Numerical Methods: Structured vs. unstructured grids

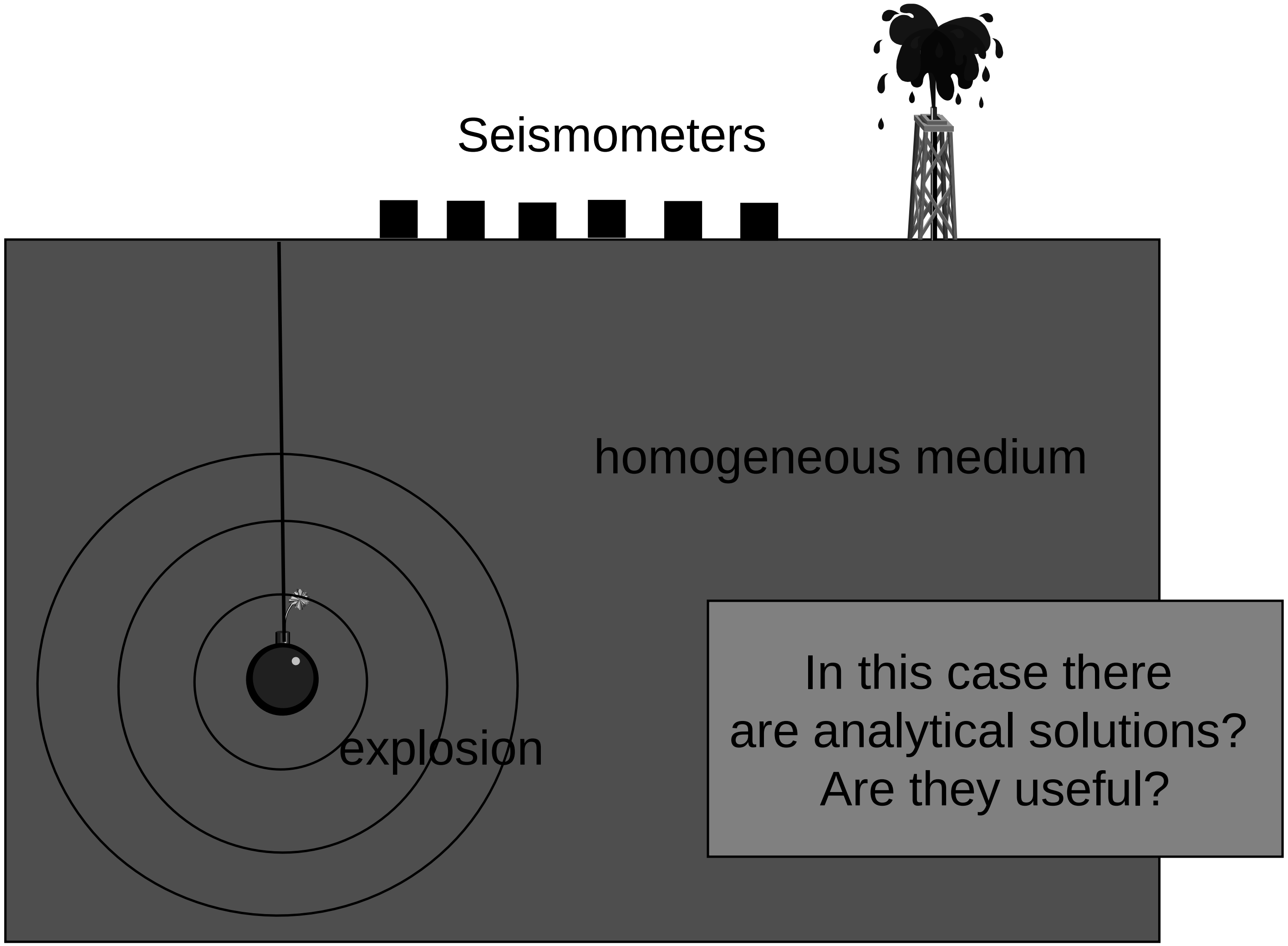
- The goals of this course
- General Introduction: Why numerical methods?
- Numerical methods and their fields of application
- Review of finite differences

Goals:

- Understanding the basics of all the “finite”s
  (differences, elements, volumes)
- The beauty: in the *linear* limit they are all really the
  same

Why numerical methods?

Example: seismic wave propagation



Why numerical methods?

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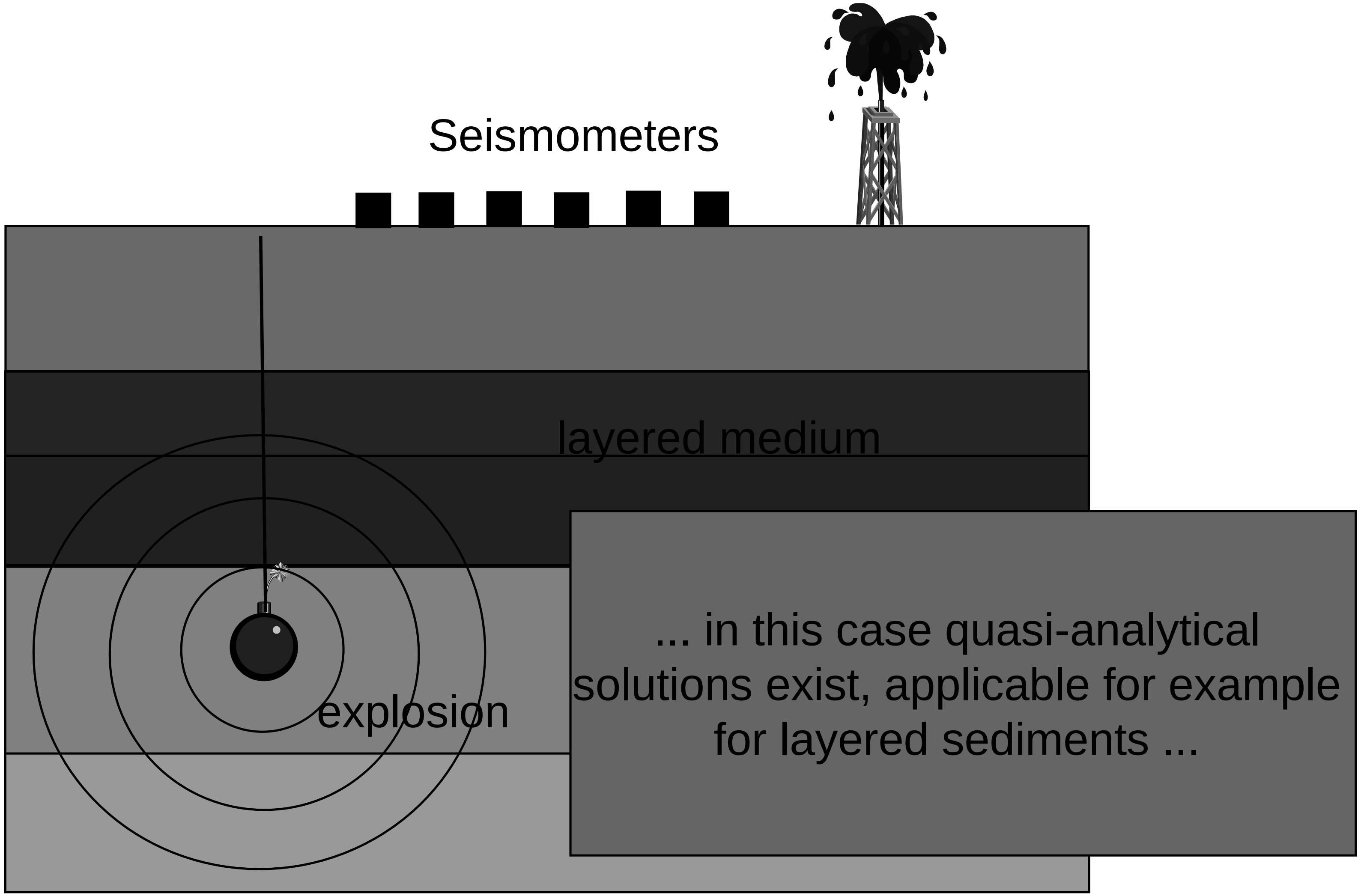

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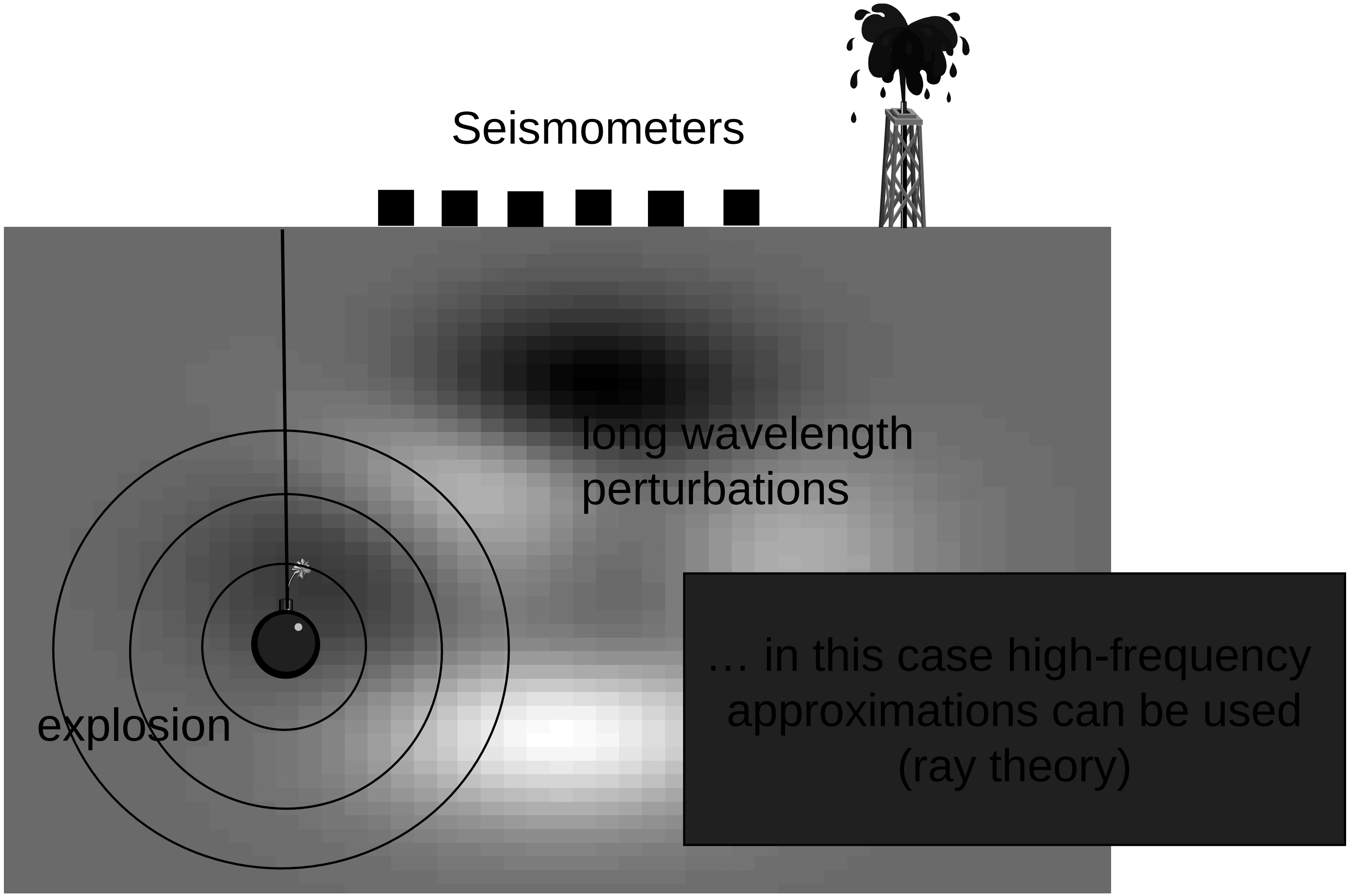
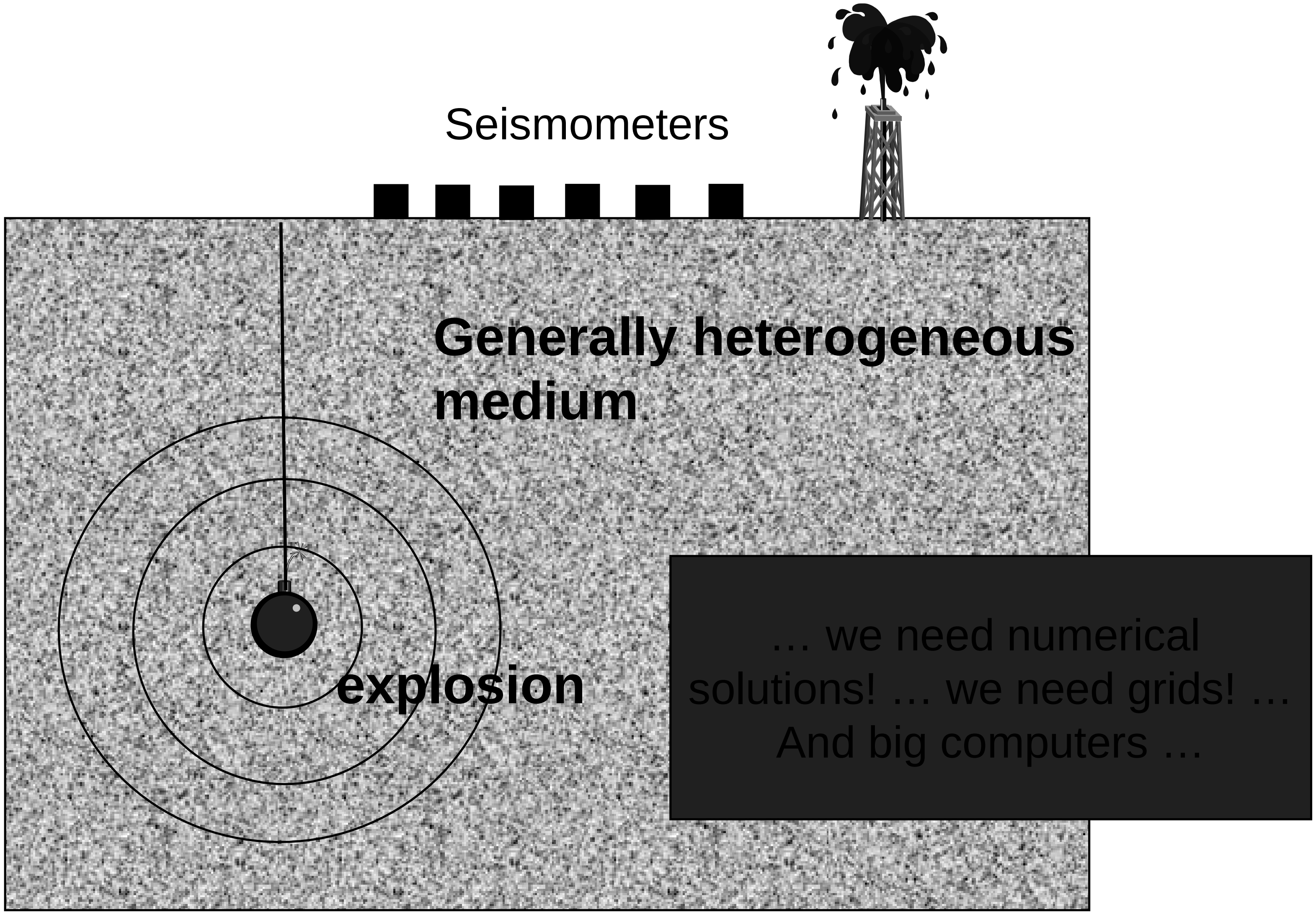


Why numerical methods

Example: seismic wave propagation



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

$$\Delta = (\partial_x^2 + \partial_y^2 + \partial_z^2)$$

P	pressure
c	acoustic wave speed
s	sources

The acoustic wave equation

- seismology
- acoustics
- oceanography
- meteorology

$$\partial_t C = k\Delta C - \mathbf{v} \bullet \nabla C - RC + p$$

C	tracer concentration
k	diffusivity
v	flow velocity
R	reactivity
p	sources

Diffusion, advection, Reaction

- geodynamics
- oceanography
- meteorology
- geochemistry
- sedimentology
- geophysical fluid dynamics

Numerical methods: fields of application

Finite differences

- time-dependent PDEs
- seismic wave propagation
- geophysical fluid dynamics
- Maxwell’s equations
- Ground penetrating radar

-> robust, simple concept, easy to parallelize, regular grids, explicit method

Finite elements

- static and time-dependent PDEs
- seismic wave propagation
- geophysical fluid dynamics
- all problems

-> implicit approach, matrix inversion, well founded, <u>irregular grids</u>, more complex algorithms, engineering problems

Finite volumes

- time-dependent PDEs
- seismic wave propagation
- mainly fluid dynamics

-> robust, simple concept, <u>irregular grids</u>, explicit method

Other Numerical methods:

Particle-based methods

- lattice gas methods
- molecular dynamics
- granular problems
- fluid flow
- earthquake simulations

-> very heterogeneous problems, nonlinear problems

Boundary element methods

- problems with boundaries (rupture)
- based in analytical solutions
- only discretization of planes

--> good for problems with special boundary conditions (rupture, cracks, etc)

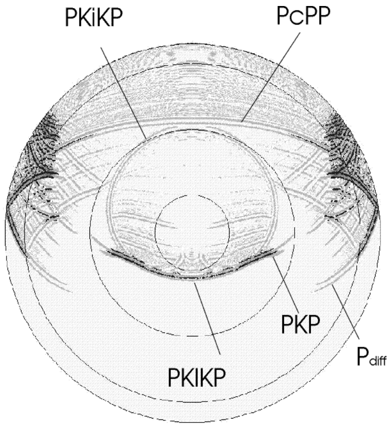
*Pseudo*spectral methods

- orthogonal basis functions
- spectral accuracy of space derivatives
- wave propagation, GPR

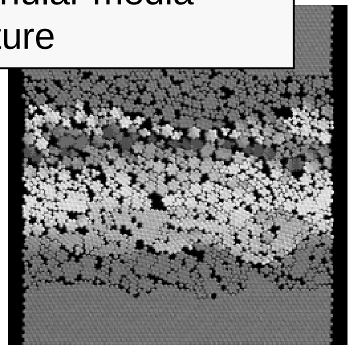
-> regular grids, explicit method, problems with discontinuities

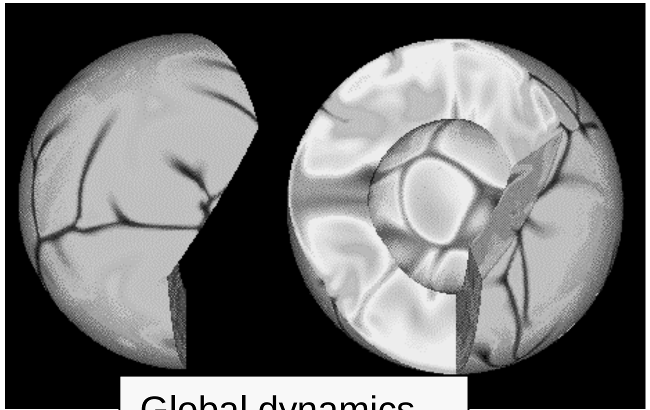
Numerical methods … in all fields of Earth sciences

Seismology

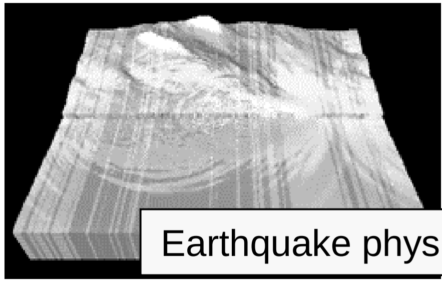


Granular media - rupture

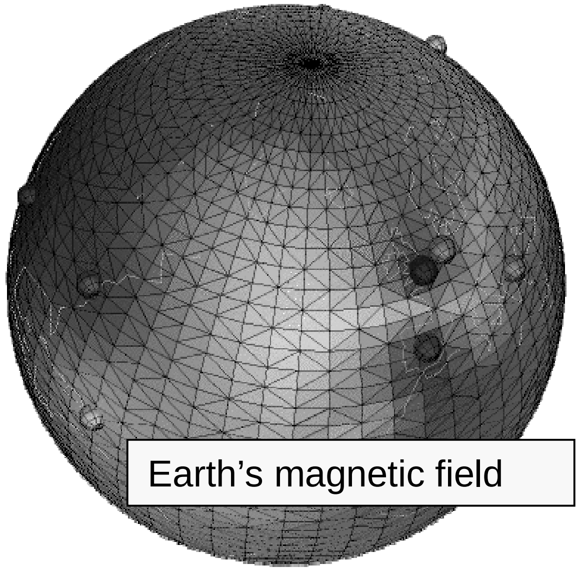




Global dynamics

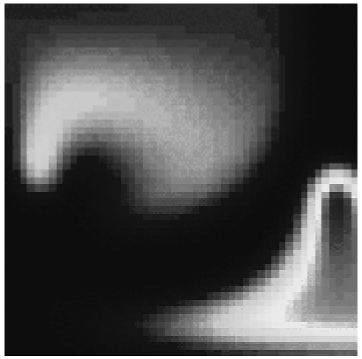


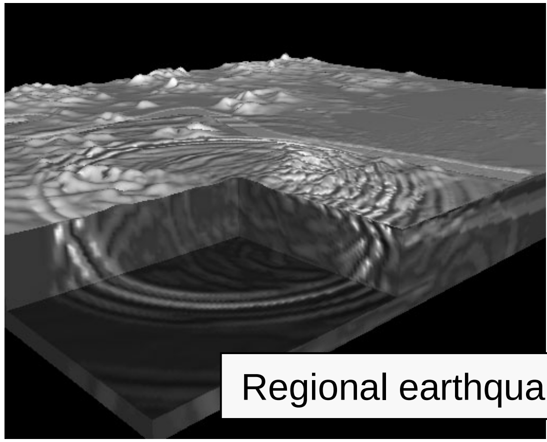
Earthquake physics



Earth’s magnetic field

Mixing - Geochemistry





Regional earthquakes

What is a finite difference?

Common definitions of the derivative of f(x):

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x) - f(x-dx)}{dx}$$

$$\partial_x f = \lim_{dx \to 0} \frac{f(x+dx) - f(x-dx)}{2dx}$$

These are all correct definitions in the limit dx->0.

But we want dx to remain <u>**FINITE**</u>

What is a finite difference?

The equivalent ***approximations*** of the derivatives are:

$$\partial_x f \approx \frac{f(x+dx) - f(x)}{dx}$$

forward difference

$$\partial_x f \approx \frac{f(x) - f(x-dx)}{dx}$$

backward difference

$$\partial_x f \approx \frac{f(x+dx) - f(x-dx)}{2dx}$$

centered difference

The **big** question:

How good are the FD approximations?

$$\approx \neq =$$

This leads us to Taylor series....

Taylor Series

... that leads to :

$$\frac{f(x+dx)-f(x)}{dx} = \frac{1}{dx}\left[\mathrm{dx} f^{'}(x) + \frac{dx^2}{2!} f^{''}(x) + \frac{dx^3}{3!} f^{'''}(x) + \ldots \right]$$

$$= f^{'}(x) + O(dx)$$

The error of the first derivative using the *forward* formulation is *of order dx*.

Is this the case for other formulations of the derivative? Let's check!

Taylor Series

... with the *centered* formulation we get:

$$\frac{f(x+dx/2)-f(x-dx/2)}{dx}=\frac{1}{dx}\left[\mathrm{dx}f^{'}(x)+\frac{dx^{3}}{3!}f^{'''}(x)+\ldots\right]$$

$$=f^{'}(x)+O(dx^{2})$$

The error of the first derivative using the centered approximation is *of order dx^2*.

This is an **important** results: it DOES matter which formulation we use. The centered scheme is more accurate!

Alternative Derivation of FD

$$af^{+} \approx af + af'dx \quad + \quad bf^{-} \approx bf - bf'dx$$

$$\Rightarrow af^{+} + bf^{-} \approx (a+b)f + (a-b)f'dx$$

Interpolation	Derivative
$\boxed{a-b=0}$	$\boxed{a+b=0}$
$\Downarrow$	$\Downarrow$
$f \approx \frac{1}{2}f^{-} + \frac{1}{2}f^{+}$	$f' \approx \frac{f^{+} - f^{-}}{2dx}$
$w_1 = 0.5, w_2 = 0.5$	$w_1 = -\frac{1}{2dx}, w_2 = \frac{1}{2dx}$
Interpolation weights	Derivative weights

Our first FD algorithm!

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

$$\Delta = (\partial_x^2 + \partial_y^2 + \partial_z^2)$$

P	pressure
c	acoustic wave speed
s	sources

Problem: Solve the 1D acoustic wave equation using the finite Difference method.

Solution:

$$p(t+dt) = \frac{c^2 dt^2}{dx^2}\left[p(x+dx) - 2p(x) + p(x-dx)\right] + 2p(t) - p(t-dt) + sdt^2$$

Problems: Stability

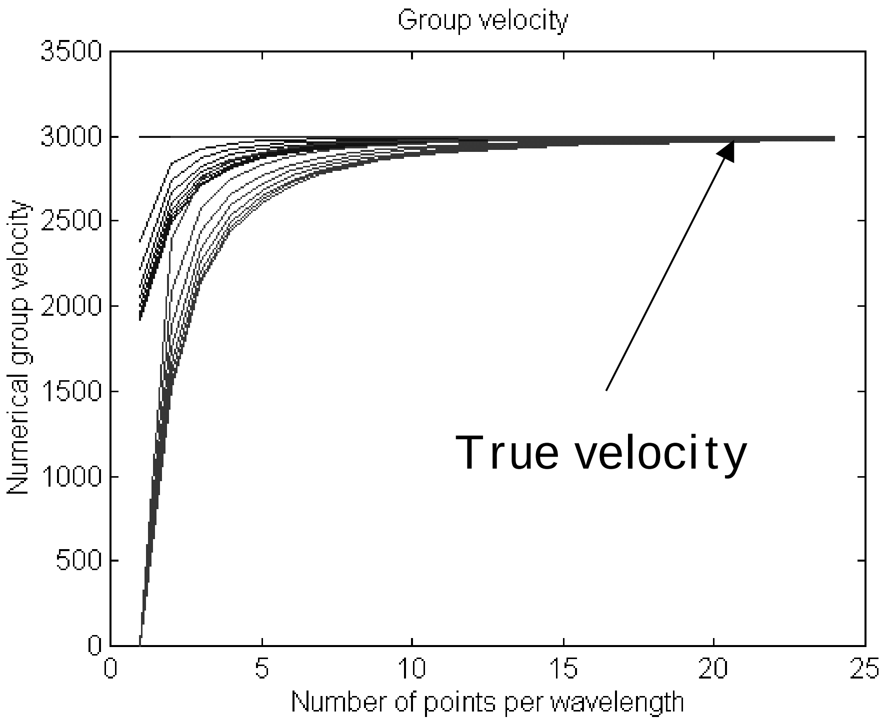
$$p(t+dt) = \frac{c^2 dt^2}{dx^2}\left[p(x+dx) - 2p(x) + p(x-dx)\right] + 2p(t) - p(t-dt) + sdt^2$$

Stability: Careful analysis using harmonic functions shows that a stable numerical calculation is subject to special conditions (conditional stability). This holds for many numerical problems.

$$\mathbf{c}\,\frac{\mathbf{dt}}{\mathbf{dx}} \leq \varepsilon \approx 1$$

Problems: Dispersion

$$p(t+dt) = \frac{c^2 dt^2}{dx^2}\left[p(x+dx) - 2p(x) + p(x-dx)\right] + 2p(t) - p(t-dt) + sdt^2$$



Dispersion: The numerical approximation has artificial dispersion, in other words, the wave speed becomes frequency dependent.
You have to find a frequency bandwidth where this effect is small.
The solution is to use sufficient grid points per wavelength.

Our first FD code!

$$p(t+dt) = \frac{c^2 dt^2}{dx^2}\left[p(x+dx) - 2p(x) + p(x-dx)\right] + 2p(t) - p(t-dt) + sdt^2$$

```
% Time stepping

for i=1:nt,

   % FD

   disp(sprintf(' Time step : %i',i));

   for j=2:nx-1
      d2p(j)=(p(j+1)-2*p(j)+p(j-1))/dx^2; % space derivative
   end
   pnew=2*p-pold+d2p*dt^2;                % time extrapolation
   pnew(nx/2)=pnew(nx/2)+src(i)*dt^2;     % add source term
   pold=p;                          % time levels
   p=pnew;
   p(1)=0;              % set boundaries pressure free
   p(nx)=0;

   % Display
   plot(x,p,'b-')
   title(' FD ')
   drawnow

end
```

Our first FD code!

$$p(t+dt) = \frac{c^2 dt^2}{dx^2}\left[p(x+dx) - 2p(x) + p(x-dx)\right] + 2p(t) - p(t-dt) + sdt^2$$

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      d2p(j)=(p(j+1)-2*p(j)+p(j-1))/dx^2; % space
derivative
   end
   pnew=2*p-pold+d2p*dt^2;                 % time
extrapolation
   pnew(nx/2)=pnew(nx/2)+src(i)*dt^2;     % add
source term
   pold=p;
                        % time levels
   p=pnew;
   p(1)=0;                                      %
set boundaries pressure free
   p(nx)=0;

   % Display
   plot(x,p,'b-')
   title(' FD ')
   drawnow

end
```

Exercises (FD):

1. Increase the time step dt manually and determine the stability limit numerically (c*dt/dx).
2. Make the medium heterogeneous. Put in a velocity contrast along the x axis with a 30% perturbation.
3. Perturb the medium (e.g. 20%) with random perturbations (dc=rand([1 nx]). What effect do you have on the propagating pulse? Do you think the result is accurate?
4. Compare the results with a simulation with 10000 time steps.

Finite Differences - Summary

Depending on the choice of the FD scheme (e.g. forward, backward, centered) a numerical solution may be more or less accurate.

Explicit finite difference solutions to differential equations are often *conditionally stable*. The correct choice of the space or time increment is crucial to enable accurate solutions.

Sometimes it is useful to employ so-called *staggered grids* where the fields are defined on separate grids which may improve the overall accuracy of the scheme.