Pseudospectral Methods

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

The goal of this lecture is to shed light at one end of the axis of FD (or convolutional) type differential operators. When one uses all information of a space-dependent field to estimate the derivative at a point one obtains spectral accuracy.

What is *pseudospectral*?

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 ω-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 matrix-matrix multiplications, fast Fourier transform (FFT), or convolutions.

Fourier Derivatives

.. 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

The 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

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

... leading to the extrapolation scheme ...

The Fourier Method: acoustic wave propagation

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

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

$$P_j^n \rightarrow \text{FFT} \rightarrow \hat{P}_\upsilon^n \rightarrow ik_\upsilon \hat{P}_\upsilon^n \rightarrow \text{FFT}^{-1} \rightarrow \partial_x P_j^n$$

multiply by 1/ρ

$$\frac{1}{\rho}\partial_x P_j^n \rightarrow \text{FFT} \rightarrow \left(\frac{1}{\rho}\partial_x \hat{P} \right)_\upsilon^n \rightarrow ik_\upsilon \left(\frac{1}{\rho}\partial_x \hat{P} \right)_\upsilon^n \rightarrow \text{FFT}^{-1} \rightarrow \partial_x \left(\frac{1}{\rho}\partial_x P_j^n \right)$$

... then extrapolate ...

… and in 3D …

$$p(t+dt) =$$

$$\rho c^2 dt^2 \boxed{\left(\partial_x \left(\frac{1}{\rho} \partial_x p \right) + \partial_y \left(\frac{1}{\rho} \partial_y p \right) + \partial_z \left(\frac{1}{\rho} \partial_z p \right) \right)}$$

$$+ 2p(t) - p(t-dt)$$

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

$$P_j^n \rightarrow \text{FFT} \rightarrow \hat{P}_\upsilon^n \rightarrow ik_\upsilon \hat{P}_\upsilon^n \rightarrow \text{FFT}^{-1} \rightarrow \partial_x P_j^n$$

$$\frac{1}{\rho} \partial_x P_j^n \rightarrow \text{FFT} \rightarrow \left(\frac{1}{\rho} \partial_x \hat{P} \right)_\upsilon^n \rightarrow ik_\upsilon \left(\frac{1}{\rho} \partial_x \hat{P} \right)_\upsilon^n \rightarrow \text{FFT}^{-1} \rightarrow \partial_x \left(\frac{1}{\rho} \partial_x P_j^n \right)$$

… FD in Matlab …

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
```

… and as PS …

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

```
function df=sder1d(f,dx)
% SDER1D(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 and Stability

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

$$\partial_x^2 p_j^n = -k^2 e^{i(kjdx - \omega ndt)}$$

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

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

Dispersion and Stability

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

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

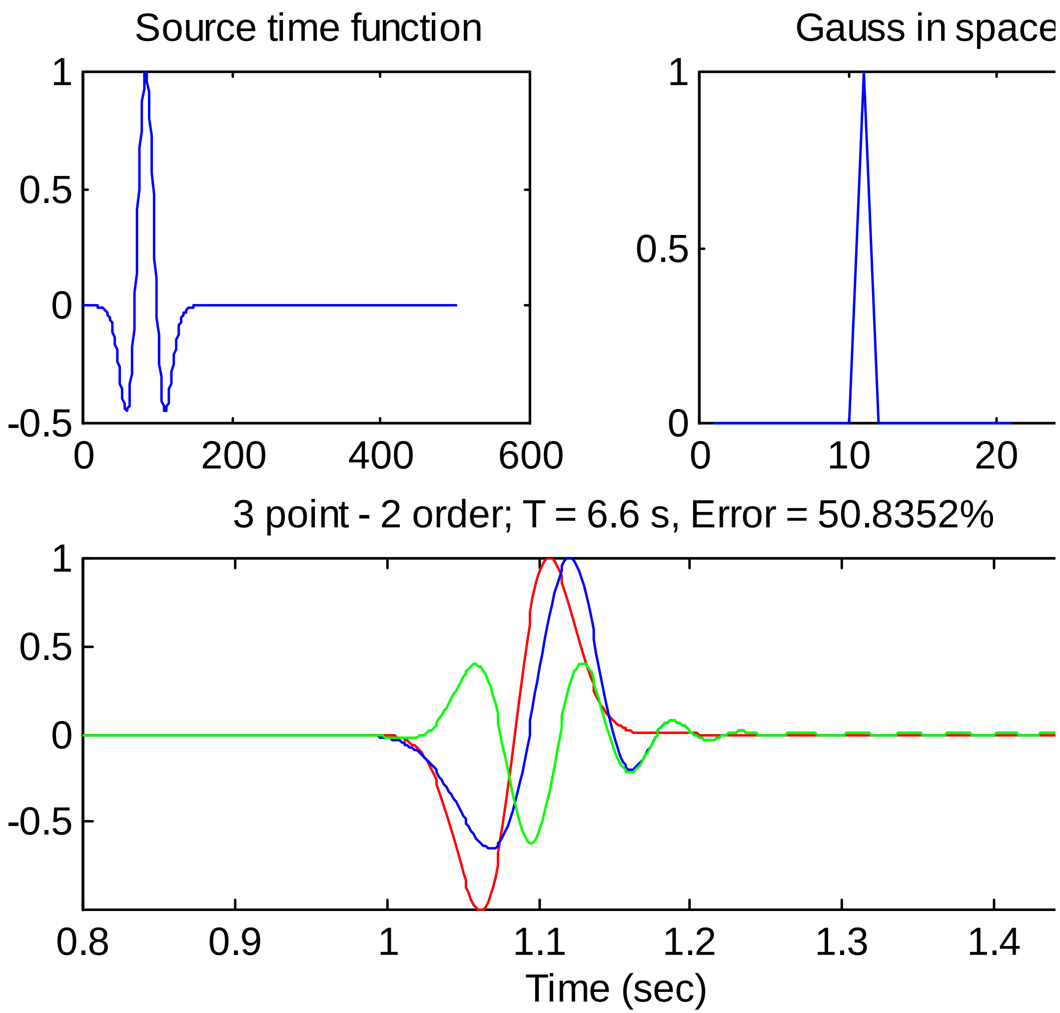
What are the consequences?

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

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

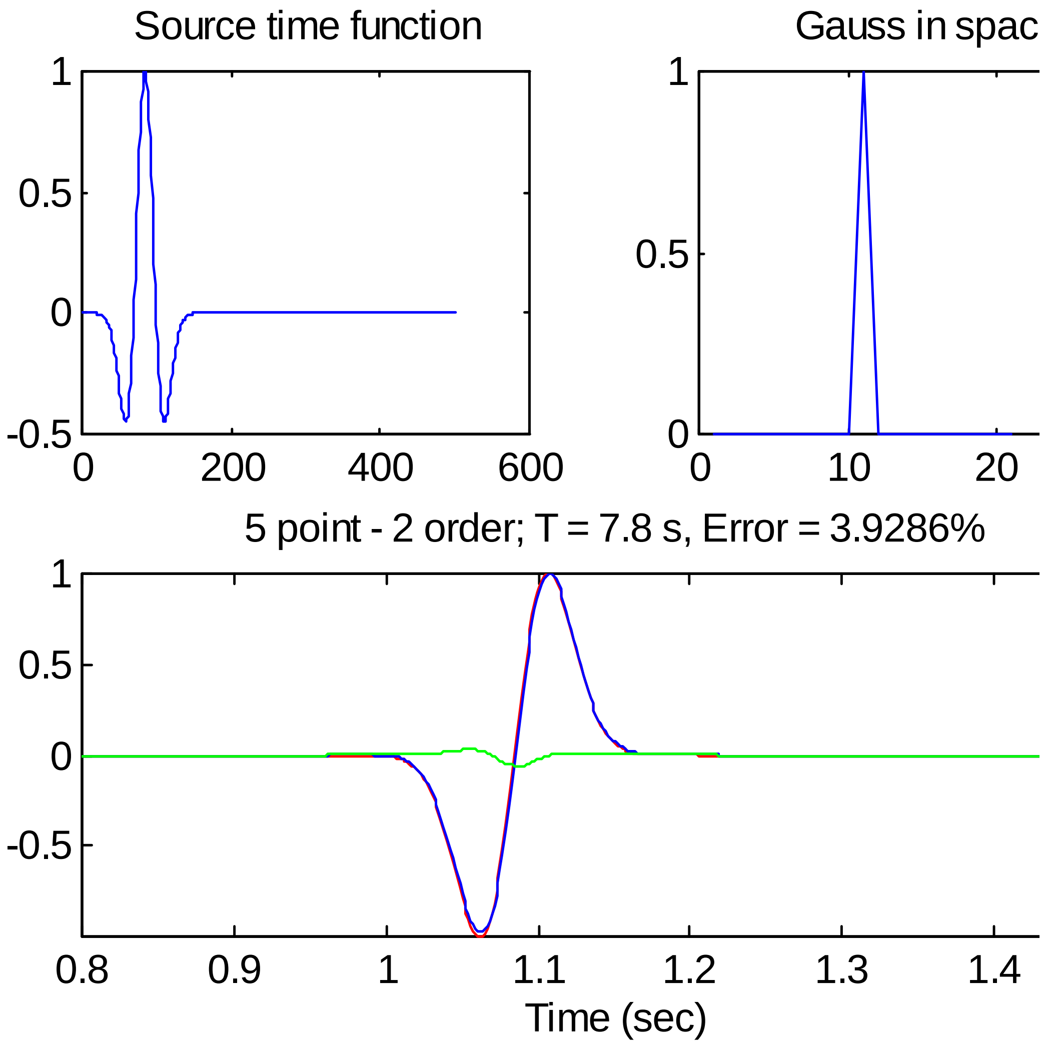
$$cdt / dx \leq 2 / \pi \approx 0.636$$

Results @ 10Hz



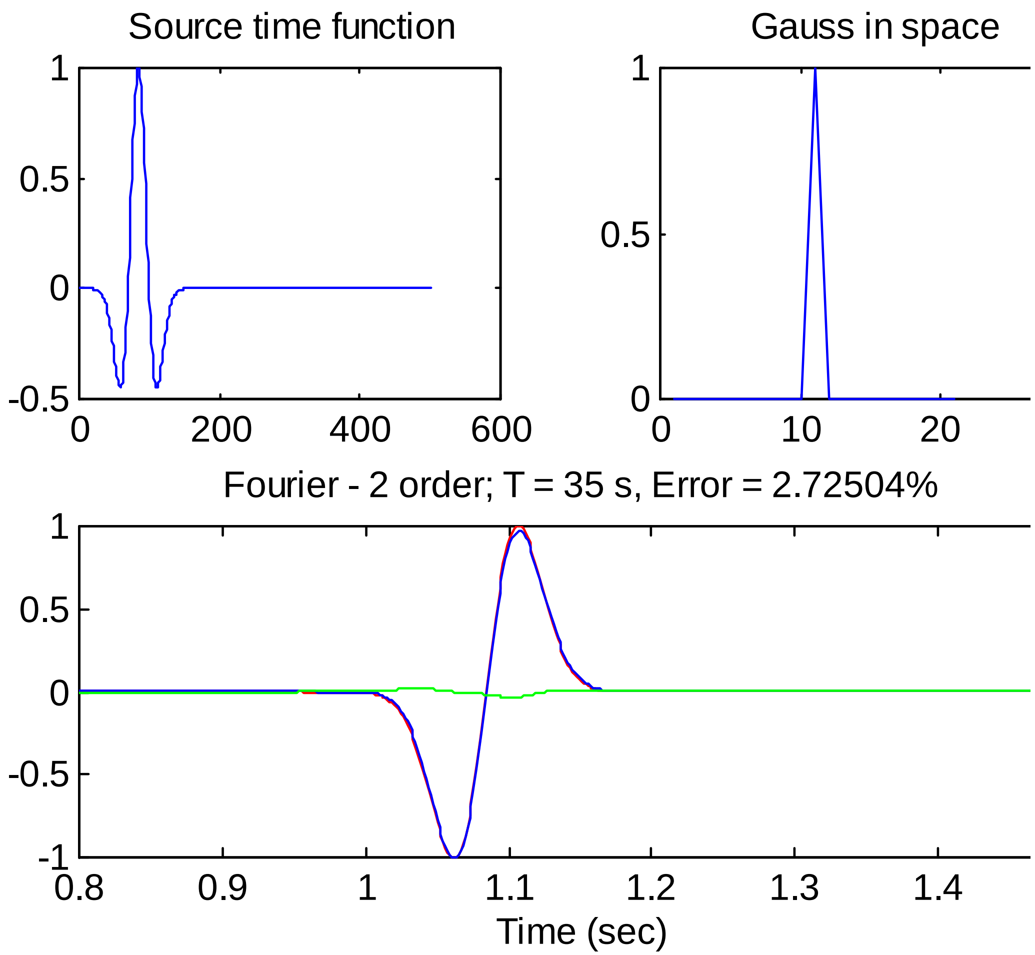
Example of acoustic 1D wave simulation.
FD3 -point operator
red-analytic; blue-numerical; green-difference

Results @ 10Hz



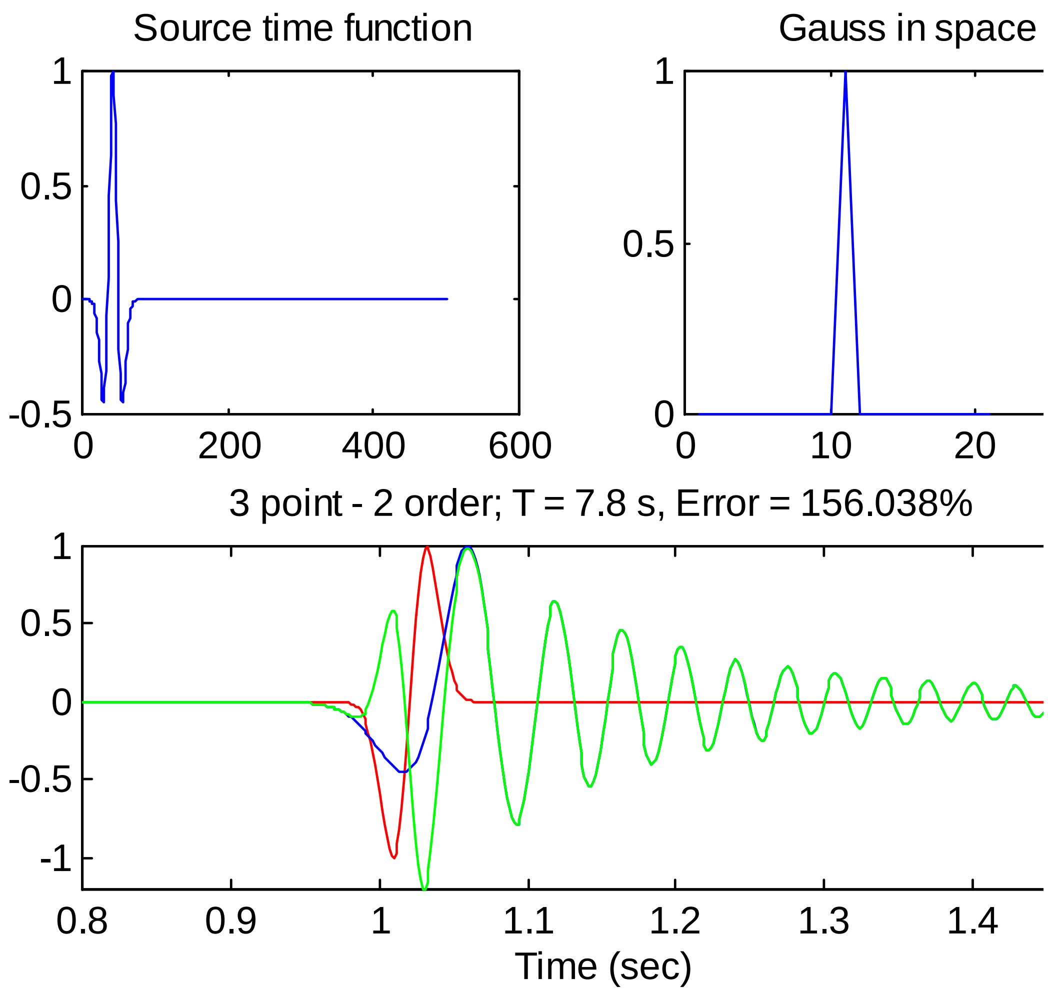
Example of acoustic 1D wave simulation.
FD 5 -point operator
red-analytic; blue-numerical; green-difference

Results @ 10Hz



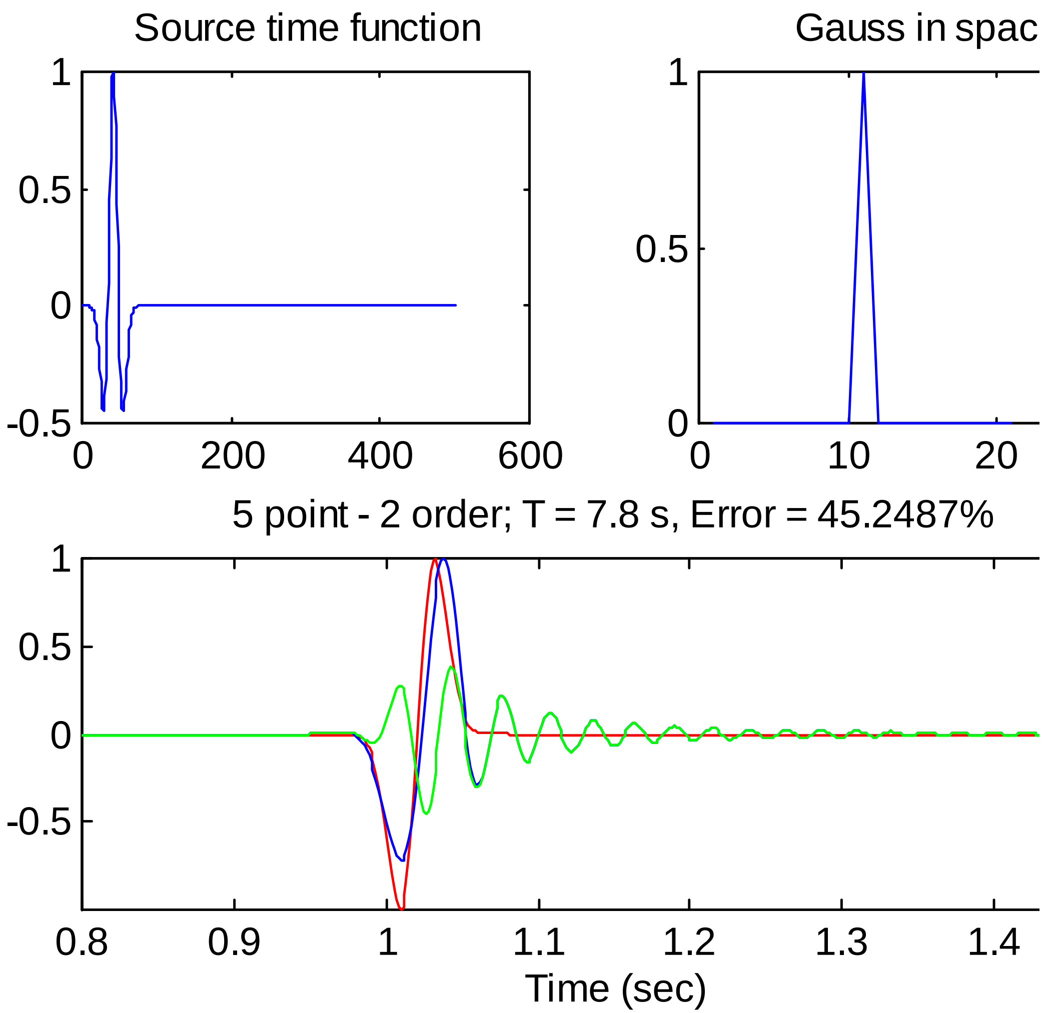
Example of acoustic 1D wave simulation.
Fourier operator
red-analytic; blue-numerical; green-difference

Results @ 20Hz



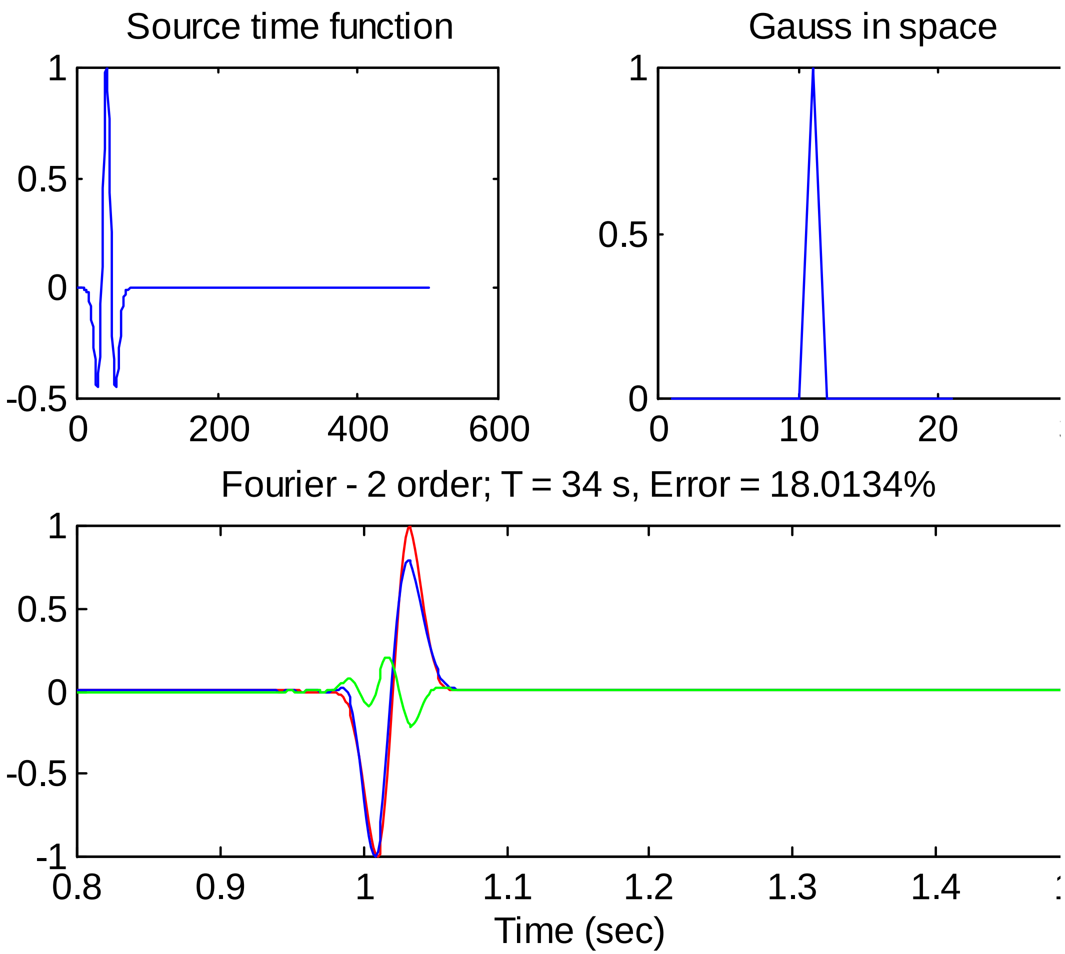
Example of acoustic 1D wave simulation.
FD3 -point operator
red-analytic; blue-numerical; green-difference

Results @ 20Hz



Example of acoustic 1D wave simulation.
FD 5 -point operator
red-analytic; blue-numerical; green-difference

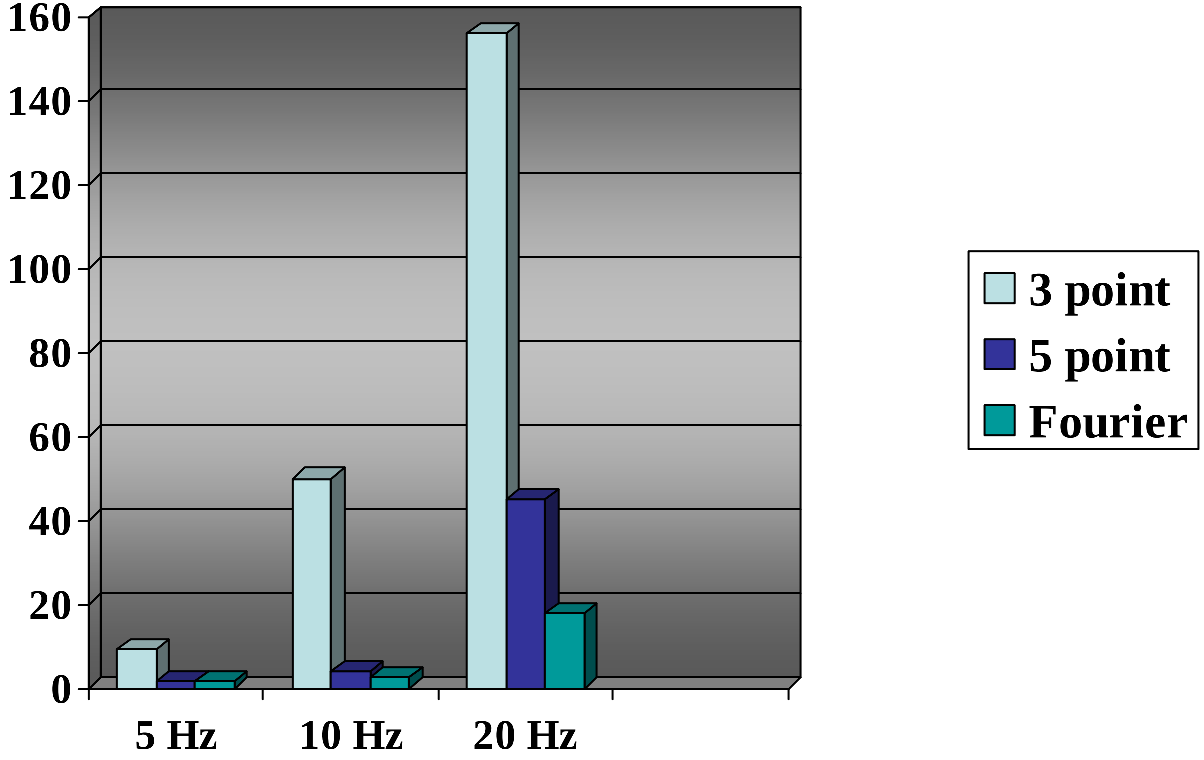
Results @ 20Hz



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

Computational Speed

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



Simulation time
5.4s
7.8s
33.0s

Numerics and Green's Functions

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 Δ being the Laplace operator. We now introduce a delta source in space and time

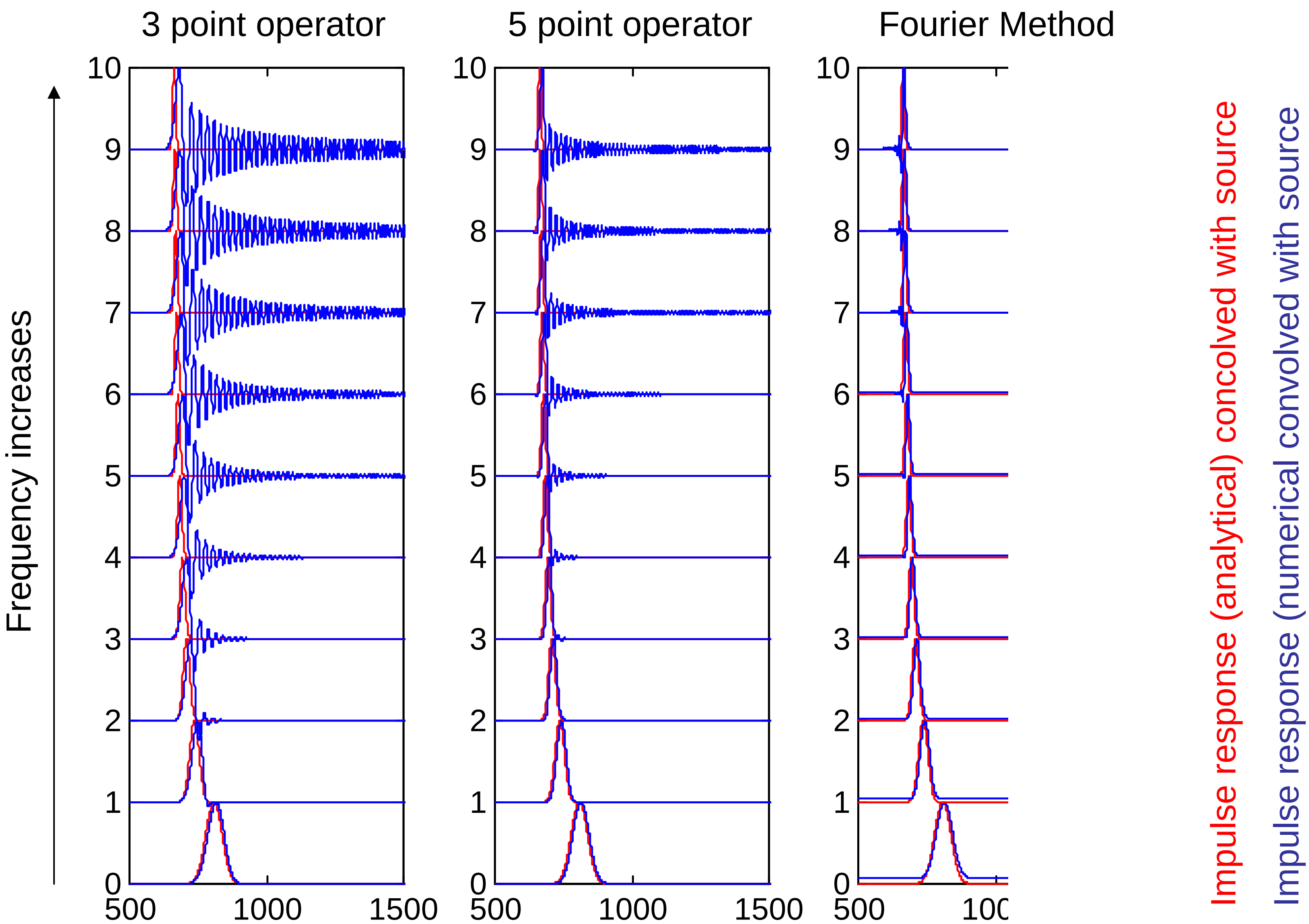
$$\partial_t^2 p = \delta(\underline{x})\delta(t) + c^2 \Delta p$$

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)

Numerical Green's functions



Pseudospectral Methods - Summary

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).

Pseudospectral methods play a minor role in seismology today but the principal of spectral accuracy plays an important role in spectral element methods