

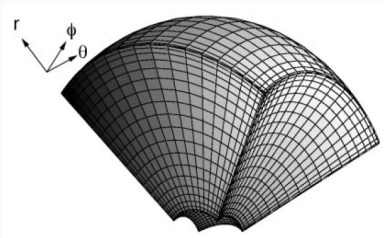
The Pseudospectral Method

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Introduction

Motivation



- **Orthogonal basis functions**, special case of FD
- **Spectral accuracy** of space derivatives
- High **memory efficiency**
- Explicit method
- **No** requirement of grid **staggering**
- Problems with strongly **heterogeneous** media

History

- Coining as transform methods as their implementation was based on the **Fourier transform** (Gazdag, 1981; Kossloff and Bayssal, 1982)
- Initial applications to the acoustic wave equation were extended to the elastic case (Kossloff et al., 1984), and to 3D (Reshef et al., 1988)
- Developing efficient time integration schemes (Tal-Ezer et al., 1987) that allowed large time steps to be used in the extrapolation procedure
- Replacing harmonic functions as bases for the function interpolation by **Chebyshev polynomials** (Kossloff et al., 1990)
- To improve the accurate modelling of curved internal interfaces and **surface topography grid stretching** as coordinate transforms was introduced and applied (Tessmer et al., 1992; Komatitsch et al., 1996)
- By mixing finite-difference operators and pseudospectral operators in the different spatial directions, the method was used for interesting seismological problems (Furumura et al., 1998b; Furumura and Kennett, 2005)

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The Pseudospectral Method in a Nutshell

The Pseudospectral method is:

- a grid point method
- a series expansion method (Fourier or Chebyshev)

Looking at the acoustic wave equation using finite-difference method leaves us with

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

The Pseudospectral Method in a Nutshell

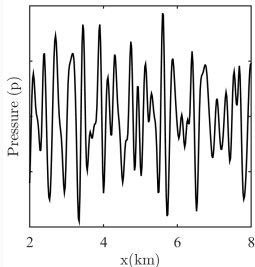
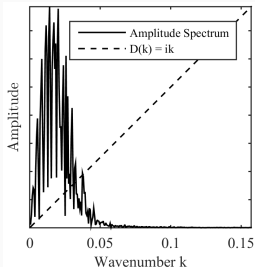
The remaining task is to calculate the space derivative on the r.h.s.

$$\partial_x^{(n)} p(x, t) = \mathcal{F}^{-1}[(-ik)^n P(k, t)]$$

where i is the imaginary unit, \mathcal{F}^{-1} is the inverse Fourier transform, and $P(k, t)$ is the spatial Fourier transform of the pressure field $p(x, t)$, k being the wavenumber.

Using discrete Fourier transform of functions defined on a regular grid, we obtain exact derivatives up to the Nyquist wavenumber $k_N = \pi/dx$.

The Pseudospectral Method in a Nutshell



Principle of the pseudospectral method based on the Fourier series

- Use of sine and cosine functions for the expansions implies periodicity
- Using Chebyshev polynomials similar accuracy of common boundary conditions (free surface, absorbing) can be achieved

The Pseudospectral Method: Ingredients

Orthogonal Functions, Interpolation, Derivative

In many situations we either...

- seek to approximate a known analytic function by an approximation
- know a function only at a discrete set of points and we would like to interpolate in between those points

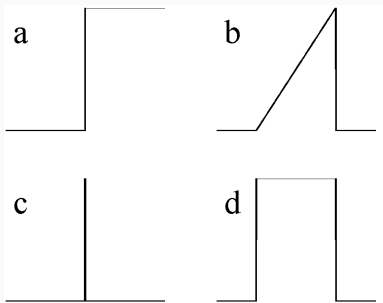
Let us start with the first problem such that our known function is approximated by a finite sum over some N basis functions Φ_i

$$f(x) \approx g_N(x) = \sum_{i=1}^N a_i \Phi_i(x)$$

and assume that the basis functions form an orthogonal set

Orthogonal Functions, Interpolation, Derivative

Why would one want to replace a known function by something else?



Dynamic phenomena are mostly expressed by PDEs

Either nature is not smooth and differentiable

mathematical functions are non-differentiable

Orthogonal Functions, Interpolation, Derivative

With the right choice of differentiable basis functions Φ_i the calculation becomes

$$\partial_x f(x) \approx \partial_x g_N(x) = \sum_{i=1}^N a_i \partial_x \Phi_i(x)$$

Consider the set of (trigonometric) basis functions

$$\cos(nx) \quad n = 0, 1, \dots, \infty$$

$$\sin(nx) \quad n = 0, 1, \dots, \infty$$

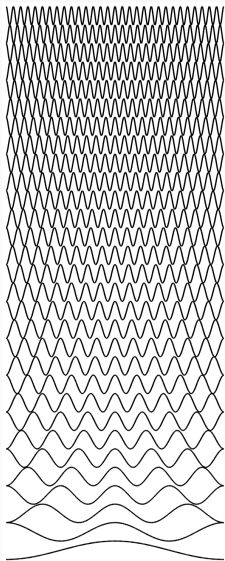
with

$$1, \cos(x), \cos(2x), \cos(3x), \dots$$

$$0, \sin(x), \sin(2x), \sin(3x), \dots$$

in the interval $[-\pi, \pi]$

Orthogonal Functions, Interpolation, Derivative



Checking whether these functions are orthogonal by evaluating integrals with all possible combinations

$$\int_{-\pi}^{\pi} \cos(jx) \cos(kx) dx = \begin{cases} 0 & \text{for } j \neq k \\ 2\pi & \text{for } j = k = 0 \\ \pi & \text{for } j = k > 0 \end{cases}$$

$$\int_{-\pi}^{\pi} \sin(jx) \sin(kx) dx = \begin{cases} 0 & \text{for } j \neq k ; j, k > 0 \\ \pi & \text{for } j = k > 0 \end{cases}$$

$$\int_{-\pi}^{\pi} \cos(jx) \sin(kx) dx = 0 \text{ for } j \geq 0, k > 0$$

Orthogonal Functions, Interpolation, Derivative

The approximate function $g_N(x)$ can be stated as

$$f(x) \approx g_N(x) = \sum_{k=0}^N a_k \cos(kx) + b_k \sin(kx)$$

By minimizing the difference between approximation $g_N(x)$ and the original function $f(x)$, the so-called l_2 -norm, the coefficients a_k, b_k can be found

$$\|f(x) - g_N(x)\|_{l_2} = \left[\int_a^b \{f(x) - g_N(x)\}^2 dx \right]^{\frac{1}{2}} = \text{Min}$$

\implies independent of the choice of basis functions

Fourier Series and Transforms

The most important concept of this section will consist of the properties of Fourier series on regular grids.

The approximate function $g_N(x)$ has the following form

$$g_N(x) = \frac{1}{2}a_0 + \sum_{k=1}^n a_k \cos(kx) + b_k \sin(kx)$$

and leads to the coefficients

$$a_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \cos(kx) dx \quad k = 0, 1, \dots, n$$
$$b_k = \frac{1}{\pi} \int_{-\pi}^{\pi} f(x) \sin(kx) dx \quad k = 0, 1, \dots, n .$$

Fourier Series and Transforms

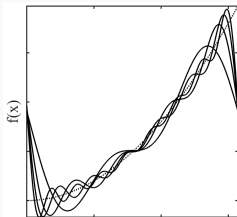
Using Euler's formulae, yields to

$$g_N(x) = \sum_{k=-n}^{k=n} c_k e^{ikx}$$

with complex coefficients c_k given by

$$\begin{aligned} c_k &= \frac{1}{2} (a_k - ib_k) \\ c_{-k} &= \frac{1}{2} (a_k + ib_k) \quad k > 0 \\ c_0 &= \frac{1}{2} a_0 . \end{aligned}$$

Fourier Series and Transforms

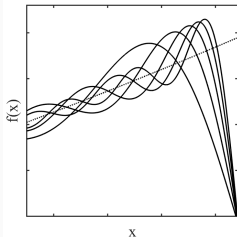


Finding the interpolating trigonometric polynomial for the periodic function

$$f(x + 2\pi) = f(x) = x^2 \quad x \in [0, 2\pi]$$

The approximation $g_N(x)$ can be obtained with

$$g_N(x) = \frac{4\pi^2}{3} + \sum_{k=1}^N \left\{ \frac{4}{k^2} \cos(kx) - \frac{4\pi}{k} \sin(kx) \right\}$$



Fourier Series and Transforms

We assume that we know our function $f(x)$ at a discrete set of points x_i given by

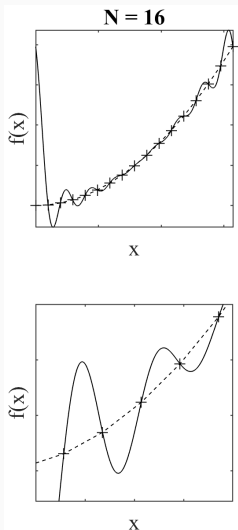
$$x_i = \frac{2\pi}{N}i \quad i = 0, \dots, N.$$

Using the "trapezoidal rule" for the integration of a definite integral we obtain for the Fourier coefficients

$$a_k^* = \frac{2}{N} \sum_{j=1}^N f(x_j) \cos(kx_j) \quad k = 0, 1, \dots, n$$

$$b_k^* = \frac{2}{N} \sum_{j=1}^N f(x_j) \sin(kx_j) \quad k = 0, 1, \dots, n$$

Fourier Series and Transforms



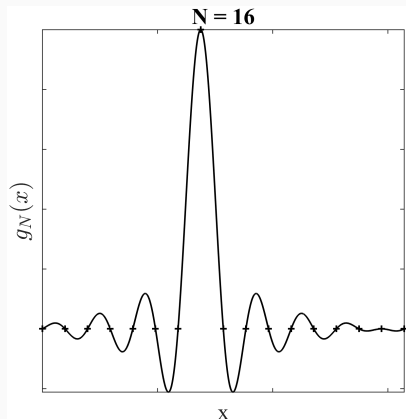
We thus obtain the specific Fourier polynomial with $N = 2n$

$$g_n^* := \frac{1}{2}a_0^* + \sum_{k=1}^{n-1} \{a_k^* \cos(kx) - b_k^* \sin(kx)\} + \frac{1}{2}a_n^* \cos(nx)$$

with the tremendously important property

$$g_n^*(x_i) = f(x_i) .$$

Cardinal functions



Discrete interpolation and derivative operations can also be formulated in terms of convolutions

It is unity at grid point x_i and zero at all other points on the discrete grid

It has the form of a *sinc*-function

Forward Transform

$$F(k) = \mathcal{F}[f(x)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Inverse Transform

$$f(x) = \mathcal{F}^{-1}[F(k)] = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{ikx} dk$$

Fourier Series and Transforms

Taking the formulation of the inverse transform to obtain the derivative of function $f(x)$

$$\begin{aligned}\frac{d}{dx}f(x) &= \frac{d}{dx} \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(k) e^{-ikx} dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} -ik F(k) e^{-ikx} dk \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} D(k) F(k) e^{-ikx} dk\end{aligned}$$

with $D(k) = -ik$

We can extend this formulation to the calculation of the $n - th$ derivative of $f(x)$ to achieve

$$F^{(n)}(k) = D(k)^n F(k) = (-ik)^n F(k)$$

Fourier Series and Transforms

Thus using the condensed Fourier transform operator \mathcal{F} we can obtain an exact n – th derivative using

$$\begin{aligned} f^{(n)}(x) &= \mathcal{F}^{-1}[(-ik)^n F(k)] \\ &= \mathcal{F}^{-1}[(-ik)^n \mathcal{F}[f(x)]] . \end{aligned}$$

Adopting the complex notation of the forward transform we gain

$$F_k = \sum_{j=0}^{N-1} f_j e^{i 2\pi jk/N} \quad k = 0, \dots, N$$

and the inverse transform

$$f_j = \frac{1}{N} \sum_{k=0}^{N-1} F_k e^{-i 2\pi jk/N} \quad j = 0, \dots, N$$

Fourier Series and Transforms

We are able to gain exact $n - th$ derivatives on our regular grid by performing the following operations on vector f_j defined at grid points x_j

$$\partial_x^{(n)} f_j = \mathcal{F}^{-1}[(-ik)^n F_k]$$

where

$$F_k = \mathcal{F}[f_j]$$

Example

We initialize a 2π -periodic Gauss-function in the interval $x \in [0, 2\pi]$ as

$$f(x) = e^{-1/\sigma^2 (x-x_0)^2}$$

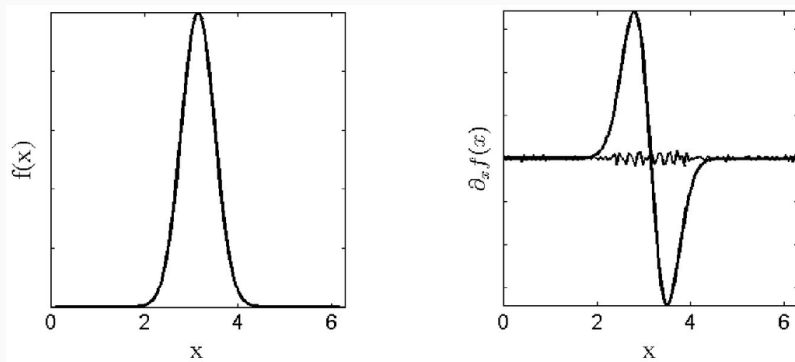
with $x_0 = \pi$ and the derivative

$$f'(x) = -2 \frac{(x - x_0)}{\sigma^2} e^{-1/\sigma^2 (x-x_0)^2}$$

Grid spacing of $dx = \frac{2\pi}{N}$ with $N = 127$ and $x_j = j \frac{2\pi}{N}$, $j = 0, \dots, N$.

```
def fourier_derivative(f, dx):  
    # Length of vector f  
    nx = np.size(f)  
    # Initialize k vector up to Nyquist wavenumber  
    kmax = np.pi/dx  
    dk = kmax/(nx/2)  
    k = np.arange(float(nx))  
    k[: int(nx/2)] = k[: int(nx/2)] * dk  
    k[int(nx/2) :] = k[: int(nx/2)] - kmax  
    # Fourier derivative  
    ff = np.fft.fft(f); ff = 1j*k*ff  
    df_num = np.real(np.fft.ifft(ff))  
    return df_num
```

Result



The Fourier Pseudospectral Method

Constant-density acoustic wave equation in 1D

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

The time-dependent part is solved using a standard 3-point finite-difference operator leading to

$$\frac{p_j^{n+1} - 2p_j^n + p_j^{n-1}}{\Delta t^2} = c_j^2 \partial_x^2 p_j^n + s_j^n$$

where upper indices represent time and lower indices space.

Calculating the 2^{nd} derivatives using the Fourier transform

$$\begin{aligned}\partial_x^2 p_j^n &= \mathcal{F}^{-1}[(-ik)^2 P_\nu^n] \\ &= \mathcal{F}^{-1}[-k^2 P_\nu^n]\end{aligned}$$

where P_ν^n is the discrete complex wavenumber spectrum at time n

leading to an exact derivative with only numerical rounding errors.

```
# -----  
# Time extrapolation  
# -----  
for it in range(nt):  
    # -----  
    # Fourier Pseudospectral Method  
    # -----  
    sd2p = fourier_derivative_2nd(sp, dx) # 2nd space derivative  
    spnew = 2*sp - spold + c**2 * dt**2 * sd2p # Time Extrapolation  
    spnew = spnew + sg*src[it]*dt**2 # Add sources  
    spold, sp = sp, spnew # Time Levels  
    sp[1] = 0; sp[nx-1] = 0 # set boundaries pressure free
```

Example

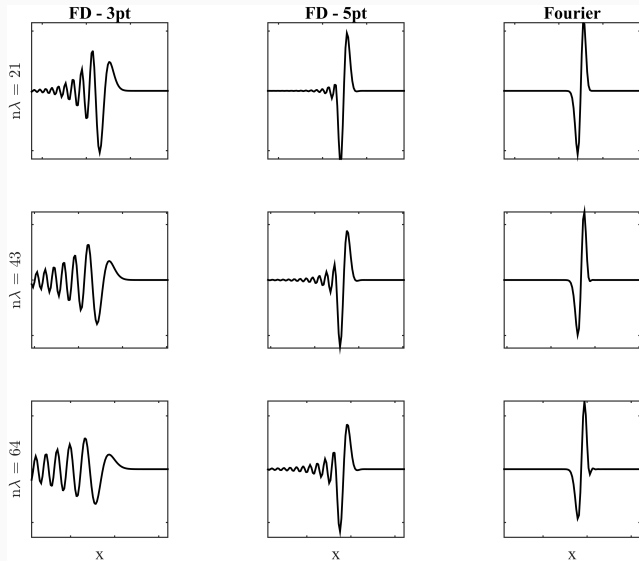
In FD method possible to initiate a point-like source at one grid point

In PS method not possible because Fourier transform of a spike-like function creates oscillations

⇒ Defining a space-dependent part of the source using a Gaussian function $e^{-1/\sigma^2(x-x_0)^2}$ with $\sigma = 2dx$, dx being the grid interval and x_0 the source location

Parameter	Value
x_{max}	1250 m
n_x	2048
c	343 m/s
dt	0.00036 s
dx	0.62 m
f_0	60 Hz
ϵ	0.2

Result



Stability, Convergence, Dispersion

To understand the behaviour of numerical approximations using discrete plane waves of the form

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

The time-dependent part can be expressed as

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

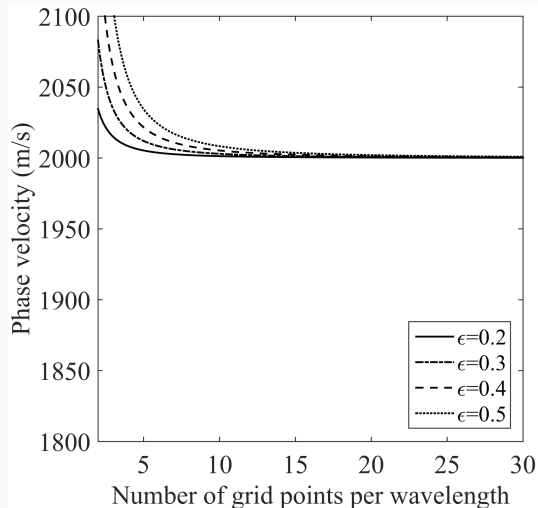
where we made use of Euler's formula and that $2 \sin^2 x = 1/2(1 - \cos 2x)$

Phase velocity $c(k)$

$$c(k) = \frac{\omega}{k} = \frac{2}{kdt} \sin^{-1}\left(\frac{kcdt}{2}\right).$$

- When dt becomes small $\sin^{-1}(kcdt/2) \approx kcdt/2$
- dx does not appear in this equation
- The inverse sine must be smaller than one the stability limit requires $k_{max}(cdt/2) \leq 1$. As $k_{max} = \pi/dx$ the stability criterion for the 1D case is $\epsilon = cdt/dx = 2/\pi \approx 0.64$

Stability, Convergence, Dispersion



Acoustic wave equation in 2D

$$\ddot{p} = c^2(\partial_x^2 p + \partial_z^2 p) + s$$

The time-dependent part is replaced by a standard 3-point finite-difference approximation

$$\frac{p_{j,k}^{n+1} - 2p_{j,k}^n + p_{j,k}^{n-1}}{dt^2} = c_{j,k}^2(\partial_x^2 p + \partial_z^2 p)_{j,k} + s_{j,k}^n$$

Using Fourier approach for approximating 2nd partial derivatives

$$\partial_x^2 p + \partial_z^2 p = \mathcal{F}^{-1}[-k_x^2 \mathcal{F}[p]] + \mathcal{F}^{-1}[-k_z^2 \mathcal{F}[p]]$$

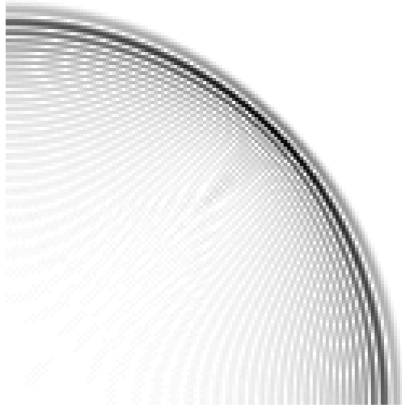
Parameter	Value
X_{max}	200 m
n_x	256
c	343 m/s
dt	0.00046 s
dx	0.78 m
f_0	200 Hz
ϵ	0.2

```
# -----  
# Time extrapolation  
# -----  
for it in range(nt):  
    # -----  
    # Fourier Pseudospectral Method  
    # -----  
    # 2nd space derivative  
    for j in np.arange(nz):  
        sd2px[:,j] = fourier_derivative_2nd(sp[:,j].T, dx)  
    for i in np.arange(nx):  
        sd2pz[i,:] = fourier_derivative_2nd(sp[i,:], dx)  
  
    # Time Extrapolation  
    spnew = 2*sp - spold + c**2 * dt**2 * (sd2px + sd2pz)  
    spnew = spnew + sg*src[it]*dt**2 # Add sources  
    spold, sp = sp, spnew # Time Levels
```


Fourier Method



Finite-Difference Method



Numerical anisotropy

Investigating the dispersion behaviour by finding solutions to monochromatic plane waves propagating in the direction $\mathbf{k} = (k_x, k_z)$

$$p_{j,k}^n = e^{i(k_x j dx + k_z k dx - \omega n dt)}$$

With Fourier method the derivatives can be calculated by

$$\partial_x p_{j,k}^n = -k_x^2 e^{i(k_x j dx + k_z k dx - \omega n dt)}$$

$$\partial_z p_{j,k}^n = -k_z^2 e^{i(k_x j dx + k_z k dx - \omega n dt)}$$

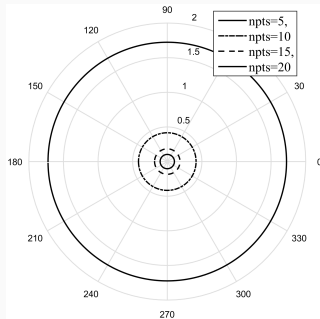
Combining this with the 3-point-operator for the time derivative

$$\partial_t^2 p_{j,k}^n = -\frac{4}{dt^2} \sin^2\left(\frac{\omega dt}{2}\right) e^{i(k_x j dx + k_z k dx - \omega n dt)}$$

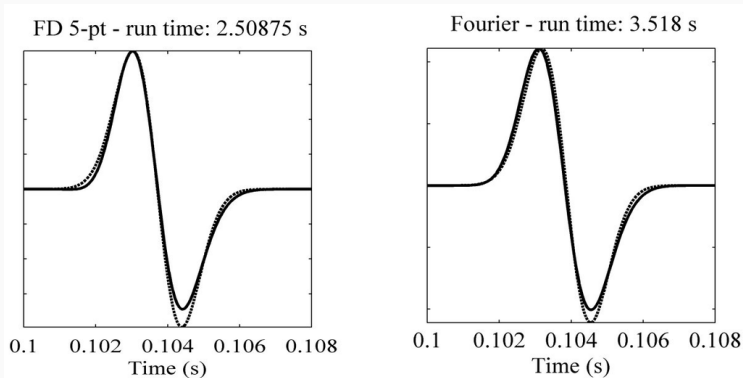
Numerical anisotropy

We obtain the numerical dispersion relation in 2D for arbitrary wave number vectors (i.e., propagation directions) \mathbf{k} as

$$c(\mathbf{k}) = \frac{\omega}{|\mathbf{k}|} = \frac{2}{|\mathbf{k}|dt} \sin^{-1} \left(\frac{cdt \sqrt{k_x^2 + k_z^2}}{2} \right).$$



Elastic 1D



Comparing memory requirements and computation speed between the Fourier method (**right**) and a 4th-order finite-difference scheme (**left**). In both cases the relative error compared to the analytical solution (misfit energy calculated by $\frac{u_{FD} - u_a}{u_a^2}$) is approximately 1%. The big difference is the number of grid points along the x dimension. The ratio is 3:1 (FD:Fourier)

Summary

- Pseudospectral methods are based on **discrete function approximations** that allow exact interpolation at so-called collocation points. The most prominent examples are the **Fourier method** based on trigonometric basis functions and the **Chebyshev method** based on Chebyshev polynomials.
- The Fourier method can be interpreted as an application of discrete Fourier series on a **regular-spaced grid**. The **space derivatives can be obtained exactly** (except for rounding errors). Derivatives can be efficiently calculated with the discrete Fourier transform requiring $n \log n$ operations.
- The Fourier method implicitly assumes **periodic behavior**. **Boundary conditions** like the free surface or absorbing behaviour are **difficult to implement**.