- Short introduction
- ≻Finite-differences
- Solutions of the acoustic wave equation
  - difference equations
- Stability and numerical dispersion
- ≻The Fourier method

**Scope:** Understand how to calculate synthetics using finite differences, we will later analyse the data (time series) in the spectral domain

# Why numerical methods



## **Partial Differential Equations in Geophysics**

$$\partial_{t}^{2} \mathbf{p} = \mathbf{c}^{2} \Delta \mathbf{p} + \mathbf{s}$$
$$\Delta = (\partial_{x}^{2} + \partial_{y}^{2} + \partial_{z}^{2})$$

Ρ	pressure
С	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: properties**



## **Other Numerical methods:**



## 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 FINITE

Calculating synthetics

## 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

What about the second or higher derivatives?

## Higher Derivatives with FD

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

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

Second Derivative

Other derivation via Taylor Series (Exercise).

Calculating synthetics



#### How good are the FD approximations?



This leads us to Taylor series....

Calculating synthetics

## **Taylor Series**

Taylor series are expansions of a function f(x) for some finite distance dx to f(x+dx)

$$f(x \pm dx) = f(x) \pm dx f'(x) + \frac{dx^2}{2!} f''(x) \pm \frac{dx^3}{3!} f'''(x) + \frac{dx^4}{4!} f''''(x) \pm \dots$$

What happens, if we use this expression for

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

## **Taylor Series**

... that leads to :

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

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:

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

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



desired x location

What is the (approximate) value of the function or its (first, second ..) derivative at the desired location ?

How can we calculate the weights for the neighboring points?

## Alternative Derivation of FD



$$f^{(i)}(x) \approx \sum_{j=1,L} w_j^{(i)} f(x_{index(j)})$$

Calculating synthetics

## Alternative Derivation of FD

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



# Our first FD algorithm (ac1d.m) !

$$\partial_{t}^{2} \mathbf{p} = \mathbf{c}^{2} \Delta \mathbf{p} + \mathbf{s}$$
  
 $\Delta = (\partial_{x}^{2} + \partial_{y}^{2} + \partial_{z}^{2})$ 

Ρ	pressure
С	acoustic wave speed
S	sources

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

#### Solution:

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

## **Problems: Stability**

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

**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.

$$\mathbf{C}\frac{\mathbf{dt}}{\mathbf{dx}} \le \varepsilon \approx 1$$

The 1-D wave equation

$$\rho(x)\partial_t^2 \mathbf{u}(\mathbf{x},\mathbf{t}) = \partial_x \left[ \mathbf{E}(\mathbf{x})\partial_x \mathbf{u}(\mathbf{x},\mathbf{t}) \right]$$

Elastic parameters E(x) vary only in one direction.

$$E(x) = \mu(x)$$
 shear waves  
 $E(x) = \lambda(x) + 2\mu(x)$  P waves

with the corresponding velocities

$$v_{S} = \sqrt{\frac{\mu}{\rho}}$$
 shear waves  
 $v_{P} = \sqrt{\frac{\lambda + 2\mu}{\rho}}$  P waves

Calculating synthetics

We want to avoid having to take derivatives of the material parameters (why?). This can be achieved by using a *velocity-stress* formulation, which leads to the following simultaneous equations:

$$\partial_t \dot{u} = \frac{1}{\rho(x)} \partial_x \tau$$
$$\partial_t \tau = E(x) \partial_x \dot{u}$$

where

$$\tau = E(x)\partial_x u$$
 stress

Let us try to use one of the previously introduced FD schemes: central difference for space and forward difference for time

Discretization: (ldt, mdx)

dx space increment, dt time increment



... leading to the following scheme:

forward 
$$\frac{\dot{u}_{m}^{l+1} - \dot{u}_{m}^{l}}{dt} = \frac{1}{\rho_{m}} \frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx} \quad \text{centered}$$
forward 
$$\frac{\tau_{m}^{l+1} - \tau_{m}^{l}}{dt} = E_{m} \frac{\dot{u}_{m+1}^{l} - \dot{u}_{m-1}^{l}}{2dx} \quad \text{centered}$$

like in the continuous case, we can make the following Ansatz:

$$f(x,t) = A\exp(ikx - iwt)$$

which in the discrete world is :

$$f_{lm} = A \exp(ikmdx - iwldt)$$



then solve

$$\tau_m^{l+1} = dt \left[ E_m \frac{\dot{u}_{m+1}^l - \dot{u}_{m-1}^l}{2dx} \right] + \tau_m^l$$

... let us assume a signal is propagating:

$$f(\tau_m^l) = A \exp(ikmdx - iwldt)$$
$$f(\dot{u}_m^l) = B \exp(ikmdx - iwldt)$$

we now put this Ansatz into the following equations ...

$$\frac{\dot{u}_{m}^{l+1} - \dot{u}_{m}^{l}}{dt} = \frac{1}{\rho_{m}} \frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx}$$
$$\frac{\tau_{m}^{l+1} - \tau_{m}^{l}}{dt} = E_{m} \frac{\dot{u}_{m+1}^{l} - \dot{u}_{m-1}^{l}}{2dx}$$

Calculating synthetics

...after some algebra (hours later) ...

$$\exp(-iwdt) = 1 \pm i \sqrt{\frac{E_m}{\rho_m}} \left(\frac{dt}{dx}\right) \sin kdx$$

What does this result tell us about the numerical solution?

$$\left|\exp(-iwdt)\right| > 1$$

for any choice of dt and dx! So  $\omega$  must be complex. But then for example:

$$f(\tau_m^l) = A \exp(ikm dx - iwl dt) = A \exp(ikm) \exp(-w^* l dt)$$

will grow exponentially as,  $\omega^*$  is real.

Calculating synthetics

Can we find a scheme that works? Let us use a centered scheme in time:

$$\frac{\dot{u}_{m}^{l+1} - \dot{u}_{m}^{l-1}}{2dt} = \frac{1}{\rho_{m}} \frac{\tau_{m+1}^{l} - \tau_{m-1}^{l}}{2dx}$$



$$\frac{\tau_m^{l+1} - \tau_m^{l-1}}{2dt} = E_m \frac{\dot{u}_{m+1}^l - \dot{u}_{m-1}^l}{2dx}$$

And again we use the following Ansatz to investigate the behavior of the numerical solution:

$$f(\tau_m^l) = A \exp(ikmdx - iwldt)$$
$$f(\dot{u}_m^l) = B \exp(ikmdx - iwldt)$$

Calculating synthetics

...again after some algebra (minutes later) ...

$$\sin w dt = \pm \sqrt{\frac{E_m}{\rho_m}} \left(\frac{dt}{dx}\right) \sin k dx$$

... has real solutions as long as

$$\sqrt{\frac{E_m}{\rho_m}} \left(\frac{dt}{dx}\right) \le 1$$

... knowing that for example ...

$$\sqrt{\frac{E_m}{\rho_m}} = v_p$$
 P-wave velocity

Calculating synthetics

... we arrive at maybe the most important result for FD schemes applied to the wave equation:



 $v_{P,S}$  is the locally homogeneous velocity. This is called a *conditionally stable* finite-difference scheme. Finding the right combination of dt and dx for a practical application, where the velocities vary in the medium is one of the most important tasks.



... leading to the FD scheme:

$$\frac{\dot{u}_{m}^{l+1/2} - \dot{u}_{m}^{l-1/2}}{dt} = \frac{1}{\rho_{m}} \frac{\tau_{m+1/2}^{l} - \tau_{m-1/2}^{l}}{dx}$$
$$\frac{\tau_{m+1/2}^{l+1} - \tau_{m+1/2}^{l}}{dt} = E_{m+1/2} \frac{\dot{u}_{m+1}^{l+1/2} - \dot{u}_{m}^{l+1/2}}{dx}$$

And again we use the following *Ansatz* to investigate the behaviour of the numerical solution:

$$f(\tau_m^l) = A \exp(ikmdx - iwldt)$$
$$f(\dot{u}_m^l) = B \exp(ikmdx - iwldt)$$

Find the corresponding stability condition (Exercise)!

Calculating synthetics

## **Staggered Grids**



Because the error is  $O(h^2)$ , the error of the centered scheme is 4 times larger.

Calculating synthetics

What does the stability criterion tell us about the quality of the numerical solution?

$$\sin\frac{\omega dt}{2} = \pm \sqrt{\frac{E_{m+1/2}}{\rho_m}} \left(\frac{dt}{dx}\right) \sin\frac{kdx}{2}$$

To answer this we need the concept of *phase velocity.* Remember we assumed a harmonic oscillation with frequency  $\omega$  and wavenumber k, for example

$$y(x,t) = \sin(kx - \omega t) = \sin(k(x - \frac{\omega}{k}t)) = \sin(\omega(\frac{k}{\omega}x - t))$$

where the phase velocity is

$$c_{phase} = \frac{\omega}{k}$$

$$\sin\frac{\omega dt}{2} = \pm \sqrt{\frac{E_{m+1/2}}{\rho_m}} \left(\frac{dt}{dx}\right) \sin\frac{kdx}{2}$$

we can first assume that dt and dx are very small, in this case :

$$sin(x) \approx x$$
 for small x

then

$$\frac{\omega}{k} = \sqrt{\frac{E_{m+1/2}}{\rho_m}} = c \qquad \text{wave speed}$$



for small dt and dx we simulate the correct velocity: The scheme is **convergent**.

How about the general case?

$$\sin \frac{\omega dt}{2} = \pm \sqrt{\frac{E_{m+1/2}}{\rho_m}} \left(\frac{dt}{dx}\right) \sin \frac{k dx}{2}$$
  
using  $k = \frac{2\pi}{\lambda}$  we obtain  
 $c(\lambda) = \frac{\omega}{k} = \frac{\lambda}{\pi dt} \sin^{-1} \left(c_0 \frac{dt}{dx} \sin \frac{\pi dx}{\lambda}\right)$ 

This formula expresses our *numerical* phase velocity as a function of the wave speed and the propagating wavelength.

## **Numerical Phase Velocity**



What we really measure in a seismogram is the group velocity:



This formula expresses our *numerical* group velocity as a function of the wave speed and the propagating wavelength.

## **Numerical Group Velocity**





## Example

Velocity 5 km/s





## **FD 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 seperate grids which may improve the overall accuracy of the scheme.

# **The Fourier Method**

- What is a *pseudo*-spectral Method?
- Fourier Derivatives
- The Fast Fourier Transform (FFT)
- The Acoustic Wave Equation with the Fourier Method
- Comparison with the Finite-Difference Method
- Dispersion and Stability of Fourier Solutions

## **Pseudospectral methods**

Spectral solutions to time-dependent PDEs are formulated in the frequency-wavenumber domain and solutions are obtained in terms of spectra (e.g. seismograms). This technique is particularly interesting for geometries where partial solutions in the  $\omega$ -k domain can be obtained analytically (e.g. for layered models).

In the pseudo-spectral approach - in a finite-difference like manner - the PDEs are solved pointwise in physical space (x-t). However, the space derivatives are calculated using orthogonal functions (e.g. Fourier Integrals, Chebyshev polynomials). They are either evaluated using matrixmatrix multiplications or the fast Fourier transform (FFT).

## **Spectral derivative**

.. let us recall the definition of the derivative using Fourier integrals ...

$$\partial_{x} f(x) = \partial_{x} \left( \int_{-\infty}^{\infty} F(k) e^{-ikx} dk \right)$$
$$= -\int_{-\infty}^{\infty} ikF(k) e^{-ikx} dk$$

... we could either ...

1) perform this calculation in the space domain by convolution

2) actually transform the function f(x) in the k-domain and back

#### Acoustic wave equation

let us take the acoustic wave equation with variable density

$$\frac{1}{\rho c^{2}} \partial_{t}^{2} p = \partial_{x} \left( \frac{1}{\rho} \partial_{x} p \right)$$

the left hand side will be expressed with our standard centered finite-difference approach

$$\frac{1}{\rho c^2 dt^2} \left[ p \left( t + dt \right) - 2 p \left( t \right) + p \left( t - dt \right) \right] = \partial_x \left( \frac{1}{\rho} \partial_x p \right)$$

... leading to the extrapolation scheme ...

#### ... pseudospectral approximation ...

$$p(t+dt) = \rho c^2 dt^2 \frac{\partial_x}{\partial_x} \left(\frac{1}{\rho} \frac{\partial_x}{\partial_x} p\right) + 2 p(t) - p(t-dt)$$

where the space derivatives will be calculated using the Fourier Method. The highlighted term will be calculated as follows:

$$P_{j}^{n} \rightarrow \text{FFT} \rightarrow \hat{P}_{v}^{n} \rightarrow ik_{v}\hat{P}_{v}^{n} \rightarrow \text{FFT}^{-1} \rightarrow \partial_{x}P_{j}^{n}$$
  
multiply by  $1/\rho$ 

$$\frac{1}{\rho}\partial_x P_j^n \to \mathrm{FFT} \to \left(\frac{1}{\rho}\partial_x \hat{P}\right)_{\nu}^n \to ik_{\nu}\left(\frac{1}{\rho}\partial_x \hat{P}\right)_{\nu}^n \to \mathrm{FFT}^{-1} \to \partial_x\left(\frac{1}{\rho}\partial_x P_j^n\right)$$

... then extrapolate ...

## ... pseudospectral approximation ...

$$p(t+dt) = \rho c^{2} dt^{2} \left[ \partial_{x} \left( \frac{1}{\rho} \partial_{x} p \right) + \partial_{y} \left( \frac{1}{\rho} \partial_{y} p \right) + \partial_{z} \left( \frac{1}{\rho} \partial_{z} p \right) \right] + 2 p(t) - p(t-dt)$$

#### ... where the following algorithm applies to each space dimension ...

$$P_{j}^{n} \rightarrow \text{FFT} \rightarrow \hat{P}_{v}^{n} \rightarrow ik_{v}\hat{P}_{v}^{n} \rightarrow \text{FFT}^{-1} \rightarrow \partial_{x}P_{j}^{n}$$
$$\frac{1}{\rho}\partial_{x}P_{j}^{n} \rightarrow \text{FFT} \rightarrow \left(\frac{1}{\rho}\partial_{x}\hat{P}\right)_{v}^{n} \rightarrow ik_{v}\left(\frac{1}{\rho}\partial_{x}\hat{P}\right)_{v}^{n} \rightarrow \text{FFT}^{-1} \rightarrow \partial_{x}\left(\frac{1}{\rho}\partial_{x}P_{j}^{n}\right)$$

## Matlab code

# let us compare the core of the algorithm - the calculation of the derivative (Matlab code)

```
function df=fder1d(f,dx,nop)
% fDER1D(f,dx,nop) finite difference
% second derivative
nx=max(size(f));
n2=(nop-1)/2;
if nop==3; d=[1 -2 1]/dx^2; end
if nop==5; d=[-1/12 4/3 -5/2 4/3 -1/12]/dx^2; end
df = [1:nx]*0;
for i=1:nop;
df=df+d(i).*cshift1d(f,-n2+(i-1));
end
```

#### Matlab code

... and the first derivative using FFTs ...

```
function df=sderld(f,dx)
% SDERlD(f,dx) spectral derivative of vector
nx=max(size(f));
% initialize k
kmax=pi/dx;
dk=kmax/(nx/2);
for i=1:nx/2, k(i)=(i)*dk; k(nx/2+i)=-kmax+(i)*dk; end
k=sqrt(-1)*k;
% FFT and IFFT
ff=fft(f); ff=k.*ff; df=real(ifft(ff));
```

.. simple and elegant ...

## Dispersion

... with the usual Ansatz

$$p_{j}^{n} = e^{i(kjdx - n\omega dt)}$$

we obtain

$$\partial_x^2 p_j^n = -k^2 e^{i(kjdx - \omega ndt)}$$
$$\partial_t^2 p_j^n = -\frac{4}{dt^2} \sin^2 \frac{\omega dt}{2} e^{i(kjdx - \omega ndt)}$$

... leading to

$$k = \frac{2}{cdt} \sin \frac{\omega dt}{2}$$

## Dispersion

$$k = \frac{2}{cdt} \sin \frac{\omega dt}{2}$$

$$\omega = \frac{2}{dt} \sin^{-1}(\frac{kcdt}{2})$$

What are the consequences?

a) when dt << 1, sin<sup>-1</sup> (kcdt/2) ≈kcdt/2 and w/k=c
-> practically no dispersion
b) the argument of asin must be smaller than one.

$$\frac{k_{\max}cdt}{2} \le 1$$

$$cdt / dx \le 2 / \pi \approx 0.636$$

## Matlab code: lectsac.m



Calculating synthetics



Calculating synthetics



Example of acoustic 1D wave simulation. Fourier operator red-analytic; blue-numerical; green-difference

Calculating synthetics



Example of acoustic 1D wave simulation. FD 3 -point operator red-analytic; blue-numerical; green-difference

Calculating synthetics





Calculating synthetics

## **Computation speed**

Difference (%) between numerical and analytical solution as a function of propagating frequency



## Green's function

The concept of Green's Functions (impulse responses) plays an important role in the solution of partial differential equations. It is also useful for numerical solutions. Let us recall the acoustic wave equation

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

with  $\Delta$  being the Laplace operator. We now introduce a delta source in space and time

$$\partial_t^2 p = \delta(\underline{x})\delta(t) + c^2\Delta p$$

the formal solution to this equation is

$$p(\underline{x},t) = \frac{1}{4\pi c^2} \frac{\delta(t - |\underline{x}|/c)}{|\underline{x}|}$$

(Full proof given in Aki and Richards, Quantitative Seismology, Freeman+Co, 1981, p. 65)

Calculating synthetics

## Green's function?

$$p(\underline{x},t) = \frac{1}{4\pi c^2} \frac{\delta(t - |\underline{x}|/c)}{|\underline{x}|}$$

In words this means (in 1D and 3D but not in 2D, why?), that in homogeneous media the same source time function which is input at the source location will be recorded at a distance r, but with amplitude proportional to 1/r.

An arbitrary source can evidently be constructed by summing up different delta - solutions. Can we use this property in our numerical simulations?

What happens if we solve our numerical system with delta functions as sources?

## Heaviside



## FD vs. Fourier



Impulse response (analytical) concolved with source Impulse response (numerical convolved with source

# 2-D acoustic wave propagation ac2d.m

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40 % FD	
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42 - disp(sprintf(' Time step : %i',it));	
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44 - for j=3:nx-2,	
45 - for k=3:nz-2,	
$46 - d2px(j,k) = (-1/12*p(j+2,k)+4/3*p(j+1,k)-5/2*p(j,k)+4/3*p(j-1,k)-1/12*p(j-2,k))/dx^{2}; & space derivative data and the second derivative derivative data and the second derivative$	
47 - d2pz(j,k)=(-1/12*p(j,k+2)+4/3*p(j,k+1)-5/2*p(j,k)+4/3*p(j,k-1)-1/12*p(j,k-2))/dx^2; % space derivative	
48 - end	
49 - end	
50 - pnew=2*p-pold+c.*c.*(d2px+d2pz)*dt^2; % time extrapolation	
51 - pnew(nx/4,nz/4)=pnew(nx/4,nz/4)+src(it)*dt^2; % add source term	
52 - pold=p; % time levels	
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## Snapshots und Seismogramme:

homogenes Medium



Snapshots

#### Snapshots und Seismogramme: Niedriggeschwindigkeitsschicht



#### Snapshots und Seismogramme: Störungszone (Verwerfung)



# Snapshots und Seismogramme:

Punktstreuung



The Fourier Method can be considered as the limit of the finite-difference method as the length of the operator tends to the number of points along a particular dimension.

The space derivatives are calculated in the wavenumber domain by multiplication of the spectrum with *ik.* The inverse Fourier transform results in an exact space derivative up to the Nyquist frequency.

The use of Fourier transform imposes some constraints on the smoothness of the functions to be differentiated. Discontinuities lead to Gibb's phenomenon.

As the Fourier transform requires periodicity this technique is particular useful where the physical problems are periodical (e.g. angular derivatives in cylindrical problems).