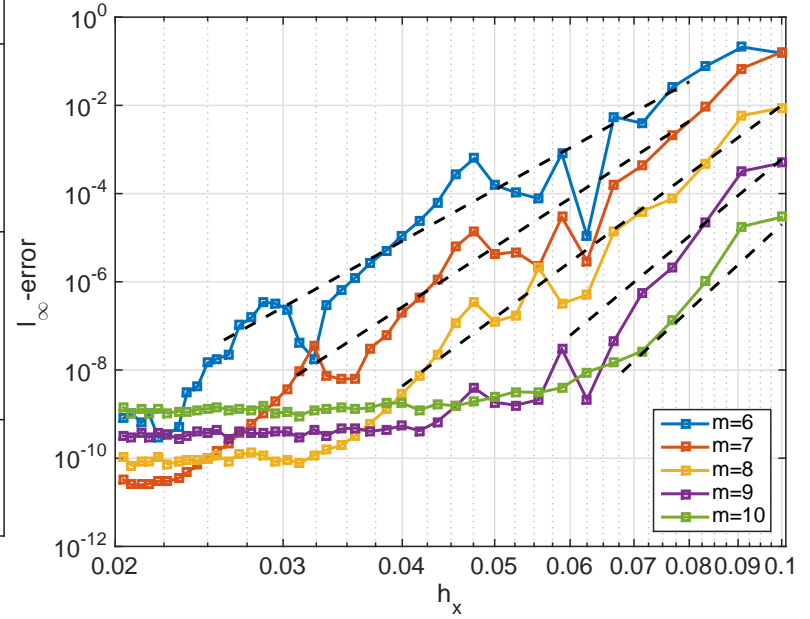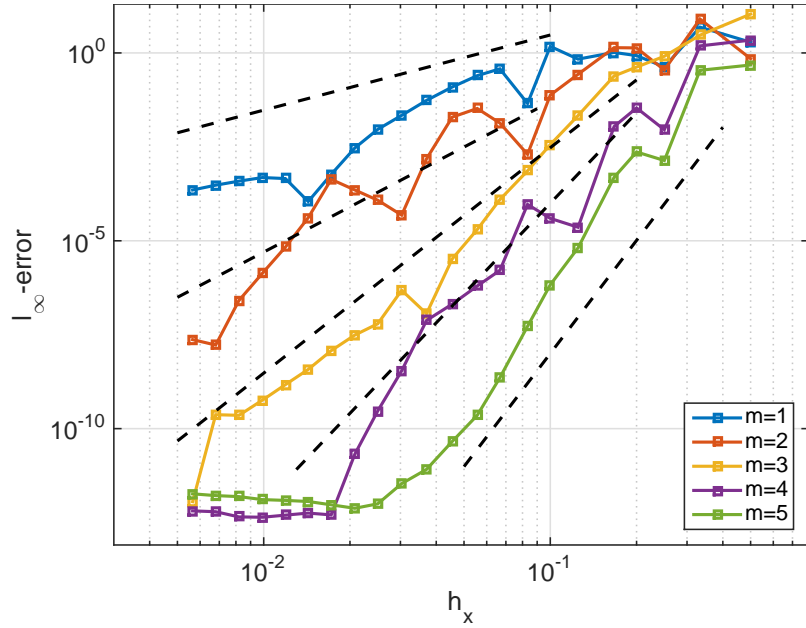
so that $\|E_\pm(\cdot, t_{n+1})\| = O(h^{2m+1})$.

3. Finally estimate the error itself:

$$\|e(\cdot, t_{n+1})\| \le \|e(\cdot, t_{n+1/2})\| + \|E_\pm(\cdot, t_{n+1})\|$$

which yields the final result.

A simple numerical experiment - evolve $\sin(\kappa\pi x) \cdot \sin(\kappa\pi y) \cdot \sin(\sqrt{2}\kappa\pi t)$ on the unit square. $\kappa = 8$ for $m = 1, \ldots, 5$ and $\kappa = 32$ for $m = 6, \ldots, 10$. The straight lines correspond to the theoretical convergence rate $2m$.

One unique feature of Hermite schemes is that the time stepping is **purely local to each cell**. At high order we can take large steps without needing any intercell communication. Thus Hermite methods are good candidates for efficient implementation on many-core platforms such as gpus.

First experiments with an implementation of conservative Hermite methods on NVIDIA P100 gpus - comparison with a 36-core Broadwell CPU. Codes are written in OCCA (www.libocca.org) so that the target device (e.g. CPU using OpenMP or gpu using CUDA) can be determined at runtime. Here the grid sizes are 280^3, 190^3 and 140^3 respectively.

m	1	2	3
GPU: Bandwidth (GB/s)	146	106	82
GPU: GFLOPS	1175	1259	1410
GPU: Time/step	.035	.052	.058
CPU: Time/step	.69	1.02	1.12

HAPPY BIRTHDAY VLADIMIR!