The Finite Difference Method

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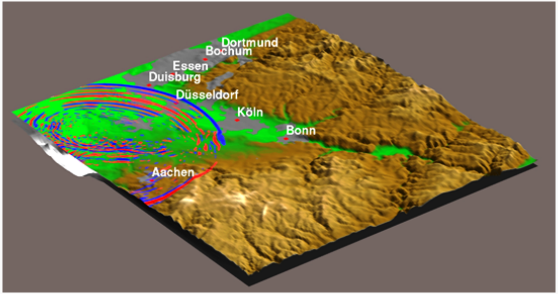
Introduction

Motivation



- Simple concept
- Robust
- Easy to parallelize
- Regular grids
- Explicit method

History

- Several Pioneers of solving PDEs with finite-difference method (Lewis Fry Richardson, Richard Southwell, Richard Courant, Kurt Friedrichs, Hans Lewy, Peter Lax and John von Neumann)
- First application to elastic wave propagation (Alterman and Karal, 1968)
- Simulating Love waves and was the frst showing snapshots of seimsic wave fields (Boore, 1970)
- Concept of staggered-grids by solving the problem of rupture propagation (Madariaga, 1976 and Virieux and Madariaga, 1982)

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- Extension to 3D because of parallel computations (Frankel and Vidale, 1992; Olsen and Archuleta, 1996; etc.)
- Application to spherical geometry by Igel and Weber, 1995; Chaljub and Tarantola, 1997 and 3D spherical sections by Igel et al., 2002
- Incorporation in the first full waveform inversion schemes initially in 2D, e.g. (Crase et al., 1990) and later in 3D (Chen et al., 2007)

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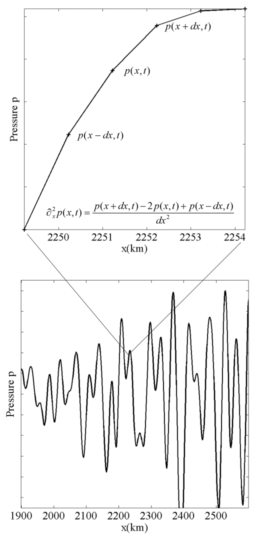
Finite Differences in a Nutshell



- Snapshot in space of the pressure field p
- Zoom into the wave field with grid points indicated by +
- Exact interpolate using Taylor series

Scalar wave equation

1D acoustic wave equation

$$\ddot{p}(x,t) = c(x)^2 \, \partial_x^2 p(x,t) + s(x,t)$$

p	pressure
c	acoustic velocity
s	source term

Approximation with a difference formula

$$\ddot{p}(x,t) \approx \frac{p(x,t+dt) - 2p(x,t) + p(x,t-dt)}{dt^2}$$

Finite Differences and Taylor Series

Finite Differences

Forward derivative

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

Centered derivative

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

Backward derivative

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

Finite Differences

Forward derivative

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

Centered derivative

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

Backward derivative

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

Finite Differences and Taylor Series

The approximate sign is important here as the derivatives at point x are not exact. Understanding the accuracy by looking at the definition of Taylor Series:

$$f(x + dx) = f(x) + f'(x)\, dx + \frac{1}{2!}\, f''(x)\, dx^2 + O(dx^3)$$

Subtraction with f(x) and division by dx leads to the definition of the forward derivative:

$$\frac{f(x+dx)-f(x)}{dx} = f'(x)\ + \frac{1}{2!}\, f''(x)\, dx + O(dx^2)$$

Finite Differences and Taylor Series

Using the same approach - adding the Taylor Series for $f(x+dx)$ and $f(x-dx)$ and dividing by $2dx$ leads to:

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

This implies a centered finite-difference scheme more rapidly converges to the correct derivative on a regular grid

$\Longrightarrow$ It matters which of the approximate formula one chooses

$\Longrightarrow$ It does not imply that one or the other finite-difference approximation is always the better one

Higher Derivatives

The partial differential equations have often 2nd (seldom higher) derivatives

Developing from first derivatives by mixing a forward and a backward definition yields

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

Higher Derivatives - Alternative derivation

Determining the weights with which the function values have to be multiplied to obtain derivative approximations ...

$$
\begin{aligned}
{\color{red}a}\, f(x+dx) &= {\color{red}a}\left[f(x) + f'(x)\,dx + \tfrac{1}{2!}\,f''(x)\,dx^2 + \ldots\right] \\
{\color{red}b}\, f(x) &= {\color{red}b}\,[f(x)] \\
{\color{red}c}\, f(x-dx) &= {\color{red}c}\left[f(x) - f'(x)\,dx + \tfrac{1}{2!}\,f''(x)\,dx^2 - \ldots\right]
\end{aligned}
$$

Higher Derivatives - Alternative derivation

How to determine a, b, and c?

$$\begin{aligned} af(x+dx) + bf(x) + cf(x-dx) \approx & \\ f(x)\,[a + b + c] & \\ +dxf'\,[a - c] & \\ +\tfrac{1}{2!}dx^2 f''\,[a + c] & \end{aligned}$$

Higher Derivatives - Alternative derivation

To obtain a 2nd derivative we require

$$\begin{aligned} a + b + c &= 0 \\ a \qquad - c &= 0 \\ a \qquad + c &= \frac{2!}{dx^2} \end{aligned}$$

Higher Derivatives - Alternative derivation

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \\ 1 & 0 & 1 \end{pmatrix}}_{\mathbf{A}} \underbrace{\begin{pmatrix} a \\ b \\ c \end{pmatrix}}_{\mathbf{w}} = \underbrace{\begin{pmatrix} 0 \\ 0 \\ \frac{2!}{dx} \end{pmatrix}}_{\mathbf{s}}$$

with solution

$$\mathbf{w} = \mathbf{A}^{-1}\mathbf{s}$$

Higher Derivatives - Solution

$$
\begin{aligned}
a &= \frac{1}{dx^2} \\
b &= -\frac{2}{dx^2} \\
c &= \frac{1}{dx^2}
\end{aligned}
$$

High-Order Operators

What happens if we extend the *domain of influence* for the derivative(s) of our function f(x)?

Let us search for a 5-point operator for the second derivative

$$f'' \approx af(x+2dx) + bf(x+dx) + cf(x) + df(x-dx) + ef(x-2dx)$$

$$\begin{aligned}
a + b + c + d + e &= 0 \\
2a + b \quad - d - 2e &= 0 \\
4a + b \quad + d + 4e &= \frac{1}{2\mathrm{d}x^2} \\
8a + b \quad - d - 8e &= 0 \\
16a + b \quad + d + 16e &= 0
\end{aligned}$$

High-Order Operators

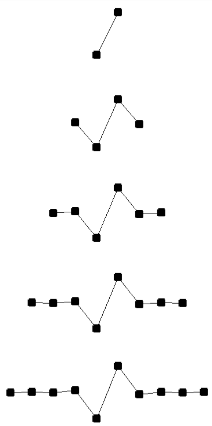
Using matrix inversion we obtain a unique solution

$$
\begin{aligned}
a &= -\frac{1}{12\mathrm{d}x^2} \\
b &= \frac{4}{3\mathrm{d}x^2} \\
c &= -\frac{5}{2\mathrm{d}x^2} \\
d &= \frac{4}{3\mathrm{d}x^2} \\
e &= -\frac{1}{12\mathrm{d}x^2} \,.
\end{aligned}
$$

with a leading error term for the 2nd derivative is $O(dx^4)$

$\implies$ Accuracy improvement

High-Order Operators



Graphical illustration of the Taylor Operators for the first derivative for higher orders

The weights rapidly become small for increasing distance to central point of evaluation

Finite-Difference Approximation of Wave Equations

Acoustic waves in 1D

To solve the wave equation, we start with the simplemost wave equation:

The constant density acoustic wave equation in 1D

$$\ddot{p} = c^2\, \partial_x^2 p + s$$

impossing pressure-free conditions at the two boundaries as

$$p(x)\,|_{x=0,L} = 0$$

Acoustic waves in 1D

The following dependencies apply:

$$\begin{aligned} p &\rightarrow p(\mathbf{x, t}) && \text{pressure} \\ c &\rightarrow c(\mathbf{x}) && \text{P-velocity} \\ s &\rightarrow s(\mathbf{x, t}) && \text{source term} \end{aligned}$$

As a first step we need to discretize space and time and we do that with a constant increment that we denote dx and dt.

$$\begin{aligned} x_j &= j\mathrm{d}x, \qquad j = 0, j_{max} \\ t_n &= n\mathrm{d}t, \qquad n = 0, n_{max} \end{aligned}$$

Acoustic waves in 1D

Starting from the continuous description of the partial differential equation to a discrete description. The upper index will correspond to the time discretization, the lower index will correspond to the spatial discretization

$$
\begin{aligned}
p_j^{n+1} &\rightarrow p(x_j, t_n + \mathrm{d}t) \\
p_j^{n} &\rightarrow p(x_j, t_n) \\
p_j^{n-1} &\rightarrow p(x_j, t_n - \mathrm{d}t) \\
p_{j+1}^{n} &\rightarrow p(x_j + \mathrm{d}x, t_n) \\
p_j^{n} &\rightarrow p(x_j, t_n) \\
p_{j-1}^{n} &\rightarrow p(x_j - \mathrm{d}x, t_n)
\end{aligned}
$$

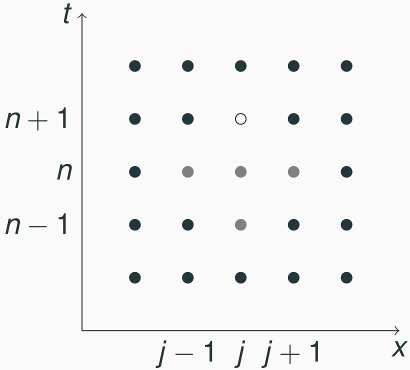
.

Acoustic waves in 1D

$$\frac{p_j^{n+1} - 2p_j^n + p_j^{n-1}}{\mathrm{d}t^2} = c_j^2 \left[\frac{p_{j+1}^n - 2p_j^n + p_{j-1}^n}{\mathrm{d}x^2} \right] + s_j^n \,.$$

the r.h.s. is defined at same time level n

the l.h.s. requires information from three different time levels



Acoustic waves in 1D

Assuming that information at time level n (the presence) and $n-1$ (the past) is known, we can solve for the unknown field p_j^{n+1}:

$$p_j^{n+1} = c_j^2 \frac{\mathrm{d}t^2}{\mathrm{d}x^2}\left[p_{j+1}^n - 2p_j^n + p_{j-1}^n\right] + 2p_j^n - p_j^{n-1} + \mathrm{d}t^2 s_j^n$$

The initial condition of our wave simulation problem is such that everything is at rest at time t = 0:

$$p(x,t)|_{t=0} = 0 \,, \ \dot{p}(x,t)|_{t=0} = 0.$$

Acoustic waves in 1D

Waves begin to radiate as soon as the source term $s(x, t)$ starts to act

For simplicity: the source acts directly at a grid point with index j_s

Temporal behaviour of the source can be calculated by Green's function

$$s(x, t) = \delta(x - x_s)\, \delta(t - t_s)$$

where x_s and t_s are source location and source time and $\delta()$ corresponds to the delta function

Acoustic waves in 1D

A delta function contains all frequencies and we cannot expect that our numerical algorithm is capable of providing accurate solutions Operating with a band-limited source-time function:

$$s(x,t) = \delta(x - x_s)\ f(t)$$

where the temporal behaviour f(t) is chosen according to our specific physical problem

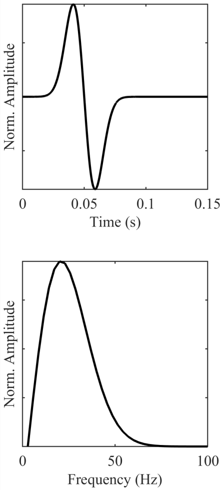
Example

Simulating acoustic wave propagation in a 10km column (e.g. the atmosphere) and assume an air sound speed of $c = 0.343 m/s$. We would like to *hear* the sound wave so it would need a dominant frequency of at least 20 Hz. For the purpose of this exercise we initialize the source time function $f(t)$ using the first derivative of a Gauss function.

$$f(t) \; = \; -8 \; f_0 \; (t - t_0) \; e^{-\frac{1}{(4 f_0)^2} \; (t - t_0)^2}$$

where t_0 corresponds to the time of the zero-crossing, f_0 is the dominant frequency

Example



- What is the minimum spatial wavelength that propagates inside the medium?
- What is the maximum velocity inside the medium?
- What is the propagation distance of the wavefield (e.g., in dominant wavelengths)?

Example

Sufficient to look at the relation between frequency and wavenumber:

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

where c is velocity, T is period, λ is wavelength, f is frequency, and $\omega = 2\pi f$ is angular frequency

dominant wavelength of $f_0 = 20Hz$

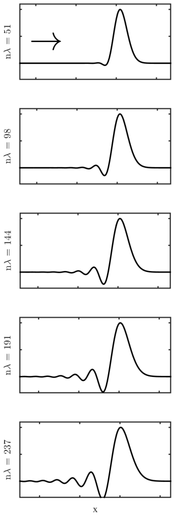
substantial amount of energy in the wavelet is at frequencies above 20 Hz

$\implies \lambda = 17m$ and $\lambda = 7m$ for frequencies $20Hz$ and $50Hz$, respectively

Python code fragment

```python
# Time extrapolation
for it in range(nt):
    # calculate partial derivatives (omit boundaries)
    for i in range(1, nx - 1):
        d2p[i] = (p[i + 1] - 2 * p[i] + p[i - 1]) / dx ** 2
    # Time extrapolation
    pnew = 2 * p - pold + dt ** 2 * c ** 2 * d2p
    # Add source term at isrc
    pnew[isrc] = pnew[isrc] +  dt ** 2 * src[it] / dx
    # Remap time levels
    pold, p = p, pnew
```

Result



Choosing a grid increment of $dx = 0.5m \longrightarrow$ about 24 points per spatial wavelength for the dominant frequency

Setting time increment $dt = 0.0012 \longrightarrow$ around 40 points per dominant period

Summary

- Replacing the partial derivatives by finite differences allows partial differential equations such as the wave equation to be solved directly for (in principle) arbitrarily heterogeneous media
- The accuracy of finite-difference operators can be improved by using information from more grid points (i.e., longer operators). The weights for the grid points can be obtained using Taylor series