Karlsruhe Institute of Technology

Seismic Modelling

1D acoustic Finite Difference Method

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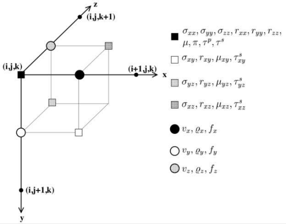
Wave equations

$$p_{ij} = \lambda\theta\delta_{ij} + 2\mu\epsilon_{ij}$$

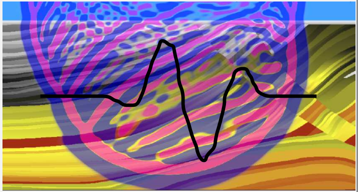
$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

$$\rho\frac{\partial^2 u_i}{\partial t^2} = \frac{\partial p_{ij}}{\partial x_j} + f_i$$

Discretization



Solutions



Motivation

1. Understand the complexity of wave propagation
2. Produce reference results to test new methods
3. Optimize acquisition geometry
4. Predict earthquake hazard
5. Kernel of many imaging methods, e.g. migration, tomography, FWI

Content of the lecture Seismic Modelling

7 lectures

1. **Introduction**
2. **Finite-Difference Method (3)**
3. **Reflectivity Method (1)**
4. **Eikonal solver (1)**
5. **Finite Element method (1)**
6. **Spectral Element method (1)**

Literature for further study

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- Book ”Computational Seismology” by Igel (2016).
- Book ” Full Seismic Waveform Modelling and Inversion” by (Fichtner 2011)

Agenda

1. Classification of methods

2. The Finite-Difference Method

2.1 FD-Approximation to the second order derivatives

2.2 Discretization of 1D second order wave equation

2.3 Dispersion analysis

Classification of modelling methods

1 Direct methods that solve the full wave equation
   - a Geological model is discretized on a numerical mesh
   - b Full solution of the wave equations in space and time
   - c Computationally very expensive (HPC)
   - d Examples are Finite-Differences , Finite elements, Spectral elements

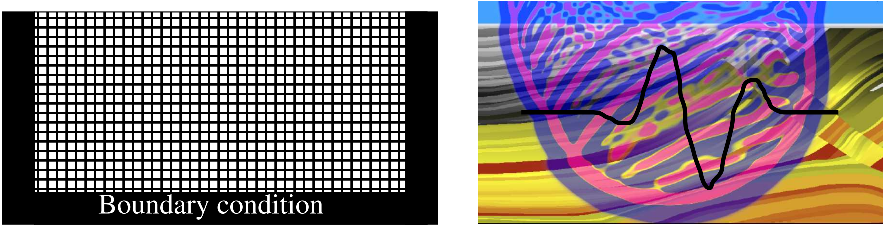

Figure 1: The Finite-Difference methods computes the full wavefield on a regular grid.

Classification of modelling methods

2 Integral-equation methods
- a Seperation of wavefield in upgoing and downgoing scattered/reflected waves
- b Superposition in performed by integration
- c Computationally very efficient
- d Examples: Kirchhoff-Modelling, Reflectivity method

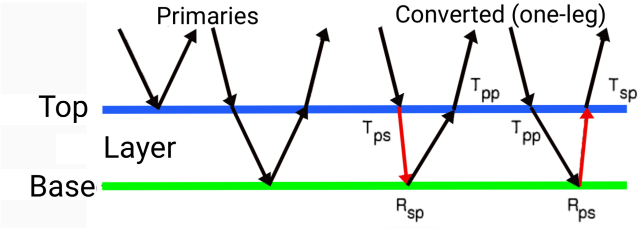

Figure 2: Integral methods superpose specific waves by numerical integration.

Classification of modelling methods

3 Ray-tracing

- (a) High-frequency approximation
- (b) Calculation of individual rays
- (c) Computationally very fast
- (d) Traveltimes reliable, amplitudes not
- (e) Examples: Ray-tracing (full ray path), Eikonal solvern (first arrivals)

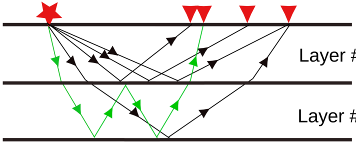

Figure 3: Individual rays are traced and their traveltime and amplitude is calculated.

Agenda

The Finite-Difference Method

The general idea of the FD-method is to replace the partial derivatives in time and space with difference equations. These can be obtained by a Taylor-series expansion.

- 🙂 The difference equations are straightforward to implement.
- 🙂 The numerical properties are well understood.
- 🙂 Wavefields in arbitrary complex media can be calculated.
- 🙂 The resulting algorithms are very fast and efficient and show excellent performance on HPCs.
- 🙁 Variable spatial and temporal discretization is problematic.

Agenda

1D wave equation

For simplicity we consider the second order 1D wave equation:

$$\frac{\partial^2 p}{\partial t^2} = c^2 \frac{\partial^2 p}{\partial x^2} \tag{1}$$

We want to approximate the second order space derivatives first.

We discretize

$$p(x) = p(mh) = p_m$$

where h denotes the grid spacing.

Finite-Difference equations for second order derivatives

We perform a Taylor series expansion around $p(x=0)=p_0$

$$p_m = p_0 + \sum_{k=1}^{N} \frac{p^{(k)} m^k h^k}{k!} \tag{2}$$

We can eliminate uneven derivatives by adding p at negative offsets m:

$$p_m + p_{-m} = 2p_0 + p^{''} m^2 h^2 + 2 \sum_{k=2}^{N} \frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!} \tag{3}$$

Finite-Difference equations for second order derivatives

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We now isolate the desired second order derivative:

$$p'' m^2 = \frac{-2p_0}{h^2} + \frac{1}{h^2}\left(p_m + p_{-m}\right) - \frac{2}{h^2}\sum_{k=2}^{N}\frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!} \tag{4}$$

We multiply each of the m equations with an (yet unknown) coefficient a_m:

$$a_m p'' m^2 = \frac{-2p_0}{h^2} a_m + \frac{1}{h^2} a_m \left(p_m + p_{-m}\right) - \frac{2}{h^2} a_m \sum_{k=2}^{N}\frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!} \tag{5}$$

Then we sum all m equations:

$$\sum_{m=1}^{M} a_m m^2 p'' = \frac{-2p_0}{h^2}\sum_{m=1}^{M} a_m + \frac{1}{h^2}\sum_{m=1}^{M} a_m \left(p_m + p_{-m}\right) - \frac{-2}{h^2}\sum_{m=1}^{M} a_m \sum_{k=2}^{N}\frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!} \tag{6}$$

Finite-Difference equations for second order derivatives

We repeat the last equation:

$$\sum_{m=1}^{M} a_m m^2 p'' = \frac{-2p_0}{h^2}\sum_{m=1}^{M} a_m + \frac{1}{h^2}\sum_{m=1}^{M} a_m\left(p_m + p_{-m}\right) - \frac{-2}{h^2}\sum_{m=1}^{M} a_m \sum_{k=2}^{N} \frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!}$$

If we choose the coefficients a_m so that

$$\sum_{m=1}^{M} a_m m^2 = 1 \quad \text{and} \quad \sum_{m=1}^{M} a_m m^{2k} = 0 \quad \text{with} \quad k = 2, ..., M$$

we obtain:

$$\begin{aligned} p'' &= \frac{-2p_0}{h^2}\sum_{m=1}^{M} a_m + \frac{1}{h^2}\sum_{m=1}^{M} a_m\left(p_m + p_{-m}\right) - \frac{-2}{h^2}\sum_{k=M+1}^{N} \frac{p^{(2k)} m^{2k} h^{2k}}{(2k)!} \\ p'' &= \frac{1}{h^2}\left(-a_0 p_0 + \sum_{m=1}^{M} a_m\left(p_m + p_{-m}\right)\right) + \mathcal{O}\left(h^{2M}\right) \quad \text{with} \quad a_0 = 2\sum_{m=1}^{M} a_m \end{aligned}$$

Finite-Difference equations for second order derivatives

The accuracy order is defined as smallest exponent of h in the error term

$$-\frac{-2}{h^2}\sum_{k=M+1}^{N}\frac{p^{(2k)}m^{2k}h^{2k}}{(2k)!}=\mathcal{O}(h^{2M})$$

which is $2(M+1)-2=2M$.
So we finally obtained the following FD aproximation for the second order derivative:

$$p'' = \frac{1}{h^2}\left(-a_0p_0+\sum_{m=1}^{M}a_m\left(p_m+p_{-m}\right)\right)+\mathcal{O}(h^{2M}) \quad \text{with} \quad a_0=2\sum_{m=1}^{M}a_m \tag{7}$$

for which we can also write

$$\boxed{p'' = \frac{1}{h^2}\left(\sum_{m=1}^{M}a_m\left(p_m+p_{-m}-2p_0\right)\right)+\mathcal{O}(h^{2M})}$$

Finite-Difference equations for second order derivatives

The coefficient can be interpreted as follows:

$$\boxed{p'' = \frac{1}{h^2}\left(\sum_{m=1}^{M} a_m\left(p_m + p_{-m} - 2p_0\right)\right) + \mathcal{O}(h^{2M})} \tag{8}$$

The length of the operator is M grid points. The order of accuracy is $2M$.

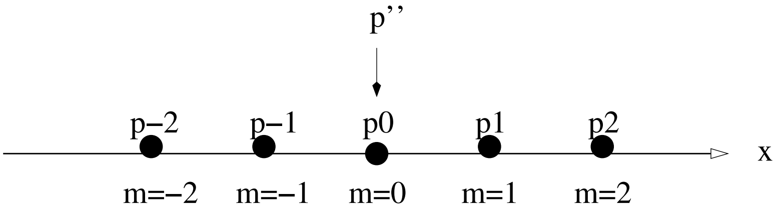

Figure 4: Illustration of the summation of adjacent pressure values to approximate the second order spatial derivative using the symmetric FD-operator given in equation 7.

Finite-Difference equations for second order derivatives

Remember that the FD coefficients a_m must be determined by

$$\sum_{m=1}^{M} a_m m^2 = 1 \quad \text{and} \quad \sum_{m=1}^{M} a_m m^{2k} = 0 \quad \text{with} \quad k = 2, \ldots, M \tag{9}$$

This resulting a_m are:

M	$a_0 = 2\sum_{m=1}^{M} a_m$	a_1	a_2	a_3	a_4	a_5	accuracy order (2M)
1	2	1					2
2	5/2	4/3	-1/12				4
3	49/18	3/2	-3/20	1/90			6
4	205/72	8/5	-1/5	8/315	-1/560		8
5	5269/1800	5/3	-5/21	5/126	-5/1008	1/3150	10

Table 1: FD-coefficients for the approx. of the second derivative (eq. 8) calculated via eq. 9.

Example: Approximation of second derivative of test function $\sin(x)$

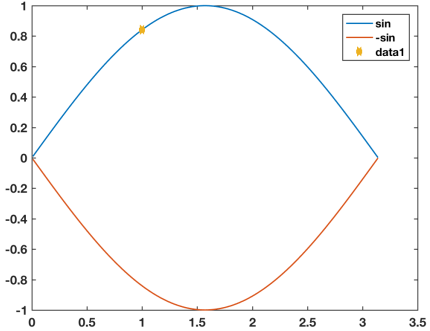

Figure 5: Test function $\sin(x)$ at $x_0 = 1.0$ and second deriviative.

- $p_{true}(x_0) = \sin(x_0)$ at $x_0 = 1.0$
- $p''_{true}(x_0) = -\sin(x_0)$.
- L1-error: $E = \|p''_{FD} - p''_{true}\|$

Approximation of second derivative of $\sin(x)$

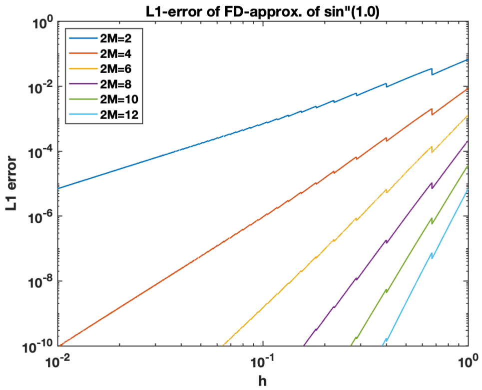

Figure 6: L1-error of FD approximation of second derivative of test function $\sin(x)$ at $x_0 = 1.0$.

- The error decreases $log(E) \propto 2M \cdot log(h)$
- The error can be reduced significantly by increasing M

Agenda

Discretization of 1D acoustic wave equation

We consider the 1-D second order wave equation

$$\frac{\partial^2 p(x,t)}{\partial t^2} = c^2 \frac{\partial^2 p(x,t)}{\partial x^2} \tag{10}$$

The pressure $p(x,t)$ at the location x at time t is discretized with $p(x,t) = p(jh, n\triangle t) = p_j^n$. According to equation 7 a second order approximation (M=1) of the second order derivatives are:

$$\frac{1}{\triangle t^2}(p_j^{n+1} - 2p_j^n + p_j^{n-1}) = \frac{c^2}{h^2}(p_{j+1}^n - 2p_j^n + p_{j-1}^n) \tag{11}$$

The resulting explicit FD-scheme the reads

$$p_j^{n+1} = 2p_j^n - p_j^{n-1} + \frac{c^2 \triangle t^2}{h^2}(p_{j+1}^n - 2p_j^n + p_{j-1}^n) \tag{12}$$

It is if second order accuracy in both time and space O(2,2). The symbol O(N,2M) denotes the accuracy order in time (N) and space (2M).

Discretization of 1D acoustic wave equation

For arbitrary order in space $2M$ but second order in time O(2,2M) the explicit FD approximation to the second order wave equations reads

$$\boxed{p_j^{n+1} = 2p_j^n - p_j^{n-1} + \frac{c^2 \triangle t^2}{h^2}\left(-a_0 p_j^n + \sum_{m=1}^{M} a_m \left(p_{j+m}^n + p_{j-m}^n\right)\right)} \tag{13}$$

- This is a very common explicit discretization of the wave equation.
- The wavefield can be calculated in a time-loop starting at $n = 0$ and then increase n by 1: $n \rightarrow n+1$. The numerical implementation is relatively straightforward.
- Typical accuracy orders in space are $2M = 2, 4, 6$.

Agenda

Dispersion analysis

We now perform a so-called dispersion analysis of the discrete 1-D wave equation:

$$\frac{1}{\triangle t^2}(p_j^{n+1} + p_j^{n-1} - 2p_j^n) = \frac{c^2}{h^2}\sum_{m=1}^{M} a_m \left(p_{j+m}^n + p_{j-m}^n - 2p_j^n\right) \tag{14}$$

We insert again a plane wave

$$p_j^n = p_0 \exp(i(kjh + \omega n \triangle t) \tag{15}$$

and obtain

$$\begin{aligned} & p_0 \exp(i(kjh + \omega n \triangle t) \left[\exp(i\omega(+\triangle t)) + \exp(i\omega(-\triangle t)) - 2\right] = \\ & \frac{c^2 \triangle t^2}{h^2} p_0 \exp(i(kjh + \omega n \triangle t) \sum_{m=1}^{M} a_m \left[\exp(ikmh) + \exp(-ikmh) - 2\right] \end{aligned}$$

Dispersion analysis

We can eliminate $p_0 \exp(i(kjh + \omega n \triangle t)$ and make the substitutions

$$\begin{aligned} z_t &= \exp(i \triangle t \omega) \\ z_x &= \exp(ikh) \\ r &= \frac{c \triangle t}{h} \quad \text{"Courant number"} \end{aligned}$$

and get

$$\left(z_t^1 + z_t^{-1} - 2\right) = r^2 \sum_{m=1}^{M} a_m \left(z_x^m + z_x^{-m} - 2\right) \tag{16}$$

Dispersion analysis

We first analyze the RHS of eq. 16 and use the Euler eq. $\exp(ix) = \cos(ix) + i\sin(ix)$

$$
\begin{aligned}
a_m\left(z_x^m + z_x^{-m} - 2\right) &= a_m\left(\exp(imkh) + \exp(-imkh) - 2\right) \\
&= 2a_m\left(\cos(mkh) - 1\right) = 2a_m\left(-2\sin^2\left(\frac{mkh}{2}\right)\right) \\
&= -4a_m\sin^2\left(\frac{mkh}{2}\right)
\end{aligned}
$$

For the LHS we obtain:

$$
\left(z_t^1 + z_t^{-1} - 2\right) = -4\sin^2\left(\frac{\omega\triangle t}{2}\right)
$$

Therefore

$$
\sin^2\left(\frac{\omega\triangle t}{2}\right) = r^2\sum_{m=1}^{M} a_m\sin^2\left(\frac{mkh}{2}\right) \tag{17}
$$

This is a ”dispersion relation” between ω and k.

Dispersion analysis

We want to solve this dispersion relation and analyze the effect on the numerical phase velocity of the waves. The numerical propagation velocity is $c_{fd} = \frac{\omega}{k}$. We can therefore write

$$\frac{c_{fd}}{c} = \frac{\frac{\omega}{k}}{c} = \frac{\frac{\omega}{k}}{\frac{rh}{\triangle t}} = \frac{\omega \triangle t}{khr} \tag{18}$$

With equation 18 we finally obtain the dispersion relation for the O(2,2M) scheme

$$\boxed{\frac{c_{fd}}{c} = \frac{\omega \triangle t}{khr} = \frac{2}{khr} \arcsin\left(r\sqrt{\sum_{m=1}^{M} a_m sin^2\left(\frac{mkh}{2}\right)}\right)} \tag{19}$$

Numerical dispersion 1D FD O(2,2)

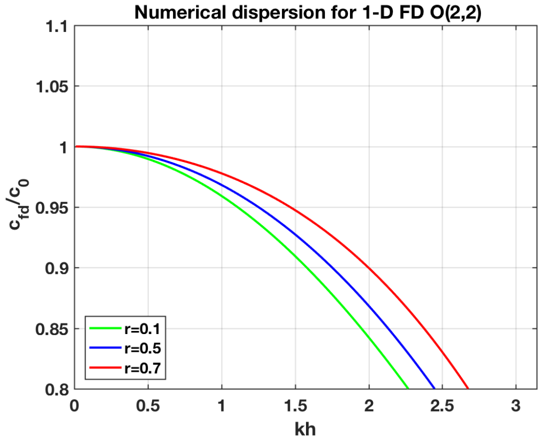

Figure 7: Numerical dispersion O(2,2) (M=1, equation 19)

- $c_{fd} < c$ for all kh.
- Velocity decrease with kh, i.e. with decreasing frequency
- For small r (small $\triangle t$) the dispersion becomes worse

Numerical dispersion 1D FD O(2,2)

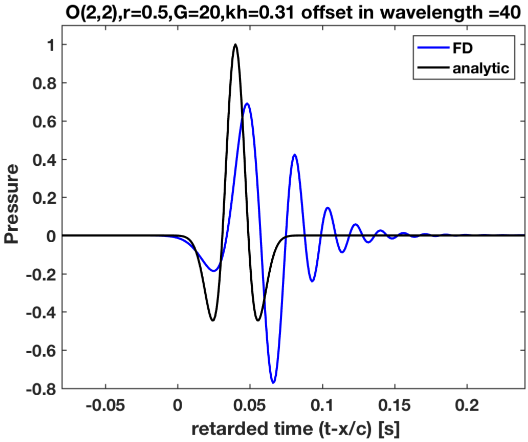

Figure 8: Seismograms for M=1 calculated via equation 13.

- Signals are dispersed
- Low frequencies arrive later
- Movie

Numerical dispersion 1D FD O(2,4)

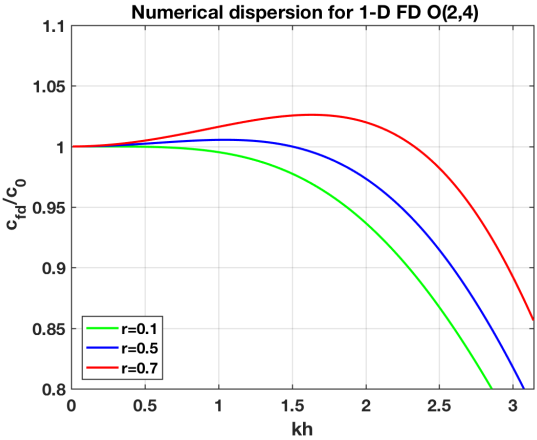

Figure 9: Numerical dispersion O(2,4) (M=2, equation 19)

- Now also $c_{fd} > c$ for some kh.
- Velocity increases for small kh, i.e. at high frequencies
- Velocity decreases for large kh, i.e. at low frequencies

Numerical dispersion 1D FD O(2,4)

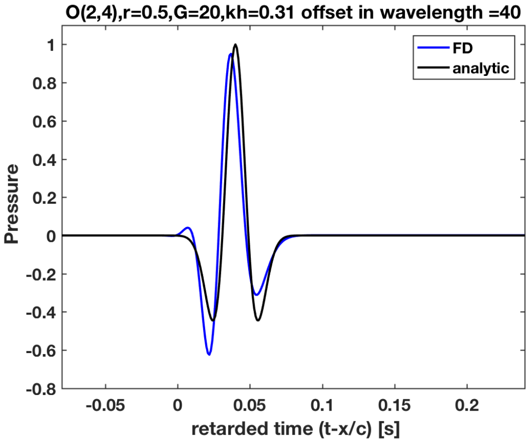

Figure 10: Seismograms for M=2 calc. via eq. 13.

- Signals are much less dispersed
- High frequencies arrive earlier
- Movie

Magic time step

Let us look again at the dispersion relation for the 1D FD O(2,2M) scheme

$$\frac{c_{fd}}{c} = \frac{\omega \triangle t}{khr} = \frac{2}{khr} \arcsin\left(r \sqrt{\sum_{m=1}^{M} a_m sin^2 (\frac{mkh}{2})} \right)$$

For second order accuracy (M=1) the dispersion relation becomes

$$\frac{c_{fd}}{c} = \frac{2}{khr} \arcsin\left(r \sin(\frac{kh}{2}) \right) \tag{20}$$

For r=1 we get

$$\frac{c_{fd}}{c} = 1 \tag{21}$$

We thus have **no error** for O(2,2) and $r = \frac{c \triangle t}{h} = 1$. The **magic time step** is

$$\triangle t_{magic} = \frac{h}{c} \tag{22}$$

Magic time step, G=20

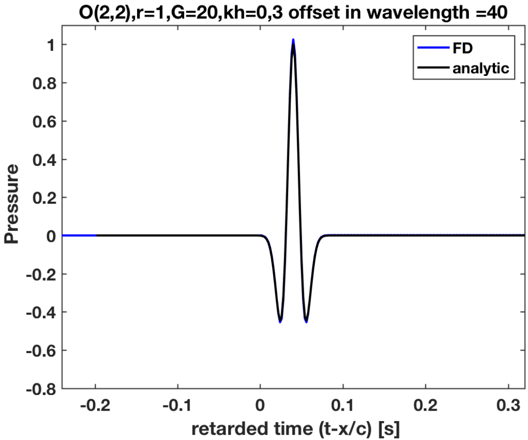

Figure 11: Seismograms for M=2 and $r = 1$.

- All frequencies propagate with $c_{fd} = c$!
- Movie

Summary

- Seismic modelling methods can be categorised into direct methods, integral methods, and ray-tracing methods
- The FD method is a direct method. The wavefield is discretized on a regular grid in space and time.
- The FD approximations for the second derivative have been obtained by Taylor series expansion.
- We derived an explicit FD scheme O(2,2M) for the 1D wave equation.
- The error in the approximation of derivatives leads to numerical dispersion. The numerical velocity becomes frequency dependent leading to precursors and/or the development of a coda.
- The O(2,2) 1D FD scheme for $r = 1$ is magic.

References

Fichtner, A. (2011), *Full Seismic Waveform Modelling and Inversion*, Springer.

Igel, H. (2016), *Computational Seismology: A Practical Introduction*, 1. edn, Oxford University Press.
URL: *https://global.oup.com/academic/product/computational-seismology-9780198717409?cc=de&lang=en&*

Questions

1. What does the term ”order of accuracy” ($2M$) mean in detail ? How can we test the ”order of accuracy” of a given algorithm numerically ?
2. What are the benefits of increasing the order of accuracy ? What are possible drawbacks ? How should we choose it ”wisely” ?
3. How can we implement equation 13 into a practical computer program (Matlab or Phython). Let us discuss the general structure of such a program.
4. How do simulation errors generally become apparent in synthetic seismograms ?
5. How can we judge if a certain FD simulation is accurate (enough) ? How can we improve the accuracy ?
6. Would you also call the specific choice of time step in equation 22 ”magic”. Do we have such a ”magic time step” also for $M > 1$ or for higher dimensions ?