Computational Seismology: What is the best strategy for my problem?

SPIN Short Course, March 30- April 1, 2022

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Format of Short Course (approx.)

- 1 - 1.5 hour blocks with lectures
- 1 hour blocks with theoretical and computational **exercises** in breakout rooms
- **Sebastian Noe** and **Dominik Strutz** help with tutorials
- **Questions** by you (always allowed during lecture!). **Interrupt** me!

Course Content

- Part I
  - Introduction - **Motivation**
  - **Fundamentals** of wave propagation (**wave equations, analytical solutions, reciprocity, superposition principle, dispersion, homogenization**)
- Part II
  - The **finite-difference** method
  - The **pseudospectral** method
  - Linear **finite-element** method
- Part III
  - The **spectral-element** method
  - The **finite-volume** method
  - The **discontinuous Galerkin** method
  - Outlook

Introduction

Goals of lecture

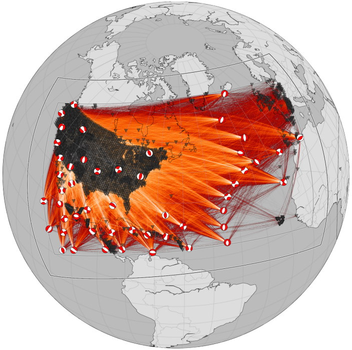
- Who needs **computational seismology**?
- What are some fundamental aspects of computational **wave propagation**?
- Is it a tough or an easy problem as far as **computational resources** are concerned?
- Which **numerical methods** are on the market, basic principles, and domains of application?
- What options do you have to get training (**Jupyter notebooks**, **COURSERA**, etc) ...?

What is Computational Seismology?

We define **computational seismology** such that it **involves the complete solution of the seismic wave propagation (and rupture) problem for arbitrary 3-D models by numerical means.**

What is not covered ... but you can do tomography with ...

- **Ray-theoretical** methods
- **Quasi-analytical** methods (e.g., normal modes, reflectivity method)
- **Frequency-domain** solutions
- **Boundary integral** equation methods
- **Discrete particle** methods



These methods are important for **benchmarking** numerical solutions!

Who needs Computational Seismology

Many problems rely on the analysis of **elastic wavefields**

- **Global seismology** and tomography of the Earth's interior
- The quantification of **strong ground motion - seismic hazard**
- The understanding of the **earthquake source process**
- The monitoring of **volcanic processes** and the forecasting of eruptions
- **Earthquake early warning** systems
- **Tsunami early warning** systems
- Local, regional, and global **earthquake services**
- Global monitoring of **nuclear tests**
- **Laboratory scale analysis** of seismic events

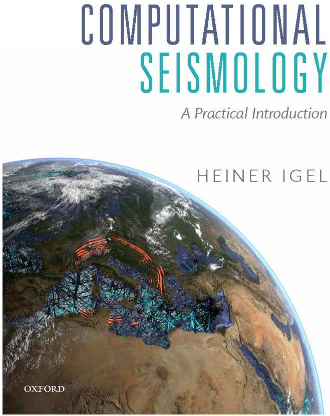
Who needs Computational Seismology (cont'd)

(...)

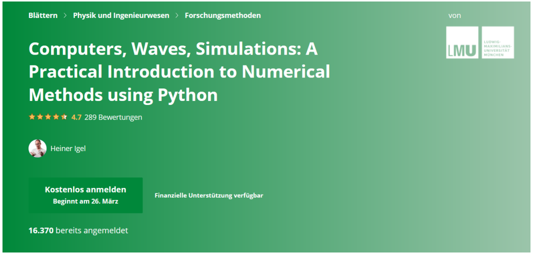
- Ocean generated **noise measurements** and cross-correlation techniques
- **Planetary seismology - Apollo, INSIGHT**
- **Exploration geophysics**, reservoir scale seismics
- **Geotechnical engineering** (non-destructive testing, small scale tomography)
- **Medical applications**, breast cancer detection, reverse acoustics

Literature

- Igel, **Computational Seismology: A Practical Introduction** (Oxford University Press, 2016)
- Shearer, **Introduction to Seismology** (3rd edition, 2019)
- Aki and Richards, **Quantitative Seismology** (1st edition, 1980)
- Mozco, **The Finite-Difference Modelling of Earthquake Motions** (Cambridge University Press)
- Fichtner, **Full Seismic Waveform Modelling and Inversion** (Springer Verlag, 2010).



9-week course in Computational wave propagation on COURSERA (free!)



Covers the finite-difference, pseudospectral, finite-element, and spectral-element method.

Why numerical methods?

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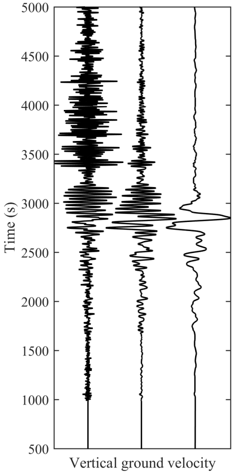
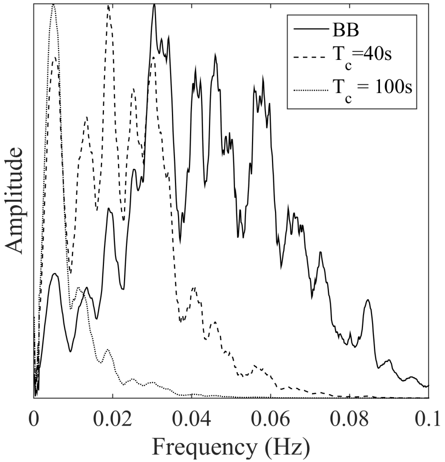
Computational Seismology, Memory, and Compute Power

Numerical solutions necessitate the discretization of Earth models. Estimate how much memory is required to store the Earth model and the required displacement fields.

Are we talking laptop or supercomputer?

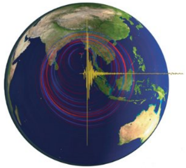
Seismic Wavefield Observations





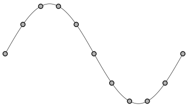
Exercise: Sampling a global seismic wavefield

- The highest frequencies that we observe for global wave fields is 1Hz.
- We assume a homogeneous Earth (radius 6371km).
- P velocity $v_p = 10km/s$ and the v_p/v_s ratio is $\sqrt{3}$
- We want to use 20 **grid points (cells) per wavelength**
- How many grid cells would you need (assume cubic cells).
- What would be their size?
- How much memory would you need to store one such field (e.g., density in single precision).



You may want to make use of

$$c = \frac{\lambda}{T} = \lambda f = \frac{\omega}{k}$$



Exercise: Solution (Matlab)

% **Earth volume**
$v_e = 4/3 * pi * 6371^3$;
% **smallest velocity (ie, wavelength)**
vp=10; vs=vp/sqrt(3);
% **Shortest Period**
T=10;
% **Shortest Wavelength**
lam=vs*T;
% **Number of points per wavelength and**
% **required grid spacing**
$nplambda = 20$;
$dx = lam/nplambda$;
% **Required number of grid cells**
$nc = v_e/(dx^3)$;
% **Memory requirement (TBytes)**
$mem = nc * 8/1000/1000/1000/1000$;

$$\text{Results } (@T = 1s): \text{ 360 TBytes}$$
$$\text{Results } (@T = 10s): \text{ 360 GBytes}$$
$$\text{Results } (@T = 100s): \text{ 360 MBytes}$$

Computational Seismology, Memory, and Compute Power

1960: 1 MFlops

1970: 10MFlops

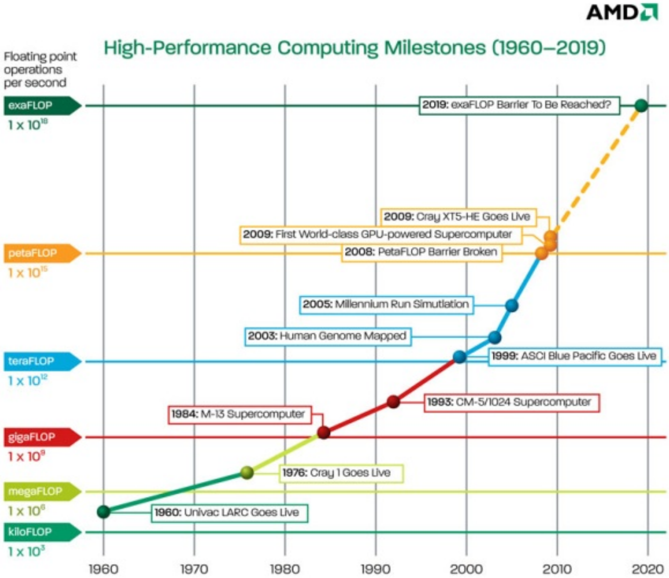
1980: 100MFlops

1990: 1 GFlops

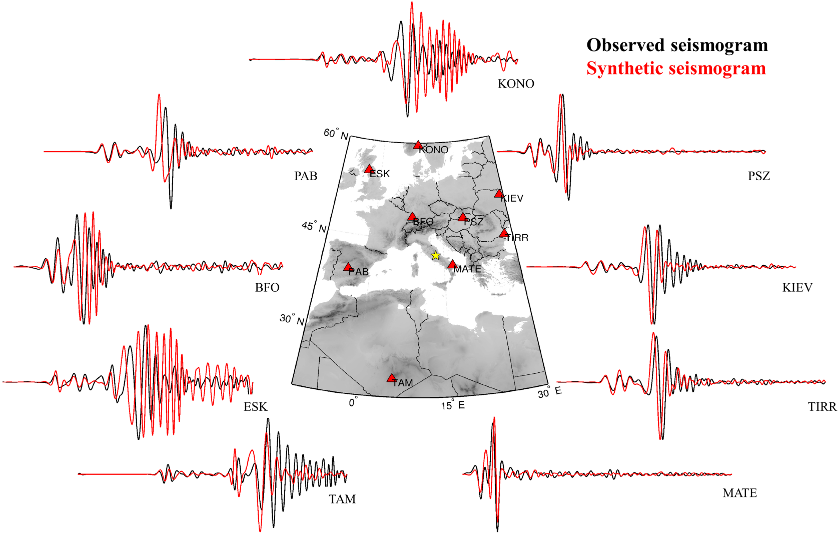
1998: 1 TFlops

2008: 1 Pflops

2021: 1 EFlops



The Ultimate Goal: Matching Wavefield Observations



A Bit of Wave Physics

Acoustic wave equation: no source

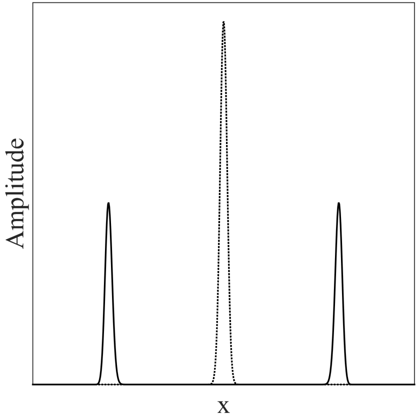
Acoustic wave equation

$$\partial_t^2 p \;=\; c^2 \Delta p + s$$

$p \rightarrow p(\mathbf{x}, t)$, pressure
$c \rightarrow c(\mathbf{x})$, velocity
$s \rightarrow s(\mathbf{x}, t)$, source term

Initial conditions

$$p(\mathbf{x}, t = 0) \;=\; p_0(\mathbf{x}, t)$$
$$\partial_t p(\mathbf{x}, t = 0) \;=\; 0$$



Snapshot of $p(\mathbf{x}, t)$ (solid line) after some time for initial condition $p_0(\mathbf{x}, t)$ (Gaussian, dashed line), 1D case.

Acoustic wave equation: external source

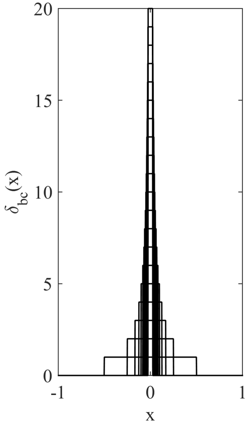
Green's Function G

$$\partial_t^2 G(\mathbf{x}, t; \mathbf{x}_0, t_0) - c^2 \Delta G(\mathbf{x}, t; \mathbf{x}_0, t_0) = \delta(\mathbf{x} - \mathbf{x}_0)\delta(t - t_0)$$

Delta function δ

$$\delta(x) = \begin{cases} \infty & x = 0 \\ 0 & x \neq 0 \end{cases}$$

$$\int_{-\infty}^{\infty} \delta(x) dx = 1 \; , \; \int_{-\infty}^{\infty} f(x)\delta(x) dx = f(0)$$



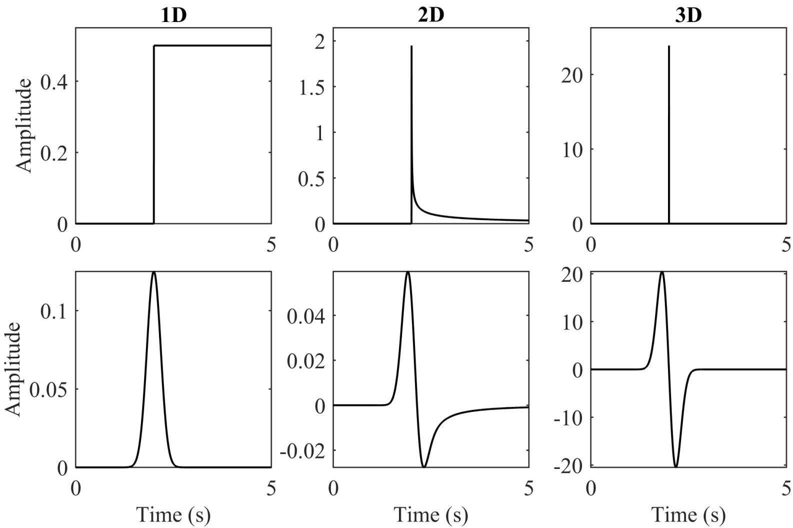
δ-generating function using boxcars.

Acoustic wave equation: analytical solutions

Green's functions for the inhomogeneous acoustic wave equation for all dimensions. $H(t)$ is the Heaviside function.

1D	2D	3D
$\frac{1}{2c}H(t-\frac{\lvert r\rvert}{c})$	$\frac{1}{2\pi c^2}\frac{H(t-\frac{\lvert r\rvert}{c})}{\sqrt{t^2-\frac{r^2}{c^2}}}$	$\frac{1}{4\pi c^2 r}\delta(t-r/c)$
$r=x$	$r=\sqrt{x^2+y^2}$	$r=\sqrt{x^2+y^2+z^2}$

Acoustic wave equation: analytical solutions



The Elastic Wave Equation

Displacement-stress formulation

$$
\begin{aligned}
\rho \partial_t^2 u_i &= \partial_j(\sigma_{ij} + M_{ij}) + f_i \\
\sigma_{ij} &= \lambda \epsilon_{kk} \delta_{ij} \; + \; 2\, \mu \epsilon_{ij} \\
\epsilon_{kl} &= \frac{1}{2}(\partial_k u_l + \partial_l u_k),
\end{aligned}
$$

Dependencies

$$
\begin{array}{lll r c l}
u_i & \rightarrow & u_i(\mathbf{x}, t) & i & = & 1,2,3 \\
v_i & \rightarrow & v_i(\mathbf{x}, t) & i & = & 1,2,3 \\
\sigma_{ij} & \rightarrow & \sigma_{ij}(\mathbf{x}, t) & i,j & = & 1,2,3 \\
\epsilon_{ij} & \rightarrow & \epsilon_{ij}(\mathbf{x}, t) & i,j & = & 1,2,3 \\
\rho & \rightarrow & \rho(\mathbf{x}) & & & \\
c_{ijkl} & \rightarrow & c_{ijkl}(\mathbf{x}) & i,j,k,l & = & 1,2,3 \\
f_i & \rightarrow & f_i(\mathbf{x}, t) & i & = & 1,2,3 \\
M_{ij} & \rightarrow & M_{ij}(\mathbf{x}, t) & i,j & = & 1,2,3,
\end{array}
$$

1-D elastic wave equation

Shear Motion

$$\rho(x)\partial_t^2 u(x,t) = \partial_x \left[\mu(x)\partial_x u(x,t)\right] \; + \; f(x,t)$$

u displacement

f external force

ρ mass density

μ shear modulus

Velocity - Stress Formulation

Defining velocity v and stress component σ as

$$\begin{aligned} \partial_t u &= v \\ \sigma &= \mu \partial_x u \end{aligned}$$

and assuming space-time dependencies leads to the wave equation

$$\begin{aligned} \rho \partial_t v &= \partial_x \sigma + f \\ \dot{\sigma} &= \mu \partial_x v \end{aligned}$$

Our unknown solution vector is

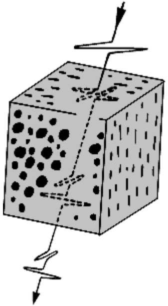
$$\mathbf{q}(x, t) = (v, \sigma)$$

Rheologies

In order of relevance

- Viscoelasticity
- Anisotropy
- Poroelasticity
- Plasticity

Anisotropy



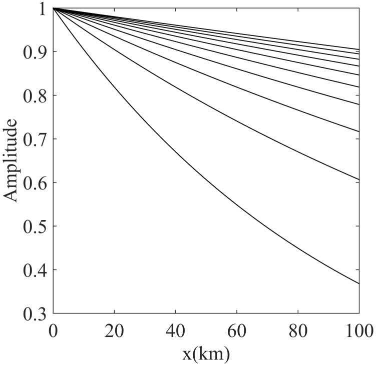
Attenuation

Amplitude decay

$$\frac{1}{Q(\omega)} = -\frac{\Delta E}{2\pi E}$$

$$A(x) = A_0 e^{-\frac{\omega x}{2cQ}}$$

Examples



Anisotropy

Generalized Hooke's Law

$$\sigma_{ij} = c_{ijkl}\,\epsilon_{kl}, \quad i,j,k,l = 1,2,3$$

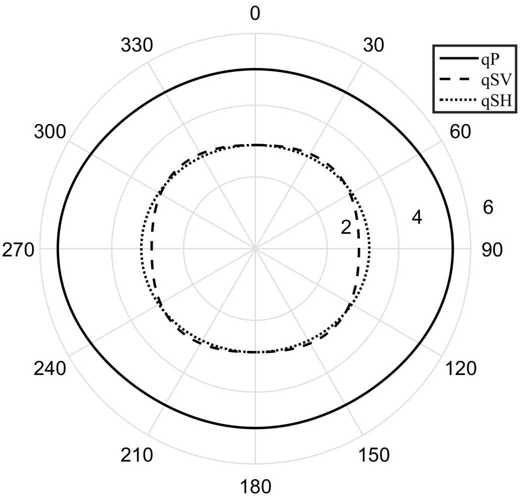
Reduced notation (Kelvin-Voight)

$$c_{pq} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{c_{11}-c_{12}}{2} \end{pmatrix}$$

Velocity variations (Thomson parameters)

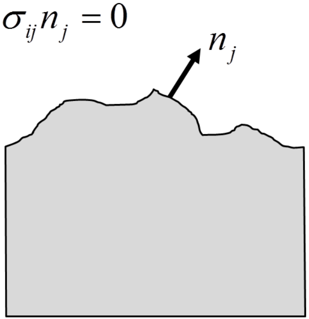
$$\begin{aligned} v_{qP}(\theta) &= v_{P0}\left(1 + \delta\sin^2(\theta)\cos^2(\theta) + \epsilon\sin^4(\theta)\right) \\ v_{qSV}(\theta) &= v_{S0}\left(1 + \frac{v_{P0}^2}{v_{S0}^2}(\epsilon - \delta)\sin^2(\theta)\cos^2(\theta)\right) \\ v_{qSH}(\theta) &= v_{S0}\left(1 + \gamma\sin^2(\theta)\right) \end{aligned} \tag{1}$$

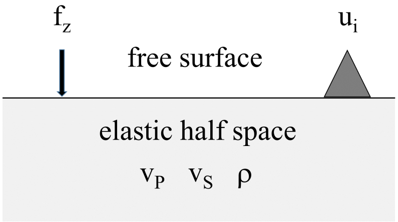
Anisotropic velocities



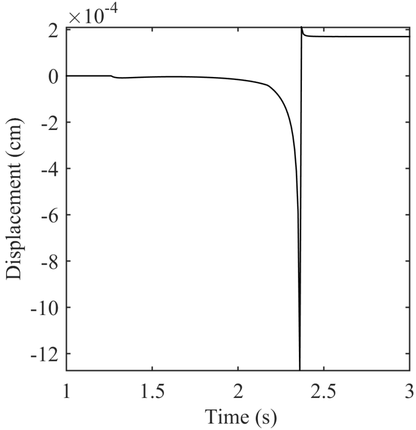
Free Surface Boundary Conditions

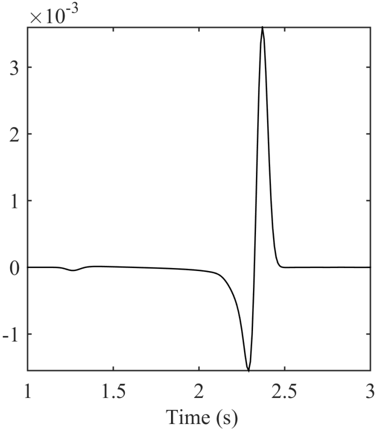
$$t_i = \sigma_{ij} n_j \quad \rightarrow \sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0$$





Lamb's Problem

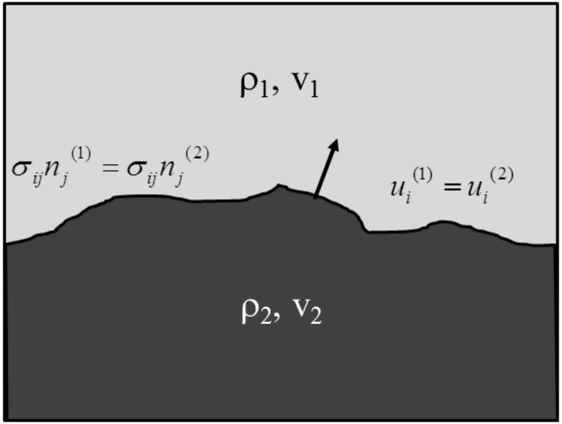




Internal Boundary Conditions

$$\sigma_{ij} n_j^{(1)} = \sigma_{ij} n_j^{(2)}$$
$$u_i^{(1)} = u_i^{(2)}$$

Internal boundary conditions need not be modelled explicitly!



Gradient, Divergence, Curl

Gradient

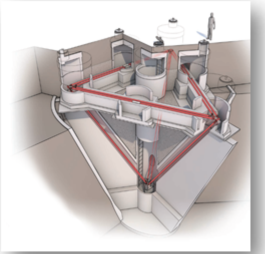
$$\nabla \mathbf{u}(\mathbf{x}, t) = \partial_j u_i(\mathbf{x}, t) \ .$$

Deformation

$$\epsilon_{ij}(\mathbf{x}, t) = \frac{1}{2}(\partial_i u_j(\mathbf{x}, t) + \partial_j u_i(\mathbf{x}, t))$$

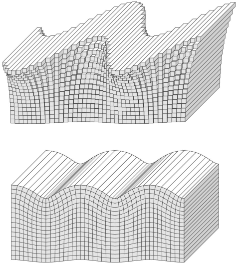
Curl

$$\frac{1}{2}\nabla \times \mathbf{u} = \frac{1}{2}\begin{pmatrix} \partial_y u_z - \partial_z u_y \\ \partial_z u_x - \partial_x u_z \\ \partial_x u_y - \partial_y u_x \end{pmatrix}$$

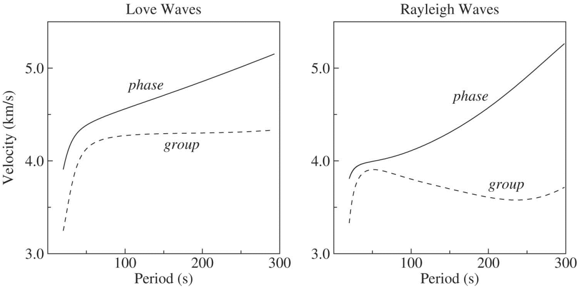


Surface Waves - Dispersion

Ralyeigh and Love Waves

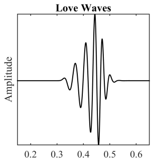


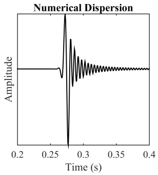
Dispersion Curves



Physical and Numerical Dispersion

Numerical Dispersion





Numerical and physical dispersion can be confused!

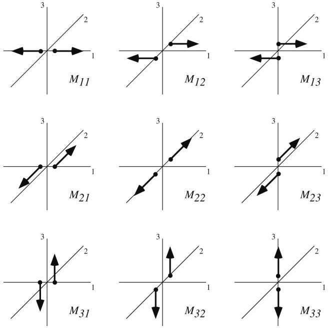
In wave simulations we have to **avoid** numerical dispersion!

The Moment Tensor

Moment Tensor

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix}$$

$$M_0 = \mu A d$$



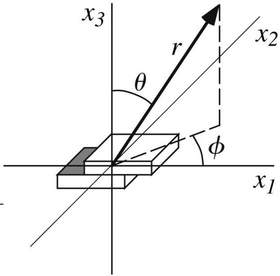
The DC analytical solution

Double Couple Green's function

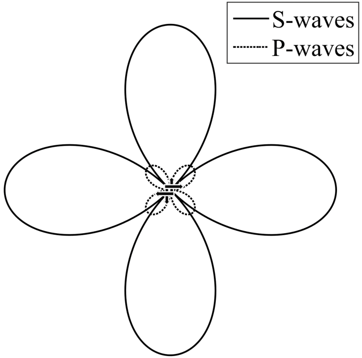
$$\boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{4\pi\rho}\boldsymbol{A}^{N}\frac{1}{r^4}\int_{r/\alpha}^{r/\beta}\tau M_0(t-\tau)d\tau +$$

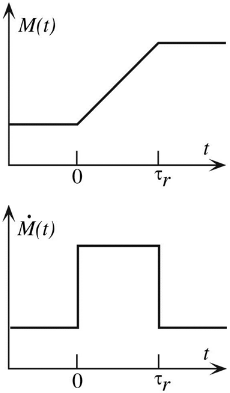
$$+\frac{1}{4\pi\rho\alpha^2}\boldsymbol{A}^{IP}\frac{1}{r^2}M_0(t-\frac{r}{\alpha}) + \frac{1}{4\pi\rho\beta^2}\boldsymbol{A}^{IS}\frac{1}{r^2}M_0(t-\frac{r}{\beta})+$$

$$+\frac{1}{4\pi\rho\alpha^3}\boldsymbol{A}^{FP}\frac{1}{r}\dot{M}_0(t-\frac{r}{\alpha}) + \frac{1}{4\pi\rho\beta^3}\boldsymbol{A}^{FS}\frac{1}{r}\dot{M}_0(t-\frac{r}{\beta})$$

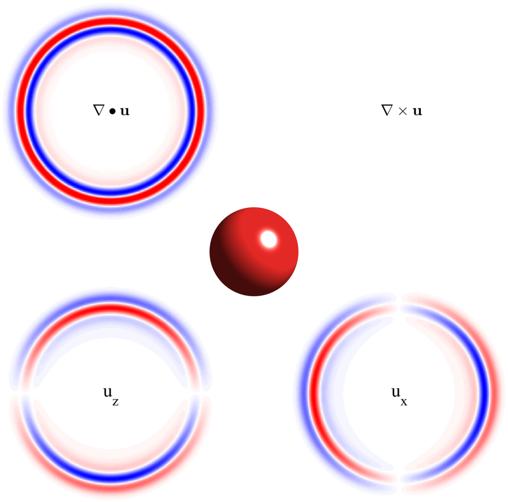


Radiation and Source Time Function

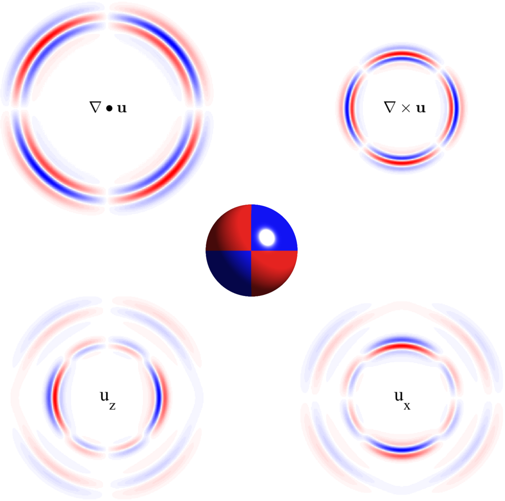




Wavefields from Moment Tensor Sources



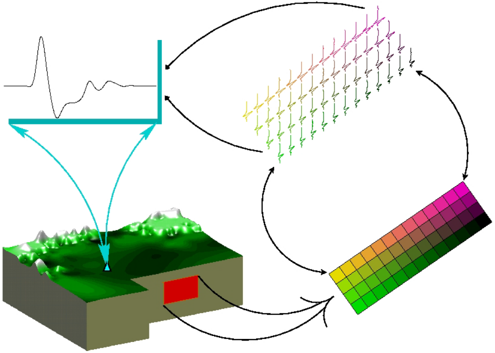
Wavefields from Moment Tensor Sources



Superposition Principle

$$v_l^r(\omega) = \sum_{k=1}^{N} \text{slip}_k \exp[-i\omega t_k(c^{rup})] G_{kl}^r(\omega) S(R, \omega)$$

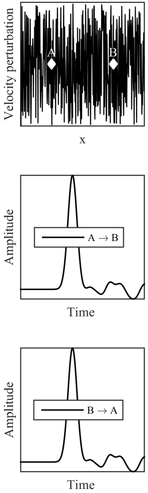
Finite sources can be simulated by summing up over point sources



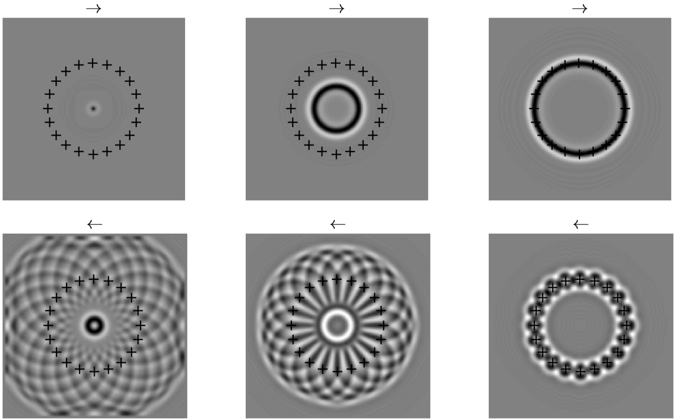
Reciprocity

$$G_{ij}(\boldsymbol{x}, t; \boldsymbol{x}_0, t_0) \;=\; G_{ji}(\boldsymbol{x}_0, -t_0; \boldsymbol{x}, -t)$$

The wave equation is symmetric in time. Source and receiver locations can be interchanged. This has dramatic consequences for modeling and inversion!



Time Reversal



it = 50 it = 100 it = 150

Wave Equation as Linear System

Seismogram for arbitrary source s(t) as convolution (exact)

$$p(\mathbf{x}, t) = G(\mathbf{x}, t, \mathbf{x}_0) \otimes s(t)$$

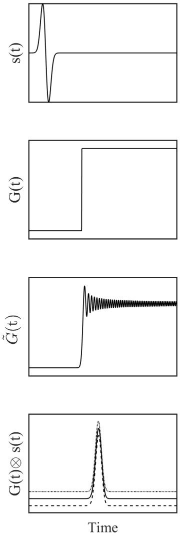
Seismogram for arbitrary source s(t) as convolution (numerical)

$$\tilde{p}(\mathbf{x}, t) = \tilde{G}(\mathbf{x}, t, \mathbf{x}_0) \otimes s(t)$$

Important consequence:

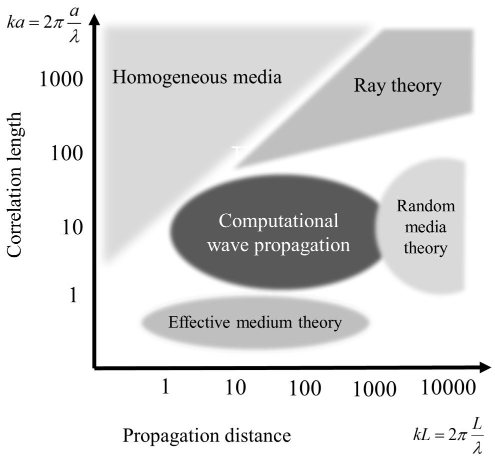
Even if your numerical Green's function $\tilde{G}(\mathbf{x}, t, \mathbf{x}_0)$ is inaccurate, the numerical solution $\tilde{p}(\mathbf{x}, t)$ might be very accurate provided the $s(t)$ is defined in the right frequency band!

Wave Equation as Linear System



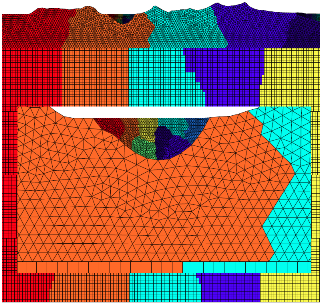
- Accurate Green's functions cannot be calculated numerically
- A numerical solver is a **linear system**
- The convolution theorem applies
- Inaccurate simulations can be filtered afterwards
- Source time functions can be altered afterwards
- ... provided the sampling is good enough ...

Spatial Scales, Scattering, Solution Strategies



- Recorded seismograms are affected by ...
- ... the ratio of seismic wavelength λ and structural wavelength *a* ...
- ... how many wavelengths are propagated ...
- strong scattering when $a \approx \lambda \rightarrow$ numerical methods
- ray theory works when $a >> \lambda$
- random medium theory necessary for strong scattering media (and long distances)

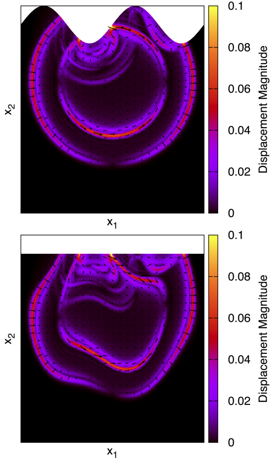
Challenges - Meshing



Human time	Simulation workflow	cpu time
15%	Design	0%
80% (weeks)	Geometry creation, meshing	10%
5%	Solver	90%

- Meshing work flow not well defined
- Still major bottleneck for simulation tasks with complex geometries
- Tetrahedral meshes easier, but ...
- Salvus?

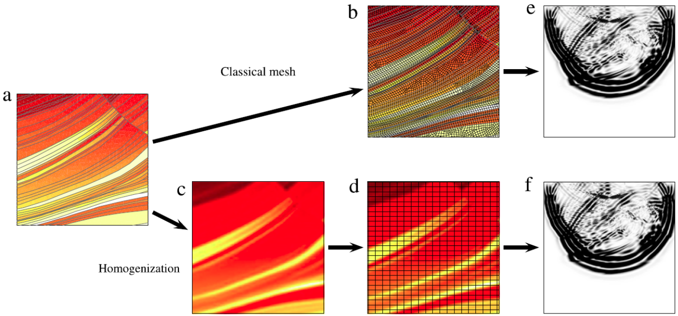
Future Strategies - Alternative Formulations



- Particle relabelling, grid stretching
- Mapping geometrical complexity onto regular grids
- Smart pre-processing rather than meshing?
- Similar concept used in summation-by-parts (SBP) algorithms (SW4)

Al-Attar and Crawford GJI 2016

Future Strategies - Homogenization



- We only *see* low-pass filtered Earth
- So why simulate models with infinite frequencies?
- Homogenisation of discontinuous model
- Renaissance of regular grid methods?

Questions?