High-order upwind methods for second-order wave equations on curvilinear and overlapping grids

Jeff Banks

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Collaborators

Bill Henshaw
Department of Mathematical Sciences
Rensselaer Polytechnic Institute

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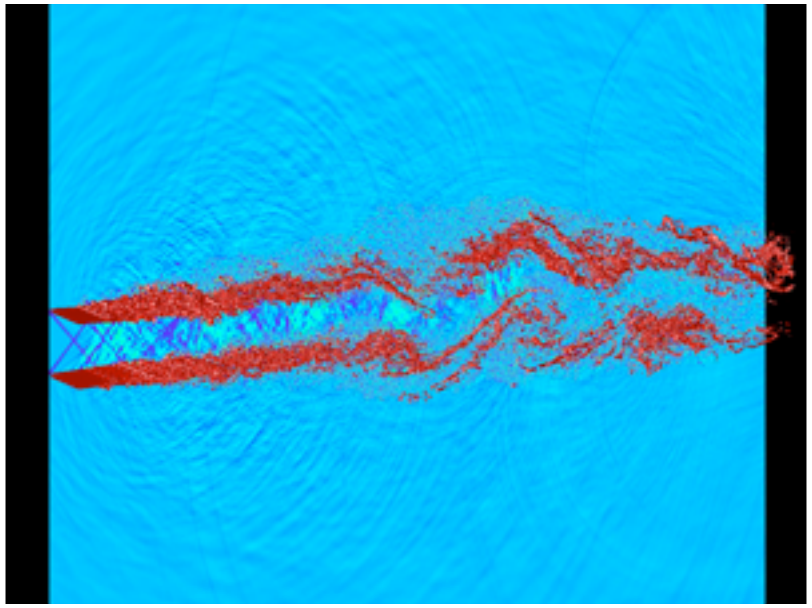
Second-order wave equations are common in many fields of science and engineering

- scalar wave propagation
  - e.g. acoustics

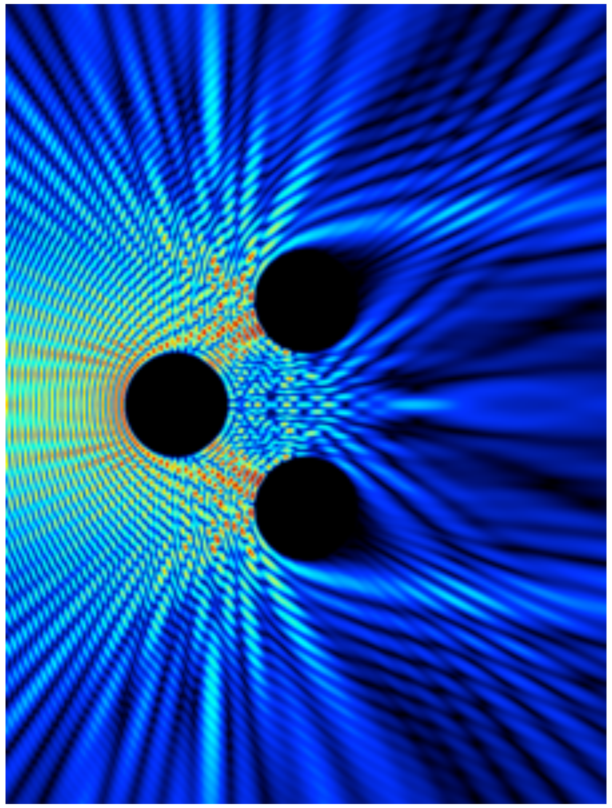
$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u$$



- systems of simple wave equations
  - e.g. electromagnetics

$$\frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{1}{\mu\epsilon}\nabla^2 \mathbf{E}$$

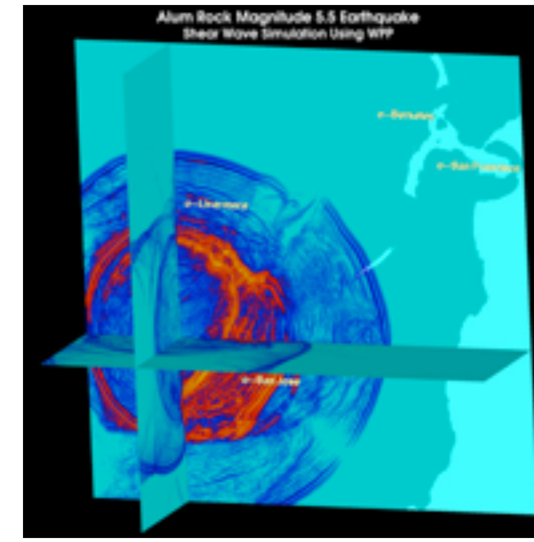
$$\frac{\partial^2 \mathbf{B}}{\partial t^2} = \frac{1}{\mu\epsilon}\nabla^2 \mathbf{B}$$



Second-order wave equations are common in many fields of science and engineering

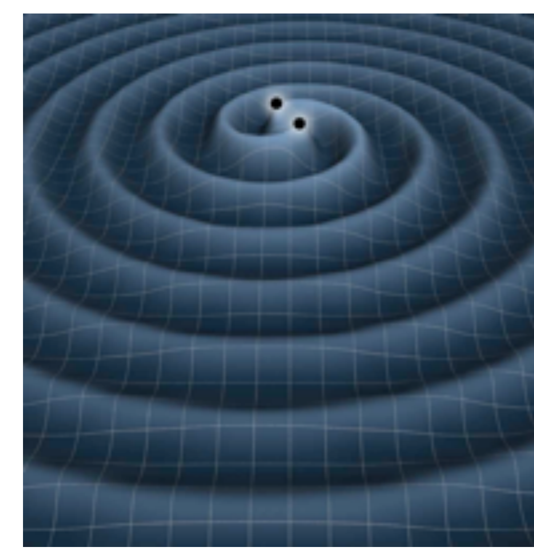
- elastic wave equation
  - e.g. seismic waves

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = (\lambda + 2\mu)\nabla(\nabla \cdot \mathbf{u}) - \mu \nabla \times (\nabla \times \mathbf{u})$$



- Einstein field equations
  - e.g. gravity waves

$$\left(-\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) \begin{pmatrix} \gamma^{tt} & \gamma^{tx} & \gamma^{ty} & \gamma^{tz} \\ \gamma^{tx} & \gamma^{xx} & \gamma^{xy} & \gamma^{xz} \\ \gamma^{ty} & \gamma^{xy} & \gamma^{yy} & \gamma^{yz} \\ \gamma^{tz} & \gamma^{xz} & \gamma^{yz} & \gamma^{zz} \end{pmatrix} = F$$



For many problems numerical dissipation mechanisms are needed, and the current state of the art for the SOS is unsatisfactory

- Stability against small perturbations
  - low order terms in the mathematical model
  - interpolation from overlapping grids
  - nonlinearity

- Discontinuities
  - discontinuous material coefficients
  - source terms with abrupt changes
  - discontinuous exact solutions

- For second-order systems, the current state of the art is ad hoc addition of numerical dissipation
  - coefficients chosen experimentally or with “expert judgement”
  - see e.g. Henshaw 2006, Hagstrom and Hagstrom 2012

- One alternative is to transform to first-order form and use “upwind methods”

Upwind methods for first-order hyperbolic systems are powerful tools that have seen extensive use and development

- CIR characteristic scheme (Courant, Isaacson and Rees 1952)

- Godunov explicitly incorporated upwinding (Godunov 1959)

- The key idea is the local incorporation of an exact solution
  - the effect is to introduce artificial viscosity (Christensen 1990)

- Since then the technique has grown
  - flux-corrected transport (Boris and Book 1983)
  - piecewise parabolic method (Colella and Woodward1984)
  - high-resolution Godunov (vanLeer 1989, Kolgan 2010)
  - discontinuous Galerkin (Cockburn and Shu 1989)
  - essentially nonoscillatory (Harten 1983)
  - weighted essentially nonoscillatory (Jiang et. al. 1996)

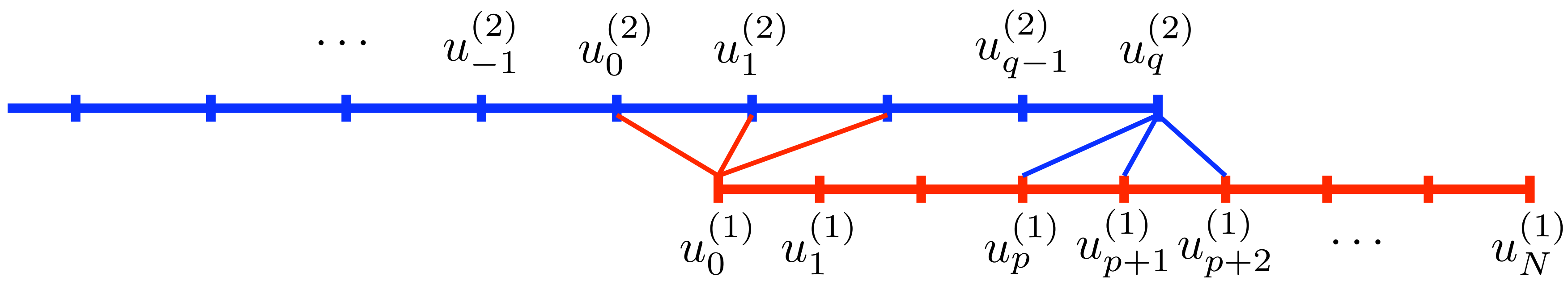
- Despite the vast literature on upwind methods, there appeared to be no attempt to generalize to wave equations in second-order form

There are many good reasons to consider second-order wave equations directly rather than simply converting to first-order form

- Converting from second- to first-order form generally increases the system size
  - from ~3 to ~6 for Maxwell's equations (Henshaw 2006)
  - from ~3 to ~10 for Elasticity (Appelo et. al. 2012)
- Converting to first-order form introduces constraint equations (e.g. St. Venant)
  - constraints are challenging in the context of discretization (Kreiss et. al. 2007)
- The Laplacian is naturally self-adjoint
  - leads to naturally compact discretizations
- Many systems occur naturally in second-order form (e.g. acoustics, elasticity, EFE)

In this talk we are primarily concerned with stability of wave equations on overlapping grids which has historically been challenging

- Consider the second order wave equation on a semi-infinite domain $x \in (-\infty, b]$
- Discretize on an overlapping grid using second order centered differences



- Define stability to mean that the solution remains uniformly bounded in time
- Normal mode theory leads to the following eigenvalue problem

$$
\begin{aligned}
&(sh_1)^2\tilde{u}^{(1)}_j = \tilde{u}^{(1)}_{j+1} - 2\tilde{u}^{(1)}_j + \tilde{u}^{(1)}_{j-1}, \quad j = 1, 2, \ldots, N-1, \\
&(sh_2)^2\tilde{u}^{(2)}_j = \tilde{u}^{(2)}_{j+1} - 2\tilde{u}^{(2)}_j + \tilde{u}^{(2)}_{j-1}, \quad j = \ldots, q-2, q-1, \\
&\tilde{u}^{(1)}_N = 0, \quad |\tilde{u}^{(2)}_j| < \infty, \\
&\tilde{u}^{(1)}_0 = \sum_{k=0}^{r} a_k \tilde{u}^{(2)}_k, \qquad \tilde{u}^{(2)}_q = \sum_{k=0}^{r} b_k \tilde{u}^{(1)}_{p+k}.
\end{aligned}
$$

Wave equation stability on overlapping grids

- Normal mode theory for the second order system says
  - Solutions to the eigenvalue problem grow as e^{st}
  - If $Re(s) > 0$, then by our definition the discretization is unstable
  - Assume a solution with parameters $(s, h_1, h_2, r, \alpha, \beta, N)$
    - Then there is a second solution with parameters $(s\gamma, h_1/\gamma, h_2/\gamma, r, \alpha, \beta, N)$
  - It is possible to find solutions numerically ... e.g.

$$h_1 = 1, \quad h_2 \approx 1.4445, \quad r = 2, \quad \alpha \approx 1.4408, \quad \beta \approx 1.2527, \quad p = 1, \quad q = 3, \quad N = 7$$

- Therefore the artificial dissipation parameter must grow with the mesh ... i.e.

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} - \frac{a_d}{h}\Big(-h^2\frac{\partial^2}{\partial x^2}\Big)^{/2}\frac{\partial u}{\partial t},$$

- A similar analysis is done for the FOS
  - The upwind dissipation has the correct form and naturally stabilizes the scheme

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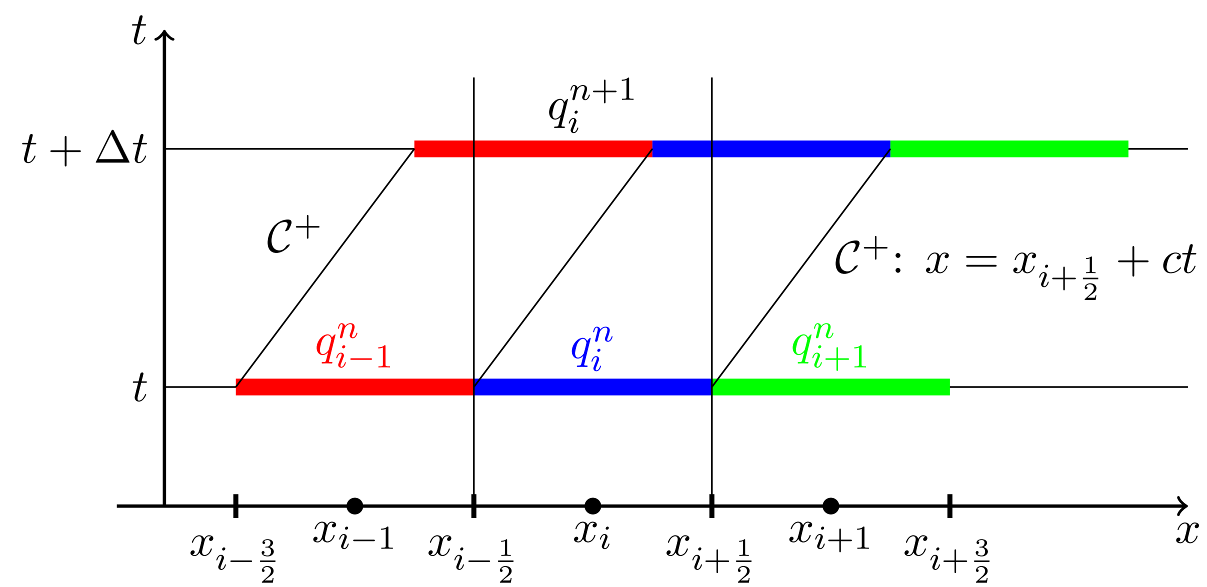
Now a reminder of how upwinding works for the advection equation (first-order formulation)

- The governing equations are

$$\frac{\partial q}{\partial t} + c\frac{\partial q}{\partial x} = 0$$
$$q(x,0) = q_0(x)$$

- Using characteristics

$$q(x,\tau) = q_i^n, \quad \text{for } x - c\tau \in (x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}})$$



- Averaging the exact solution at the next time level gives

$$\boxed{\begin{aligned} q_i^{n+1} &= \frac{1}{h_x}\left[c\Delta t q_{i-1}^n + (h_x - c\Delta t)q_i^n\right], \\ &= q_i^n - \frac{c\Delta t}{h_x}(q_i^n - q_{i-1}^n) \end{aligned}}$$

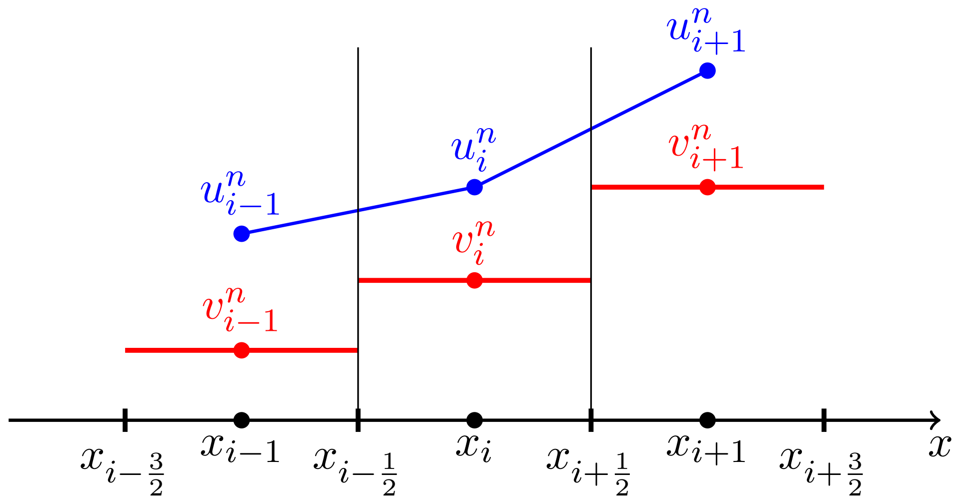
We can follow a similar procedure for the second-order wave equation

- The governing equations are

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}, \qquad -\infty < x < \infty,$$

$$u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = v(x,0) = v_0(x)$$

- Using d'Alembert's solution



$$u(x,\tau) = \frac{1}{2}\left(u_0(x+c\tau) + u_0(x-c\tau)\right) + \frac{1}{2c}\int_{x-c\tau}^{x+c\tau} v_0(\xi)d\xi,$$

$$v(x,\tau) = \frac{\partial}{\partial t}u(x,\tau) = \frac{c}{2}\left(u_0'(x+c\tau) - u_0'(x-c\tau)\right) + \frac{1}{2}\left(v_0(x+c\tau) - v_0(x-c\tau)\right)$$

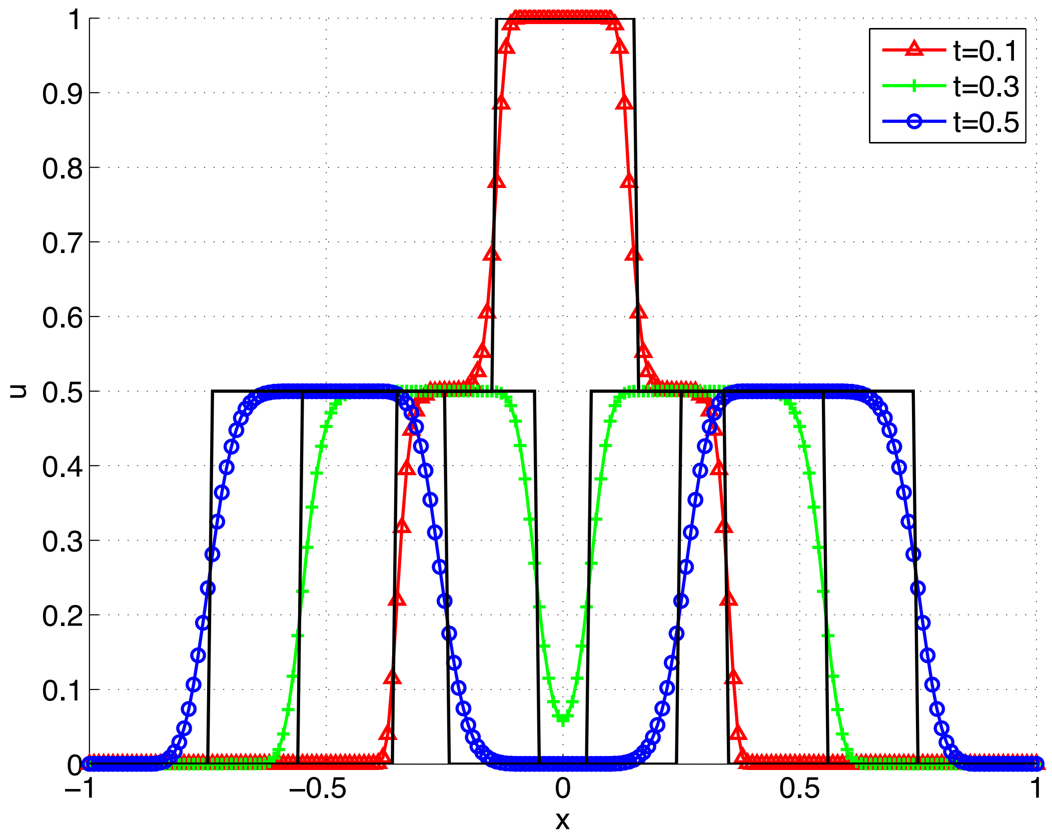
- Averaging at the next time level gives

$$\boxed{\begin{aligned} u_i^{n+1} &= u_i^n + \Delta t\ v_i^n + (\frac{c^2\Delta t^2}{2} + \frac{h_x^2}{8})D_+D_-u_i^n + \frac{c\Delta t^2}{4}\ h_x D_+D_-v_i^n, \\ v_i^{n+1} &= v_i^n + c^2\Delta t\ D_+D_-u_i^n + \frac{c\Delta t}{2}\ h_x D_+D_-v_i^n \end{aligned}}$$

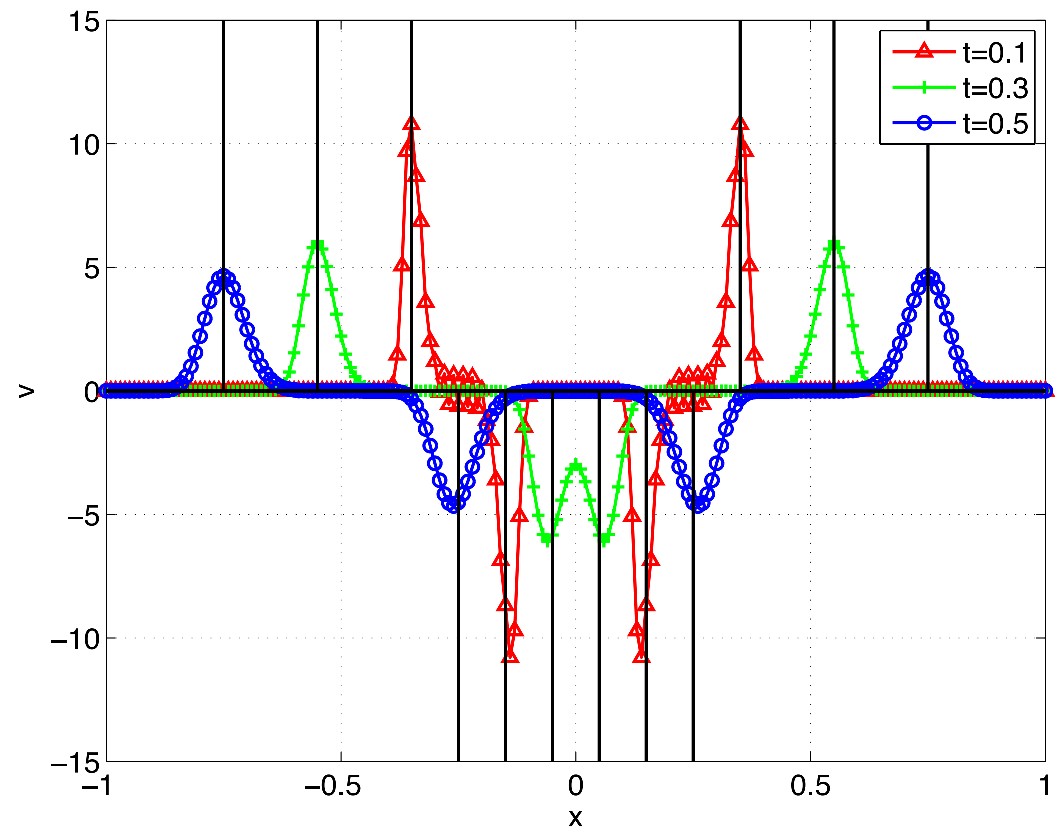
$$D_+w_i = (w_{i+1} - w_i)/h_x \qquad D_-w_i = (w_i - w_{i-1})/h_x$$

This method is 1st order accurate and behaves very well for hard problems

- Results for a top-hat initial condition (note the delta functions in V)



position

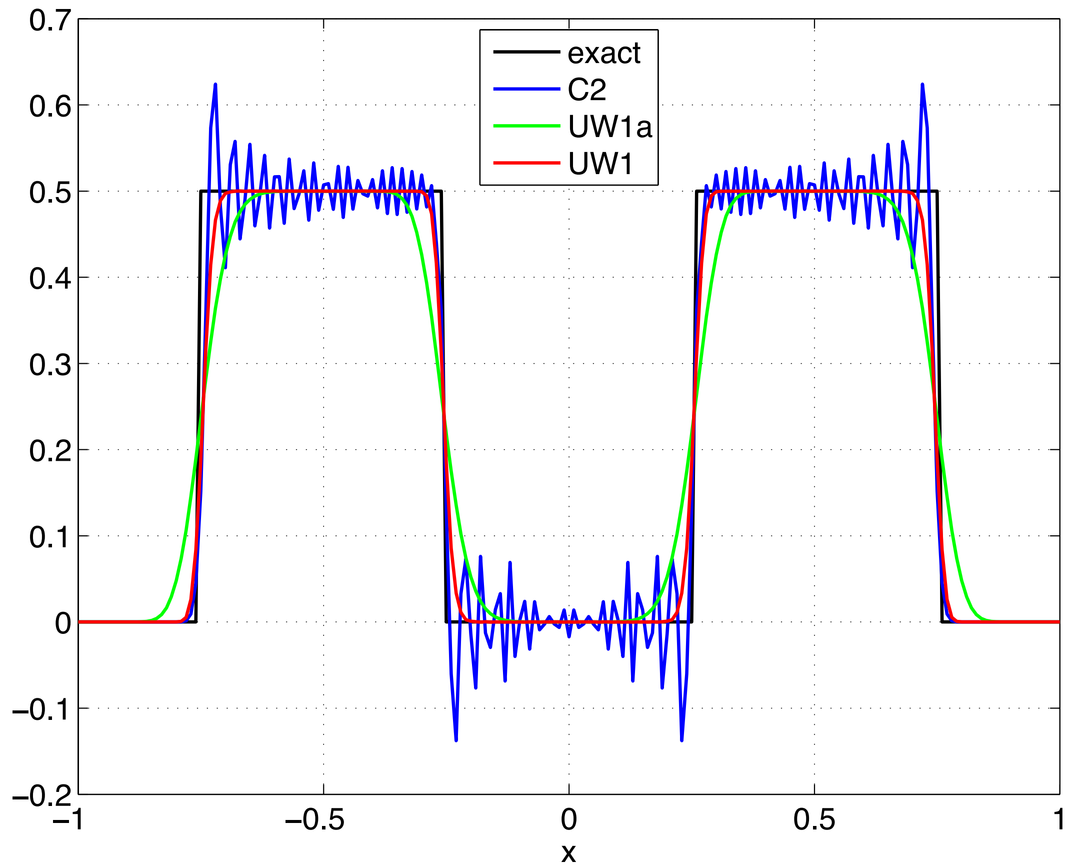


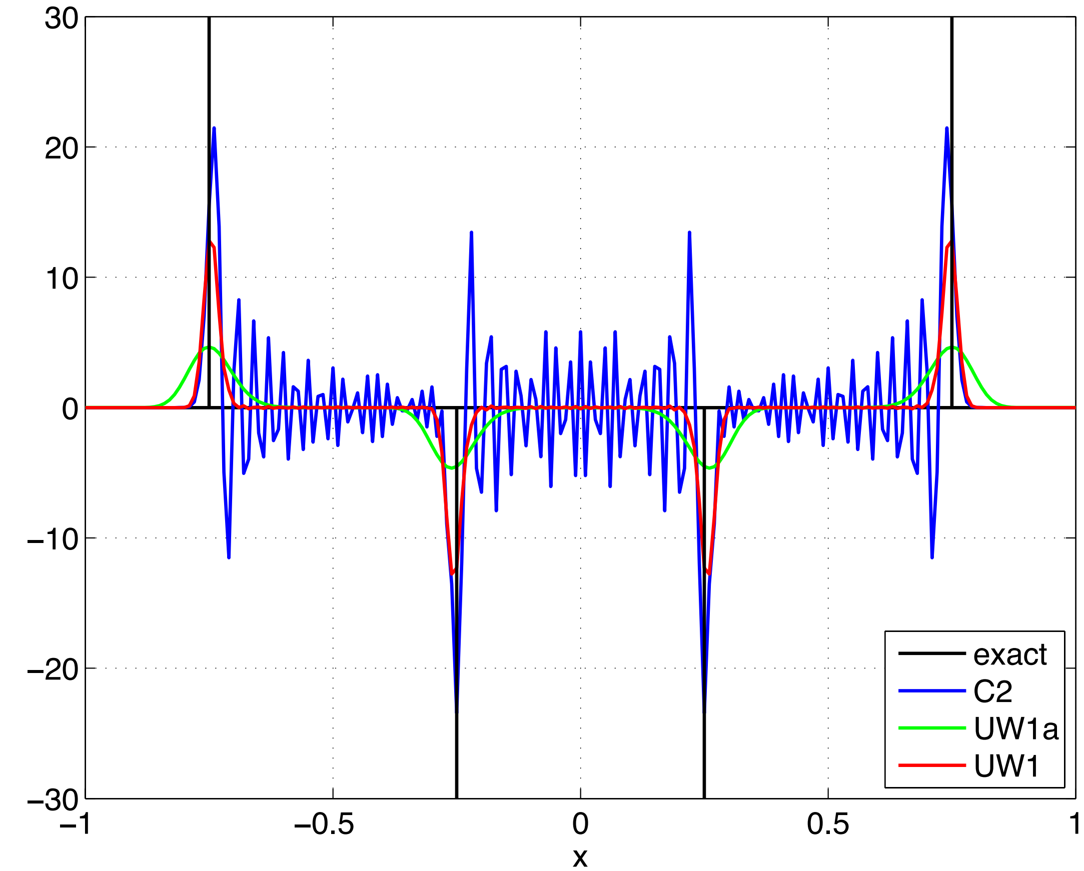
velocity

A comparison with standard centered scheme illustrates the effect of upwinding

- The centered scheme is

$$\frac{u_i^{n+1} - 2u_i^n + u_i^{n-1}}{\Delta t^2} = c^2 D_+ D_- u_i^n$$





In order to be practical (higher order, higher dimensions, variable coefficients, nonlinearity, etc ...), a more general construction is needed

- Start by recasting (note this equation is still second-order in space)

$$\begin{bmatrix} u \\ v \end{bmatrix}_t = \begin{bmatrix} 0 \\ c^2 u_x \end{bmatrix}_x + \begin{bmatrix} v \\ 0 \end{bmatrix}$$

- Integrate the v equation in time

$$v(x,t) = v(x,0) + c^2 \int_0^t \frac{\partial^2 u}{\partial x^2}(x,\tau)\, d\tau$$

- Define exact flux function so that

$$\frac{\partial^2 u}{\partial x^2}(x,t) = D_+ f(x - \frac{h_x}{2}, t), \qquad f(x,t) \equiv \mathcal{D}_x \frac{\partial u}{\partial x}(x,t)$$

- where $\mathcal{D}_x$ is defined to satisfy

$$\frac{\partial w}{\partial x}(x) = D_+ \left(\mathcal{D}_x w(x - \frac{h_x}{2}) \right)$$

The incorporation of upwinding comes in the definition of the numerical flux function using d'Alembert's solution

- Recall that the d'Alembert solution is

$$u(x, t+\tau) = \frac{1}{2}\left(u(x+c\tau, t) + u(x-c\tau, t)\right) + \frac{1}{2c}\int_{x-c\tau}^{x+c\tau} v(\xi, t)\,d\xi$$

- Now take $\tau \to 0$, assume u is smooth, and differentiate in space

$$\boxed{\frac{\partial^p}{\partial x^p}u(x, t+) = \frac{\partial^p}{\partial x^p}u(x, t) + \frac{1}{2c}\left[\frac{\partial^{p-1}}{\partial x^{p-1}}v(x+, t) - \frac{\partial^{p-1}}{\partial x^{p-1}}v(x-, t)\right]}$$

- This exact local solution is embedded into the definition of the flux

$$\check{f}(x+\frac{h_x}{2}, t^n+\tau) \equiv \mathcal{D}_x\frac{\partial u}{\partial x}(x_{i+\frac{1}{2}}, t^n+\tau) + \frac{1}{2c}\left[\mathcal{D}_x v^+(x_{i+\frac{1}{2}}, t^n+\tau) - \mathcal{D}_x v^-(x_{i+\frac{1}{2}}, t^n+\tau)\right]$$

- Cauchy-Kowalewski to get a single step high-order scheme

- M-point Gaussian quadrature is used to evaluate the fluxes

These single-step high-order accurate schemes can be compactly expressed

- For example, the fully discrete 4th order scheme is

$$v_i^{n+1} = v_i^n + c^2\Delta t\ G_i(k_0 = 1, k_1 = \frac{1}{2}, k_2 = \frac{1}{3}, k_4 = \frac{1}{4})$$
$$u_i^{n+1} = u_i^n + \Delta t v_i^n + c^2\Delta t^2\ G_i(k_0 = \frac{1}{2}, k_1 = \frac{1}{6}, k_2 = \frac{1}{12}, k_3 = \frac{1}{18})$$

where

$$G_i(k_p) = k_0 D_{4h}^{(2)} u_i^n + k_1 \Delta t D_{4h}^{(2)} v_i^n + \frac{k_2}{2} c^2 \Delta t^2 (D_+D_-)^2 u_i + \frac{k_3}{6} c^2 \Delta t^3 (D_+D_-)^2 v_i$$
$$+ \left(\frac{5k_0}{288c} h_x^5 - \frac{k_2}{12} c\Delta t^2 h_x^3\right)(D_+D_-)^3 v_i + \left(-\frac{k_1}{8} c\Delta t h_x^3 + \frac{k_3}{12} c^3 \Delta t^3 h_x\right)(D_+D_-)^3 u_i$$
$$D_{4h}^{(2)} = D_+D_-(1 - \frac{h_x^2}{12} D_+D_-)$$

- Furthermore, the modified equation is found to be

$$\frac{\partial^2 U}{\partial t^2} = c^2 \frac{\partial^2 U}{\partial x^2} + c^2 h_x^4\ M_4(\lambda)\frac{\partial^6 U}{\partial x^6} + c h_x^5\ C_4(\lambda)\frac{\partial^7 U}{\partial t \partial x^6} + \mathcal{O}((\Delta t + h_x)^6)$$

$$M_4(\lambda) = \frac{1}{2600}(-24 - 135\lambda + 60\lambda^2 + 45\lambda^3 - 16\lambda^4)$$

$$C_4(\lambda) = \frac{1}{864}(15 + 12\lambda^2 - 12\lambda^3 - 14\lambda^4 + 4\lambda^5)$$

The fourth order scheme can be analyzed using normal modes

Theorem: The fourth-order upwind method is 4th order accurate and stable under the restriction

$$\lambda = \frac{c\Delta t}{h_x}\Lambda_4 \qquad\qquad \Lambda_4 \approx 1.09$$

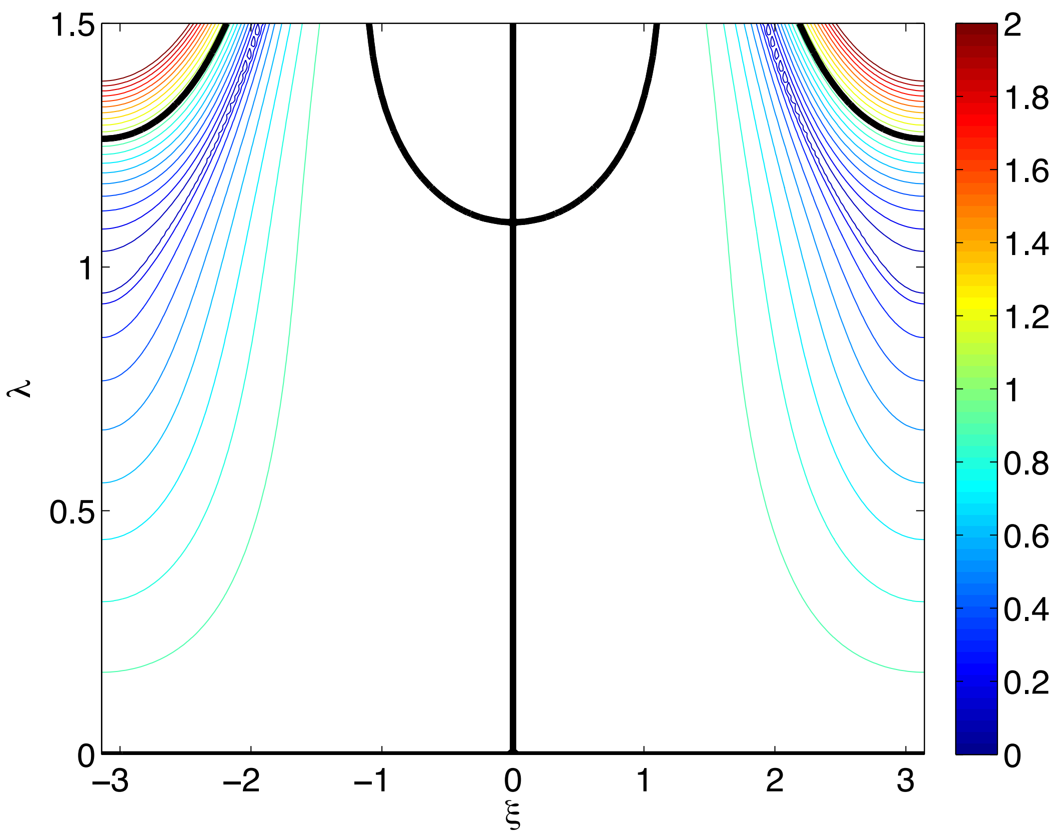
where Λ_4 is the smallest root of

$$4\Lambda_4^5 - 14\Lambda_4^4 - 12\Lambda_4^3 + 12\Lambda_4^2 + 15 = 0$$

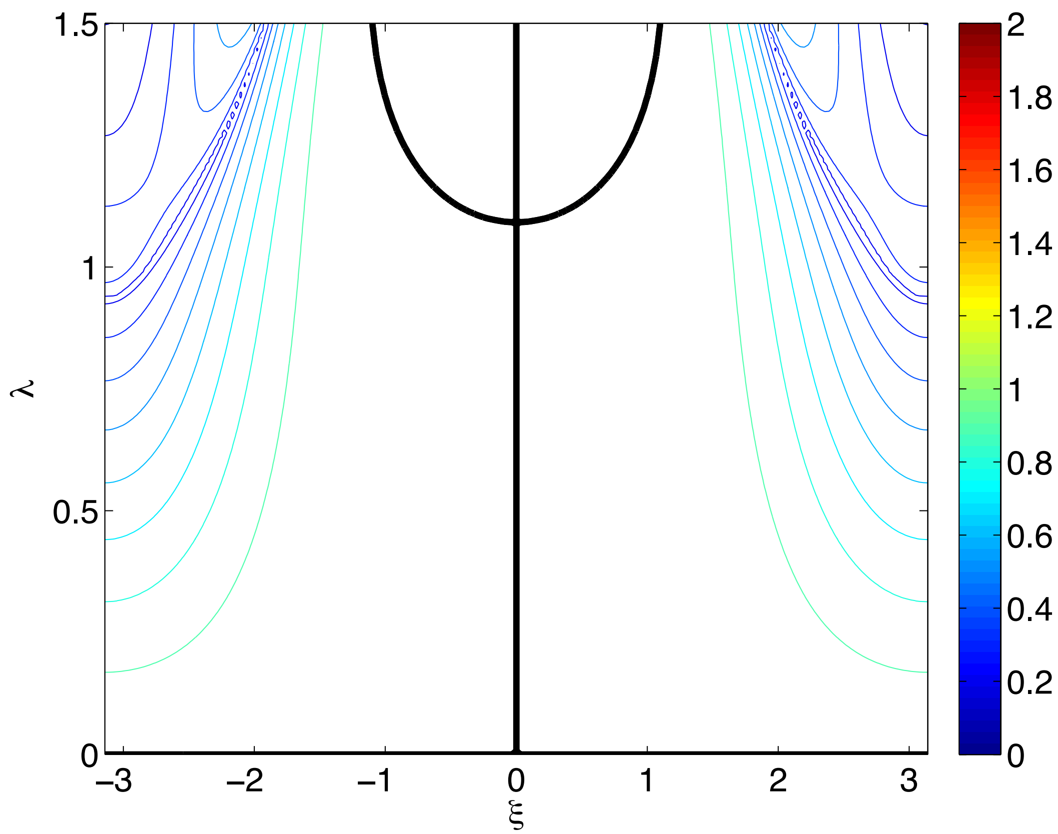
For small wave numbers the amplification factor is easily seen to be

$$z_{\pm} = 1 \pm i\lambda\xi + \frac{1}{2}(i\lambda\xi)^2 \pm \frac{1}{3!}(i\lambda\xi)^3 + \frac{1}{4!}(i\lambda\xi)^4 \pm i\frac{\lambda}{2}M_4(\lambda)\xi^5 + \mathcal{O}(\xi^6)$$

magnitude of root 1



magnitude of root 2



The generating procedure generalizes to multiple dimensions and curvilinear grids

- Consider a constant coefficient wave equation in d dimensions

$$\frac{\partial^2 u}{\partial t^2} = L(u)$$

$$L(u) \equiv c^2 \Delta u$$

- On a curvilinear grid defined by $\mathbf{x} = \mathbf{G}(\mathbf{r})$ the operator can be written

$$L(u) = \frac{1}{J} \sum_{m=1}^{d} \sum_{n=1}^{d} \frac{\partial}{\partial r_m} \left(J A^{mn} \frac{\partial u}{\partial r_n} \right)$$

- where

$$A^{mn} = c^2 \sum_{\mu=1}^{d} \frac{\partial r_m}{\partial x_\mu} \frac{\partial r_n}{\partial x_\mu}$$

As before, upwinding is incorporated by embedding the d'Alembert solution

- First we recast the system to explicitly identify a flux

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ \dot{u} \end{bmatrix} = \begin{bmatrix} \dot{u} \\ 0 \end{bmatrix} + \frac{1}{J}\sum_{m=1}^{d} \frac{\partial}{\partial r_m}\begin{bmatrix} 0 \\ \sum_{n=1}^{d} JA^{mn}\frac{\partial u}{\partial r_n} \end{bmatrix}$$

- Now we identify exact differential difference formulae, e.g.

$$\dot{u}(\mathbf{x}, t^{n+1}) = \dot{u}(\mathbf{x}, t^n) + \frac{\Delta t}{J}\sum_{m=1}^{d} D_{+r_m}\frac{1}{\Delta t}\int_0^{\Delta t}\check{f}_{r_m}(\mathbf{x}, t^n+\tau)\,d\tau$$

- Finally the d'Alembert solution is embedded

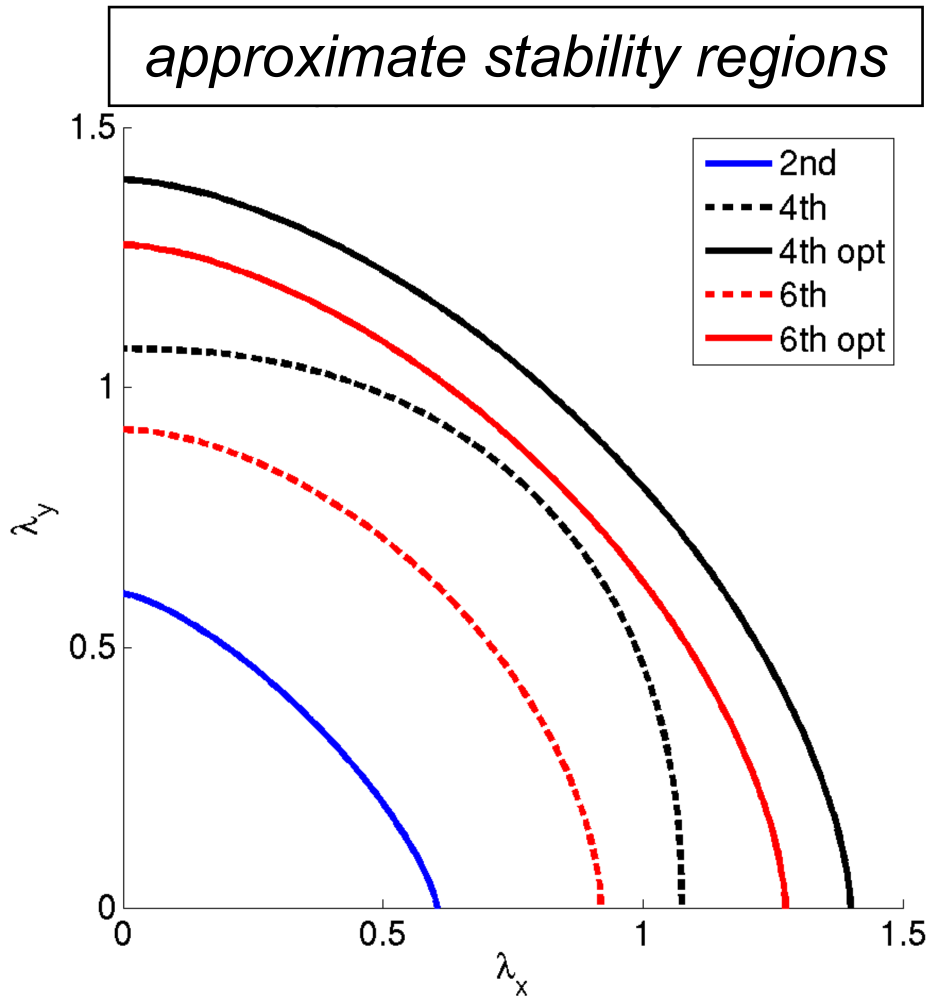
$$\boxed{\begin{aligned}\check{f}_{r_m}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m}, t^n+\tau) \equiv{}& \sum_{n=1}^{d}\mathcal{D}_{r_m} JA^{mn}\frac{\partial u}{\partial r_n}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m}, t^n+\tau) \\ &+ \mathcal{D}_{r_m}\frac{J\sqrt{A^{mm}}}{2}\left(\dot{u}^{r_m^+}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m}, t^n+\tau) - \dot{u}^{r_m^-}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m}, t^n+\tau)\right)\end{aligned}}$$

Time-step stability bounds in high dimension are derived using normal modes

- The actual stability bounds are quite complex so we instead fit simplified bounds

$$\sum_{n=1}^{d} \lambda_n^\sigma = \Lambda_{\max}^\sigma \qquad\qquad \lambda_n = \frac{c\Delta t}{h_n}$$

- For high-order, we can also increase the maximal stable time-step by leveraging the observation that the upwind dissipation need not be time accurate



Before moving on to some numerical results, lets make a few observations

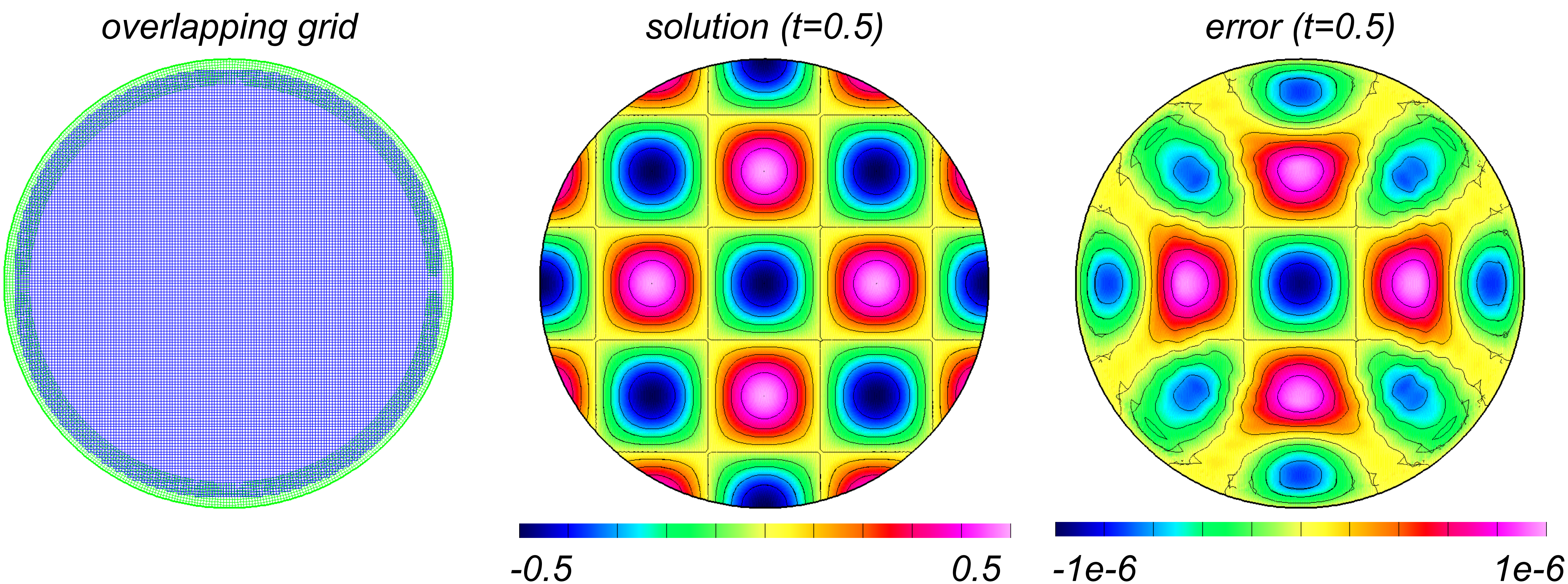
- One aspect I did not talk about is nonlinear limiting (high-resolution)
  - this has been explored for 2nd order schemes using MinMod
  - there is a lot of additional exploration that could be done here

- The upwind flux is necessary for stability for all but the 2nd order scheme

- Except for 1st order scheme, the operators are dispersive at leading order

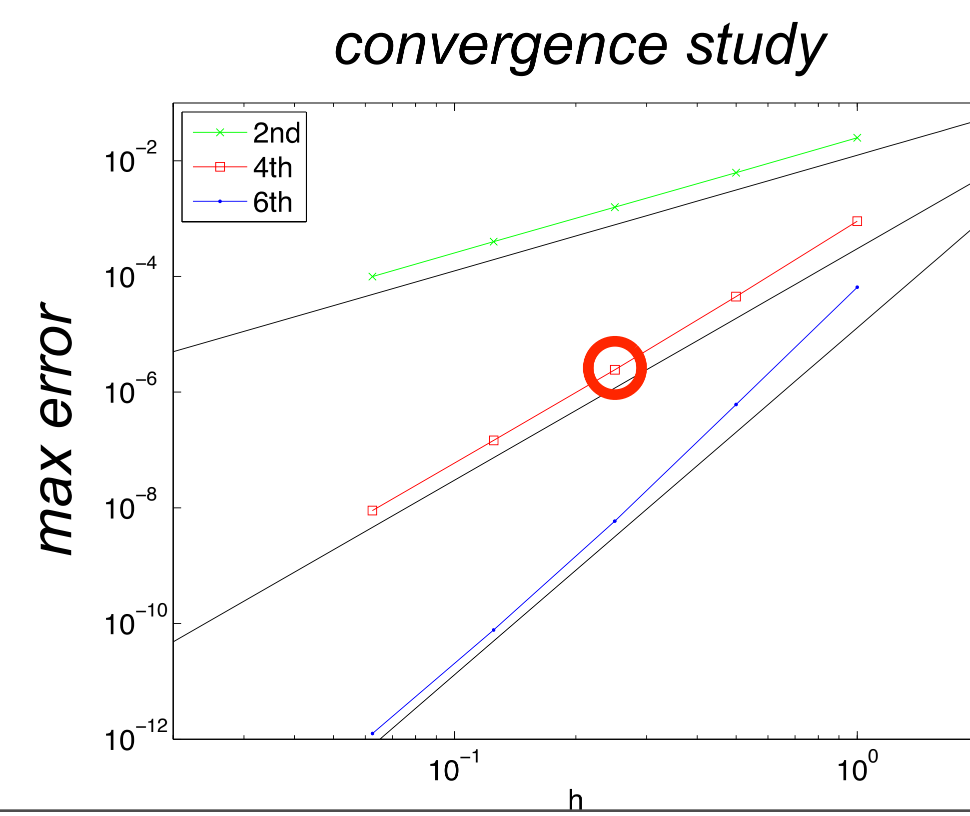
- In developing the methods, I've made extensive use of Maple
  - implemented a discrete calculus
  - automatic code generation
  - automatic normal mode analysis and MEs
  - structure of the generated code is highly cache efficient

Trigonometric twilight zone exact solutions verify the accuracy of the solvers



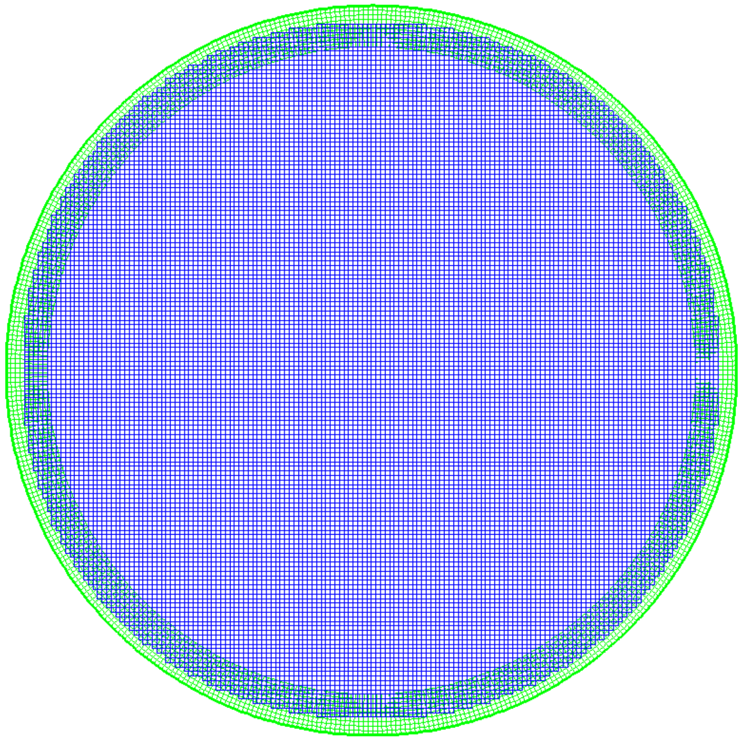
- TZ (AKA manufactured solutions) illustrates accuracy and stability for the sosup formulation on overlapping grids

- schemes of order 2-6 have been implemented and verified

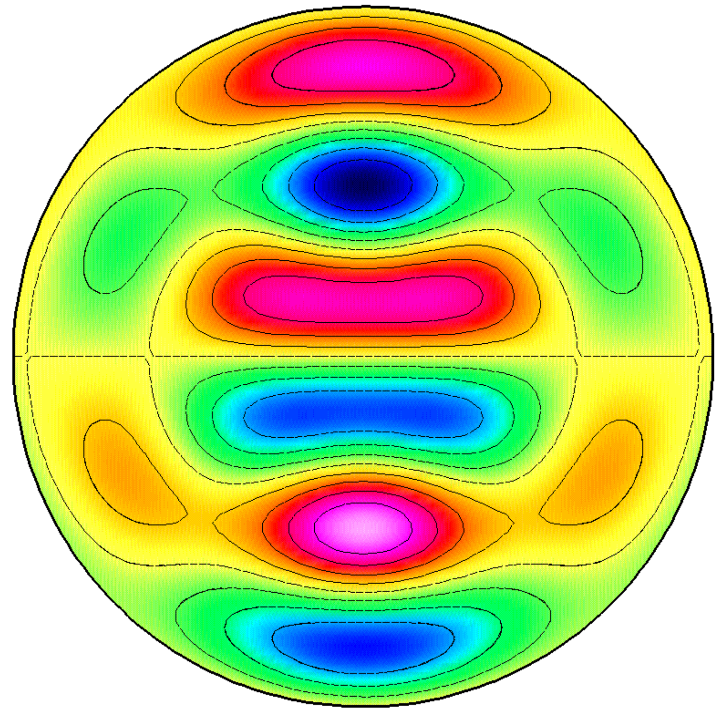


Eigenmodes of Maxwell's equations on a disk with perfect conducting boundaries

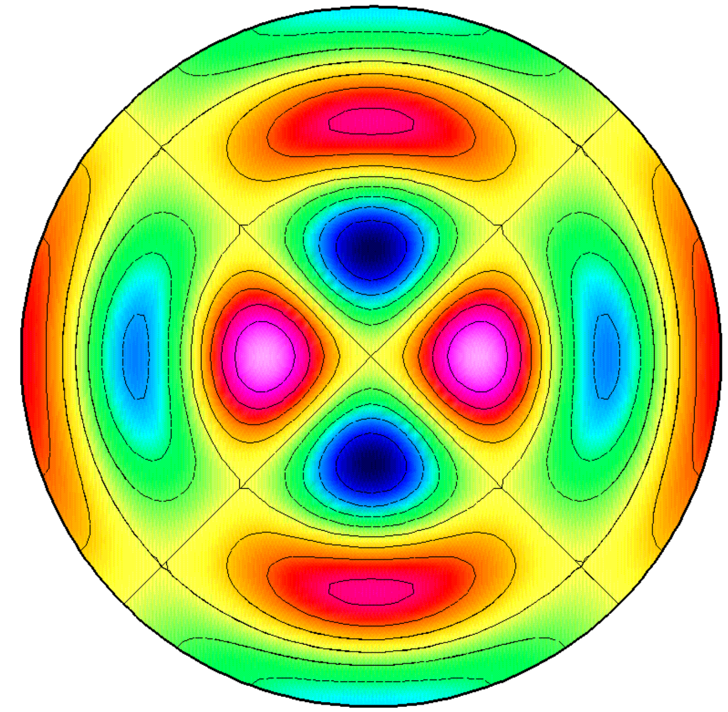
overlapping grid



EX, t=0.5

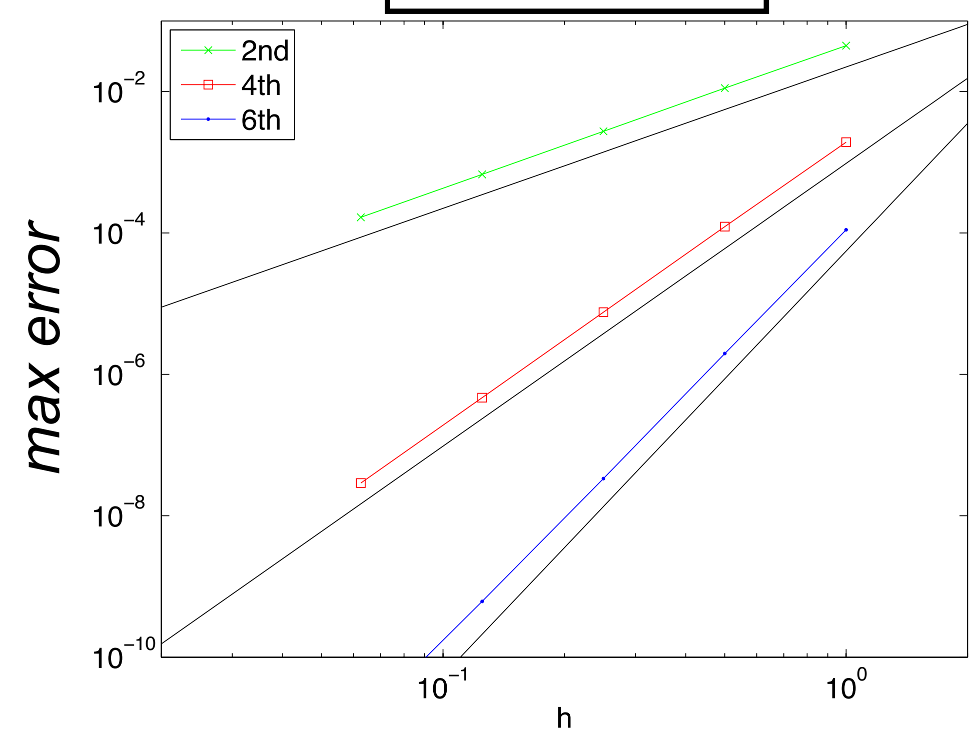


HZ, t=0.5



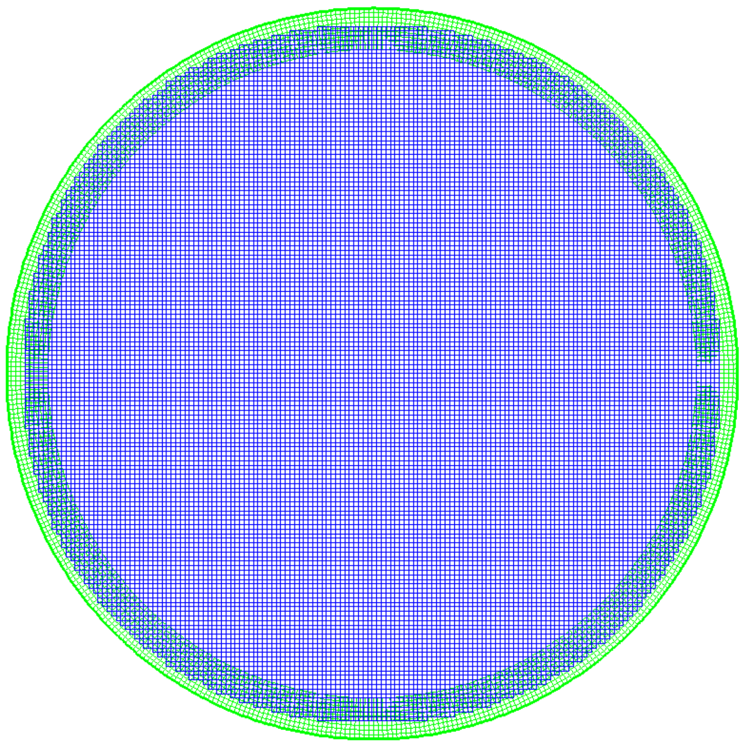
- The solvers are further verified for an exact solution to Maxwells equations on a disk
- Exact Dirichlet boundary conditions are used

Dirichlet BCs

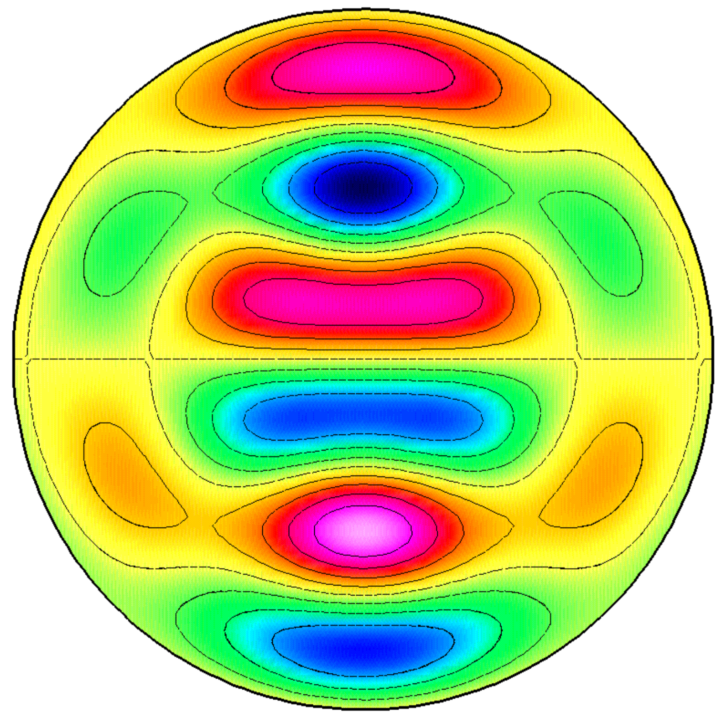


Eigenmodes of Maxwell's equations on a disk with perfect conducting boundaries

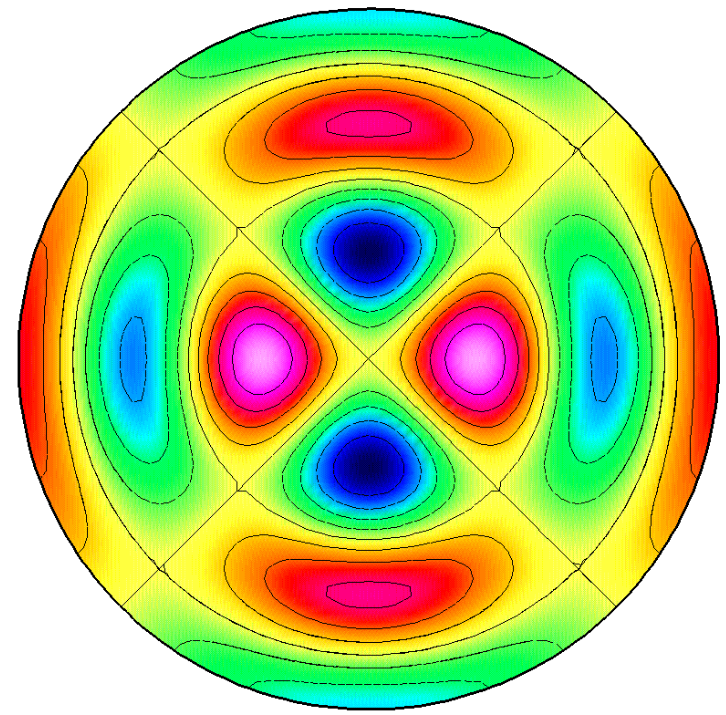
overlapping grid



EX, t=0.5



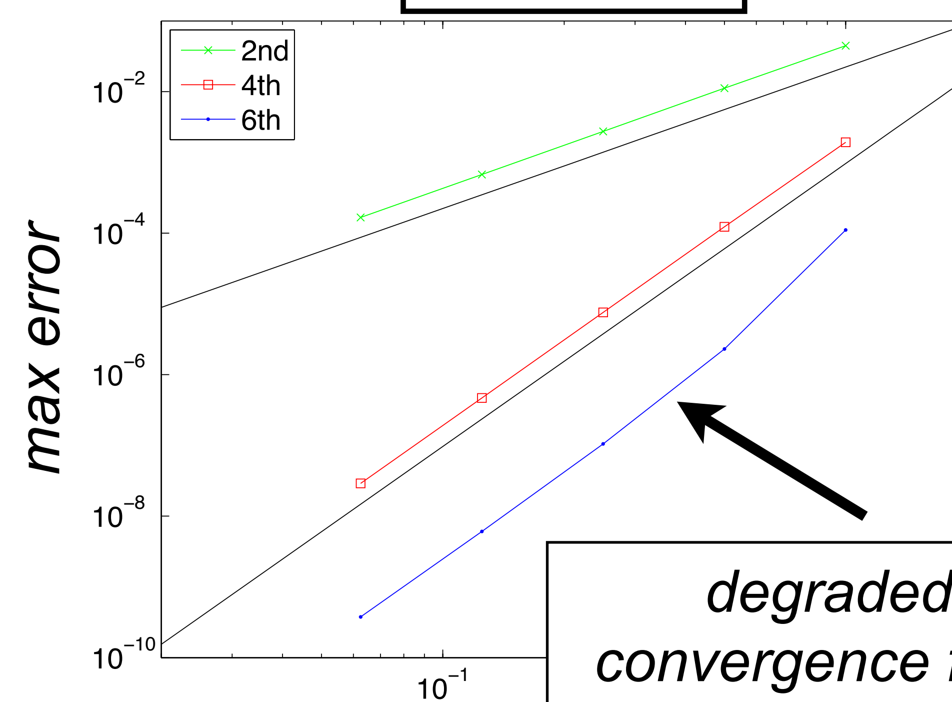
HZ, t=0.5



- Perfect electric conducting (PEC) boundary conditions have been implemented up to 4th order accuracy

- Therefore the 6th order results degrade to 4th order but they are approximately 50x more accurate than 4th order results

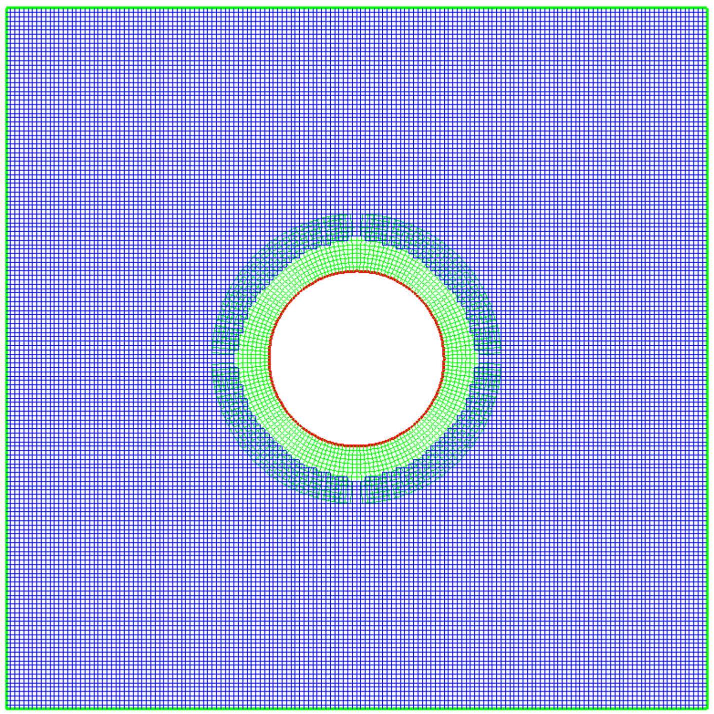
PEC BCs



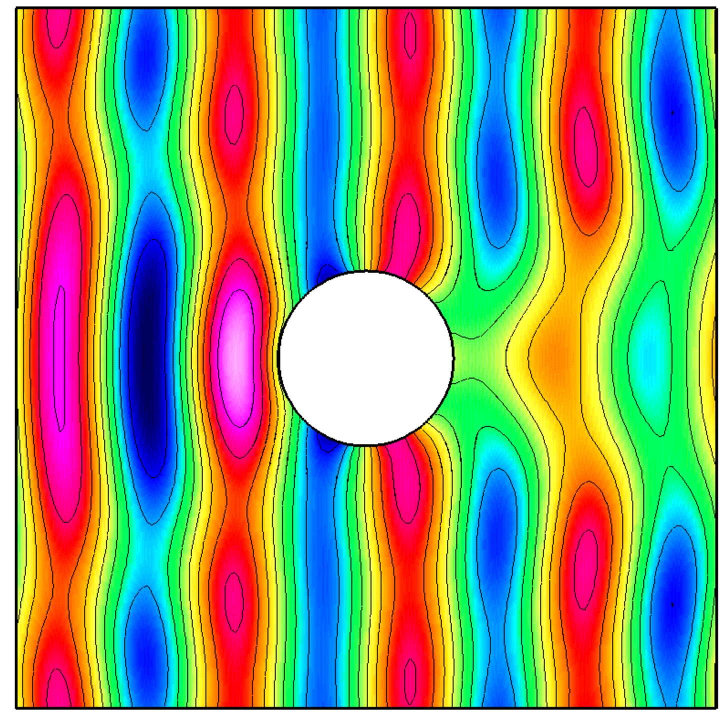
degraded convergence from 4th order BC

Electromagnetic diffraction off a perfectly conducting cylinder

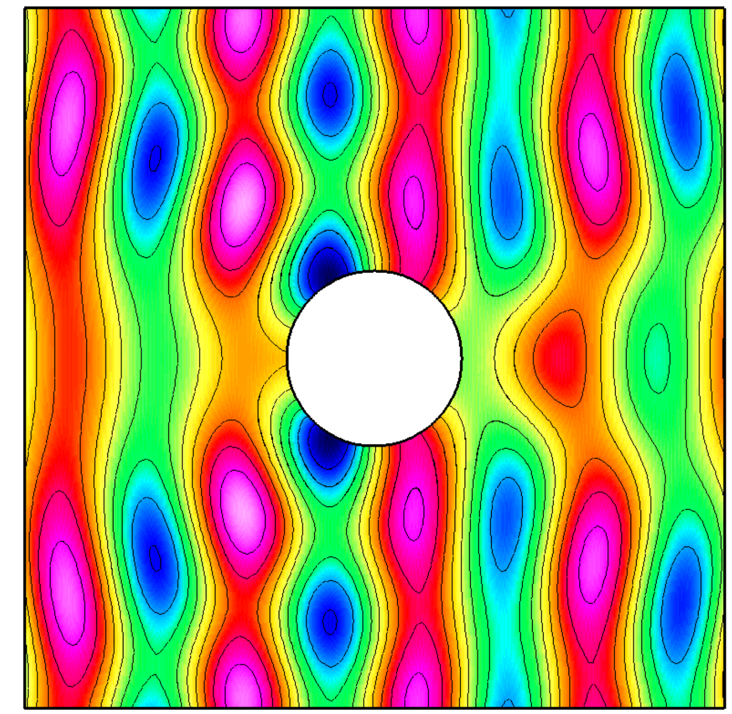
overlapping grid



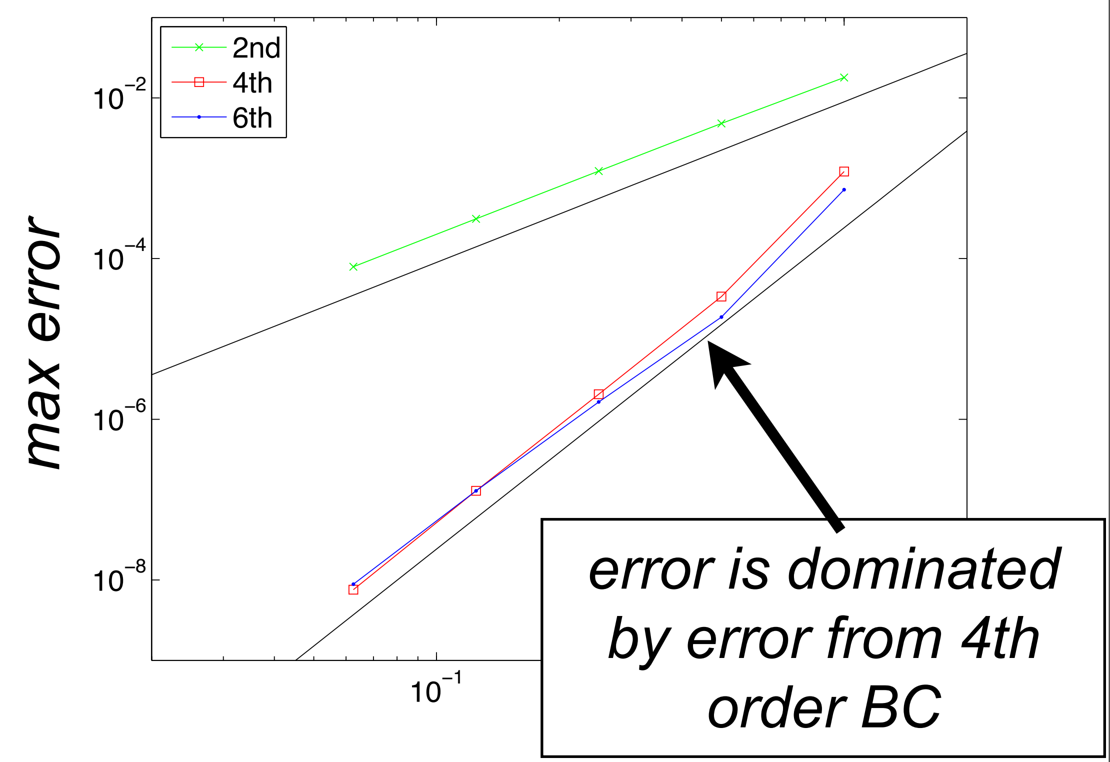
EY, t=1



HZ, t=1



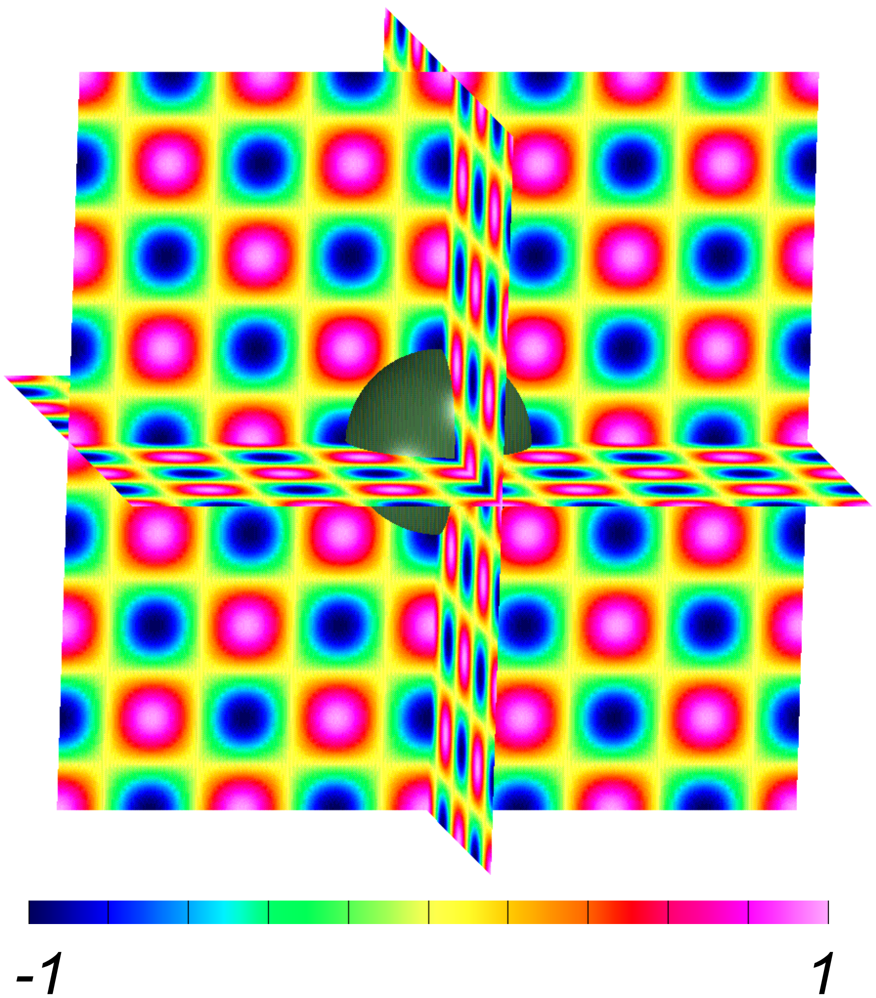
convergence study

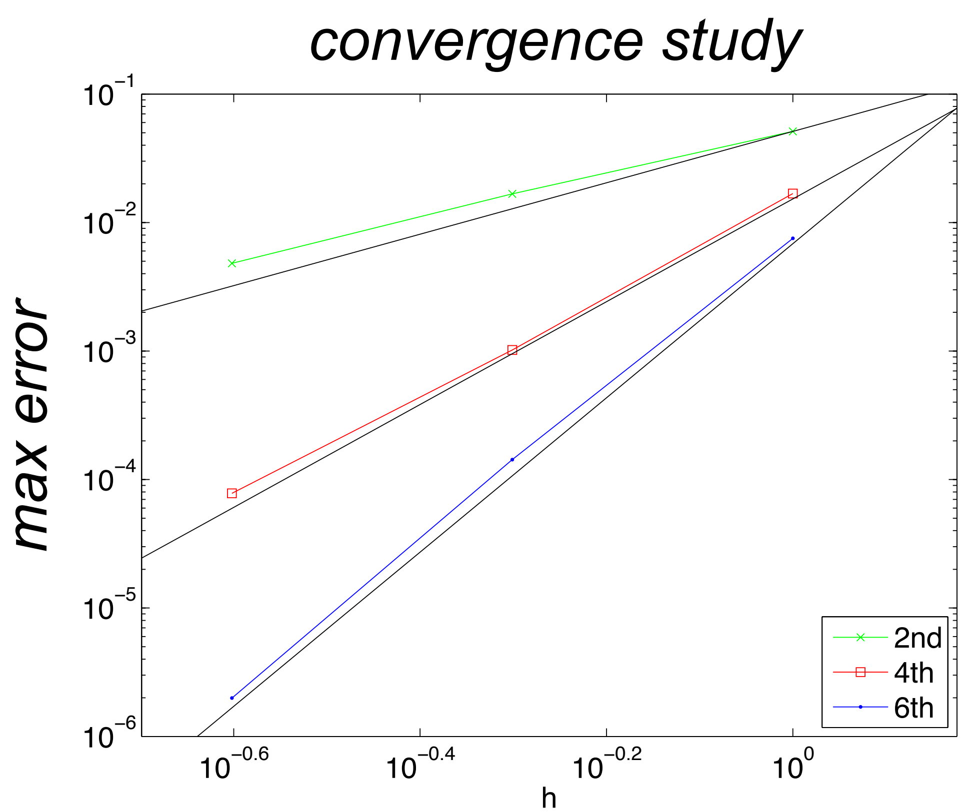


- Diffraction by a PEC cylinder also has a known exact solution

- Note that the results from the 6th order code are dominated by the 4th order accurate BC

Trigonometric twilight zone verifies the accuracy of the solvers in 3D

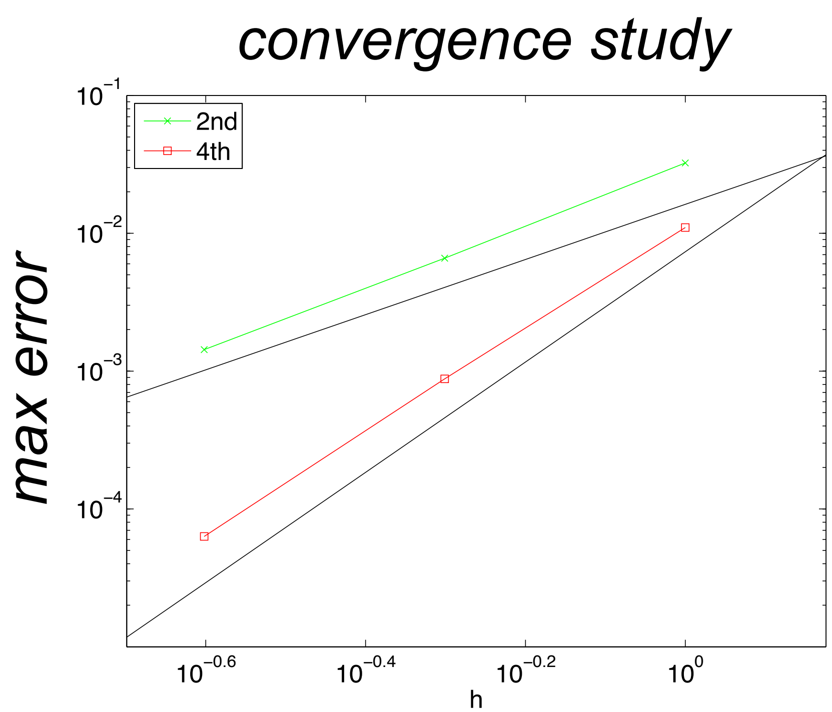


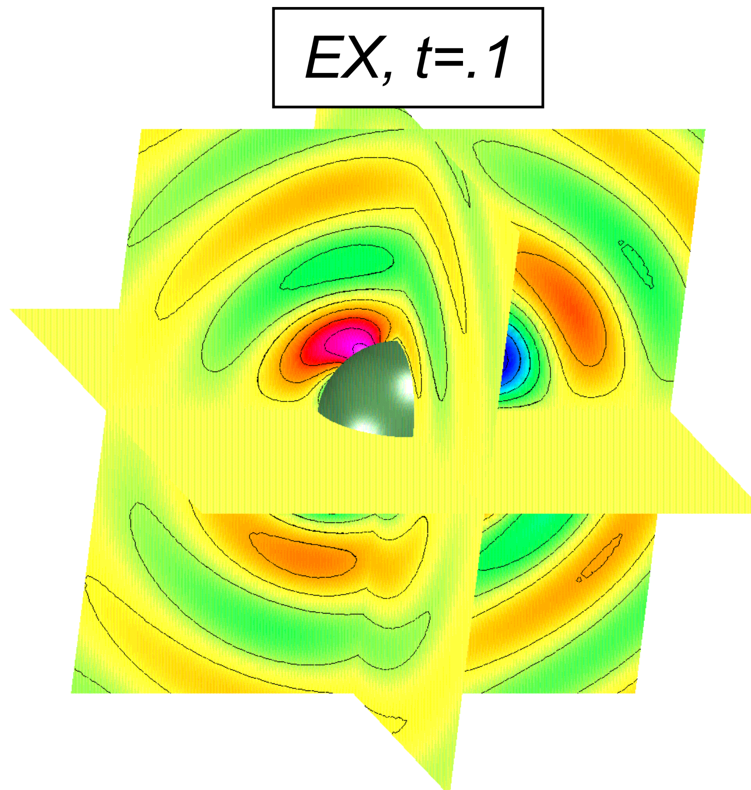


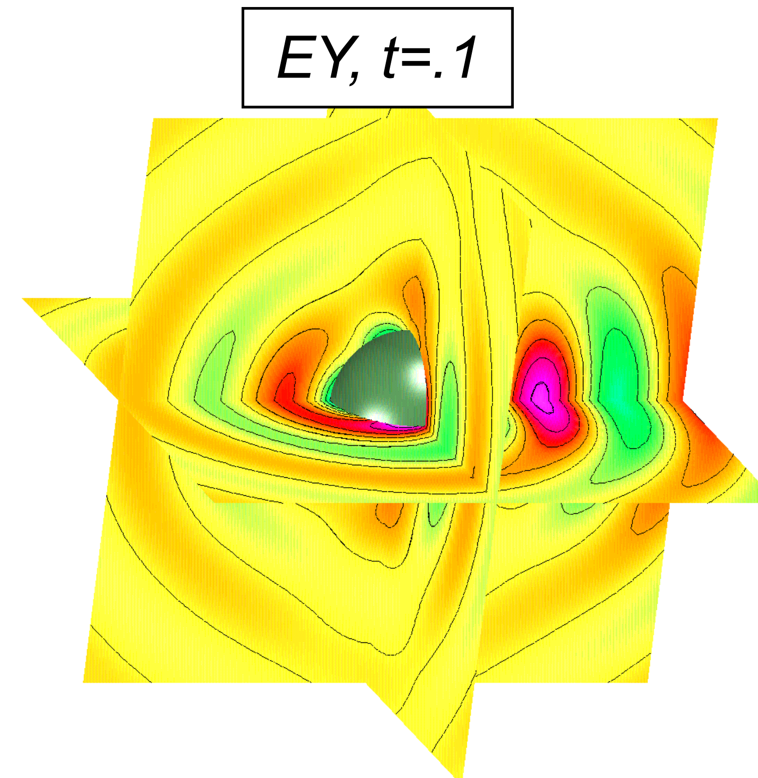
- Solvers of order 2-6 have been implemented and verified

- Stability against overlapping grid perturbations is seen for all cases

Electromagnetic diffraction off a perfectly conducting sphere







- In 3 space dimensions we have preliminary calculations for PEC sphere

- Results from the 2nd and 4th order codes show the expected behavior in terms of accuracy and stability

- The 6th order physical BCs needs further work

Summary

- By embedding the exact solution of a local problem, we generate stable and high order accurate schemes for wave propagation

- These schemes are robust and shown to be stable in the presence of overlapping grid interpolation boundaries

- The schemes have been implemented into an electromagnetics capability using Overture

Future Work

- High-order boundary conditions for Maxwell
- Variable coefficients
- More complex systems of equations such as linear elasticity
- Multidomain problems (light propagation through optics, FSI)
- Nonlinear elasticity