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Optimally Accurate Finite Difference Operators

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Background

- Developing efficient and accurate numerical methods for computing synthetic seismograms for realistic models is an important research topic.

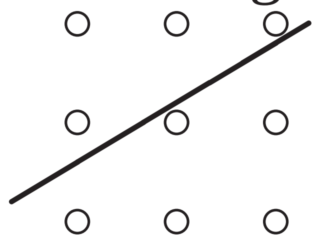
- Evaluation of accuracy should be based on rigorous theory.

- Evaluation of accuracy should be a forethought, not an afterthought.

- Accuracy is particularly important for application to waveform inversion for Earth structure and earthquake source parameters.

Overview of this presentation

1. Formal analysis of error
2. Criterion for optimally accurate operators
3. Derivation of optimally accurate operators
4. Optimally accurate operators for lithological discontinuities that do not coincide with the numerical grid.



5. Where do we go from here?

Published Results

Weak (Galerkin) Form of Equation of Motion:

Geller, R. J., and Ohminato, T., 1994, *Geophys. J. Int.*, **116**, 421–446.

Theory for Optimally Accurate (OPT) Operators:

Geller, R. J., and Takeuchi, N., 1995, *Geophys. J. Int.*, **123**, 449–470.

1-D Time Domain FDM (OPT2):

Geller, R. J., and Takeuchi, N., 1998, *Geophys. J. Int.*, **135**, 48–62.

2-D and 3-D Time Domain FDM (OPT2):

Takeuchi, N., and Geller, R.J., 2000, *Phys. Earth Planet. Int.*, **119**, 99–131.

Comparison of FDM (OPT2) to PSM:

Mizutani, H., Geller, R. J., and Takeuchi, N., 2000, *Phys. Earth Planet. Int.*, **119**, 75–97.

Accurate Treatment of Source Term:

Takeuchi, N., and Geller, R. J., 2003. *Geophys. J. Int.*, **154**, 852–866.

Accuracy metric

- We want to quantify the accuracy of synthetic seismograms:

$$\text{Relative solution error} = \frac{|(\text{numerical solution}) - (\text{exact solution})|}{|\text{exact solution}|}$$

- Relative solution error can be defined and evaluated for arbitrarily heterogeneous media, whereas numerical dispersion of phase velocity can be defined and evaluated only for homogeneous media.

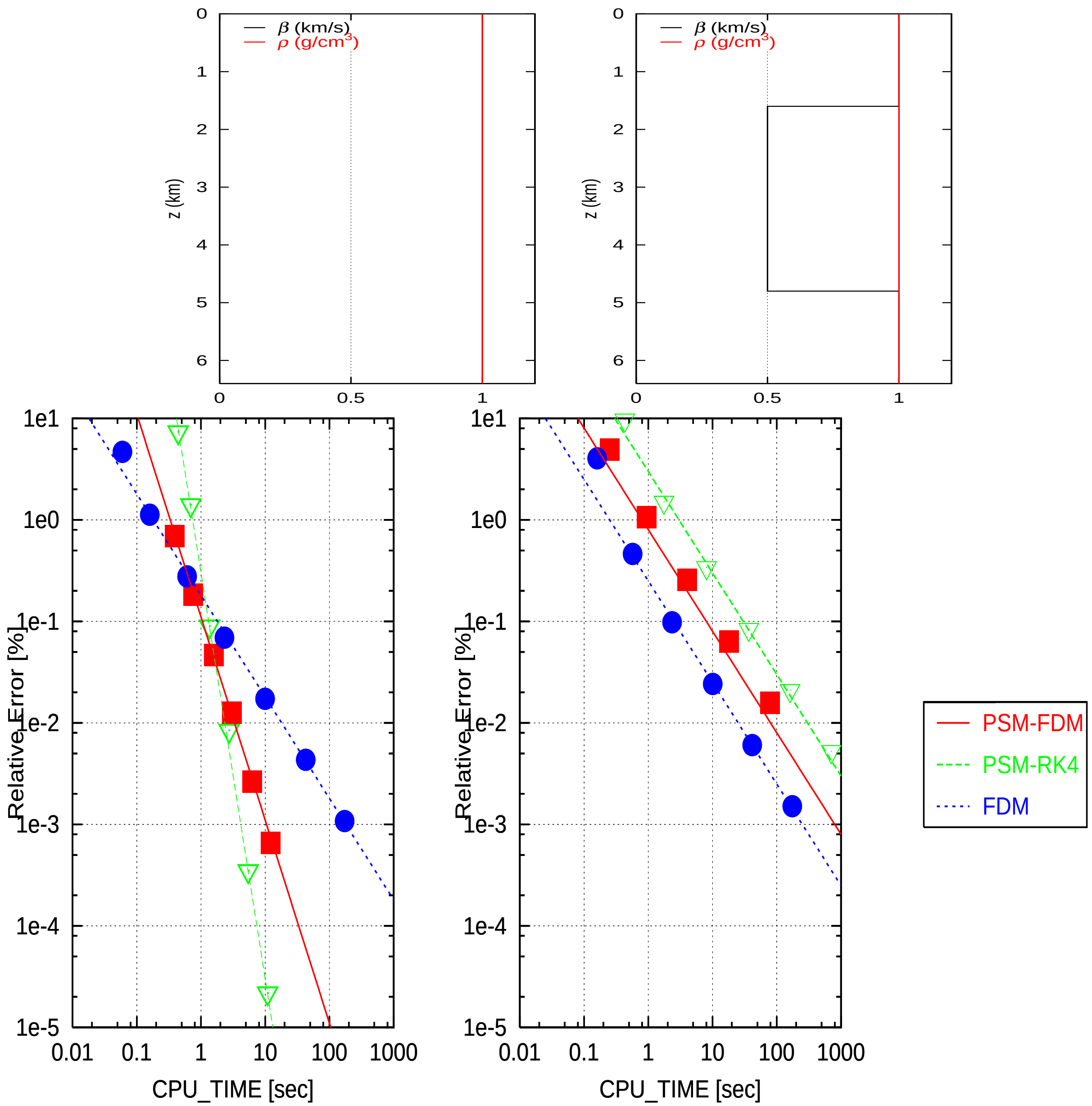
Comparison of computational methods I

- Methods must be evaluated for heterogeneous cases, not just homogeneous

- Cost-performance criteria:
  1. Minimum CPU time to achieve specified accuracy

     or

  2. Smallest error for a given CPU time



Formal evaluation of solution error I

Exact

$$\left(\omega^2 \mathbf{T}^{(0)} - \mathbf{H}^{(0)}\right) \mathbf{u}^{(0)} = -\mathbf{f}^{(0)}$$

$$\begin{aligned} \mathbf{T}^{(0)}, \mathbf{H}^{(0)} &= \text{Exact mass, stiffness matrix} \\ \mathbf{u}^{(0)} &= \text{Exact solution} \\ \mathbf{f}^{(0)} &= \text{Exact body force} \end{aligned}$$

Numerical

$$\left(\omega^2 \mathbf{T} - \mathbf{H}\right) \mathbf{u} = -\mathbf{f}$$

$$\begin{aligned} \mathbf{T} = \mathbf{T}^{(0)} + \delta\mathbf{T} &: \text{Numerical mass matrix} \\ \mathbf{H} = \mathbf{H}^{(0)} + \delta\mathbf{H} &: \text{Numerical stiffness matrix} \\ \mathbf{u} = \mathbf{u}^{(0)} + \delta\mathbf{u} &: \text{Numerical solution} \\ \mathbf{f} = \mathbf{f}^{(0)} + \delta\mathbf{f} &: \text{Numerical body force} \end{aligned}$$

Formal evaluation of solution error II

Using the 1st order Born approximation, we estimate the error of the numerical solution $\delta\mathbf{u}$ as:

$$\delta\mathbf{u} = -\left(\omega^2\mathbf{T}^{(0)} - \mathbf{H}^{(0)}\right)^{-1}\left(\omega^2\delta\mathbf{T} - \delta\mathbf{H}\right)\mathbf{u}^{(0)}$$

We formally expand the numerical solution in the normal mode basis:

$$\mathbf{u} = \sum_m c_m \mathbf{u}_m$$

where $\mathbf{u}_m$ are the eigenfunctions. c_m are the expansion coefficients, and ω_m (used in the next slide) are the corresponding eigenfrequencies. (Note: In this presentation we neglect the force term, which is handled in basically the same way.)

Formal evaluation of solution error III

We obtain

$$\text{Solution error} = \frac{|\delta \mathbf{u}|}{|\mathbf{u}^{(0)}|} = \left| \frac{\omega^2 \delta T_{mm} - \delta H_{mm}}{\omega^2 - \omega_m^2} \right|$$

$$= |\delta T_{mm}| \left| \frac{\omega^2 - \delta H_{mm}/\delta T_{mm}}{\omega^2 - \omega_m^2} \right|$$

where $\delta T_{mm} = \mathbf{u}_m^T \delta \mathbf{T} \mathbf{u}_m$, $\delta H_{mm} = \mathbf{u}_m^T \delta \mathbf{H} \mathbf{u}_m$.

To achieve optimal accuracy, the numerical operators should satisfy

$$\omega_m^2 \delta T_{mm} - \delta H_{mm} \approx 0.$$

For operators that satisfy this criterion the solution error is

$$\text{solution error} \approx |\delta T_{mm}|\,.$$

Example: 1-D Homogeneous case

$$\mathbf{H} = \frac{\mu}{\Delta z}\begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}$$

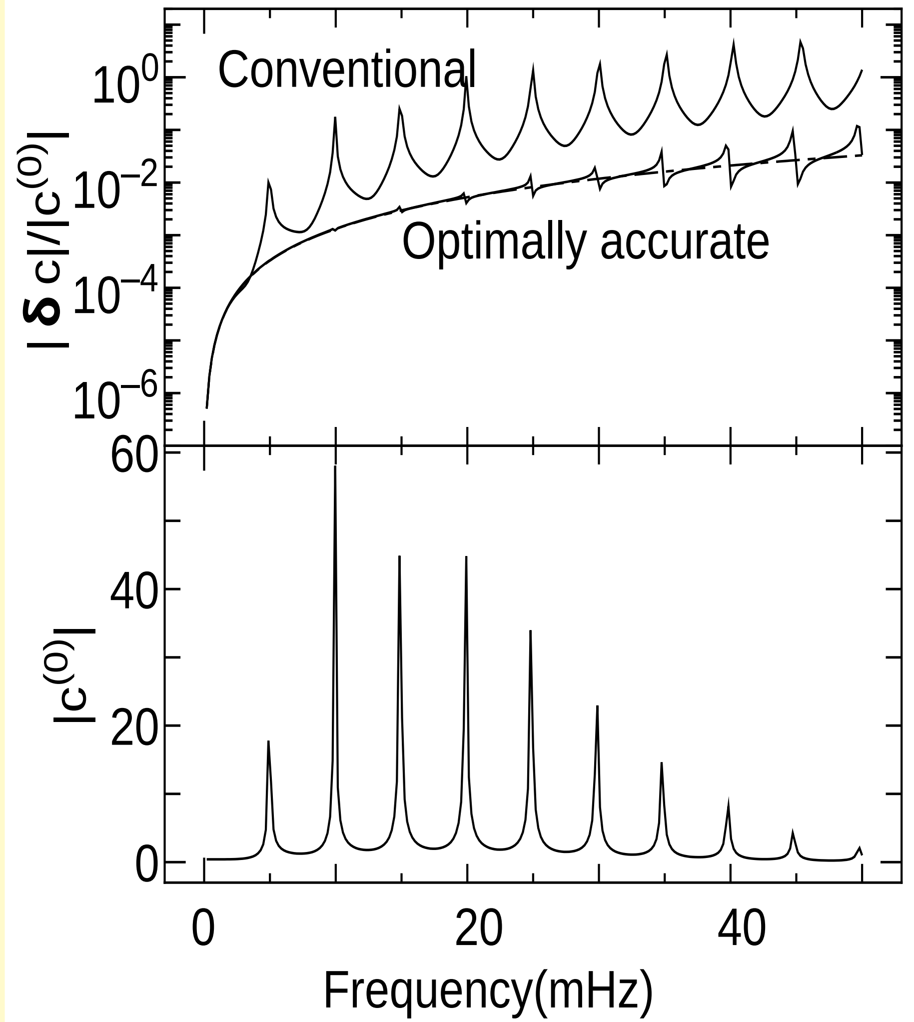
Conventional

$$\mathbf{T} = \rho\Delta z \begin{pmatrix} \frac{1}{3} & \frac{1}{6} & & & \\ \frac{1}{6} & \frac{4}{6} & \frac{1}{6} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{6} & \frac{4}{6} & \frac{1}{6} \\ & & & \frac{1}{6} & \frac{1}{3} \end{pmatrix}$$

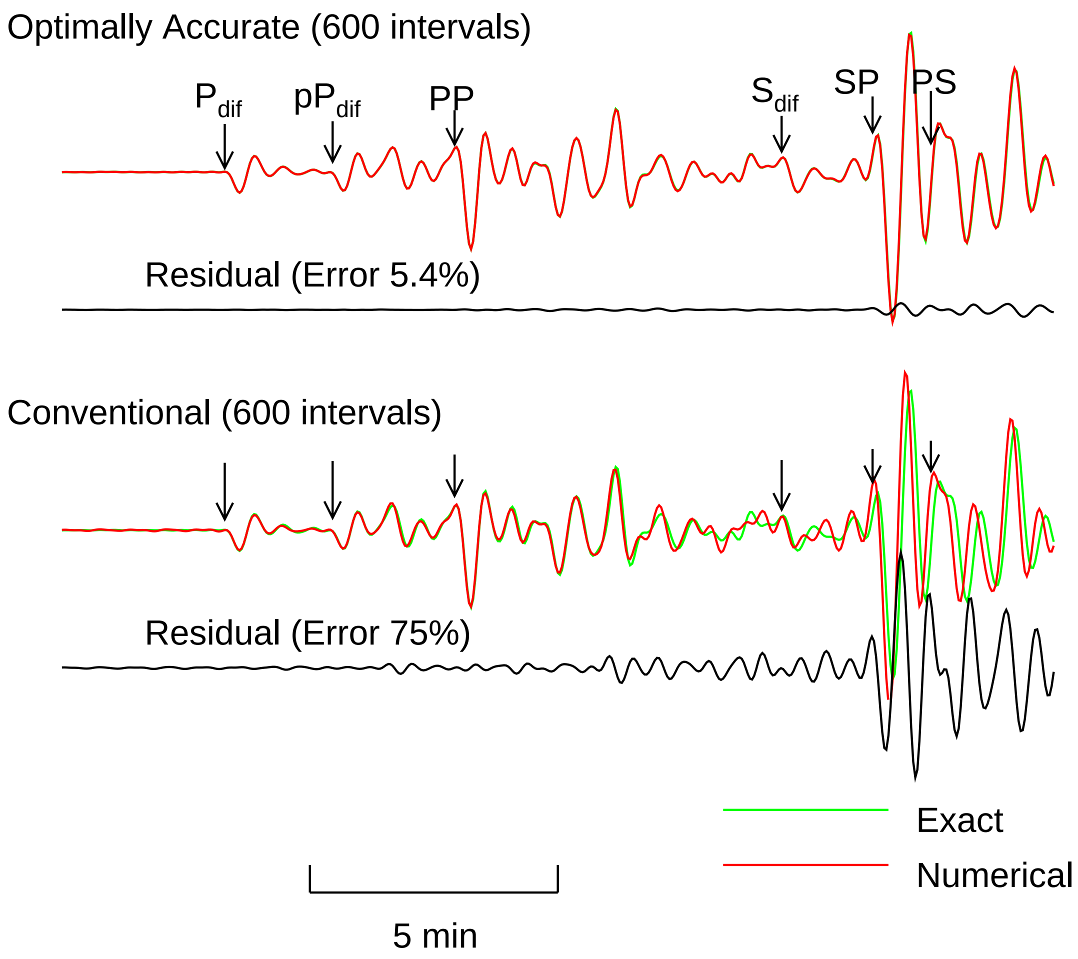
Optimally accurate

$$\mathbf{T} = \rho\Delta z \begin{pmatrix} \frac{5}{12} & \frac{1}{12} & & & \\ \frac{1}{12} & \frac{10}{12} & \frac{1}{12} & & \\ & \ddots & \ddots & \ddots & \\ & & \frac{1}{12} & \frac{10}{12} & \frac{1}{12} \\ & & & \frac{1}{12} & \frac{5}{12} \end{pmatrix}$$

The above operators approximately satisfy the general criterion for optimal accuracy.



Example: Whole Earth Model



Solution error is reduced by a factor of about 15 without increasing CPU time.

How much accuracy do we need?

- Each user can select the accuracy level depending on the application.

- For waveform inversion, the misfit will probably be between 10% and 2%, so the accuracy of the synthetics should probably be between 1% and 0.2%.

- Optimally accurate schemes allow estimates of relative error (as a function of frequency and grid size) before calculations are made.

Boundary error vs. Basic error

We divide the operator error into two parts

$$
\begin{aligned}
(\text{operator error})_m &= \left[\omega_m^2 \delta\mathbf{T} - \delta\mathbf{H}\right] \mathbf{u}_m \\
&= (\text{“Basic error”})_m + (\text{“Boundary error”})_m
\end{aligned}
$$

To satisfy the criterion for optimal accuracy we require

$$
\mathbf{u}_m^T \left[(\text{“Basic error”})_m + (\text{“Boundary error”})_m\right] \approx 0.
$$

But actually as long as $(\text{“Basic error”})_m = 0$, it's OK if $(\text{“Boundary error”})_m \neq 0$, as long as it's small.

The explanation is a bit complicated. Please trust me for now. We'll come back to this if time permits.

Physical interpretation

Criterion for optimally accurate operators:

$$\omega_m^2 \delta T_{mm} - \delta H_{mm} \approx 0 \tag{1}$$

Error in eigenfrequency due to errors in numerical operators (1st order perturbation theory):

$$-2\omega_m \delta\omega_m \approx \omega_m^2 \delta T_{mm} - \delta H_{mm} \tag{2}$$

Comparing (1) and (2), operators that satisfy (1) have

$$\delta\omega_m \approx 0$$

to lowest order.

Physical interpretation II

- One generally accepted criterion for accuracy of numerical operators is minimization of numerical dispersion of phase velocity.
- This criterion is reasonable, but can only be applied to a homogeneous medium.
- Minimization of the errors of the eigenvalues ($\delta\omega_m \approx 0$) is the appropriate generalization to arbitrarily heterogeneous media.

Time-domain schemes

Conventional

$\mathbf{A}^0 =$

$\frac{\rho}{\Delta t^2} \times$

$t+\Delta t$		1	
t		-2	
$t-\Delta t$		1	
	$x-\Delta x$	x	$x+\Delta x$

$\mathbf{K}^0 =$

$\frac{\mu}{\Delta x^2} \times$

$t+\Delta t$			
t	1	-2	1
$t-\Delta t$			
	$x-\Delta x$	x	$x+\Delta x$

Optimally accurate

$\mathbf{A} =$

$\frac{\rho}{\Delta t^2} \times$

$t+\Delta t$	$1/12$	$10/12$	$1/12$
t	$-2/12$	$-20/12$	$-2/12$
$t-\Delta t$	$1/12$	$10/12$	$1/12$
	$x-\Delta x$	x	$x+\Delta x$

$\mathbf{K} =$

$\frac{\mu}{\Delta x^2} \times$

$t+\Delta t$	$1/12$	$-2/12$	$1/12$
t	$10/12$	$-20/12$	$10/12$
$t-\Delta t$	$1/12$	$-2/12$	$1/12$
	$x-\Delta x$	x	$x+\Delta x$

Predictor-corrector scheme

To avoid implicit computation, we use a predictor-corrector scheme, where $\mathbf{A} = \mathbf{A}^0 + \delta\mathbf{A}$, $\mathbf{K} = \mathbf{K}^0 + \delta\mathbf{K}$.

$$\left(\mathbf{A}^0 - \mathbf{K}^0\right)\mathbf{u}^0 = \mathbf{f}$$

$$\left(\mathbf{A}^0 - \mathbf{K}^0\right)\delta\mathbf{u} = -\left(\delta\mathbf{A} - \delta\mathbf{K}\right)\mathbf{u}^0$$

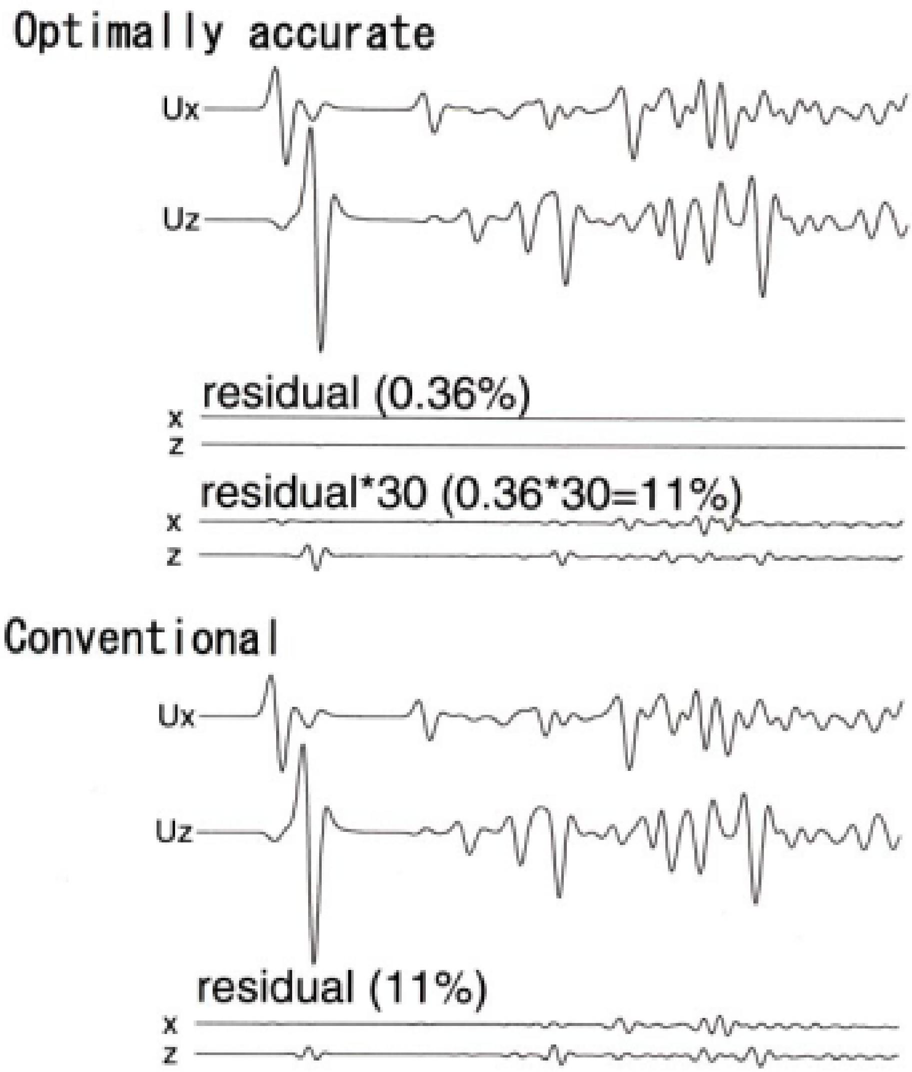
- Solve for $\mathbf{u}^0$ at each time step
- Compute $\delta\mathbf{u}$ for initial conditions

$$\delta\mathbf{u}(x,t) = \delta\mathbf{u}(x,t-\Delta t) = 0$$

- Update $\mathbf{u}^0$

$$\mathbf{u}^{\mathbf{0}}(x,t+\Delta t) \leftarrow \mathbf{u}^{\mathbf{0}}(x,t+\Delta t) + \delta\mathbf{u}(x,t+\Delta t)$$

Example: Time-domain FDM for 2-D P-SV



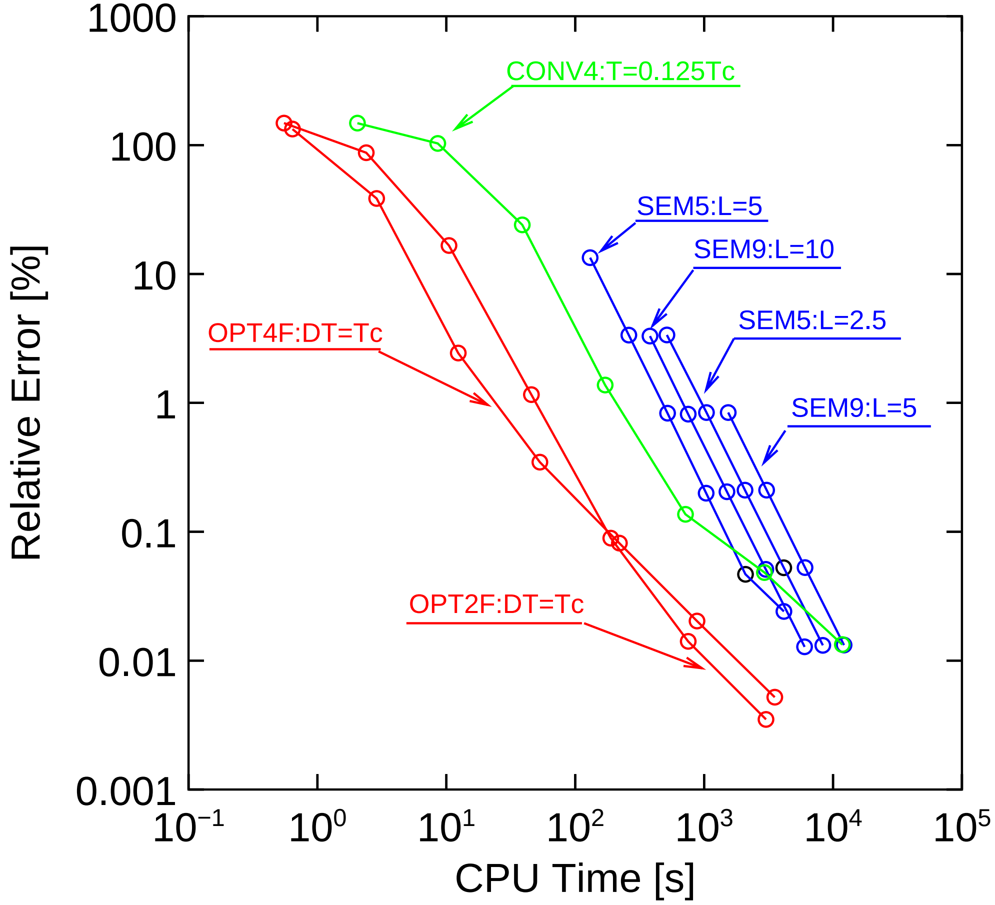
CPU time required to obtain the same accuracy (optimally accurate vs. conventional scheme):

1/47 (2-D problem)

1/100 or less (3-D problem)*

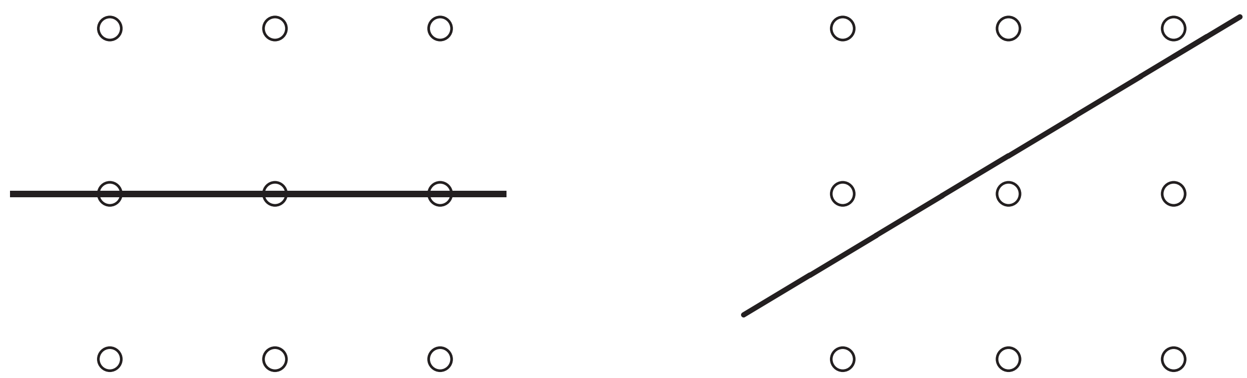
*estimate

- Performance of conventional (2,4) schemes can be improved by deriving an OPT (2,4) scheme.
- Superiority of OPT4 over CONV4 is clearcut.
- OPT2 appears preferable to OPT4 due to ease of programming, ability to handle velocity gradients, narrower memory bandwidth, etc.
- SEM performance can probably be improved by using OPT scheme for time derivatives, but probably will still underperform OPT2.



Arbitrary discontinuous boundaries

- Geller and Takeuchi (1995, 1998) and Takeuchi and Geller (2000) derived optimally accurate $O(\Delta x^2)$ operators for media with lithological discontinuities that coincide with the numerical grid.
- We can also derive optimally accurate $O(\Delta x^2)$ operators for the media with lithological discontinuities that do not coincide with the numerical grid.



Deriving numerical operators

For the local region with a discontinuity between grid points:

1. Calculate exact local matrix elements in normal mode basis

$$A_{mm}^{(0)} = \omega_m^2 T_{mm}^{(0)} - H_{mm}^{(0)}.$$

2. Derive special series expansion

3. Derive local numerical operators **T** and **H** to eliminate $O(\Delta x)$ error,

$$A_{mm} = \omega_m^2 T_{mm} - H_{mm} = A_{mm}^{(0)} + O(\Delta x^2).$$

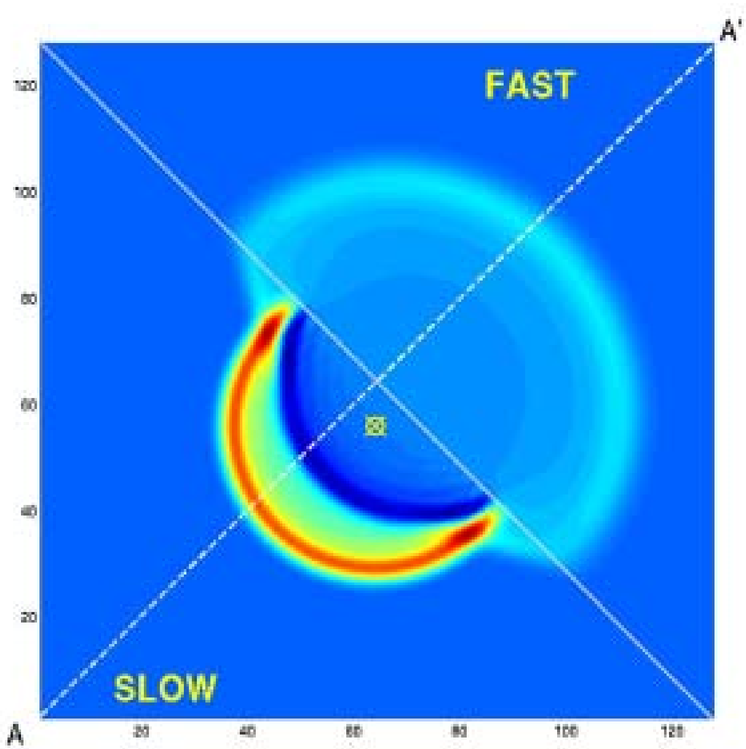
where

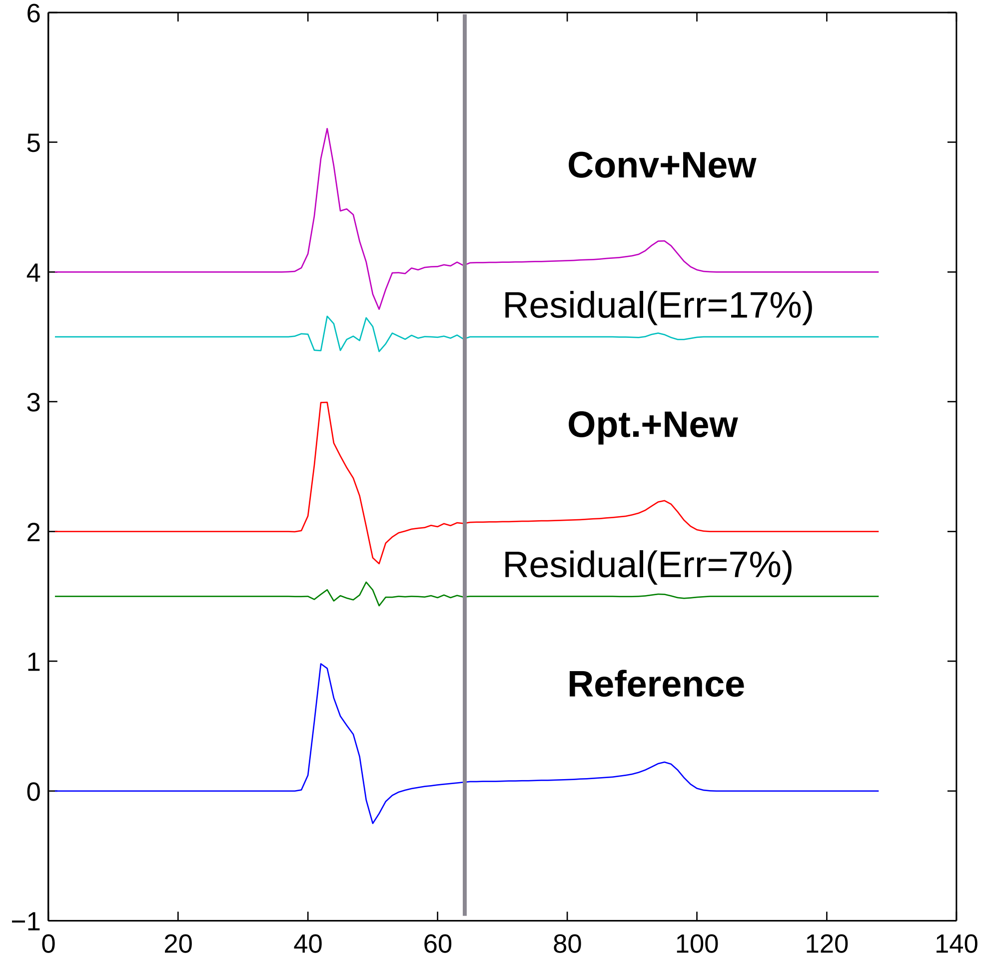
$$T_{mm} = \mathbf{u}_m^T \mathbf{T} \mathbf{u}_m, \;\; H_{mm} = \mathbf{u}_m^T \mathbf{H} \mathbf{u}_m,$$

and $\mathbf{u}_m$ is the eigenfunction in the local region.

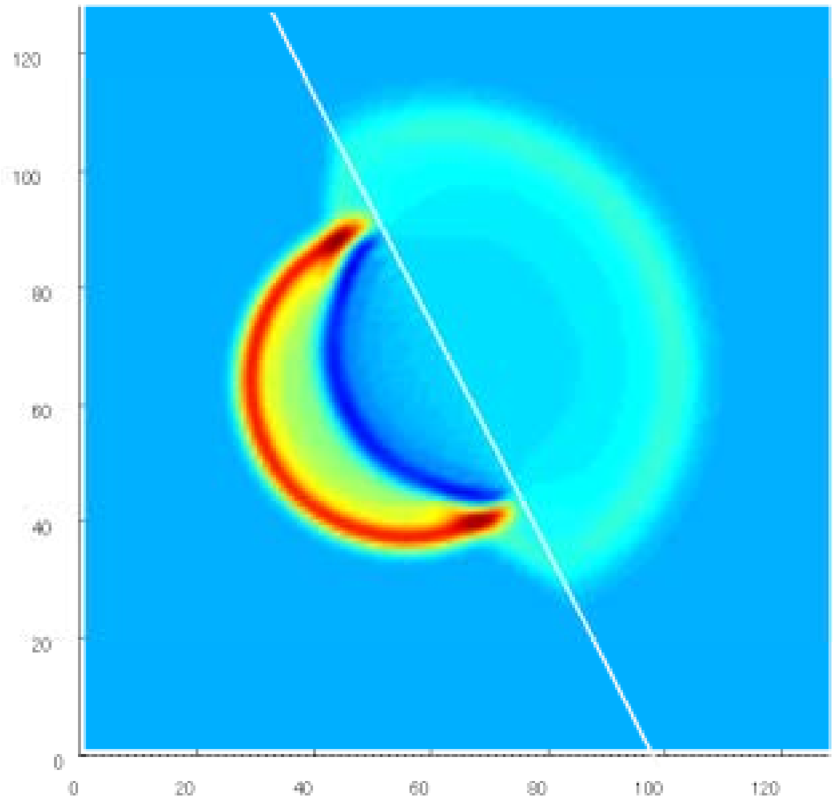
Application to 2D SH problem

The lithological discontinuity has a 45° dip and does not coincide with the numerical grid:

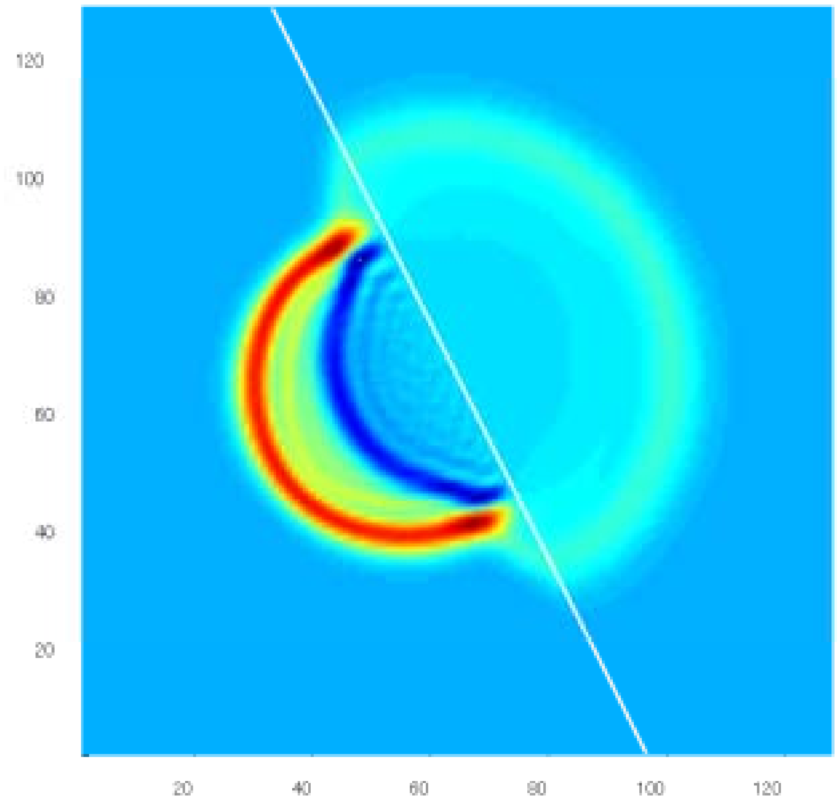




Opt. + New



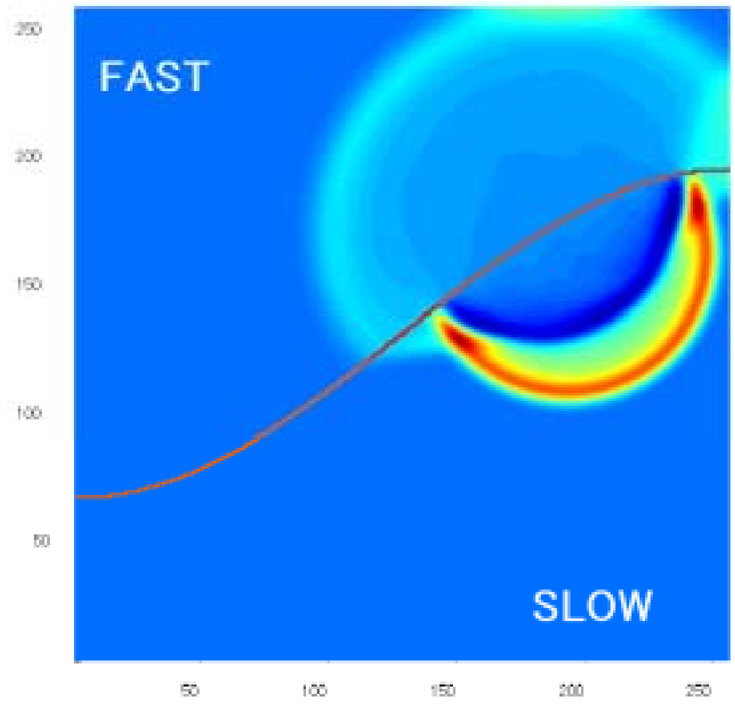
Opt. + Stair boundary



Stair boundary case has large error due to artificial diffraction.

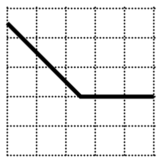
Curved boundary (2-D SH)

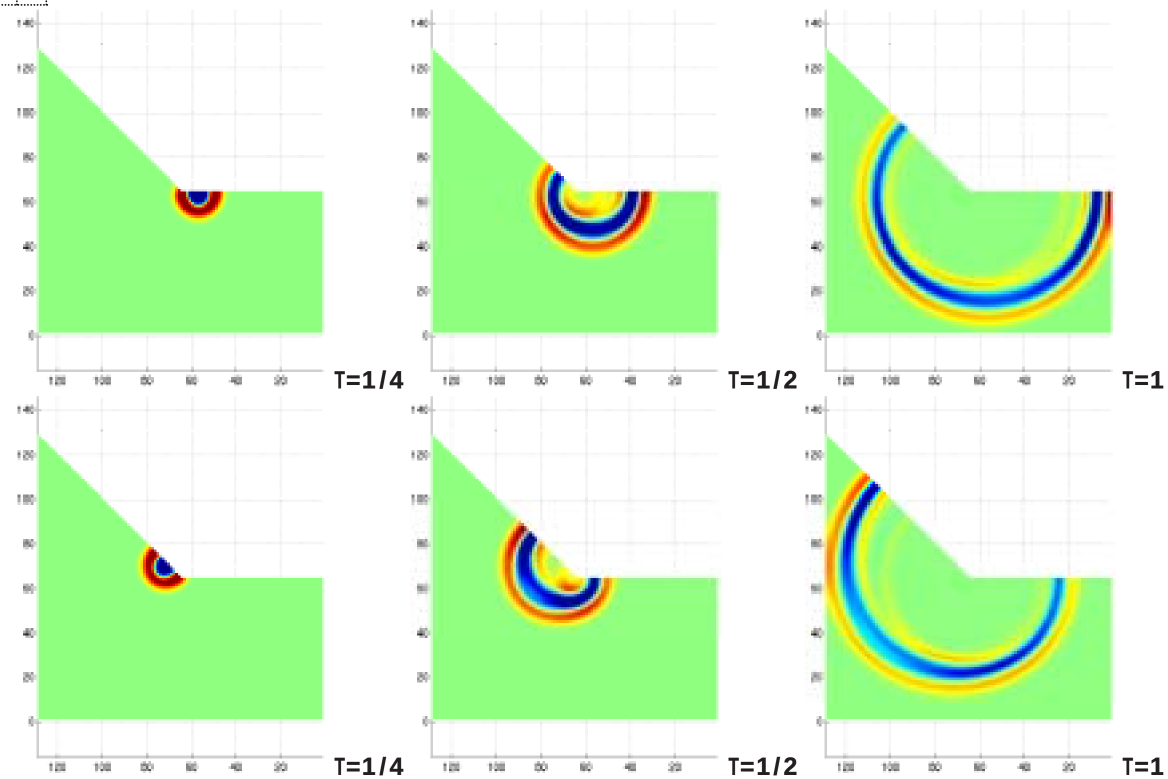
The curved lithological discontinuity does not coincide with the numerical grid:



Arbitrary free surface (2-D SH)

Freesurface does not coincide with grid (Preliminary result)





Perspectives

- FDM and FEM historically have been derived in very different ways.
- However, optimally accurate operators can be found directly by deriving operators that satisfy the general criterion.
- Many FD methods are afflicted by boundary condition problems, but the framework of this research can be used to derive accurate and stable boundary elements.

Does anyone care about accuracy?

- Many people are continuing to use non-optimally accurate FDM codes
- Inertia may be a factor–everyone wants to continue using their own codes
- But quantification of accuracy doesn’t seem to be regarded as important (“pretty good” synthetics are OK).
- Also, optimally accurate methods may be regarded as “too difficult” for students (or professors!).
- If there is actually a demand for optimally accurate codes, please let us know!

Conclusions and future research

Conclusions:

- Formal error estimates for numerical solutions
- General criterion for optimally accurate operators
- Optimally accurate computational schemes (time domain and frequency domain) for FD2, FD4 and SEM

Future Research:

- Massive parallelization
- Fluid-solid boundary, anisotropy, Q
- Waveform inversion
- Spherical coordinates