Muhong Zhou

Rice University, Houston, TX *2011.8 - present*

M.A., Ph.D. candidate in Computational and Applied Mathematics

- Ph.D.: *A Stable Composite Staggered Grid Finite Difference Scheme for Anisotropic Elastic Wave Simulations*
- M.A.: *Wave Equation Based Stencil Optimizations on a Multi-Core CPU*, 2014

Zhejiang University, Hangzhou, China *2007.8 - 2011.7*

B.Sc. in Mathematics and Applied Mathematics

A Stable Composite Staggered Grid Finite Difference Scheme for Elastic Wave Simulations (TRIP Annual Review Meeting)

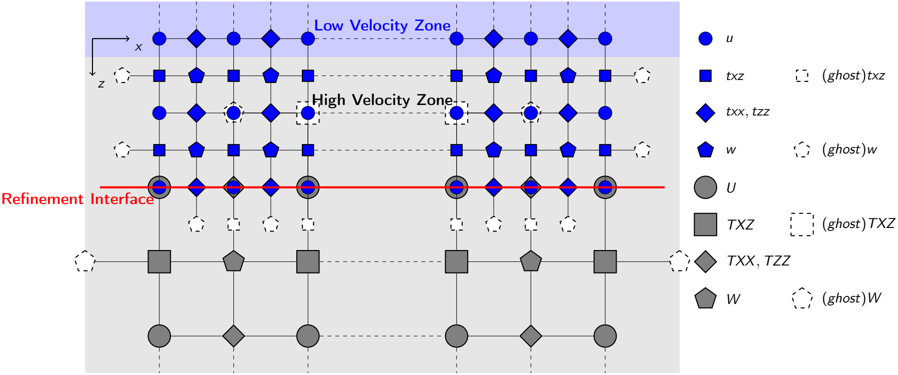
Muhong Zhou

CAAM, Rice University

April 25, 2016

I. Motivation of Using a Composite Grid

- Composite grid scheme uses less computing and memory resources than the uniform grid scheme
- Using a coarse grid in a high velocity region will not cause grid dispersion



II. Motivation of Seeking Stability

- Numerical stability: output error is bounded by the input error
- Lax-Richtmyer Equivalence Theorem: For a linear consistent scheme, stability and convergence are equivalent
- Tool to build stability: energy method

Previous Work and My Contribution

Previous papers on the energy method to build stability:

- [Petersson and Sjögreen, 2010][1] finite difference scheme, composite collocated grid, second order wave equation
- [Rodríguez, 2008][2] finite element scheme, composite staggered grid, first order wave equation system

My contribution:

- use the energy method to build a stable composite staggered grid finite difference scheme for first order wave equation system

[1] Petersson and Sjögreen, *Stable grid refinement and singular source discretization for seismic wave simulations*, 2010

[2] Rodríguez, *A spurious-free space-time mesh refinement for elastodynamics*, 2008

Previous Work and My Contribution

Previous papers on the energy method to build stability:

- [Petersson and Sjögreen, 2010][1] finite difference scheme, composite collocated grid, second order wave equation
- [Rodríguez, 2008][2] finite element scheme, composite staggered grid, first order wave equation system

My contribution:

- use the energy method to build a stable composite staggered grid finite difference scheme for first order wave equation system

[1] Petersson and Sjögreen, *Stable grid refinement and singular source discretization for seismic wave simulations*, 2010

[2] Rodríguez, *A spurious-free space-time mesh refinement for elastodynamics*, 2008

Steps to Use the Energy Method to Get Stability

1. Formulate the energy: $E[s_1, ..., s_m](t)$,
   where $s_i(t)(i = 1, ..., m)$ denote simulation variables

When the source is absent, make sure:

2. the energy is non increasing over time:
   $E[s_1, ..., s_m](t_2) \leq E[s_1, ..., s_m](t_1)$, for $t_2 \geq t_1$

3. the energy is bounded above and below by simulation variables:
   $a \sum_{i=1}^{m} \|s_i(t)\|^2 \leq E[s_1, ..., s_m](t) \leq b \sum_{i=1}^{m} \|s_i(t)\|^2$, $a, b > 0$

---

2 and 3 yield stability:

$$a \sum_{i=1}^{m} \|s_i(T)\|^2 \overset{3}{\leq} E[s_1, ..., s_m](T) \overset{2}{\leq} E[s_1, ..., s_m](0) \overset{3}{\leq} b \sum_{i=1}^{m} \|s_i(0)\|^2$$

2D Example

Isotropic elastic wave equation in first order form:

$$\begin{aligned}
\rho\dot{u} &= txx_x + txz_z + s_1 \\
\rho\dot{w} &= txz_x + tzz_z + s_2 \\
\dot{txx} &= (\lambda + 2\mu)u_x + \lambda w_z \\
\dot{tzz} &= \lambda u_x + (\lambda + 2\mu)w_z \\
\dot{txz} &= \mu(u_z + w_x)
\end{aligned}$$

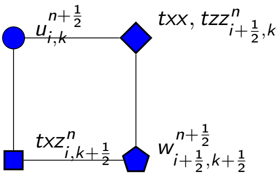
Energy in the continuous time-space:

Kinetic energy: $k(t) = \frac{1}{2}\iint \rho(u^2 + w^2)\mathrm{d}x\mathrm{d}z$

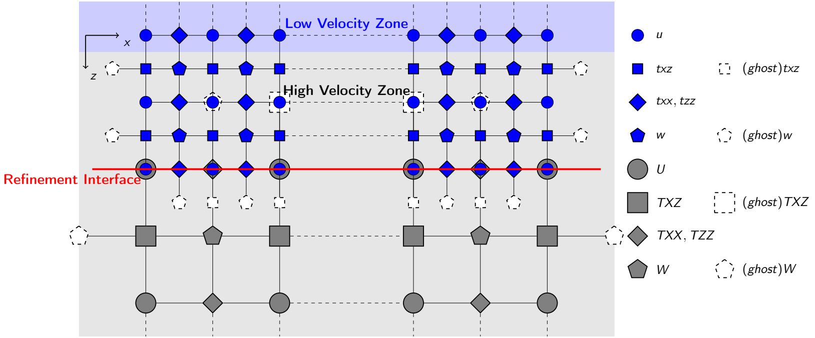
Strain energy: $s(t) = \frac{1}{2}\iint txx \cdot \epsilon xx + tzz \cdot \epsilon zz + 2txz \cdot \epsilon xz \, \mathrm{d}x\mathrm{d}z$

When the source is absent, $e(t) = k(t) + s(t)$ satisfies $\dot{e}(t) = 0$.

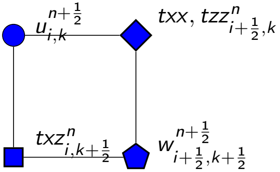
A 2D Composite Staggered Grid with (2,2) FDM



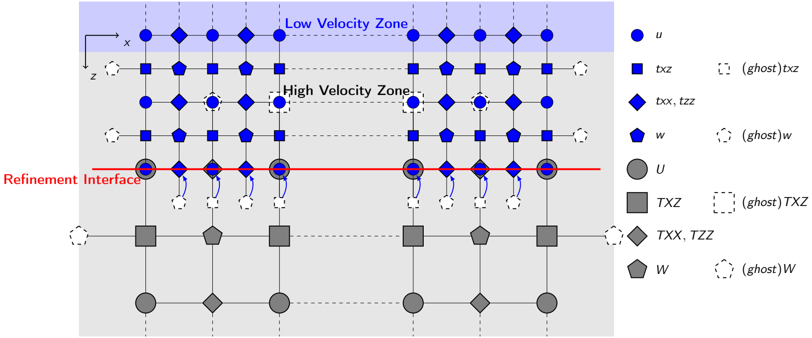
$$
\begin{cases}
u_{i,k}^{n+\frac{1}{2}} & i = 0, \ldots, nx; k = 0, \ldots, nz \\
txx, tzz_{i+\frac{1}{2},k}^{n} & i = 0, \ldots, nx-1; k = 0, \ldots, nz \\
txz_{i,k+\frac{1}{2}}^{n} & i = 0, \ldots, nx; k = 0, \ldots, nz-1 \\
w_{i+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} & i = 0, \ldots, nx-1; k = 0, \ldots, nz-1
\end{cases}
$$



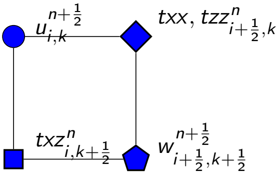
A 2D Composite Staggered Grid with (2,2) FDM



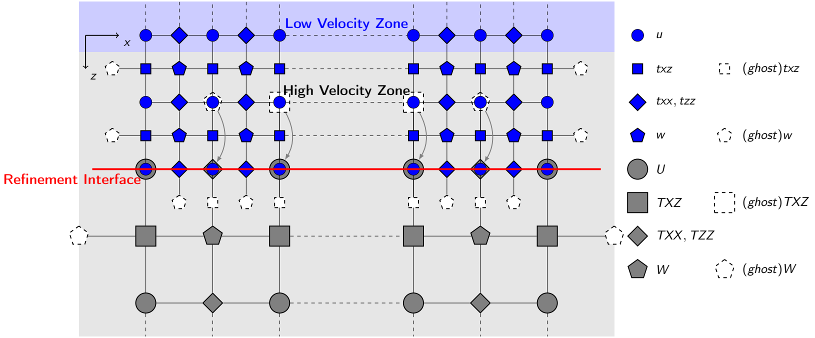
$$
\begin{cases}
u^{n+\frac{1}{2}}_{i,k} & i = 0, \ldots, nx;\ k = 0, \ldots, nz \\
txx, tzz^{n}_{i+\frac{1}{2},k} & i = 0, \ldots, nx-1;\ k = 0, \ldots, nz \\
txz^{n}_{i,k+\frac{1}{2}} & i = 0, \ldots, nx;\ k = 0, \ldots, nz-1 \\
w^{n+\frac{1}{2}}_{i+\frac{1}{2},k+\frac{1}{2}} & i = 0, \ldots, nx-1;\ k = 0, \ldots, nz-1
\end{cases}
$$



A 2D Composite Staggered Grid with (2,2) FDM



$$\begin{cases} u_{i,k}^{n+\frac{1}{2}} & i=0,\dots,nx;\ k=0,\dots,nz \\ txx, tzz_{i+\frac{1}{2},k}^{n} & i=0,\dots,nx-1;\ k=0,\dots,nz \\ txz_{i,k+\frac{1}{2}}^{n} & i=0,\dots,nx;\ k=0,\dots,nz-1 \\ w_{i+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} & i=0,\dots,nx-1;\ k=0,\dots,nz-1 \end{cases}$$



Define Discrete Energy $e^n = k^n + s^n$

Define inner products (or quadrature rules) on the grid:

$$\langle u^1, u^2\rangle_u = h^2 \sum_{i=0}^{nx} \sum_{k=0}^{nz} \alpha_i \alpha_k u^1_{i,k} u^2_{i,k} \approx \iint u^1 u^2 \mathrm{d}x\mathrm{d}z$$

$$\langle w^1, w^2\rangle_w = h^2 \sum_{i=0}^{nx-1} \sum_{k=0}^{nz-1} w^1_{i+\frac{1}{2},k+\frac{1}{2}} w^2_{i+\frac{1}{2},k+\frac{1}{2}} \approx \iint w^1 w^2 \mathrm{d}x\mathrm{d}z$$

$$\langle txz^1, txz^2\rangle_{txz} = h^2 \sum_{i=0}^{nx} \sum_{k=0}^{nz-1} \alpha_i txz^1_{i,k+\frac{1}{2}} txz^2_{i,k+\frac{1}{2}} \approx \iint txz^1 txz^2 \mathrm{d}x\mathrm{d}z$$

where $\alpha_{i/k} = \frac{1}{2}$ at two ends of axis i/k, and 1 elsewhere.

$$k^n = \frac{1}{2}\langle \rho u^{n+\frac{1}{2}}, u^{n-\frac{1}{2}}\rangle_u + \frac{1}{2}\langle \rho w^{n+\frac{1}{2}}, w^{n-\frac{1}{2}}\rangle_w \approx \frac{1}{2}\iint \rho(u^2 + w^2)\mathrm{d}x\mathrm{d}z$$

$$s^n = \frac{1}{2}h^2 \sum_{i=0}^{nx-1} \sum_{k=0}^{nz} \alpha_k \begin{pmatrix} txx^n_{i+\frac{1}{2},k} \\ tzz^n_{i+\frac{1}{2},k} \end{pmatrix}^T \begin{pmatrix} (\lambda+2\mu)_{i+\frac{1}{2},k} & \lambda_{i+\frac{1}{2},k} \\ \lambda_{i+\frac{1}{2},k} & (\lambda+2\mu)_{i+\frac{1}{2},k} \end{pmatrix}^{-1} \begin{pmatrix} txx^n_{i+\frac{1}{2},k} \\ tzz^n_{i+\frac{1}{2},k} \end{pmatrix}$$

$$+ \frac{1}{2}\langle \frac{1}{\mu} txz^n, txz^n\rangle_{txz} \approx \frac{1}{2}\iint txx \cdot \epsilon xx + tzz \cdot \epsilon zz + 2txz \cdot \epsilon xz \,\mathrm{d}x\mathrm{d}z$$

Define Discrete Energy $e^n = k^n + s^n$

Define inner products (or quadrature rules) on the grid:

$$\langle u^1, u^2 \rangle_u = h^2 \sum_{i=0}^{nx} \sum_{k=0}^{nz} \alpha_i \alpha_k u^1_{i,k} u^2_{i,k} \approx \iint u^1 u^2 \mathrm{d}x\mathrm{d}z$$

$$\langle w^1, w^2 \rangle_w = h^2 \sum_{i=0}^{nx-1} \sum_{k=0}^{nz-1} w^1_{i+\frac{1}{2},k+\frac{1}{2}} w^2_{i+\frac{1}{2},k+\frac{1}{2}} \approx \iint w^1 w^2 \mathrm{d}x\mathrm{d}z$$

$$\langle txz^1, txz^2 \rangle_{txz} = h^2 \sum_{i=0}^{nx} \sum_{k=0}^{nz-1} \alpha_i txz^1_{i,k+\frac{1}{2}} txz^2_{i,k+\frac{1}{2}} \approx \iint txz^1 txz^2 \mathrm{d}x\mathrm{d}z$$

where $\alpha_{i/k} = \frac{1}{2}$ at two ends of axis i/k, and 1 elsewhere.

$$k^n = \frac{1}{2}\langle \rho u^{n+\frac{1}{2}}, u^{n-\frac{1}{2}} \rangle_u + \frac{1}{2}\langle \rho w^{n+\frac{1}{2}}, w^{n-\frac{1}{2}} \rangle_w \approx \frac{1}{2} \iint \rho(u^2 + w^2)\mathrm{d}x\mathrm{d}z$$

$$s^n = \frac{1}{2} h^2 \sum_{i=0}^{nx-1} \sum_{k=0}^{nz} \alpha_k \begin{pmatrix} txx^n_{i+\frac{1}{2},k} \\ tzz^n_{i+\frac{1}{2},k} \end{pmatrix}^T \begin{pmatrix} (\lambda+2\mu)_{i+\frac{1}{2},k} & \lambda_{i+\frac{1}{2},k} \\ \lambda_{i+\frac{1}{2},k} & (\lambda+2\mu)_{i+\frac{1}{2},k} \end{pmatrix}^{-1} \begin{pmatrix} txx^n_{i+\frac{1}{2},k} \\ tzz^n_{i+\frac{1}{2},k} \end{pmatrix}$$
$$+ \frac{1}{2}\langle \frac{1}{\mu} txz^n, txz^n \rangle_{txz} \approx \frac{1}{2} \iint txx \cdot \epsilon xx + tzz \cdot \epsilon zz + 2txz \cdot \epsilon xz \, \mathrm{d}x\mathrm{d}z$$

Energy Conservation Condition

1. Compute energy difference on the fine grid $e^n - e^{n-1}$:

$$h\Delta t \sum_{i=1}^{nx-1} u_{i,nz}^{n-\frac{1}{2}} \frac{\overline{txz_{i,nz}^{n}} + \overline{txz_{i,nz}^{n-1}}}{2} + h\Delta t \sum_{i=0}^{nx-1} \overline{w_{i+\frac{1}{2},nz}^{n-\frac{1}{2}}} \frac{tzz_{i+\frac{1}{2},nz}^{n} + tzz_{i+\frac{1}{2},nz}^{n-1}}{2}$$

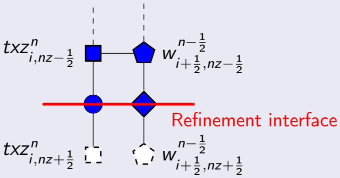
2. Compute energy difference on the coarse grid $E^n - E^{n-1}$:

$$-H\Delta t \sum_{i=1}^{NX-1} U_{i,0}^{n-\frac{1}{2}} \frac{\overline{TXZ_{i,0}^{n}} + \overline{TXZ_{i,0}^{n-1}}}{2} - H\Delta t \sum_{i=0}^{nx-1} \overline{W_{i+\frac{1}{2},0}^{n-\frac{1}{2}}} \frac{TZZ_{i+\frac{1}{2},0}^{n} + TZZ_{i+\frac{1}{2},0}^{n-1}}{2}$$

Averaging operator $\bar{(\cdot)}$:

$$\overline{txz_{i,nz}^{n}} = \frac{1}{2}\left(txz_{i,nz+\frac{1}{2}}^{n} + txz_{i,nz-\frac{1}{2}}^{n}\right)$$

$$\overline{w_{i+\frac{1}{2},nz}^{n-\frac{1}{2}}} = \frac{1}{2}\left(w_{i+\frac{1}{2},nz+\frac{1}{2}}^{n-\frac{1}{2}} + w_{i+\frac{1}{2},nz-\frac{1}{2}}^{n-\frac{1}{2}}\right)$$



Energy Conservation Condition

1. Compute energy difference on the fine grid $e^n - e^{n-1}$:

$$h\Delta t \sum_{i=1}^{nx-1} u_{i,nz}^{n-\frac{1}{2}} \frac{\overline{txz_{i,nz}^{n}} + \overline{txz_{i,nz}^{n-1}}}{2} + h\Delta t \sum_{i=0}^{nx-1} \overline{w_{i+\frac{1}{2},nz}^{n-\frac{1}{2}}} \frac{tzz_{i+\frac{1}{2},nz}^{n} + tzz_{i+\frac{1}{2},nz}^{n-1}}{2}$$

2. Compute energy difference on the coarse grid $E^n - E^{n-1}$:

$$-H\Delta t \sum_{i=1}^{NX-1} U_{i,0}^{n-\frac{1}{2}} \frac{\overline{TXZ_{i,0}^{n}} + \overline{TXZ_{i,0}^{n-1}}}{2} - H\Delta t \sum_{i=0}^{nx-1} \overline{W_{i+\frac{1}{2},0}^{n-\frac{1}{2}}} \frac{TZZ_{i+\frac{1}{2},0}^{n} + TZZ_{i+\frac{1}{2},0}^{n-1}}{2}$$

Energy Conservation Condition

Then the total energy is conserved (i.e., $e^n + E^n = e^{n-1} + E^{n-1}$) as long as for any m, n,

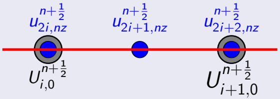
$$h \sum_{i=1}^{nx-1} u_{i,nz}^{n-\frac{1}{2}} \overline{txz_{i,nz}^{m}} = H \sum_{i=1}^{NX-1} U_{i,0}^{n-\frac{1}{2}} \overline{TXZ_{i,0}^{m}}$$

$$h \sum_{i=0}^{nx-1} \overline{w_{i+\frac{1}{2},nz}^{n-\frac{1}{2}}} tzz_{i+\frac{1}{2},nz}^{m} = H \sum_{i=0}^{NX-1} \overline{W_{i+\frac{1}{2},0}^{n-\frac{1}{2}}} TZZ_{i+\frac{1}{2},0}^{m}$$

Assume H=2h, decouple $$h\sum_{i=1}^{nx-1} u_{i,nz}^{n-\frac{1}{2}}\overline{txz_{i,nz}^{m}} = H\sum_{i=1}^{NX-1} U_{i,0}^{n-\frac{1}{2}}\overline{TXZ_{i,0}^{m}} \qquad (*)$$

Transmission condition (u, w, txz, tzz):

1 $$\begin{cases} u_{2i,nz}^{n+\frac{1}{2}} = U_{i,0}^{n+\frac{1}{2}} \\ u_{2i+1,nz}^{n+\frac{1}{2}} = \frac{1}{2}(U_{i,0}^{n+\frac{1}{2}} + U_{i+1,0}^{n+\frac{1}{2}}) \end{cases}$$



Plugging 1 back into (∗) yields

2 $$2\overline{TXZ_{i,0}^{n}} = \overline{txz_{2i,nz}^{n}} + \frac{1}{2}(\overline{txz_{2i+1,nz}^{n}} + \overline{txz_{2i-1,nz}^{n}})$$

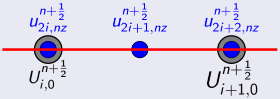
(Energy conserving interpolation): 1 and 2 together form a strictly diagonally dominant linear equation system for ghost data $(txz_{i,nz+\frac{1}{2}}^{n}, TXZ_{i,-\frac{1}{2}}^{n})$.

Energy Conserving Interpolation

Assume H=2h, decouple $$h\sum_{i=1}^{nx-1} u_{i,nz}^{n-\frac{1}{2}}\overline{txz_{i,nz}^{m}} = H\sum_{i=1}^{NX-1} U_{i,0}^{n-\frac{1}{2}}\overline{TXZ_{i,0}^{m}} \qquad (*)$$

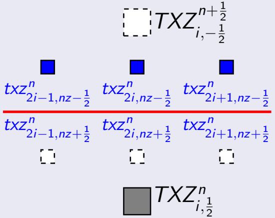
Transmission condition (u, w, txz, tzz):

$$\boxed{1}\begin{cases} u_{2i,nz}^{n+\frac{1}{2}} = U_{i,0}^{n+\frac{1}{2}} \\ u_{2i+1,nz}^{n+\frac{1}{2}} = \frac{1}{2}\left(U_{i,0}^{n+\frac{1}{2}} + U_{i+1,0}^{n+\frac{1}{2}}\right) \end{cases}$$



Plugging $\boxed{1}$ back into $(*)$ yields

$$\boxed{2}\; 2\overline{TXZ_{i,0}^{n}} = \overline{txz_{2i,nz}^{n}} + \frac{1}{2}\left(\overline{txz_{2i+1,nz}^{n}} + \overline{txz_{2i-1,nz}^{n}}\right)$$



(Energy conserving interpolation): $\boxed{1}$ and $\boxed{2}$ together form a strictly diagonally dominant linear equation system for ghost data $(txz_{i,nz+\frac{1}{2}}^{n}, TXZ_{i,-\frac{1}{2}}^{n})$.

Qualify for Boundedness

With energy conserving interpolation, Cauchy-Schwarz inequality

$$E^n + e^n \geq \underbrace{\frac{1}{2}(\langle \rho u^{n-\frac{1}{2}}, u^{n-\frac{1}{2}} \rangle_u - \frac{\Delta t(\gamma_1 + \gamma_2)}{h} \| u^{n-\frac{1}{2}} \|_u^2)}_{\text{implies } \Delta t < \frac{h\rho_{\min}}{\gamma_1 + \gamma_2}}$$

$$+ \underbrace{\frac{1}{2}(\langle \frac{txx^n}{2(\lambda+\mu)}, txx^n \rangle_{txx} - \frac{\Delta t}{h\gamma_1} \| txx^n \|_{txx}^2)}_{\text{implies } \Delta t < \frac{h\gamma_1}{2(\lambda+\mu)_{\max}}}$$

$$+ \ldots$$

γ_1, γ_2, ...: free parameters resulted from C-S, have same unit as $\sqrt{\kappa\rho}$

$$\Delta t < \max_{\gamma_1, \gamma_2, \ldots} \{\min\{\frac{h\rho_{\min}}{\gamma_1 + \gamma_2}, \frac{h\gamma_1}{2(\lambda+\mu)_{\max}}, \ldots\}\}$$

Qualify for Boundedness

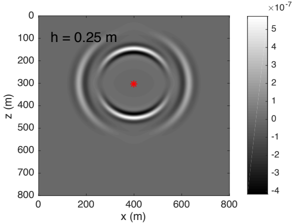
$$\Delta t < \max_{\gamma_1, \gamma_2, \ldots} \{\min\{\frac{h\rho_{\text{min}}}{\gamma_1 + \gamma_2}, \frac{h\gamma_1}{2(\lambda + \mu)_{\text{max}}}, \ldots\}\}$$

- Sufficient condition for stability vs. CFL condition (necessary condition for stability)
- Depends on both density and velocity vs. CFL condition (depends on velocity only)
- In isotropic homogenous medium, this upper bound reduces to CFL condition:

$$\Delta t < \max_{\gamma_1, \gamma_2} \{\min\{\frac{h\rho}{\gamma_1 + \gamma_2}, \frac{h\gamma_1}{2(\lambda + \mu)}, \frac{h\gamma_2}{2\mu}\}\} = h\sqrt{\frac{\rho}{2(\lambda + 2\mu)}} = \frac{h}{\sqrt{2}V_p} \text{ (CFL)}$$

Results: Compare Horizontal Velocity

- 20 Hz Ricker wavelet; delay time: 0.05 s
- $V_p = 1500$ m/s, $V_s = 1000$ m/s, $\rho = 1000$ kg/m^3
- Snapshot is taken at T = 0.2 s



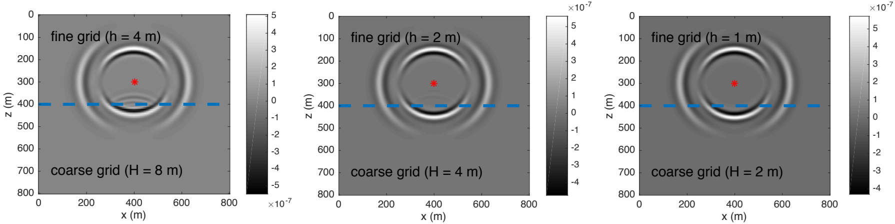
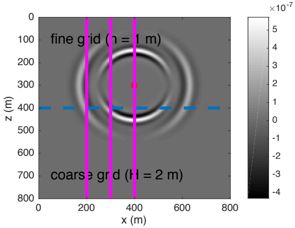
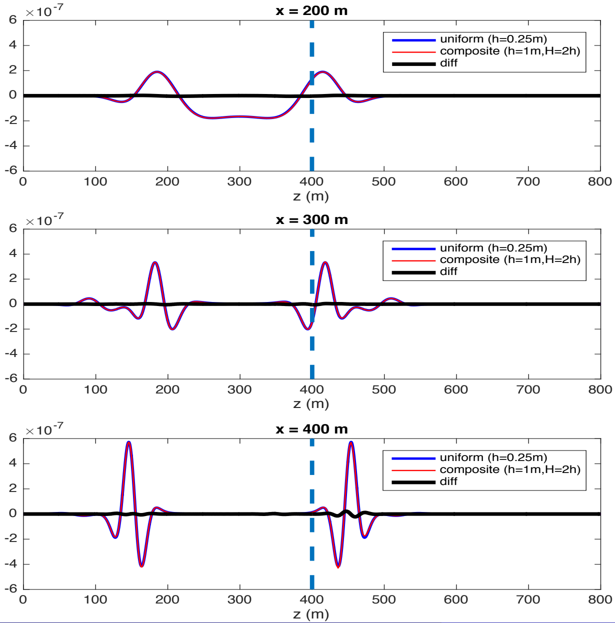


Figure: [top right] uniform grid solution (h=0.25m);
[bottom] composite grid solutions (h = 4, 2, 1m, H=2h).

Results: Compare Vertical Traces

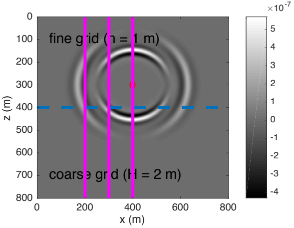


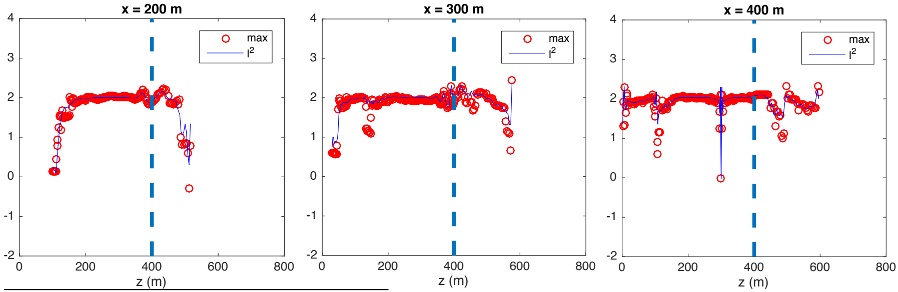


Results: Estimate Convergence Rate[3] (Tails Truncated)

- Estimate convergence rate at x = 200, 300, 400m
- $R(z) = log_2(\frac{\|u_h(z) - u_{h/2}(z)\|}{\|u_{h/2}(z) - u_{h/4}(z)\|})$ with h = 2, 1, 0.5 m

  where $\|u(z)\|_{l^2} = \sqrt{\sum_k |u(z, t_k)|^2}$ or $\|u(z)\|_\infty = \max_k |u(z, t_k)|$.

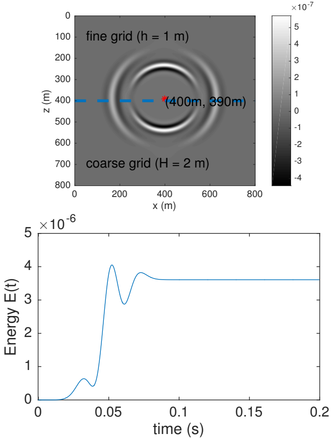




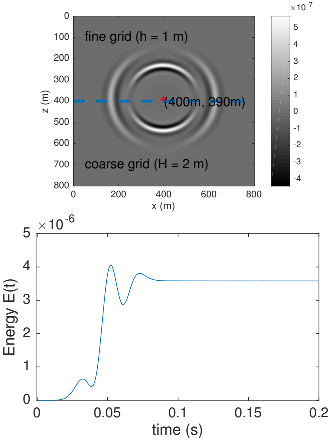
[3] Bencomo, *Joint model and minimal-source full waveform inversion for seismic imaging under general anisotropic sources, 2015*

Source: (400 m, 390 m)

Energy Conserving Interpolation



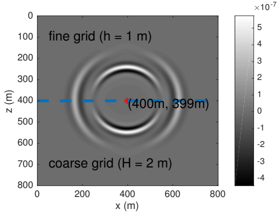
Intuitive Interpolation

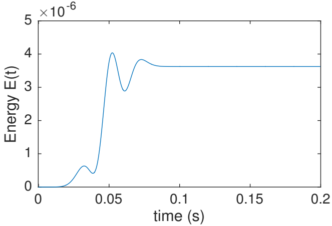


Results: Energy Conserving vs. Intuitive Interpolation

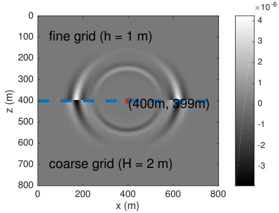
Source: (400 m, 399 m)

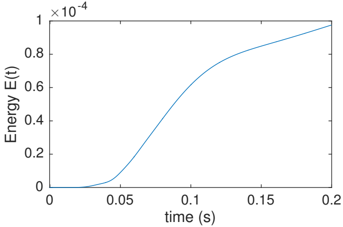
Energy Conserving Interpolation





Intuitive Interpolation





Summary and Future Work

Summary

- Proposed a numerically stable composite staggered grid FDM
- Achieved stability by implementing the energy conserving interpolation on the interface ghost data
- Demonstrated an upper bound on the time step
- Numerically verified the convergence rate for (2,2) scheme

Future Work

- Load into IWAVE, parallelization, performance tuning
- Elasto-acoustic coupling
- Towards high-order scheme

Thank You!
Q&A