Accurate Finite Difference Schemes for Constant Density Acoustics

Mass Lumping and Stencil Coefficient Optimization

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Agenda

- Finite element (FE) methods for constant density acoustics
  - FE discretization
  - Explicit scheme of same accuracy via mass lumping
  - Numerical examples
- Stencil coefficient optimization
  - Optimization approach
  - Optimization at zero frequency
  - Optimization and mass lumping
- Future work

Previously ...

Constant density acoustic wave equation:

$$\frac{1}{c^2(x)} p_{tt}(x,t) - \nabla^2 p(x,t) = 0$$

Goals:

- Regular rectangular grids – typical for seismic numerical experiments
- Very large-scale problems $\rightsquigarrow$ coarse computational grids (a few g/p per wavelength)
- Explicit finite difference (FD) schemes
- **Want to "preserve" subgrid information** (provided analytically or on a fine grid)

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Finite Element Method

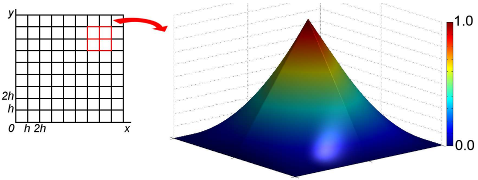
Weak formulation:

$$\int_\Omega \frac{p_{tt}(x,t)v(x)}{c^2(x)} + \int_\Omega \nabla p(x,t)\cdot\nabla v(x) = 0, \quad \forall v \in V$$

Discretization:

1. Finite-dimensional space $V := V_h$
2. Basis $\{v_1, \ldots, v_N\}$ in V_h
3. Solution represented as $p(x,t) = \sum_j \hat{p}_j(t)\, v_j(x)$

E.g.: Q^1 nodal basis functions – tensor products of 1D piecewise linear "hat" functions on a chosen grid.



Finite Element Method

Semi-discrete problem:

$$M\hat{p}_{tt} + S\hat{p} = 0, \quad \hat{p} = [\hat{p}_1, \hat{p}_2, \ldots]^T$$

$$m_{ij} = \int_\Omega \frac{v_i(x)\, v_j(x)}{c^2(x)}, \quad s_{ij} = \int_\Omega \nabla v_i(x) \cdot \nabla v_j(x)$$

Second-order discretization in time:

$$M\hat{p}^{n+1} = 2M\hat{p}^n - M\hat{p}^{n-1} - \Delta t^2 S\hat{p}^n$$

FE discretization properties:

- Stiffness matrix $S = \{s_{ij}\}$ same as 2nd order FD "cross" stencil after order-preserving numerical integration.
- 2nd order scheme for solutions smooth (bandlimited) in time, even for discontinuous $c(x)$
- **Implicit** (non-diagonal M) difference scheme

Explicit System

Mass lumping:

- Mass matrix M is replaced with a diagonal one: $\mathrm{diag}(m_1, \ldots, m_N)$
- Simplest rule: $m_i = \sum_j m_{ij}$ (P^1 or Q^1 elements)

  (more sophisticated involve Gauss-Lobatto quadrature, see Cohen 2001)

Theoretical result:

- Constant density acoustic wave equation
- Solutions *smooth in time*
- Arbitrary discontinuous coefficients ($\log c$ measurable and bounded)

THEN: mass-lumped approximation with Q^1 elements *preserves the convergence order 2*

NB (numerical result):

Replacing stiffness matrix S with a higher-order FD stencil does not change convergence order

Mass-lumped FE Using Q^1 Elements

Computationally equivalent to FD method of 2-2K order:

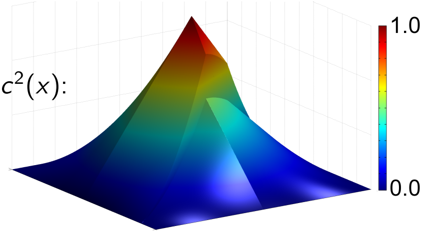
$$\hat{p}^{n+1} = 2\hat{p}^n - \hat{p}^{n-1} + \Delta t^2 (m^{-1} S)\hat{p}$$

- **Explicit** scheme
- Special stencil coefficients (averaged over elements):

$$m_i = \sum_j m_{ij} = \int_\Omega \frac{v_i(x)}{c^2(x)}$$

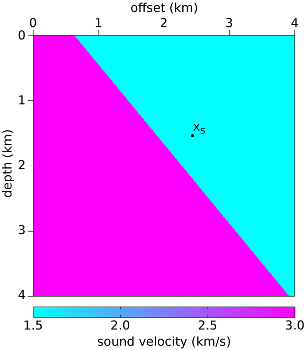
- Second order for solutions smooth (bandlimited) in time, even for discontinuous $c(x)$

$v_i(x)/c^2(x)$:



Example 1: Dipping Interface

- Domain: 4 km × 4 km
- Simulation time: 0.5 s
- Source: Ricker, 15 Hz
- Discretization: 3.33 m grid



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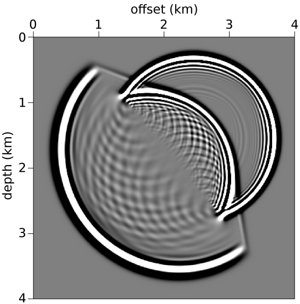
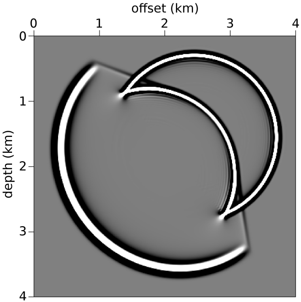
Same FLOP counts and execution times!



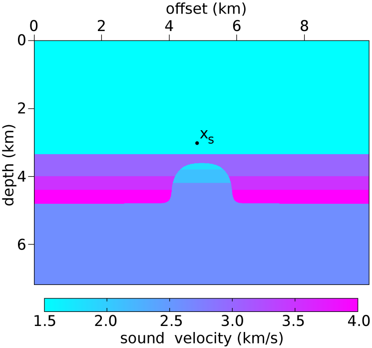
FD, 2-2



Lumped Q^1 FE, 2-4

Example 2: Dome Model

- Domain: 7 km × 4.2 km;
- Simulation time: 0.7 s
- Source: Ricker, 15 Hz
- Discretization: 10 m grid



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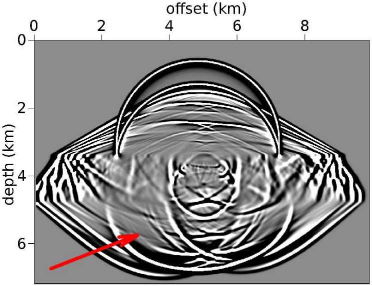
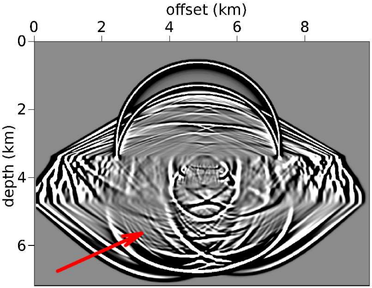


Lumped Q^1 FE, 2-8



FD, 2-8

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Stencil Coefficient Optimization

Idea:

- Modification of FD coefficients to improve scheme accuracy over a given source frequency bandwidth.
- Numerical phase or group velocity error is minimized.
- Allows coarser grids / more compact stencil.
- NB: formal scheme order is actually reduced.
- History:
  - **Holberg 1987**, Mittet et al. 1988, Kindelan et al. 1990
  - Jastram et al. 1993 – weight based on source spectrum
  - Etgen 2007 – considered spatial and temporal errors
  - Many others

Mass lumping and coefficient optimization:

- Preserving convergence rate of the standard lumped scheme?
- Optimized scheme behavior at interfaces?
- Practical applicability to real problems (coarse grids): how to choose the optimized functional?

Numerical Group and Phase Velocities

1D "2-2K" scheme:

$$\frac{p(x,t+\tau)+p(x,t-\tau)-2p(x,t)}{c^2\tau^2} =$$

$$= \frac{1}{h^2}\sum_{j=1}^{n} a_j[p(x+jh,t)+p(x-jh,t)-2p(x,t)]$$

Frequency domain:

$$\frac{\cos\omega\tau - 1}{c^2\tau^2} = \frac{1}{h^2}\sum_{j=1}^{n} a_j[\cos kjh - 1],$$

$$\omega[\mathbf{a},c,h,\nu](k) = \frac{c}{\nu h}\arccos\Big(1+\nu^2\sum_{j=1}^{n} a_j[\cos kjh - 1]\Big)$$

where $\nu = c\tau/h$ denotes the Courant number.

Numerical velocities: $v_{gr} = \frac{\partial\omega}{\partial k}, \quad v_{ph} = \frac{\omega}{k}$

Optimization

Numerical scheme is improved by minimizing weighted error $E[\mathbf{a}](\kappa)$:

$$\hat{\mathbf{a}} = \underset{\mathbf{a}\in\Omega}{\text{argabsmin}} \left\| W(\kappa)\, E[\mathbf{a}](\kappa) \right\|_{L^p[\kappa_0,\kappa_1]},$$

where $\kappa = kh$ ($\kappa = \pi$ corresponds to the Nyquist wavenumber).

E.g., minimization of the phase velocity error:

$$E_{ph}[\mathbf{a}](\kappa) = 1 - \frac{v_{\mathrm{ph}}[\mathbf{a}, c, \nu](\kappa)}{c},$$
$$\Omega = \left\{ \mathbf{a} \in \mathbb{R}^n \;:\; v_{\mathrm{ph}}[\mathbf{a}, c, \nu](\kappa) \in \mathbb{R},\;\; \forall\kappa \right\}.$$

Convergence study ($\tau, h \to 0$) is equivalent to $\kappa_0, \kappa_1 \to 0$ (assuming fixed, limited bandwidth source).

Therefore, it is reasonable to investigate $E[\mathbf{a}](\kappa)$ as $\kappa \to 0$

0-minimized Schemes

Taylor expansion of numerical phase velocity at $\kappa = 0$:

$$v_{\mathrm{ph}}[\mathbf{a}, c, \nu](\kappa) =$$

$$= c \left(\sum_{j=1}^{n} j^2 a_j \right)^{1/2} [1 + \kappa^2 R_2 + \kappa^4 R_4 + \ldots + \kappa^{2m} R_{2m} + \mathrm{O}(\kappa^{2m+2})]$$

Minimization around zero frequency leads to:

$$c \left(\sum_{j=1}^{n} j^2 a_j \right)^{1/2} [1 + \kappa^2 R_2 + \kappa^4 R_4 + \ldots + \kappa^{2m} R_{2m}] = c$$

Therefore:

$$\left(\sum_{j=1}^{n} j^2 a_j \right)^{1/2} = 1$$

$$R_2 = 0$$

$$R_4 = 0$$

$$\vdots$$

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0-minimized Schemes

$$R_2 = \frac{1}{24}\left[\nu^2 \sum_{j=1}^{n} j^2 a_j - \frac{\sum_{j=1}^{n} j^4 a_j}{\sum_{j=1}^{n} j^2 a_j}\right],$$

$$R_4 = \frac{1}{16}\left[\frac{3\nu^4}{40}\left(\sum_{j=1}^{n} j^2 a_j\right)^2 - \frac{1}{72}\left(\frac{\sum_{j=1}^{n} j^4 a_j}{\sum_{j=1}^{n} j^2 a_j}\right)^2 - \frac{\nu^2}{12}\sum_{j=1}^{n} j^4 a_j + \frac{1}{45}\frac{\sum_{j=1}^{n} j^6 a_j}{\sum_{j=1}^{n} j^2 a_j}\right],$$

$$\begin{aligned}
R_6 = \frac{1}{128}\Bigg[&\frac{5\nu^6}{56}\left(\sum_{j=1}^{n} j^2 a_j\right)^3 - \frac{1}{216}\left(\frac{\sum_{j=1}^{n} j^4 a_j}{\sum_{j=1}^{n} j^2 a_j}\right)^3 + \frac{\nu^2}{45}\sum_{j=1}^{n} j^6 a_j \\
&- \frac{\nu^4}{8}\left(\sum_{j=1}^{n} j^2 a_j\right)\left(\sum_{j=1}^{n} j^4 a_j\right) + \frac{1}{135}\frac{\left(\sum_{j=1}^{n} j^4 a_j\right)\left(\sum_{j=1}^{n} j^6 a_j\right)}{\left(\sum_{j=1}^{n} j^2 a_j\right)^2} \\
&+ \frac{\nu^2}{72}\frac{\left(\sum_{j=1}^{n} j^4 a_j\right)^2}{\sum_{j=1}^{n} j^2 a_j} - \frac{1}{315}\frac{\sum_{j=1}^{n} j^8 a_j}{\sum_{j=1}^{n} j^2 a_j}\Bigg].
\end{aligned}$$

0-minimized Scheme Coefficients

a_0	-2
a_1	1
a_0	$-5/2 + 1/2\nu^2$
a_1	$4/3 - 1/3\nu^2$
a_2	$-1/12 + 1/12\nu^2$
a_0	$-49/18 + 7/9\nu^2 - 1/18\nu^4$
a_1	$3/2 - 13/24\nu^2 + 1/24\nu^4$
a_2	$-3/20 + 1/6\nu^2 - 1/60\nu^4$
a_3	$1/90 - 1/72\nu^2 + 1/360\nu^4$
a_0	$-205/72 + 91/96\nu^2 - 4/48\nu^4 + 1/288\nu^6$
a_1	$8/5 - 61/90\nu^2 + 29/360\nu^4 - 1/360\nu^6$
a_2	$-1/5 + 169/720\nu^2 - 13/360\nu^4 + 1/720\nu^6$
a_3	$8/315 - 1/30\nu^2 + 1/120\nu^4 - 1/2520\nu^6$
a_4	$-1/560 + 7/2880\nu^2 - 1/1440\nu^4 + 1/20160\nu^6$

Black color – standard FD coefficients.

Red color – corrections from minimization.

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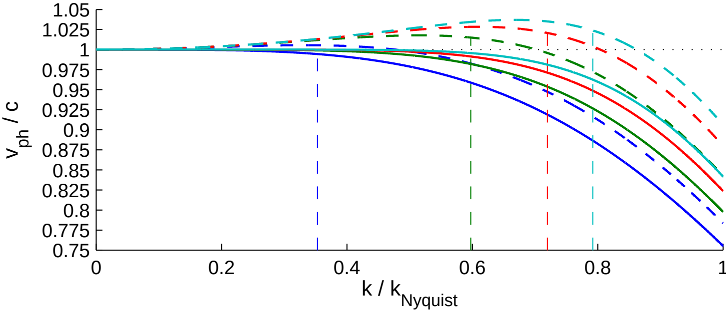
0-minimized Scheme Properties

- Stable if $\nu \leq 1$ (stability criteria for the 3-point scheme)
- "Interpolate" between higher-order schemes ($\nu = 0$) and 3-point scheme ($\nu = 1$)
- In case of the homogeneous wave equation, scheme with $2K + 1$ points is of order $2K$ both in time and space
- Coefficients can be efficiently computed "on the fly"

Numerical Velocities



Courant number $\nu = 1/2$

Solid – optimized scheme, dashed – standard scheme

Blue color – 2-4 scheme

Green color – 2-6 scheme

Red color – 2-8 scheme

Cyan color – 2-10 scheme

Mass Lumping + Optimized Coefficients

- Single interface, $c_\mathrm{l} = 1.5$ km/sec and $c_\mathrm{r} = 4.5$ km/sec
- Ricker source wavelet with 15 Hz peak frequency
- Simulation time 5.333 sec.
- Coarsest grid step 6.25 m.
- Courant number $\nu = 1/2$

Ref.	Non-opt.		Opt., original $c(x)$		Opt., lumped $c(x)$	
	RMS error	Ratio	RMS error	Ratio	RMS error	Ratio
1	$6.1 \cdot 10^{-1}$	–	$8.7 \cdot 10^{-2}$	–	$8.7 \cdot 10^{-2}$	–
2	$1.9 \cdot 10^{-1}$	3.26	$4.2 \cdot 10^{-3}$	21.0	$4.2 \cdot 10^{-3}$	20.8
4	$4.7 \cdot 10^{-2}$	4.02	$1.3 \cdot 10^{-3}$	3.27	$1.1 \cdot 10^{-3}$	3.71
8	$1.2 \cdot 10^{-2}$	4.04	$4.6 \cdot 10^{-4}$	2.76	$3.5 \cdot 10^{-4}$	3.28
16	$2.9 \cdot 10^{-3}$	3.99	$2.1 \cdot 10^{-4}$	2.19	$1.5 \cdot 10^{-4}$	2.25
32	$7.2 \cdot 10^{-3}$	4.01	$8.4 \cdot 10^{-5}$	2.49	$6.0 \cdot 10^{-5}$	2.54
64	$1.8 \cdot 10^{-4}$	3.99	$4.7 \cdot 10^{-5}$	1.78	$2.9 \cdot 10^{-5}$	2.08

NB. In case of continuous $c(x)$ 2nd order is preserved.

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Future Work

Lumping:

- First order systems (via mixed FEs) $\rightsquigarrow$ elastics

Lumping + Coefficient optimization:
more questions than answers ...

- Keeping second order of the original mass-lumped method
- Multiple dimensions
- Improving minimized functional for coarse grids

THANK YOU!