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

CHEESE Short Course, October 31, 2025

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Introduction

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

What you get ...

- Basic ideas of **discretization**, **size** of a problem, designing a solution
- The fundamentals of **wave propagation** (what should I see in a wavefield?)
- What is in the **engine** of simulation algorithms?
- What are the major parameters, where are **dangers** and **traps**?
- What is a good strategy **to know my simulation is right**?
- What is the difference between the various approaches, **pros and cons**?
- What are the **simplest programs** to see how things work?

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- **Classic approaches** like ray tracing or reflectivity methods
- **Codes** for 3D solutions
- Beamforming

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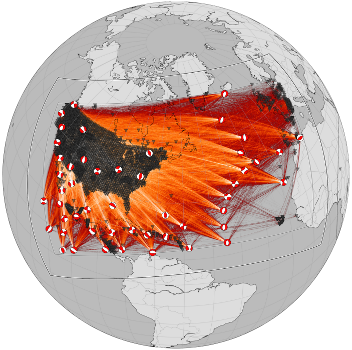
What is Computational Seismology?

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
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- **Environmental** seismology
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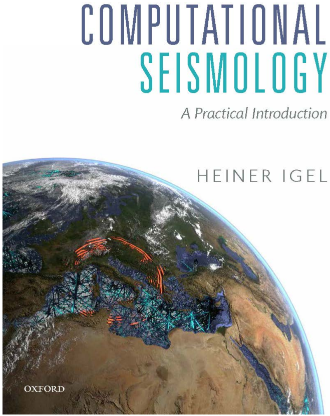

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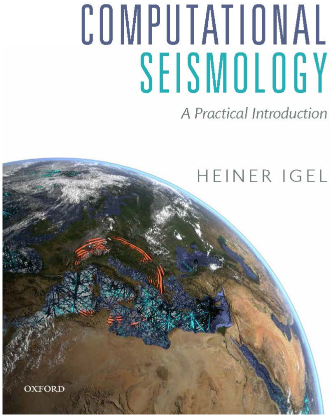

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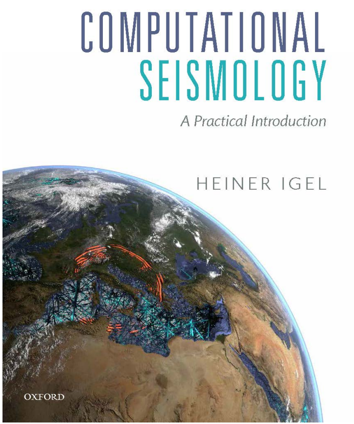

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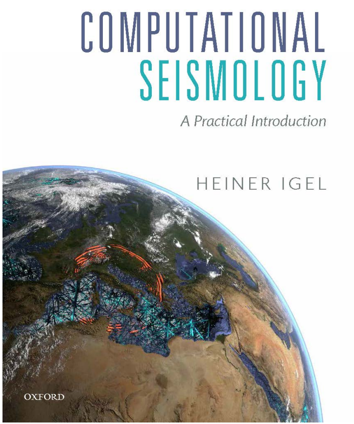

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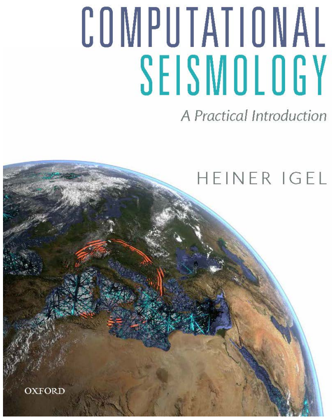
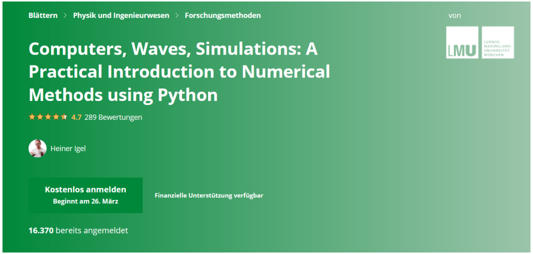


9-week course in Computational wave propagation on COURSERA (free!)



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

Why numerical methods?

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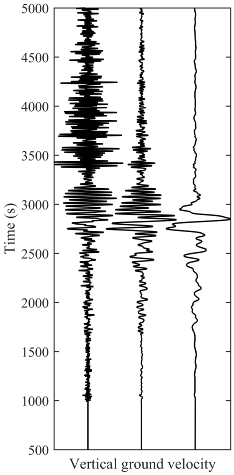
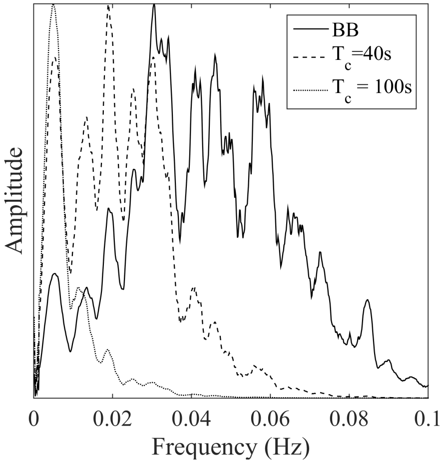
Computational Seismology, Memory, and Compute Power

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 $v_p = 10 km/s$ 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).
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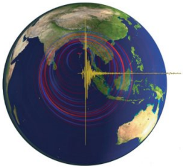

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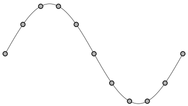

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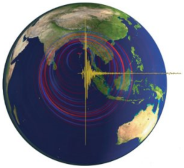

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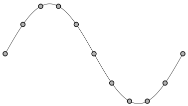

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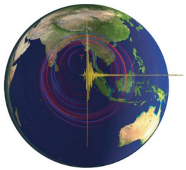

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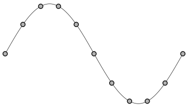

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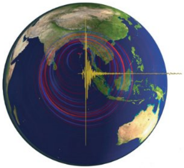

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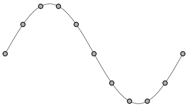

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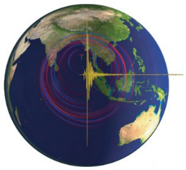

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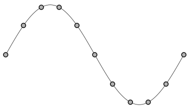

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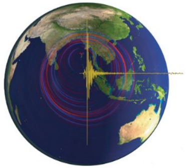

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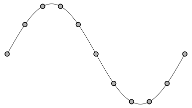

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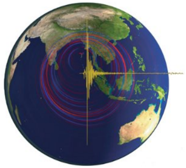

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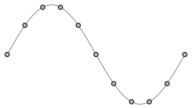


Exercise:

```
# Physics

# Earth's Velocity (S waves have smaller wavelength)
c = 10./np.sqrt(3)  # km/s

# Target Frequency
T = 1.  # Hz  (1 Hz is usually the highets frequency of global wave fields)

# Wavelength
lam = c * T   # in km

print(' Wavelength: ', lam, ' km ')
```

```
Wavelength:  5.773502691896258  km
```

```
# Computational method
npts = 20  # number of grid points per wavelength

# Required spatial discretization
dx = lam/npts # in km

# Size of a volume cell
dv = dx**3    # in km**3

print(' Size of Volume Cell',dv, 'km**3 ')
```

```
Size of Volume Cell 0.024056261216234418 km**3
```

```
# Memory requirement (Volume Earth / dv * 8 bytes)
mem = 4./3.*np.pi*6371**3/dv*8

print(' Memory requirement : ', mem/1000/1000/1000/1000, 'TBytes')
```

```
Memory requirement :  360.22452769668104 TBytes
```

Take a few minutes **with your neighbor** to think of your current or future simulation problem (whatever physical process). What is the **physical scale** of the problem? **2D or 3D**? What are the **wavelengths** involved? How much **memory** per field (elastic parameters, displacement)? **Laptop or supercomputer**?

Exercise: Solution

```
# Physics

# Earth's Velocity (S waves have smaller wavelength)
c = 10./np.sqrt(3)  # km/s

# Target Frequency
T = 1.  # Hz  (1 Hz is usually the highets frequency of global wave fields)

# Wavelength
lam = c * T   # in km

print(' Wavelength: ', lam, ' km ')
```

```
Wavelength:  5.773502691896258  km
```

```
# Computational method
npts = 20  # number of grid points per wavelength

# Required spatial discretization
dx = lam/npts # in km

# Size of a volume cell
dv = dx**3    # in km**3

print(' Size of Volume Cell',dv, 'km**3 ')
```

```
Size of Volume Cell 0.024056261216234418 km**3
```

```
# Memory requirement (Volume Earth / dv * 8 bytes)
mem = 4./3.*np.pi*6371**3/dv*8

print(' Memory requirement : ', mem/1000/1000/1000/1000, 'TBytes')
```

```
Memory requirement :  360.22452769668104 TBytes
```

Results ($@T = 1s$) : 360 TBytes

Results ($@T = 10s$) : 360 GBytes

Results ($@T = 100s$) : 360 MBytes

Computational Seismology, Memory, and Compute Power

1960: 1 MFlops

1970: 10MFlops

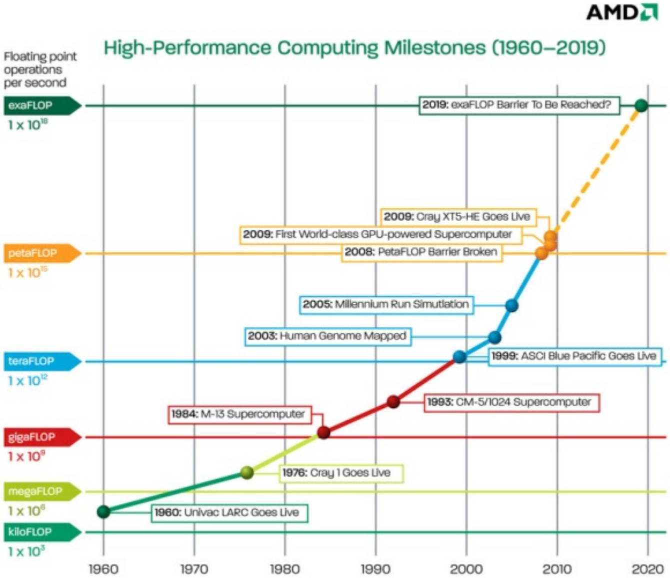
1980: 100MFlops

1990: 1 GFlops

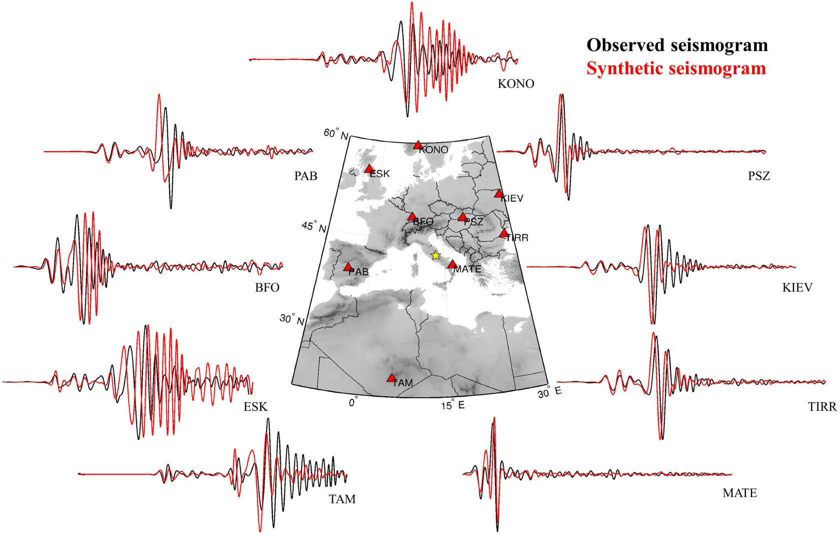
1998: 1 TFlops

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

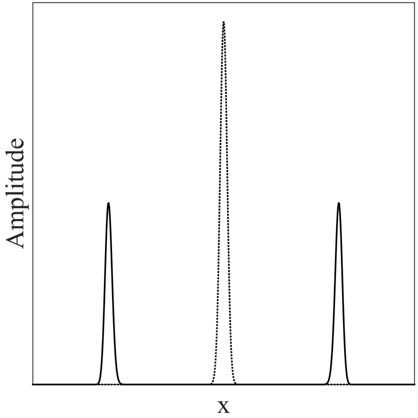
$$\partial_t^2 p \;=\; c^2 \Delta p + s$$

$p \rightarrow p(\mathbf{x}, t)$, 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

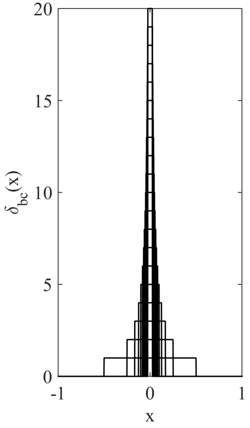
Green's Function G

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

Delta function δ

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

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



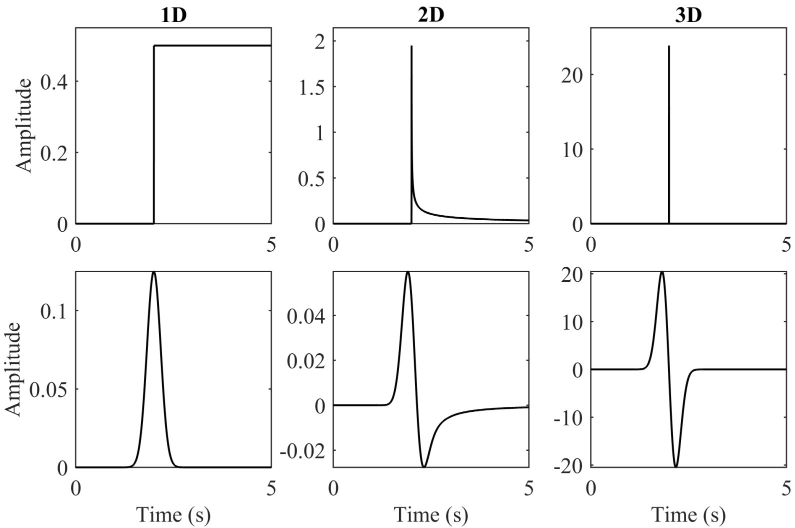
δ-generating function using boxcars.

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

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

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

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

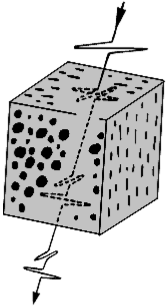
Our unknown solution vector is

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

In order of relevance

- Viscoelasticity
- Anisotropy
- Poroelasticity
- Plasticity

Anisotropy



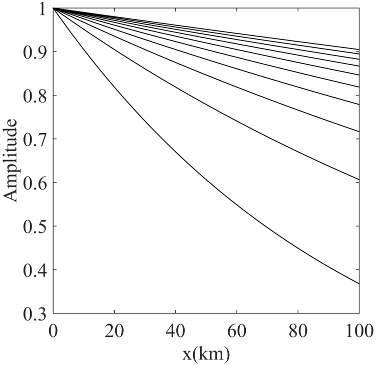
Attenuation

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

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

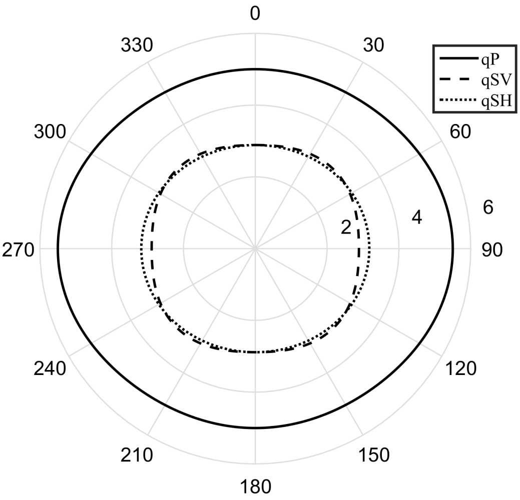
Reduced notation (Kelvin-Voight)

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

Velocity variations (Thomson parameters)

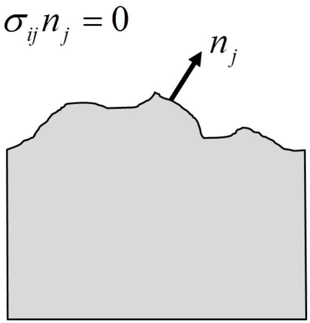
$$\begin{aligned} v_{qP}(\theta) &= v_{P0}\left(1 + \delta \sin^2(\theta)\cos^2(\theta) + \epsilon \sin^4(\theta)\right) \\ v_{qSV}(\theta) &= v_{S0}\left(1 + \frac{v_{P0}^2}{v_{S0}^2}(\epsilon - \delta)\sin^2(\theta)\cos^2(\theta)\right) \\ v_{qSH}(\theta) &= v_{S0}\left(1 + \gamma \sin^2(\theta)\right)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

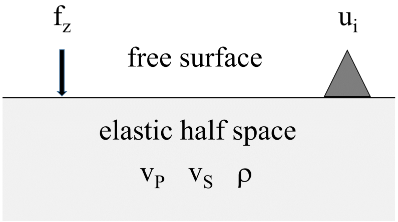
Anisotropic velocities



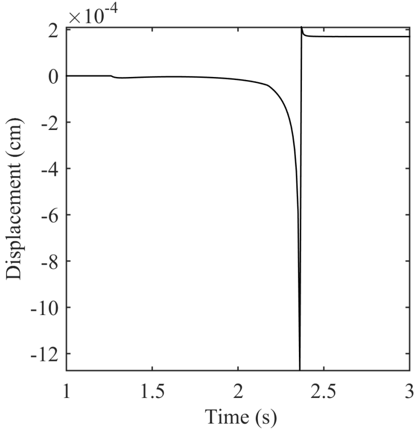
Free Surface Boundary Conditions

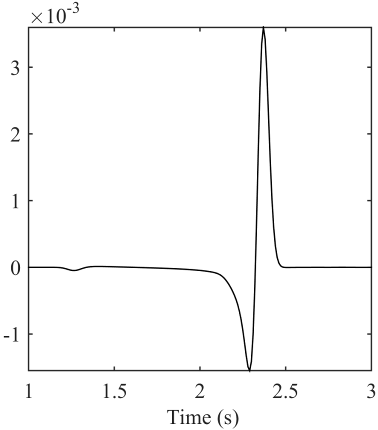
$$t_i = \sigma_{ij} n_j \quad \rightarrow \sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0$$





Lamb's Problem

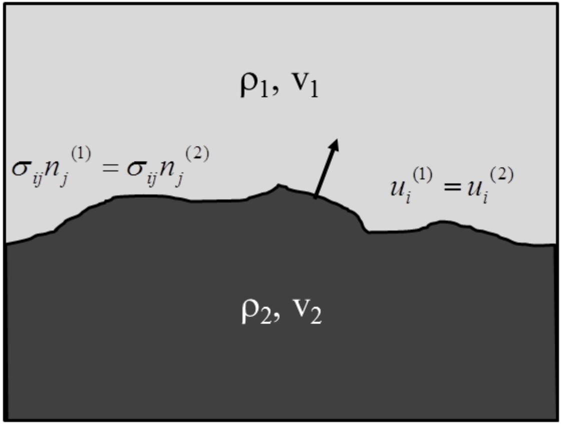




Internal Boundary Conditions

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

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

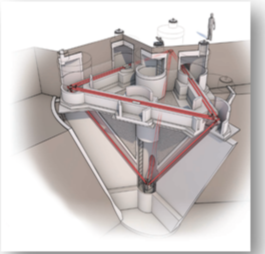
$$\epsilon_{ij}(\mathbf{x}, t) = \frac{1}{2}(\partial_i u_j(\mathbf{x}, t) + \partial_j u_i(\mathbf{x}, t))$$

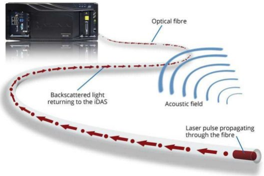
Curl

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

Divergence

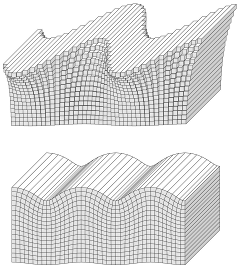
$$\nabla \mathbf{u} = \partial_x u_x + \partial_y u_y + \partial_z u_z$$



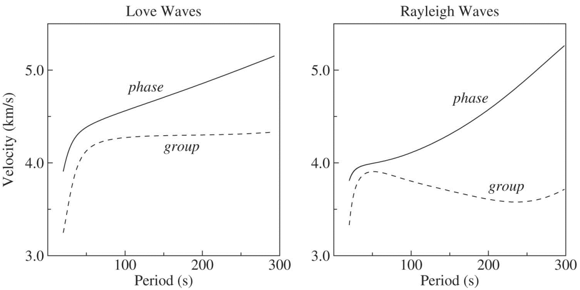


Surface Waves - Dispersion

Ralyeigh and Love Waves

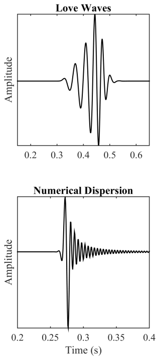


Dispersion Curves



Physical and Numerical Dispersion

Numerical Dispersion



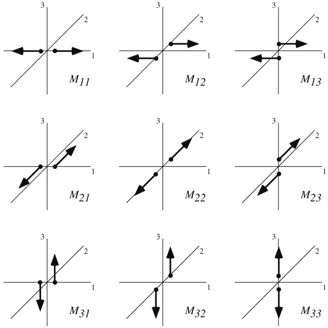
Numerical and physical dispersion can be confused!

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

Moment Tensor

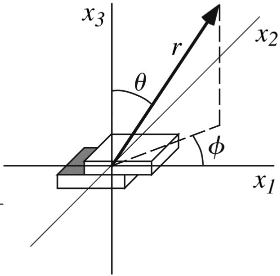
$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix}$$

$$M_0 = \mu \, A \, d$$

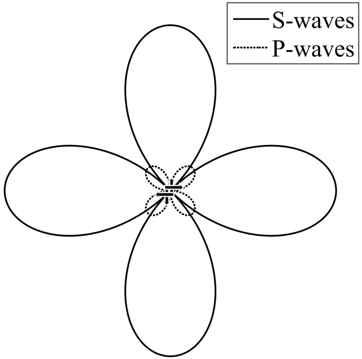


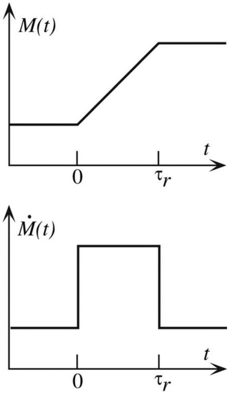
Double Couple Green's function

$$\boldsymbol{u}(\boldsymbol{x},t) = \frac{1}{4\pi\rho}\boldsymbol{A}^{N}\frac{1}{r^4}\int_{r/\alpha}^{r/\beta}\tau M_0(t-\tau)d\tau +$$
$$+\frac{1}{4\pi\rho\alpha^2}\boldsymbol{A}^{IP}\frac{1}{r^2}M_0(t-\frac{r}{\alpha}) + \frac{1}{4\pi\rho\beta^2}\boldsymbol{A}^{IS}\frac{1}{r^2}M_0(t-\frac{r}{\beta})+$$
$$+\frac{1}{4\pi\rho\alpha^3}\boldsymbol{A}^{FP}\frac{1}{r}\dot{M}_0(t-\frac{r}{\alpha}) + \frac{1}{4\pi\rho\beta^3}\boldsymbol{A}^{FS}\frac{1}{r}\dot{M}_0(t-\frac{r}{\beta})$$

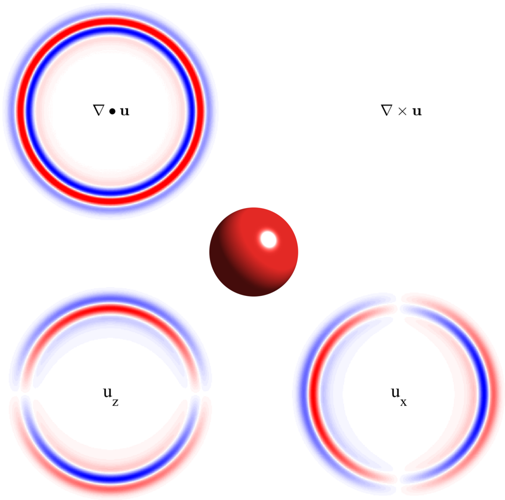


Radiation and Source Time Function

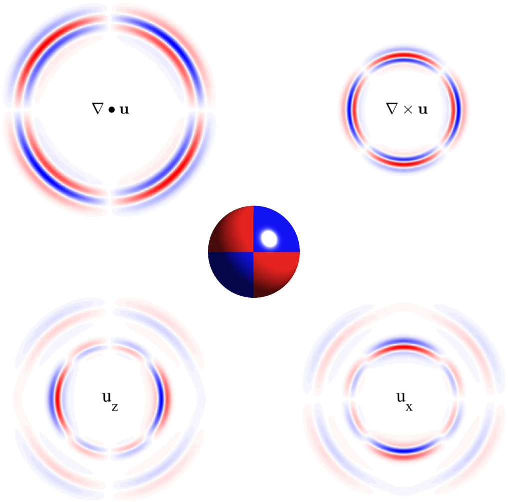




Wavefields from Moment Tensor Sources



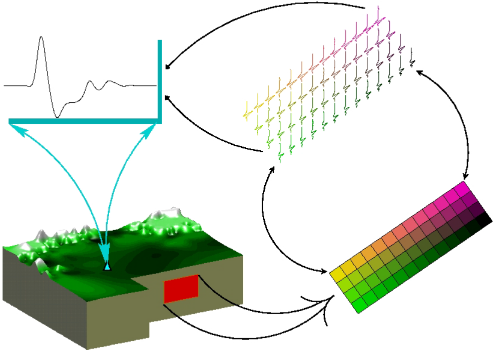
Wavefields from Moment Tensor Sources



Superposition Principle

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

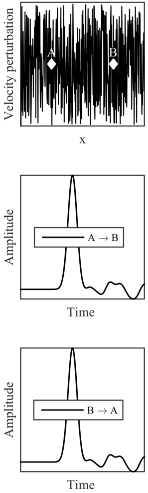
Finite sources can be simulated by summing up over point sources



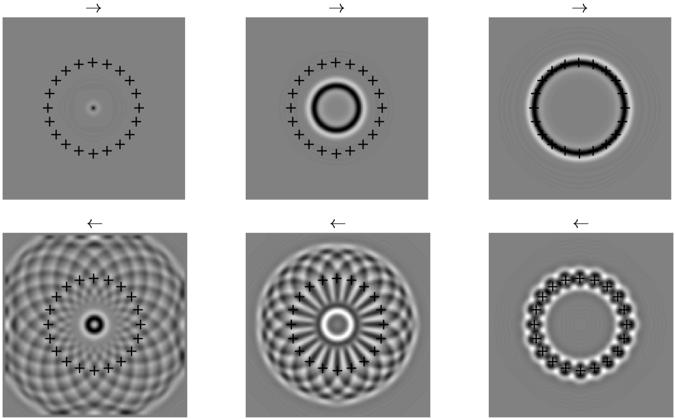
Reciprocity

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

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

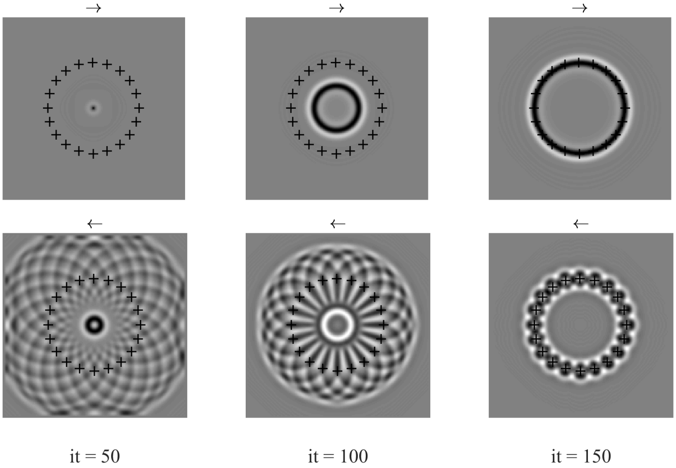


Time Reversal



it = 50 it = 100 it = 150

Time Reversal - Exercise



On github run the Jupyter Notebook 03_time_reversal_reciprocity and change the number of receivers.

Wave Equation as Linear System

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

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

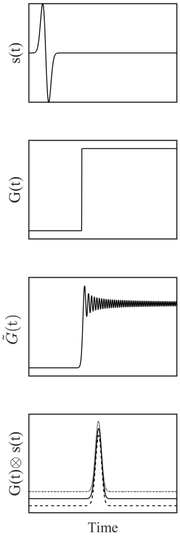
Seismogram for arbitrary source s(t) as convolution (numerical)

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

Important consequence:

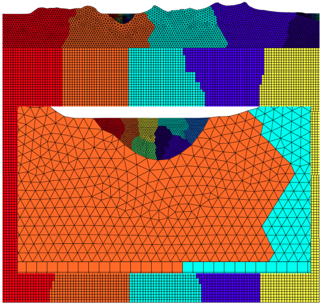
Even if your numerical Green's function $\tilde{G}(\mathbf{x}, t, \mathbf{x}_0)$ is inaccurate, the numerical solution $\tilde{p}(\mathbf{x}, t)$ might be very accurate provided the $s(t)$ is defined in the right frequency band!

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 ...

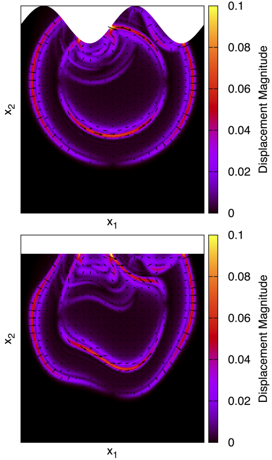
Challenges - Meshing



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?

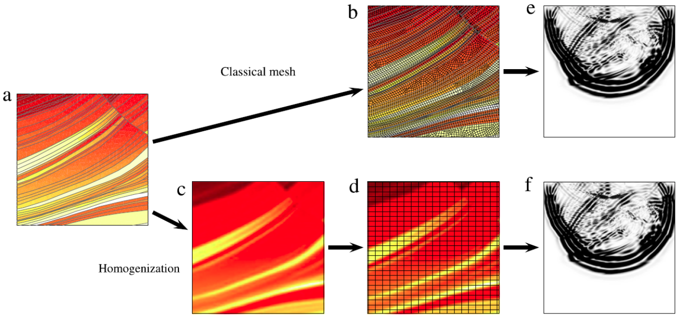
Future Strategies - Alternative Formulations



Al-Attar and Crawford GJI 2016

- 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)

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?