Spectral Methods in Seismic Modelling

by

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Why pseudospectral modelling?

- High accuracy
  - — numerical dispersion & attenuation are almost eliminated
- Few grid points per minimum wavelength
  - — allows for numerical models with coarse grids
- Computational efficiency
  - — reduces storage memory & computational time

Equation of motion

Equation of motion:

$$\varrho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i$$

Stress-strain relation:

$$\sigma_{ij} = c_{ijkl}\varepsilon_{kl}$$

Strain tensor:

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

Isotropic stress-strain relation:

$$\sigma_{ij} = \lambda \varepsilon_{kk}\delta_{ij} + 2\mu\varepsilon_{ij}$$

Acoustic wave equations

Definition of pressure:

$$\sigma_{ij} = -p\delta_{ij}$$

Variable density wave equation:

$$\frac{\partial}{\partial x}\left(\frac{1}{\varrho}\frac{\partial p}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{\varrho}\frac{\partial p}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{1}{\varrho}\frac{\partial p}{\partial z}\right) = \frac{1}{\varrho c^2}\frac{\partial^2 p}{\partial t^2}$$

Constant density wave equation

$$\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2} = \frac{1}{c^2}\frac{\partial^2 p}{\partial t^2}$$

Numerical solution

For solving the wave equation using computers we need to define:

1) the discrete time derivative operator:

$$\frac{\partial}{\partial t} \longrightarrow \mathsf{D}_t$$

2) the discrete space derivative operators:

$$\frac{\partial}{\partial x} \longrightarrow \mathsf{D}_x$$

$$\frac{\partial}{\partial y} \longrightarrow \mathsf{D}_y$$

$$\frac{\partial}{\partial z} \longrightarrow \mathsf{D}_z$$

Numerical solution (cont'd)

The discrete space derivative operators D_N can be obtained by differentiating the assumed expansion:

$$u(x) \approx u_N(x) = \sum_{k=0}^{N} \hat{u}_k \, \varphi_k(x)$$

The basis (trial) functions $\varphi_k(x)$ are given, $\hat{u}_k$ must be determined.

In the spectral methods the chosen basis functions are orthogonal:

- periodic problems –> trigonometric functions e^{ikx} ,
- non-periodic problems –> Chebyshev T_k or Legendre L_k polynomials .

Numerical solution (cont'd)

The pseudo-spectral (collocation, interpolation) methods are based on the *collocation constraint* :

$$u_N(x_i) = u(x_i)\ , \quad i = 0, \ldots,\ N,$$

where the x_i are $N+1$ collocation points.
Namely,

$$\sum_{k=0}^{N} \hat{u}_k\, \varphi_k(x_i) = u(x_i)\ , \quad i = 0, \ldots,\ N,$$

which determines the $N+1$ coefficients $\hat{u}_k$.

For the existence of $\hat{u}_k$, the collocation points must satisfy

$$det\{\varphi_k(x_i)\} = 0.$$

Numerical solution (cont'd)

The collocation constraint is not used in practice.

The $N+1$ coefficients $\hat{u}_k$ are obtained explicitly using:

- special sets $\{x_i\}$, of collocation points,
- the associated discrete orthogonality property of $\varphi_k(x_i)$.

Numerical solution (cont'd)

The collocation constraint allows for expressing the approximant in terms of $u_N(x_i)$, the values at the collocation points:

$$u_N(x) = \sum_{i=0}^{N} u_N(x_i)\ \phi_i(x) \ \left(= \sum_{k=0}^{N} \hat{u}_k\ \varphi_k(x) \right)$$

where $\phi_i(x)$ are the Lagrange basis (cardinal basis, shape functions), polynomials based on the grid points $\{x_i\}$:

- <u>trigonometric</u> polynomials in the Fourier case,
- <u>algebraic</u> polynomials in the Chebyshev & Legendre case .

Numerical solution (cont'd)

The differentiation can be expressed in terms of the derivative values at the collocation points $u_N^{'}(x_i)$:

$$\partial_x u_N(x) = \sum_{i=0}^{N} u_N(x_i)\ \partial_x \phi_i(x)\ = \sum_{i=0}^{N} u_N^{'}(x_i)\ \phi_i(x)$$

where

$$u_N^{'}(x_i) = \sum_{j=0}^{N} (\mathsf{D}_N)_{ij}\ u_N(x_j)$$

in matrix form

$$U_N^{'} = \mathsf{D}_N\ U_N$$

Numerical solution (cont'd)

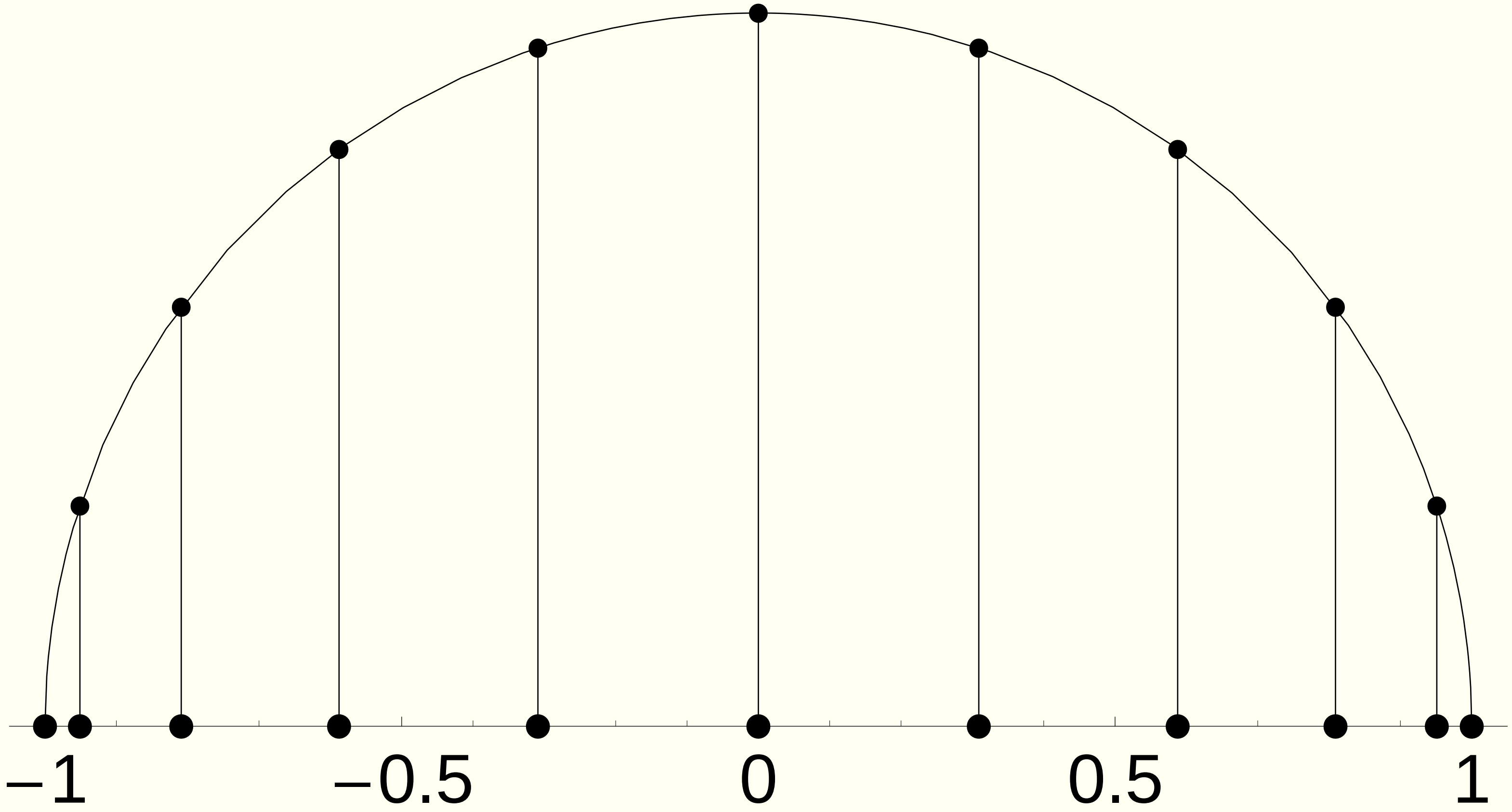
The pseudo-spectral error is decreasing faster than *any* power of N :

$$Pseudo - spectral\ error \approx O[(\frac{1}{N})^N]$$

Infinite order or exponential or spectral convergence due to:

- optimum basis choice (orthogonal polynomials),
- optimum collocation points (no Runge phenomenon),
- global influence of the high-order polynomials over the *whole* domain .

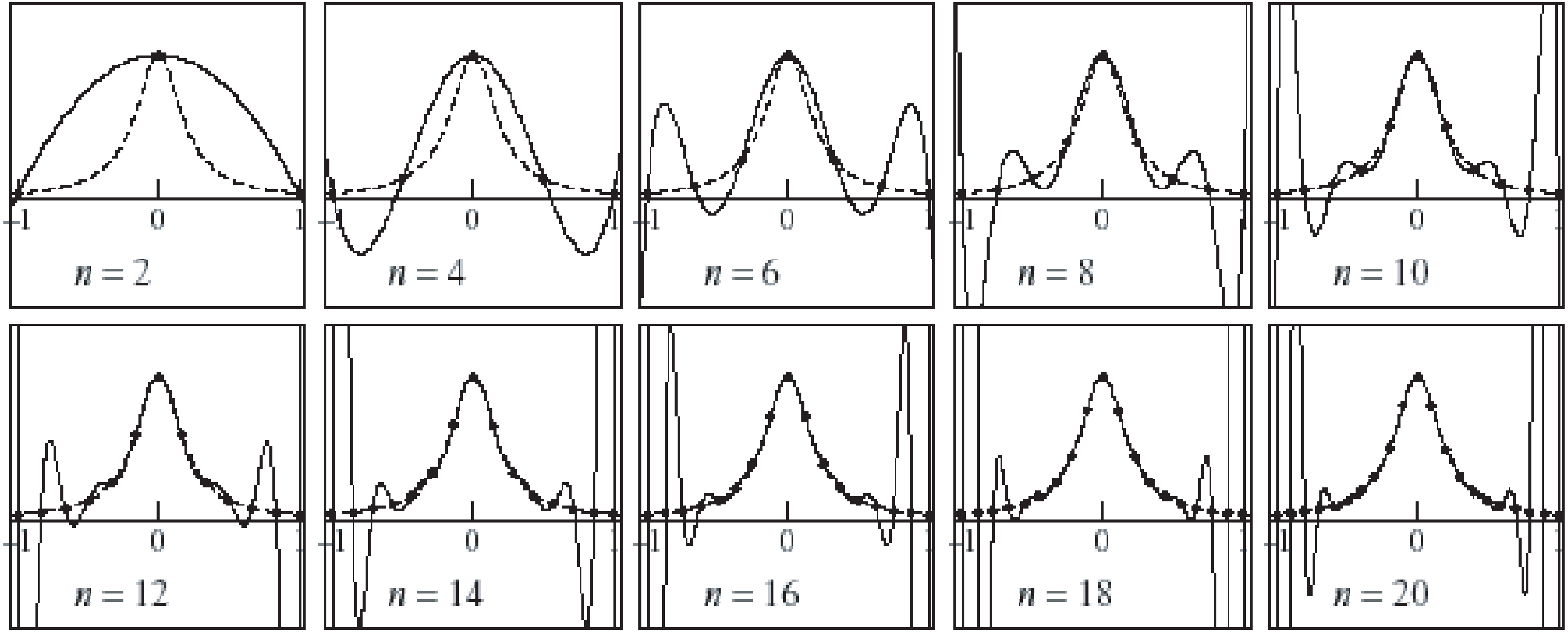
Numerical solution (cont'd)



Chebyshev-Gauss-Lobatto points

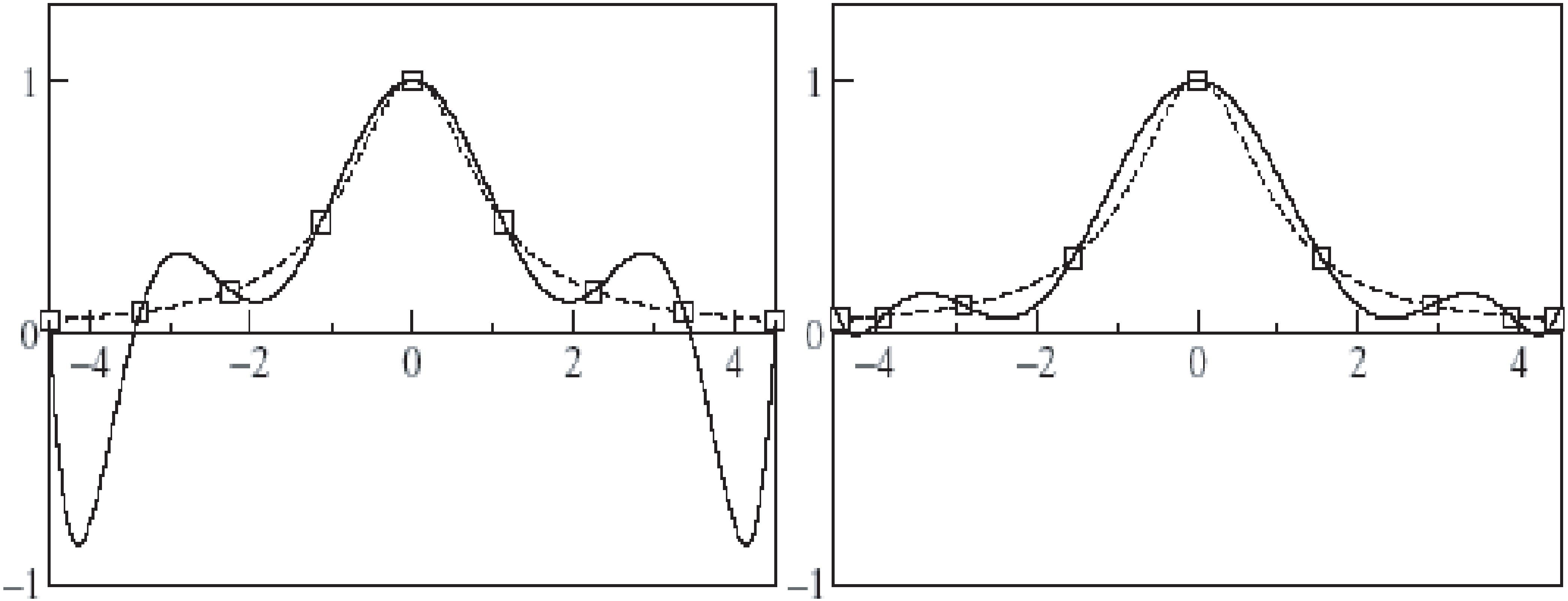
Not equispaced, Clustered towards the ends, Uneven grid

Numerical solution (Runge phenomenon)



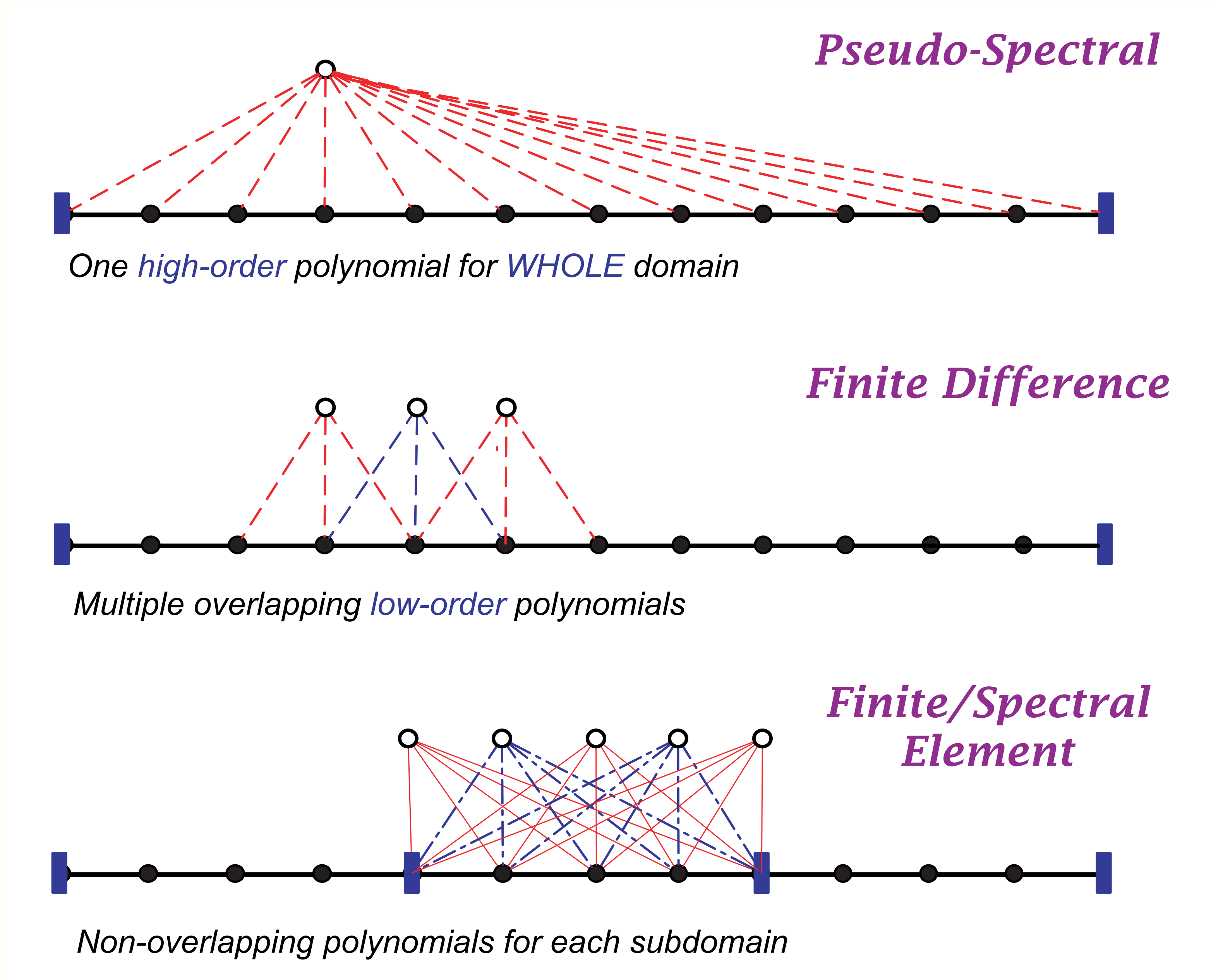
Big errors always near the endpoints

Numerical solution (Runge phenomenon)



Equispaced points «—— 9 ——» Chebyshev points

Numerical solution (cont'd)



Fourier derivative

The Fourier transform is defined by:

$$H(\omega) = \int_{-\infty}^{+\infty} h(t) e^{-i\omega t} dt$$

and its inverse by:

$$h(t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} H(\omega) e^{+i\omega t} d\omega$$

Fourier derivative (cont'd)

Taking the derivative yields:

$$\frac{d}{dt}h(t) = \frac{d}{dt}\left[\frac{1}{2\pi}\int_{-\infty}^{+\infty} H(\omega)e^{+i\omega t}d\omega\right]$$

Using Leibniz' rule yields:

$$\begin{aligned}\frac{d}{dt}h(t) &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{\partial}{\partial t}\left[H(\omega)e^{+i\omega t}\right]d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^{+\infty} i\omega H(\omega)e^{+i\omega t}d\omega\end{aligned}$$

Therefore:

$$h'(t) \quad \Longleftrightarrow \quad i\omega H(\omega)$$

Fourier derivative (cont'd)

The discrete Fourier transform pair reads:

$$H_n = \sum_{k=0}^{N-1} h_k e^{-i\frac{2\pi}{N}nk}$$

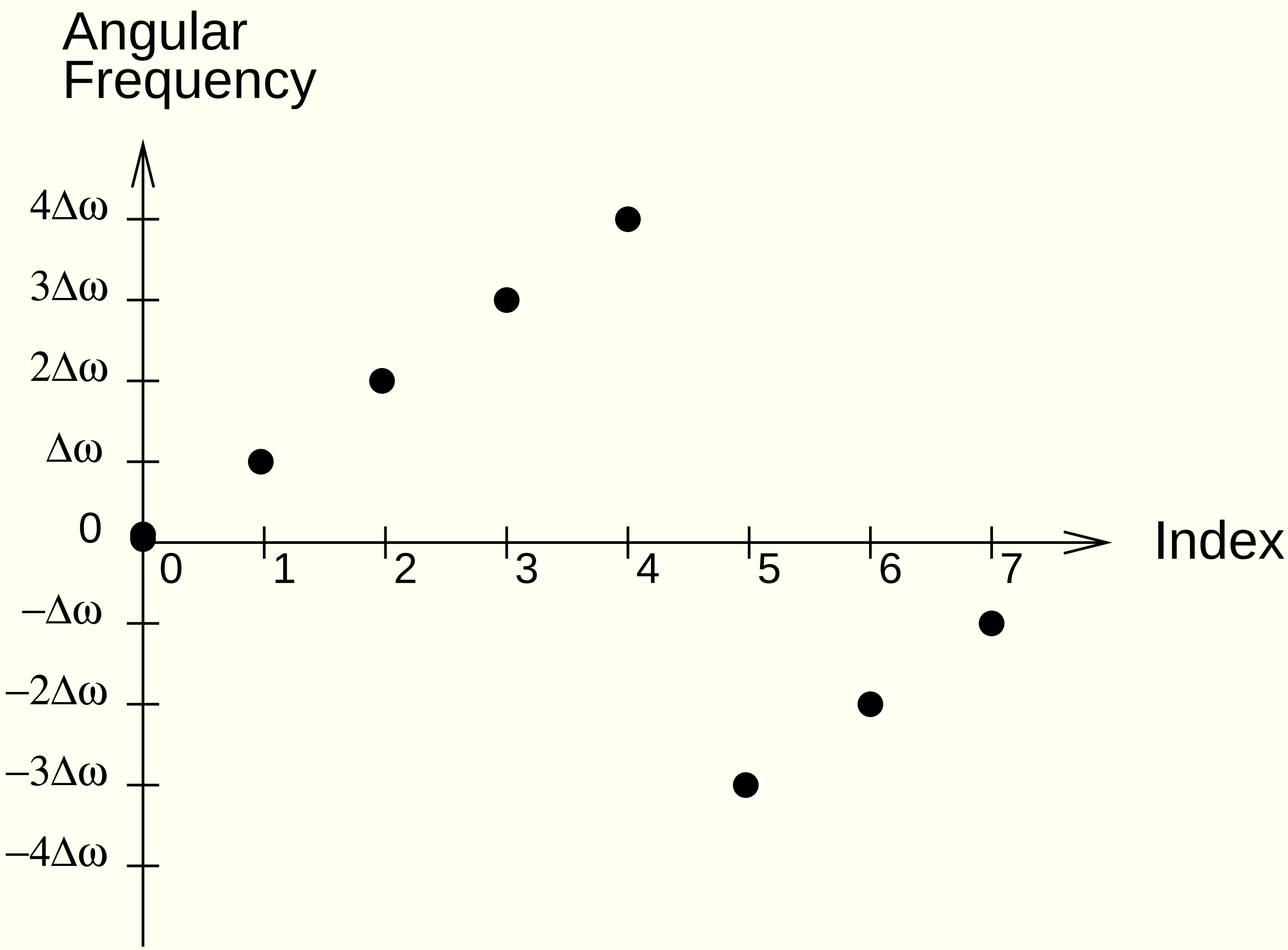
and

$$h_n = \frac{1}{N}\sum_{k=0}^{N-1} H_k e^{+i\frac{2\pi}{N}nk}$$

where $h_n = h(t_n), \qquad n = 0, \ldots, N-1$ with $t_n = n \cdot \Delta t$
and $H_n = H(\omega_n), \qquad n = 0, \ldots, N-1$ with $\omega_n = n \cdot \Delta\omega$

Fourier derivative (cont'd)

$$\omega_n = \begin{cases} \frac{2\pi}{N\Delta t} n & \text{if } n = 0, \ldots, [N/2], \\ \frac{-2\pi}{N\Delta t}(N-n) & \text{if } n = [N/2]+1, \ldots, N-1 \end{cases}$$



Fourier derivative (cont'd)

Procedure for Fourier derivative:

$$h_n \xrightarrow{DFT} H_n \longrightarrow i\omega_n H_n \xrightarrow{DFT^{-1}} h'_n$$

Fourier derivative (cont'd)

Simultaneous calculation of the derivatives of two real functions:

Two real functions: $g(t)$, $h(t)$

One complex function: $f(t) = g(t) + ih(t)$

Derivative of complex function: $f'(t) = g'(t) + ih'(t)$

Derivatives of two real functions: $g'(t)$, $h'(t)$

Fourier derivative (cont'd)

Derivatives of even and odd order:

consider real function $f(t)$

- $Re\ [H(\omega)]$: even
- $Im\ [H(\omega)]$: odd

$f(\omega) = \omega$: odd

if we multiply $H(\omega)$ by $i\omega$

- $Re\ [i\omega H(\omega)]$: even
- $Im\ [i\omega H(\omega)]$: odd

Fourier derivative (cont'd)

The discrete spectrum is:

$$H_n = \sum_{k=0}^{N-1} h_k e^{-i\frac{2\pi}{N}nk}$$

Nyquist component, where N is even:

$$H_{N/2} = \sum_{k=0}^{N-1} h_k e^{-i\frac{2\pi}{N}\frac{N}{2}k}$$

$$= \sum_{k=0}^{N-1} h_k e^{-i\pi k}$$

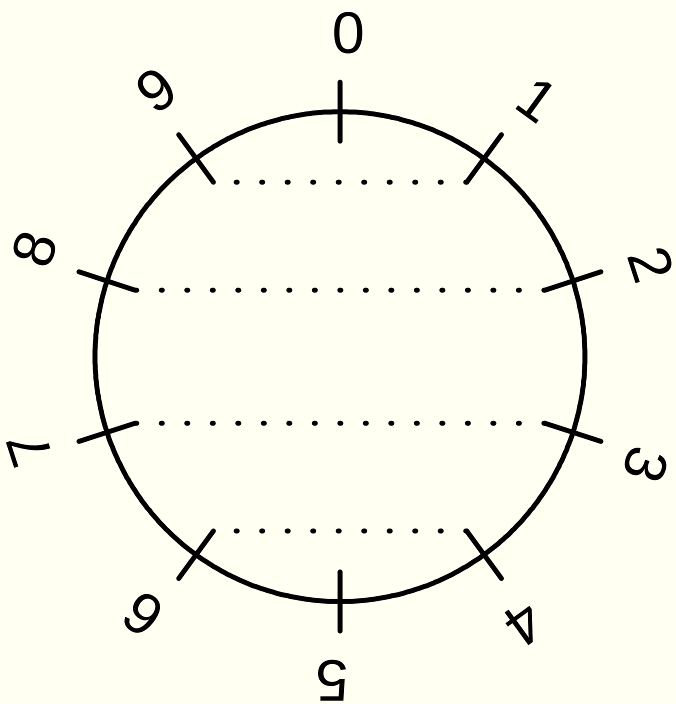
$e^{-i\pi k} = \pm 1 \quad \Longrightarrow \quad$ Nyquist component always is real!

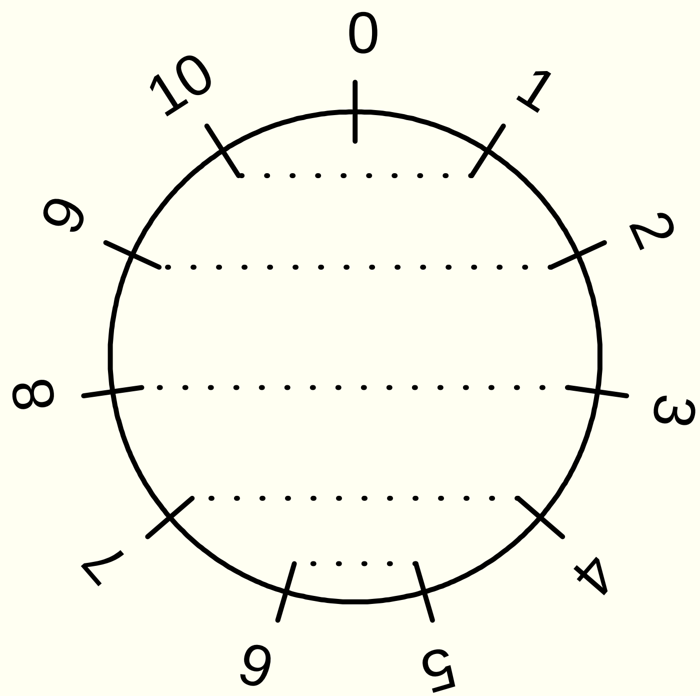
Fourier derivative (cont'd)

Multiplying the real Nyquist component by $i\omega$ results in a purely imaginary Nyquist component of the derivative.

However, the Nyquist component of a real function should have a real Nyquist component. This is a contradiction!

Solution: Use of Fourier transform of odd order, where the Nyquist frequency is not present.





Chebyshev derivative

A function can be represented by Chebyshev polynomials:

$$f(x) = \sum_{k=0}^{\infty} a_k T_k(x)$$

Likewise, a discrete function $f(x_j)$ can be approximated by:

$$f(x_j) = \sum_{k=0}^{N} a_k T_k(x_j),\ j = 0, \ldots, N$$

where the non-equidistant abscissas are:

$$x_j = \cos \frac{\pi j}{N},\ j = 0, \ldots, N.$$

Chebyshev derivative (cont'd)

The idea is to calculate the derivative of $f(x_j)$ by

- finding the coefficients a_k of $f(x_j)$
- calculate coefficients b_k of the derivative from the a_k
- calculate the function $f'(x_j)$ from the b_k

Chebyshev derivative (cont'd)

The coefficients a_k are given by:

$$a_k = \frac{2}{N} \sum_{j=0}^{N} \alpha_j f(x_j) T_k(x_j) \cdot \begin{cases} 1 & \text{if } k \neq 0 \wedge k \neq N, \\ 1/2 & \text{if } k = 0 \vee k = N \end{cases}$$

with

$$\alpha_j = \begin{cases} 1/2 & \text{if } j = 0 \vee j = N, \\ 1 & \text{else} \end{cases}$$

Expressing T_k in terms of cosine-functions

$$T_k(x_j) = \cos\left(\frac{kj\pi}{N}\right)$$

and substituting $\frac{2}{N}\alpha_j f(x_j)$ by $g(x_j)$

Chebyshev derivative (cont'd)

We find

$$a_k = \sum_{j=0}^{N} g(x_j) \cdot \cos\left(\frac{kj\pi}{N}\right) \cdot \alpha_k$$

This is similar to the real part of a DFT.

Extension to $2N$ function values, where $g(x_j) = 0,\ j = N+1, \ldots, 2\,N-1$ (zero padding) yields:

$$a_k = \sum_{j=0}^{2N-1} g(x_j) \cdot \cos\left(k\frac{j2\pi}{2N}\right) \cdot \alpha_k,\ k = 0, \ldots, N$$

Apart from α_k, this is exactly the real part of the discrete Fourier transform of $g(x_j)$

Chebyshev derivative (cont'd): b_k

Starting from

$$g(x) = \sum_{k=0}^{N} a_k T_k(x)$$

the derivative is

$$g'(x) = \sum_{k=0}^{N} a_k T_k'(x)$$

or

$$g'(x) = \sum_{k=0}^{N} b_k T_k(x)$$

We search for a relation between the coefficients a_k and b_k

Chebyshev derivative (cont'd): b_k

Equating the last two right hand sides and comparing respective terms of $T_k(x)$ yields:

$$b_{k-1} = b_{k+1} + 2ka_k$$

and

$$b_0 = b_2/2 + a_1$$

Starting with $b_{N+1} = b_N = 0$, by the downward recurrence all $\quad b_k, \quad k = N, \ldots, 2 \quad$ can be calculated.

From these the derivative can finally be calculated:

$$g'(x) = \sum_{k=0}^{N} b_k T_k(x)$$

Chebyshev derivative (the physical space)

A function can be approximated by Lagrange (-Chebyshev) interpolation polynomials:

$$f(x) = \sum_{i=0}^{N} f(x_i)\, \phi_i(x) \; \left(= \sum_{k=0}^{N} a_k T_k(x) \right).$$

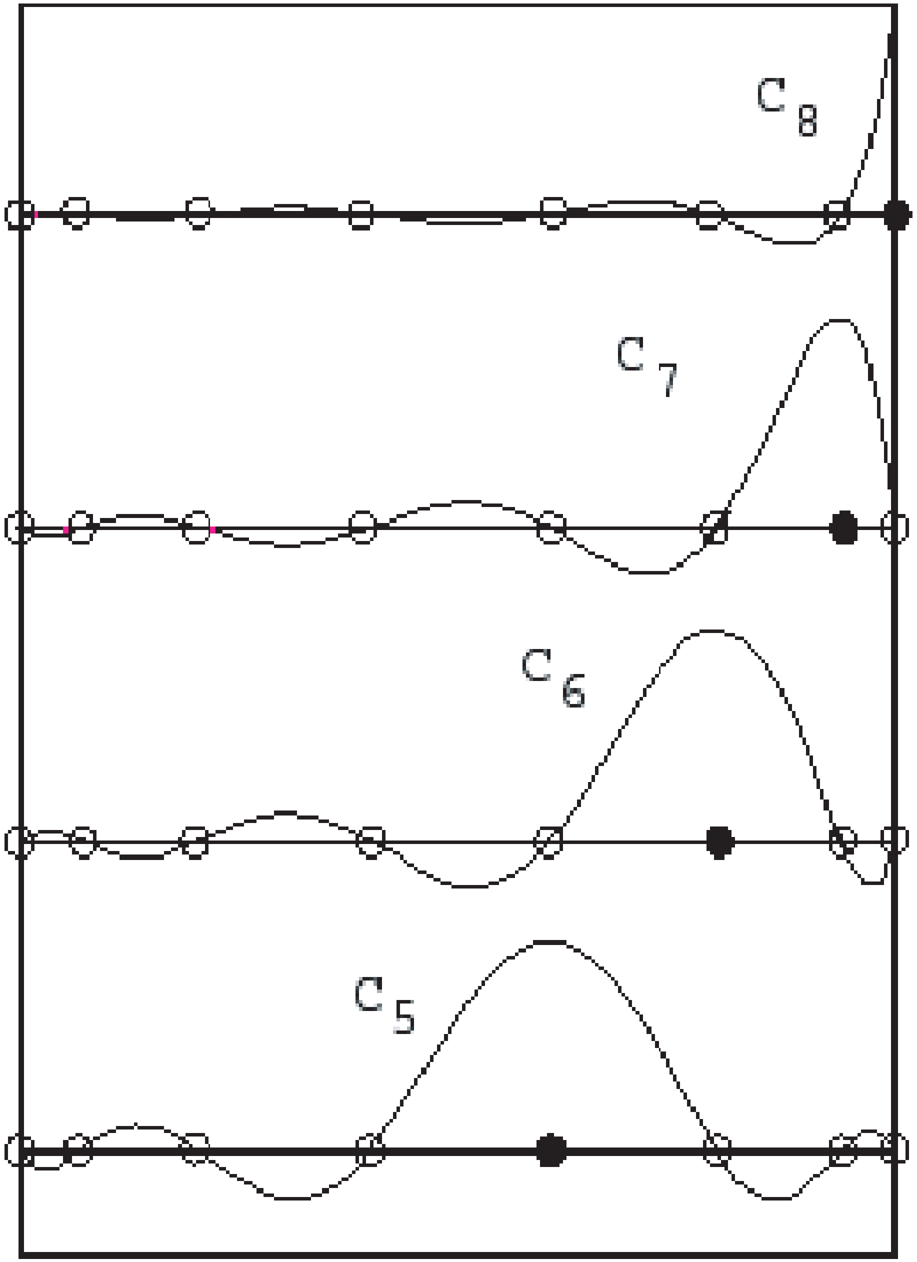
The shape functions $\phi_i(x)$ are polynomials of degree N and satisfy the conditions:

$$\phi_i(x_j) = \delta_{ij}, \quad i, j = 0, \ldots, N.$$

and are based on the Chebyshev-Gauss-Lobatto grid points $\{x_i\}$:

$$x_i = \cos \frac{\pi i}{N}, \quad i = 0, \ldots, N.$$

Chebyshev derivative (Shape functions)



Chebyshev derivative (cont'd)

$\{x_i\}$ Chebyshev-Gauss-Lobatto points properties:

- extremal points of Chebyshev polynomials $T_N(x)$,
- zeros of the polynomial $(1-x^2)\,T'_N(x)$,
- for $x \to x_i$:

$$\frac{(1-x^2)\,T'_N(x)}{x-x_i} \to (-1)^{i+1}\,\bar{c}_i\,N^2,$$

where $\bar{c}_i = \{2\ (i=0,N)\ \ \|\ \ 1\ (i \neq 0,N)\}$.

Chebyshev derivative (cont'd)

Chebyshev shape functions $\phi_i(x)$:

$$\phi_i(x) = \frac{(-1)^{i+1}\,(1-x^2)\,T_N'(x)}{\bar{c}_i\,N^2\,(x-x_i)}$$

Chebyshev differentiation matrix D_N:

$$(\mathsf{D}_N)_{ij} = \left(\frac{d\phi_j}{dx}\right)_{x_i}, \qquad i,j = 0,\ldots,N$$

Chebyshev derivative (cont'd)

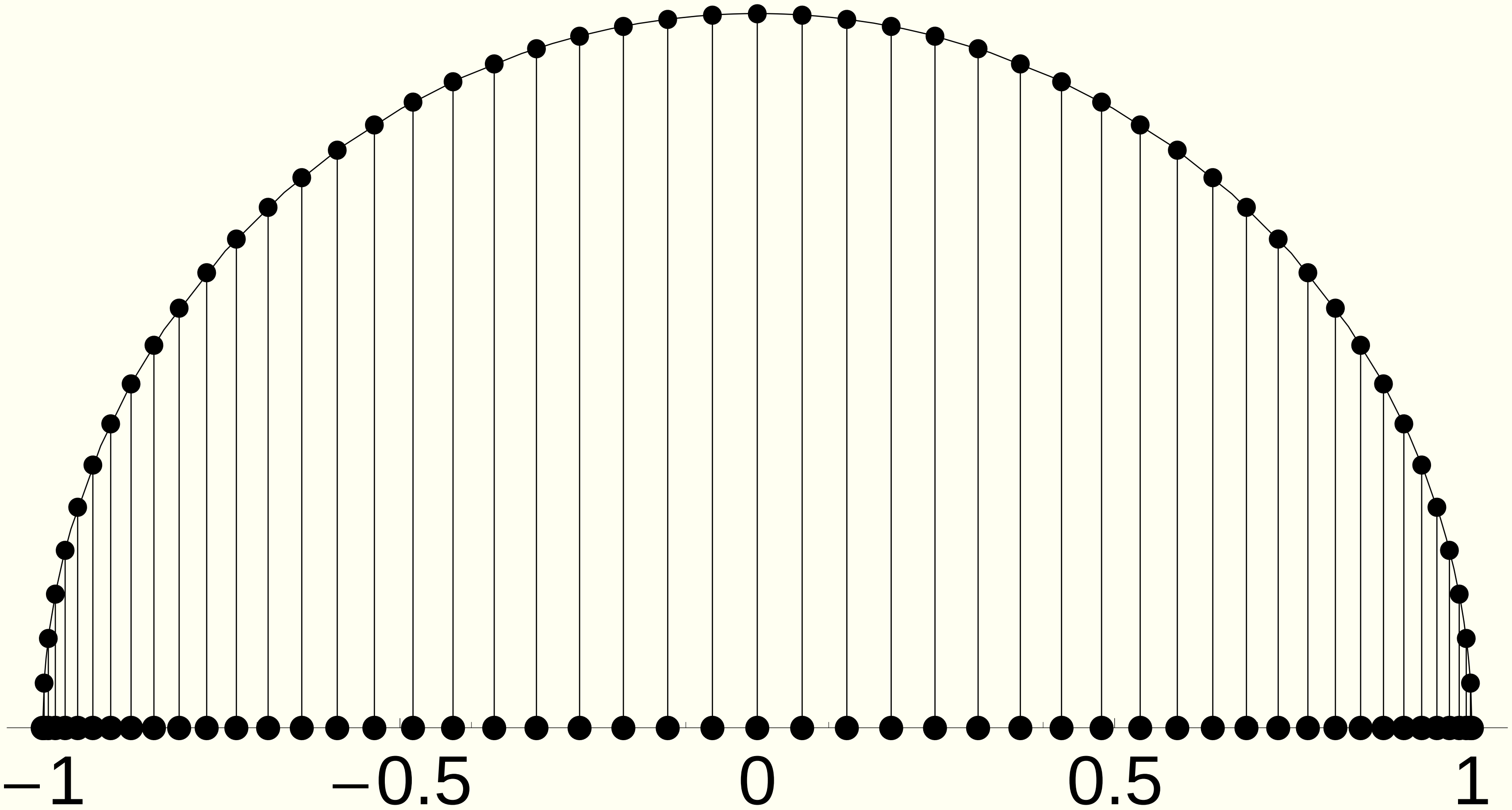
Chebyshev differentiation matrix D_N:

$$
\begin{aligned}
(\mathsf{D}_N)_{ij} &= \frac{\bar{c}_i}{\bar{c}_j}\,\frac{(-1)^{i+j}}{x_i - x_j}\;, \qquad && i \neq j\;, \\
(\mathsf{D}_N)_{ii} &= -\frac{x_i}{2(1-x_i^2)}\;, \qquad && i \neq 0, N\;, \\
(\mathsf{D}_N)_{00} &= -\,(\mathsf{D}_N)_{NN} \;=\; \frac{1}{6}\,(2\,N^2+1).
\end{aligned}
$$

Warning !!!

Possible round-off errors with endpoint values for large N.

Chebyshev derivative (cont'd)



Chebyshev-Gauss-Lobatto points

Chebyshev derivative (first cure)

More accurate Chebyshev differentiation matrix D_N:

$$
\begin{aligned}
(\mathsf{D}_N)_{ij} &= \frac{\bar{c}_i}{2\,\bar{c}_j}\,\frac{(-1)^{i+j}}{\sin\frac{\pi(i+j)}{2N}\,\sin\frac{\pi(i-j)}{2N}}\;, \qquad i \neq j\;, \\
(\mathsf{D}_N)_{ii} &= -\frac{1}{2}\,\frac{\cos\frac{\pi}{N}i}{\sin^2\frac{\pi}{N}i}\;, \qquad i \neq 0, N\;, \\
(\mathsf{D}_N)_{00} &= -\,(\mathsf{D}_N)_{NN} = \frac{1}{6}\,(2\,N^2+1), \\
(\mathsf{D}_N)_{0N} &= -\,(\mathsf{D}_N)_{N0} = \frac{1}{2}\,(-1)^N.
\end{aligned}
$$

Minimize the round-off errors by using trigonometrical identities to express the quantity $(x_i - x_j)$ and $(1 - x_i^2)$.

Chebyshev derivative (second cure)

A further reduction of the round-off errors by using the identity:

$$\sum_{j=0}^{N} (\mathsf{D}_N)_{ij} = 0 \;, \qquad\qquad i = 0, \ldots, N \;.$$

<u>Even more accurate</u> Chebyshev differentiation matrix D_N:

$$(\mathsf{D}_N)_{ij} \quad = \quad \frac{\bar{c}_i}{2\,\bar{c}_j} \, \frac{(-1)^{i+j}}{\sin\frac{\pi(i+j)}{2N} \sin\frac{\pi(i-j)}{2N}} \;, \qquad i \neq j \;,$$

$$(\mathsf{D}_N)_{ii} \quad = \quad -\sum_{\substack{j=0 \\ j\neq i}}^{N} (\mathsf{D}_N)_{ij} \;, \qquad\qquad i = 0, \ldots, N \;.$$

Chebyshev derivative (cont'd)

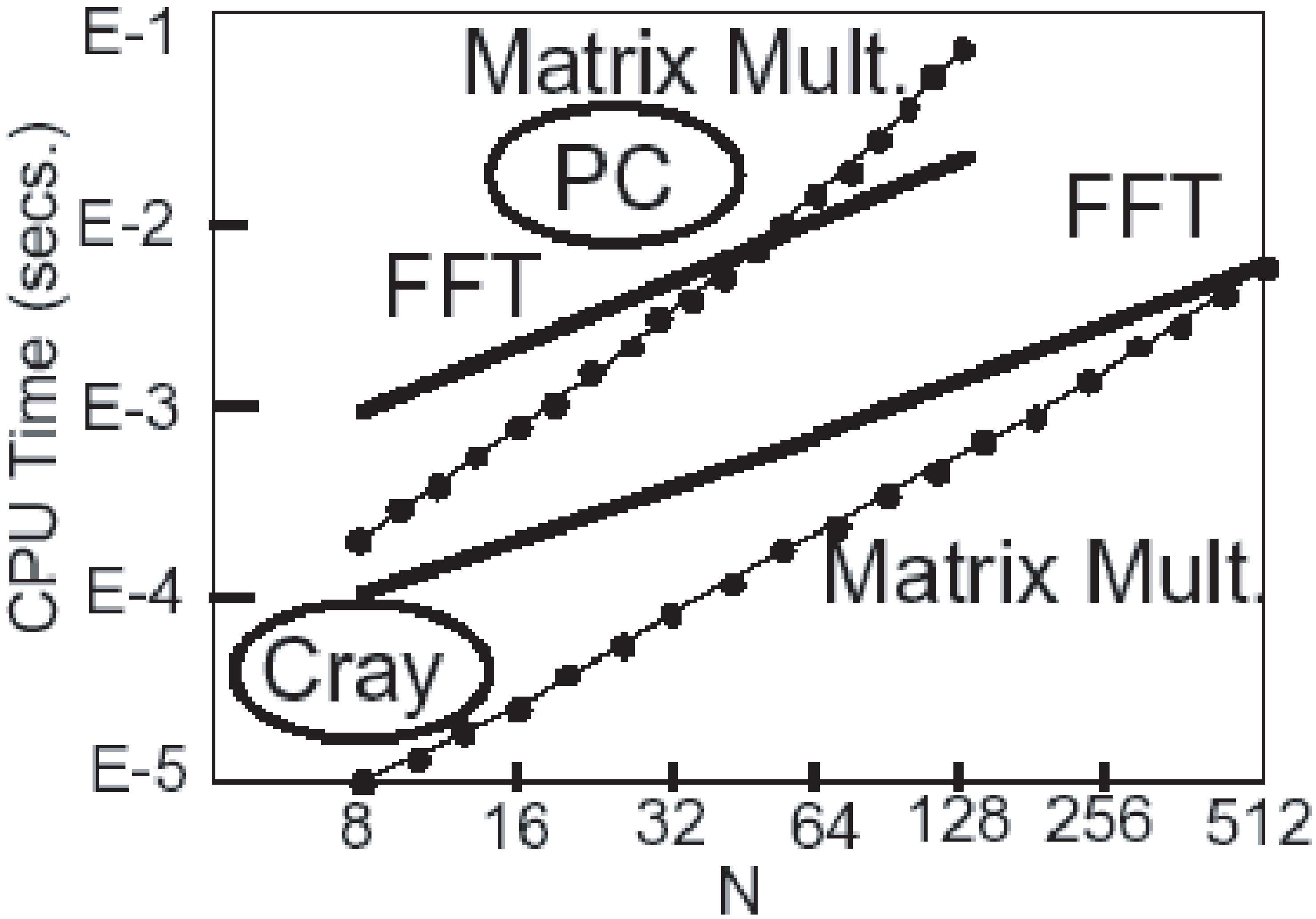
The differentiation by matrix-vector multiplication

$$f_i' = \sum_{j=0}^{N} (\mathsf{D}_N)_{ij}\, f_j$$

can be efficient for a set of points $\{x_i\}$:

- in the range of 100 - 500,
- using vector machines or super-scalar machines,
- using BLAS optimized routines.

Chebyshev derivative (cont'd)



Accuracy

Accuracy of the numerical solution depends on errors generated by:

(1) Numerical dispersion

Different Fourier modes in numerical schemes travel at different speeds (they should travel at the same speed).

(2) Gibbs-type oscillations

Spurious high-frequency oscillations are generated by sharp interfaces , rapid variations and discontinuities in the medium.

They are a consequence of the discretization order of the differentiation operator.

Accuracy (cont'd): d/dx

Assume <u>periodicity</u> and $N+1$ <u>equi-spaced</u> $(h = \Delta x = 2\pi/N)$ gridpoints within the period $[0, 2\pi]$.

Range of the allowed Fourier modes in the grid $\longrightarrow$ $-\frac{\pi}{h} \leq k \leq \frac{\pi}{h}$.

For a mode e^{ikx} the derivative d/dx is :

Exact (PS)

$$\frac{d}{dx} e^{ikx} = ike^{ikx}$$

Second-order FD

$$D_2 \, e^{ikx} = \frac{e^{ik(x+h)} - e^{ik(x-h)}}{2h} = i \, \frac{sinkh}{h} \, e^{ikx} = i\gamma_2(kh)k \, e^{ikx}$$

Accuracy (cont'd): d/dx

The multiplicative factor $\gamma_p(kh)$ can be computed for all the centered *p* th-order FD schemes D_p, $p = 2, 4, 6, \ldots$:

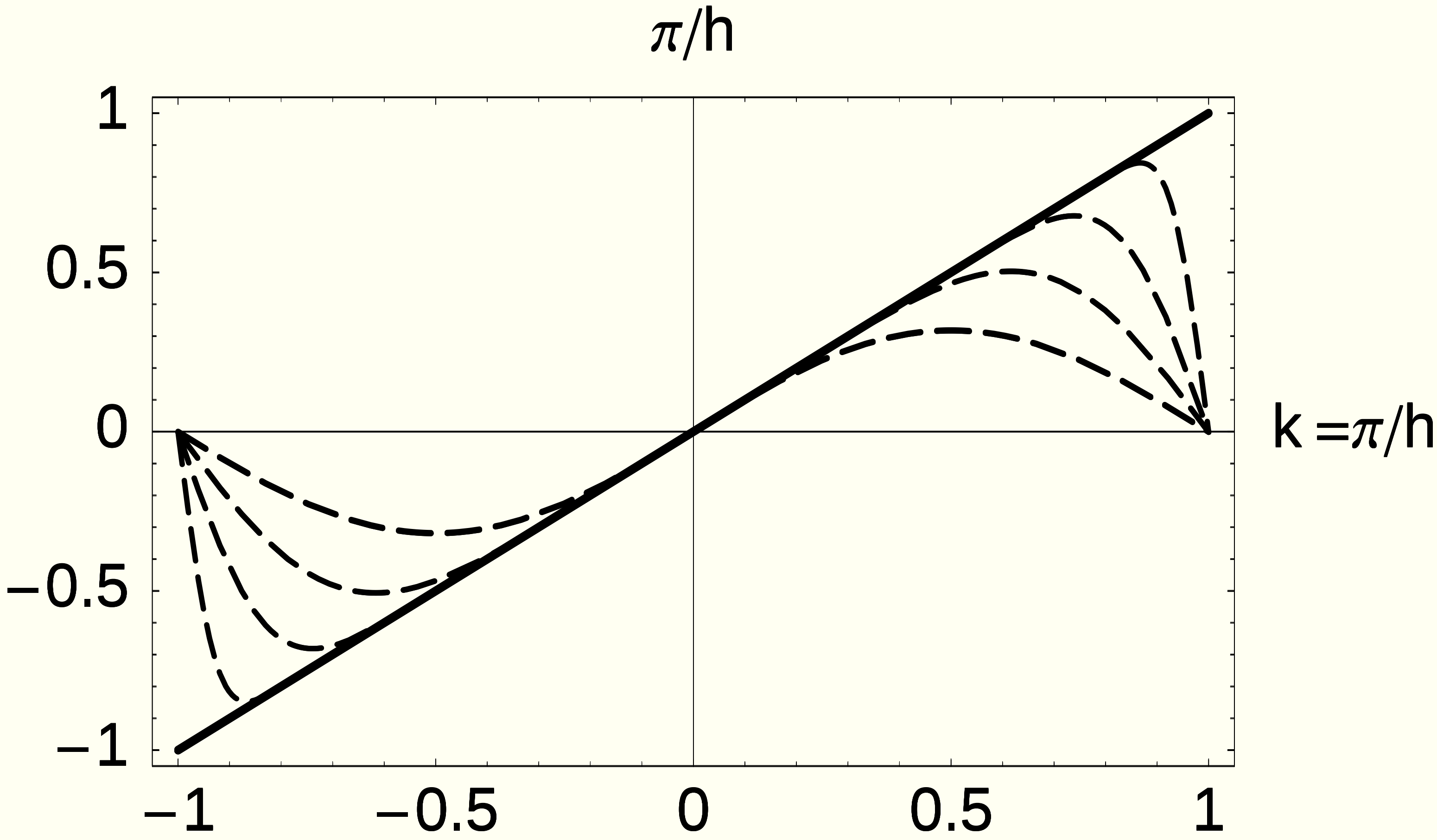
$$\gamma_p(kh) = \frac{\sin kh}{kh} \sum_{l=0}^{p/2-1} \frac{(l!)^2}{(2l+1)!} 2^{2l} \left(\sin \frac{kh}{2}\right)^{2l}$$

- High Fourier modes have an incorrect multiplicative factor.

- As $p \longrightarrow \infty$ there is convergence to correct values (PS) .

Accuracy (cont'd)

Multiplicative factor of different approximations for d/dx:



Exact (PS), 2nd Order, 6th Order, 20th Order, 120th Order

Accuracy (cont'd)

Consider the model problem:

$$\frac{\partial u}{\partial t} + c\,\frac{\partial u}{\partial x} \;=\; 0 \qquad \text{with} \qquad u(x,0) \;=\; e^{ikx}$$

The solution is :

$$u(x,t) \;=\; e^{ik(x - c\,t)}$$

On the grid points :

$$\frac{d\tilde{u}_j(t)}{dt} + ic\,\gamma_p(kh)k\,\tilde{u}_j(t) \;=\; 0 \qquad \text{with} \qquad \tilde{u}_j(0) \;=\; e^{ikx_j}$$

The solution is :

$$\tilde{u}_j(t) \;=\; e^{ik(x_j - c\,\gamma_p(kh)t)}$$

Accuracy (cont'd)

The error (phase) $e_p = \| u - \tilde{u} \|$ is:

$$e_p = \| e^{ik(x_j - c\,t)} - e^{ik(x_j - c\,\gamma_p(kh)t)} \| = \| e^{ikc\,t} - e^{ikc\,\gamma_p(kh)t} \|$$

or

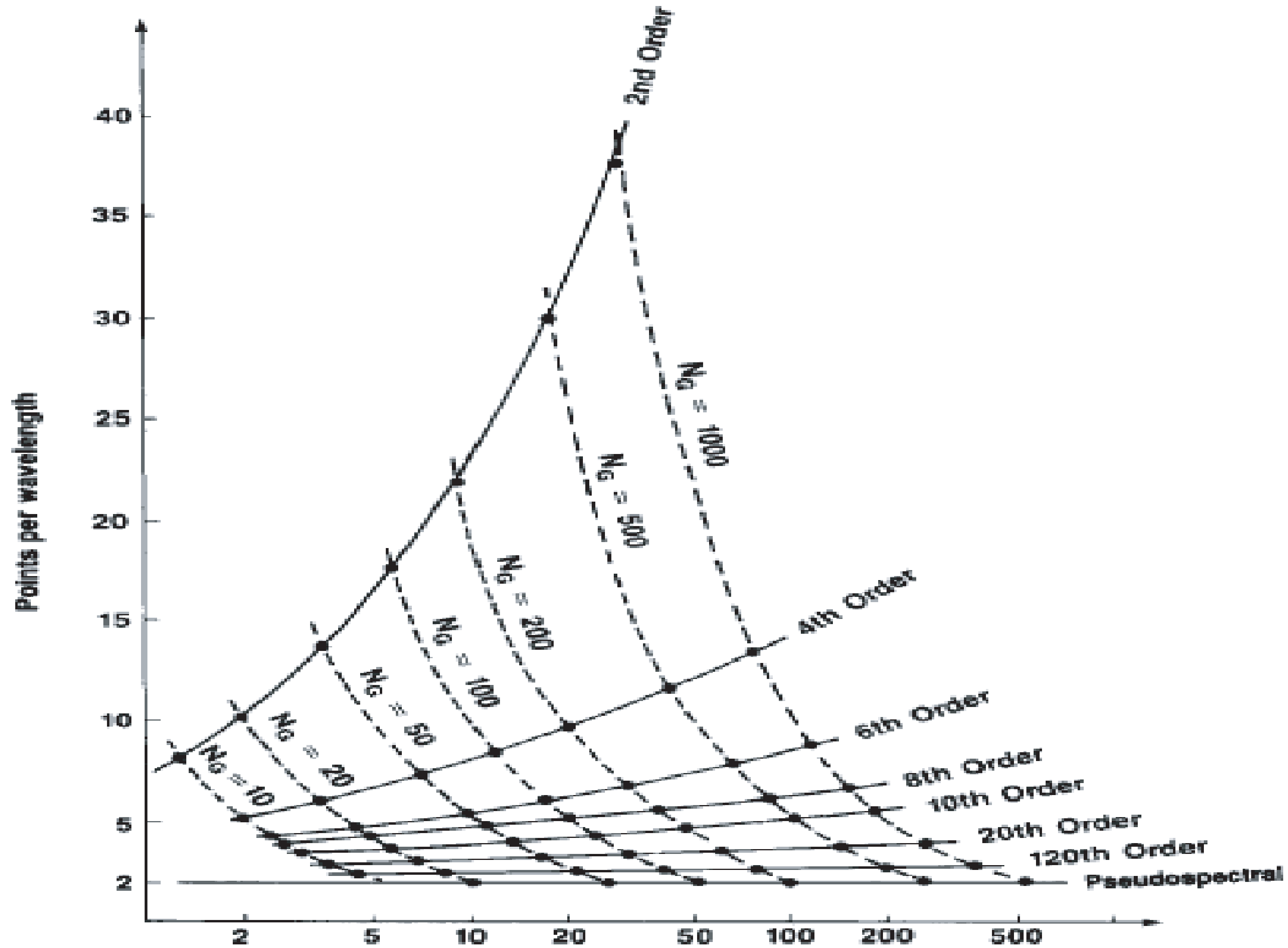
$$e_p = k\,c\,t\,[1 - \gamma_p(kh)] + O\left[(kh)^{p+2}\right]$$

We study the error after q period in time ($t = 2\pi q/(kc)$) and when it is smaller than a given tolerance $e_p \leq \epsilon$.

The number of grid points per wavelength is :

$$G = \frac{\lambda}{\Delta x} = \frac{N_G}{k} = \frac{2\pi}{hk}$$

Accuracy (cont'd): at final time (Fornberg, 1987)



Propagation dist. in # of Wavelengths for highest wave mode

Dispersion and stability

Stability analysis in the following is performed for the 1D and 2D finite difference and the Fourier method with FD time integration.

It is done for a constant velocity medium.
This usually is sufficient, since it is only necessary to maintain stability for the highest velocity. For lower velocities the schemes are then automatically stable.

Due to the truncation error of FD operators numerical grid dispersion is present. It depends on the discretization and on the order of the FD operator.

Dispersion and stability: 1D FD

1D wave equation:

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

FD approximation:

$$\frac{p_j^{n+1} - 2p_j^n + p_j^{n-1}}{(\Delta t)^2} = c^2 \, \frac{p_{j+1}^n - 2p_j^n + p_{j-1}^n}{(\Delta x)^2}$$

Inserting the harmonic solution

$$p_j^n = e^{i(kj\Delta x - \omega n \Delta t)}$$

we get

Dispersion and stability (cont'd): 1D FD

$$\frac{e^{i(kj\Delta x-\omega(n+1)\Delta t)} - 2e^{i(kj\Delta x-\omega n\Delta t)} + e^{i(kj\Delta x-\omega(n-1)\Delta t)}}{(\Delta t)^2}$$

$$= c^2 \; \frac{e^{i(k(j+1)\Delta x-\omega n\Delta t)} - 2e^{i(kj\Delta x-\omega n\Delta t)} + e^{i(k(j-1)\Delta x-\omega n\Delta t)}}{(\Delta x)^2}$$

The left side can further be simplified:

$$e^{i(kj\Delta x)} \cdot \left(e^{-i\omega(n+1)\Delta t} - 2e^{-i\omega n\Delta t} + e^{-i\omega(n-1)\Delta t}\right)/(\Delta t)^2$$

$$= e^{i(kj\Delta x-\omega n\Delta t)} \cdot \left(e^{-i\omega\Delta t} - 2 + e^{i\omega\Delta t}\right)/(\Delta t)^2$$

$$= e^{i(kj\Delta x-\omega n\Delta t)} \cdot \left(-4\sin^2\frac{\omega\Delta t}{2}\right)/(\Delta t)^2$$

Dispersion and stability (cont'd): 1D FD

Similarly we simplify the right hand side and get:

$$\frac{e^{i(kj\Delta x-\omega n\Delta t)}\cdot\left(-4\sin^2\frac{\omega\Delta t}{2}\right)}{(\Delta t)^2}=c^2\,\frac{e^{i(kj\Delta x-\omega n\Delta t)}\cdot\left(-4\sin^2\frac{k\Delta x}{2}\right)}{(\Delta x)^2}$$

Further simplification leads to:

$$\frac{\sin^2\frac{\omega\Delta t}{2}}{(\Delta t)^2}=c^2\,\frac{\sin^2\frac{k\Delta x}{2}}{(\Delta x)^2}$$

Solving for $\omega(k)$ yields the dispersion relation:

$$\omega(k)=\frac{2}{\Delta t}\arcsin\left(\frac{c\Delta t}{\Delta x}\sin\frac{k\Delta x}{2}\right)$$

Stability, if argument of $\arcsin$ not larger than unity $\Rightarrow \dfrac{c\Delta t}{\Delta x} <= 1$

Dispersion and stability (cont'd): 1D Fourier

In case of the Fourier method we have:

$$\frac{p_j^{n+1} - 2p_j^n + p_j^{n-1}}{(\Delta t)^2} = -k^2 c^2 p_j^n$$

Inserting the harmonic solution as before:

$$\frac{-4\sin^2\frac{\omega \Delta t}{2}}{(\Delta t)^2} = -k^2 c^2$$

Solving for ω we find the dispersion relation:

$$\omega(k) = \frac{2}{\Delta t}\arcsin\frac{kc\Delta t}{2}$$

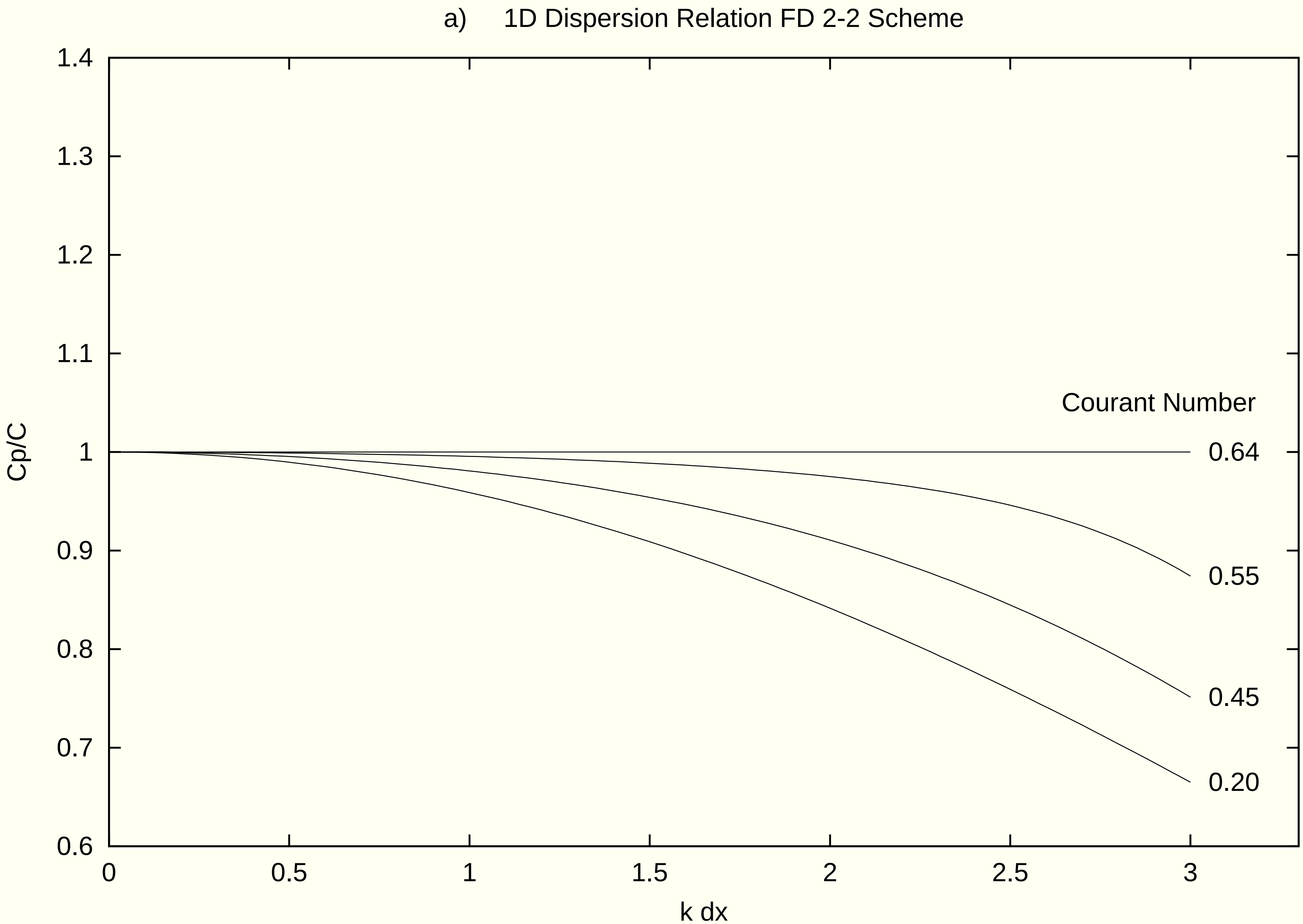
Dispersion and stability (cont'd): 1D Fourier

For the Fourier derivative $k_{max} = \frac{\pi}{\Delta x}$ holds.

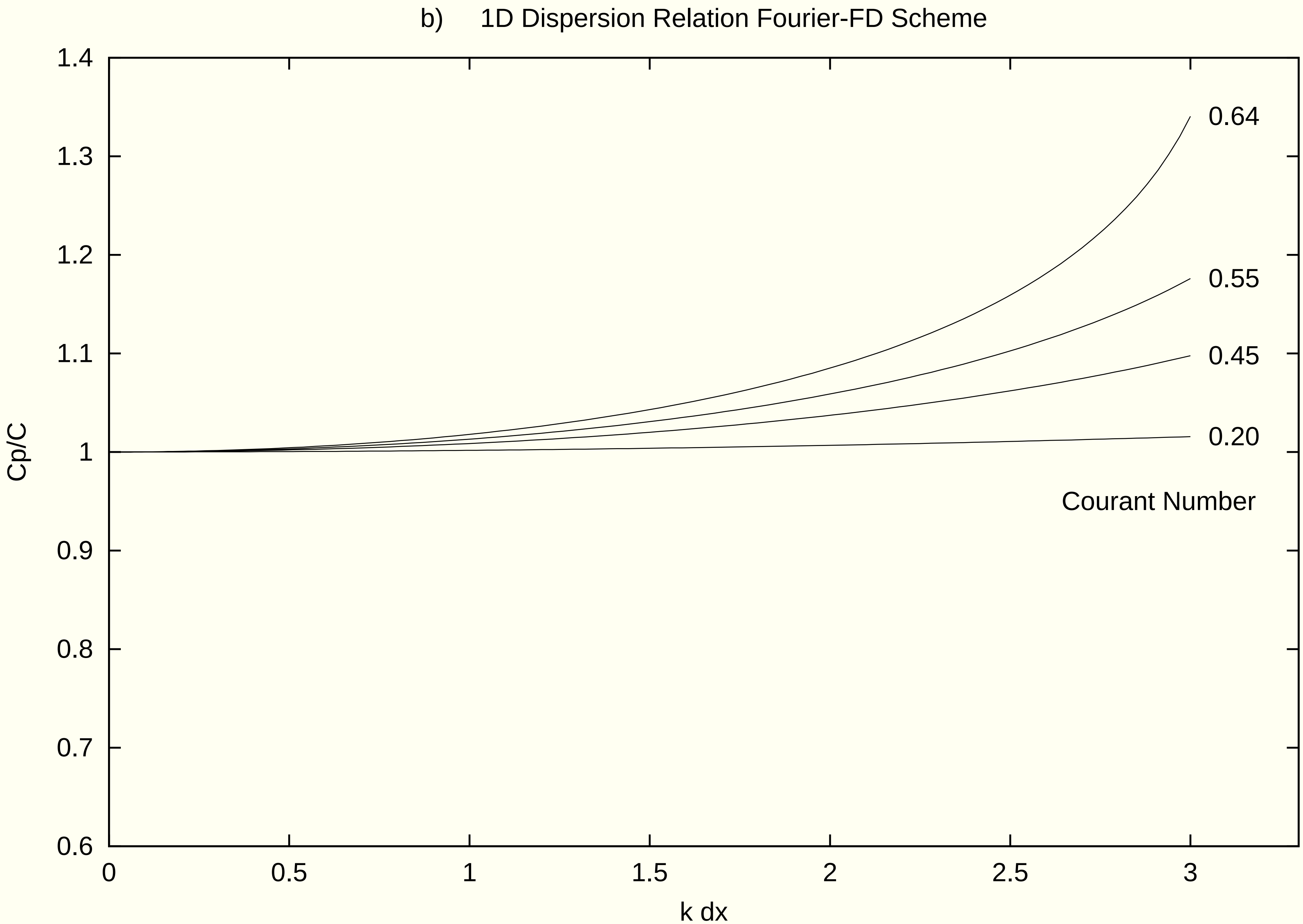
Inserting this into the argument of the $\arcsin$, we find that stability is maintained, if

$$\frac{\pi}{2} \frac{c \cdot \Delta t}{\Delta x} \leq 1 \quad \Rightarrow \quad \alpha \leq \frac{2}{\pi} \approx 0.64$$

Dispersion and stability (cont'd): 1D dispersion



Dispersion and stability (cont'd): 1D dispersion



Dispersion and stability: 2D FD

2D wave equation:

$$\frac{\partial^2 p}{\partial t^2} = c^2 \left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial z^2} \right)$$

According to the 1D FD case we obtain:

$$\frac{\sin^2 \frac{\omega \Delta t}{2}}{(\Delta t)^2} = c^2 \left(\frac{\sin^2 \frac{k_x \Delta x}{2}}{(\Delta x)^2} + \frac{\sin^2 \frac{k_z \Delta z}{2}}{(\Delta z)^2} \right)$$

and with $k_x = k \cos \vartheta, k_z = k \sin \vartheta$ and $\Delta x = \Delta z = \Delta$

$$\frac{\sin^2 \frac{\omega \Delta t}{2}}{(\Delta t)^2} = \frac{c^2}{\Delta^2} \left(\sin^2 \left(\frac{\Delta k \cos \vartheta}{2} \right) + \sin^2 \left(\frac{\Delta k \sin \vartheta}{2} \right) \right)$$

Dispersion and stability (cont'd): 2D FD

Solving for ω yields

$$\omega(k) = \frac{2}{\Delta t} \arcsin \left(\frac{c\Delta t}{\Delta} \cdot \sqrt{\sin^2\left(\frac{\Delta k \cos\vartheta}{2}\right) + \sin^2\left(\frac{\Delta k \sin\vartheta}{2}\right)} \right)$$

Stability is maintained, if $\frac{c\Delta t}{\Delta} \cdot \sqrt{2} \leq 1$.

A n-dimensional scheme is stable, if $\frac{c\Delta t}{\Delta} \cdot \sqrt{n} \leq 1$.

Dispersion and stability (cont'd): 2D Fourier

According to the 1D Fourier case we obtain:

$$\frac{-4\sin^2\frac{\omega\Delta t}{2}}{(\Delta t)^2} = c^2\left(-k_x^2 - k_z^2\right) \quad \text{or} \quad \frac{\sin\frac{\omega\Delta t}{2}}{\Delta t} = \frac{c\sqrt{k_x^2+k_z^2}}{2}$$

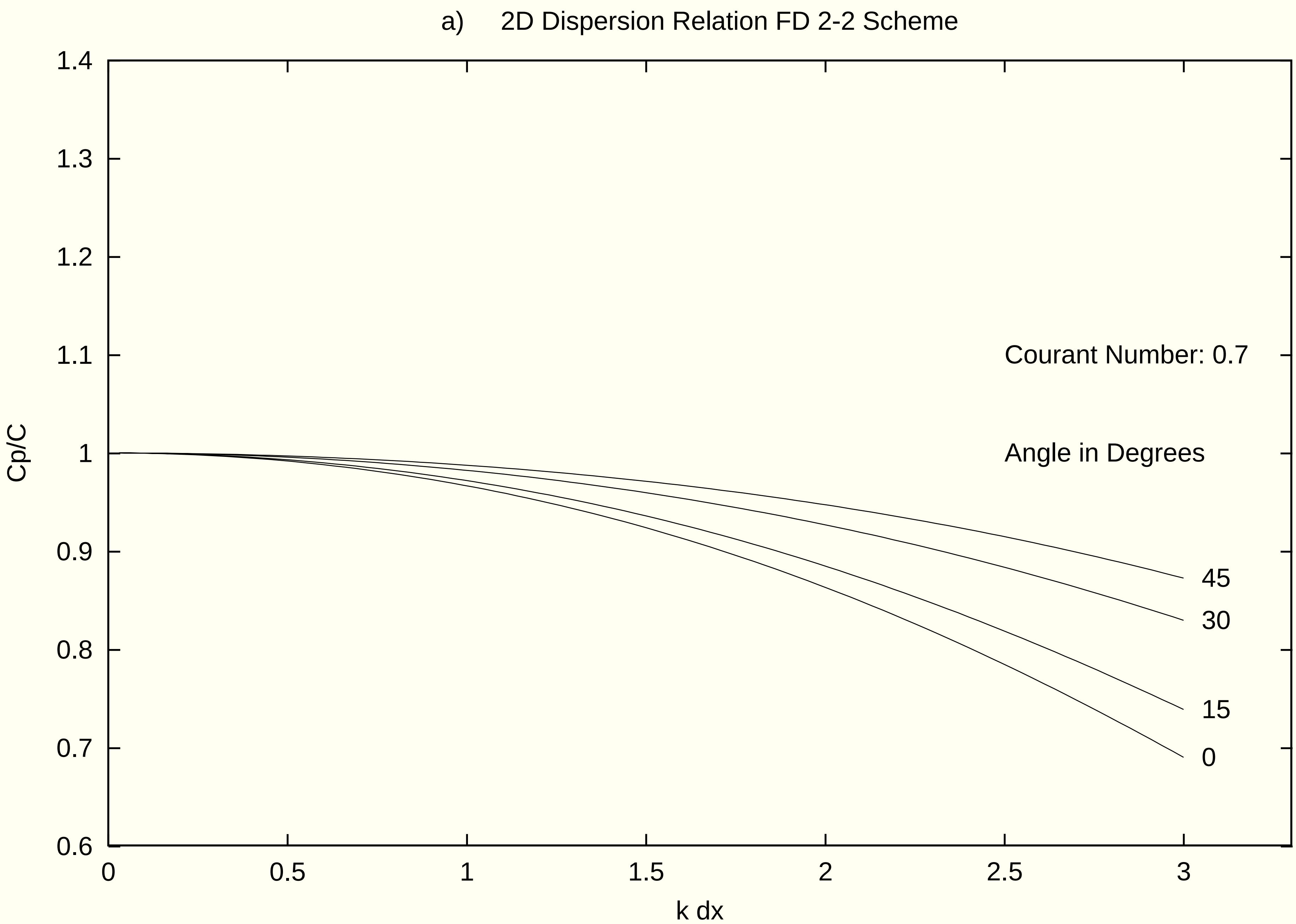
Solving for ω we obtain the dispersion relation:

$$\omega(k) = \frac{2}{\Delta t}\arcsin\left(\frac{c\sqrt{k_x^2+k_z^2}\Delta t}{2}\right)$$

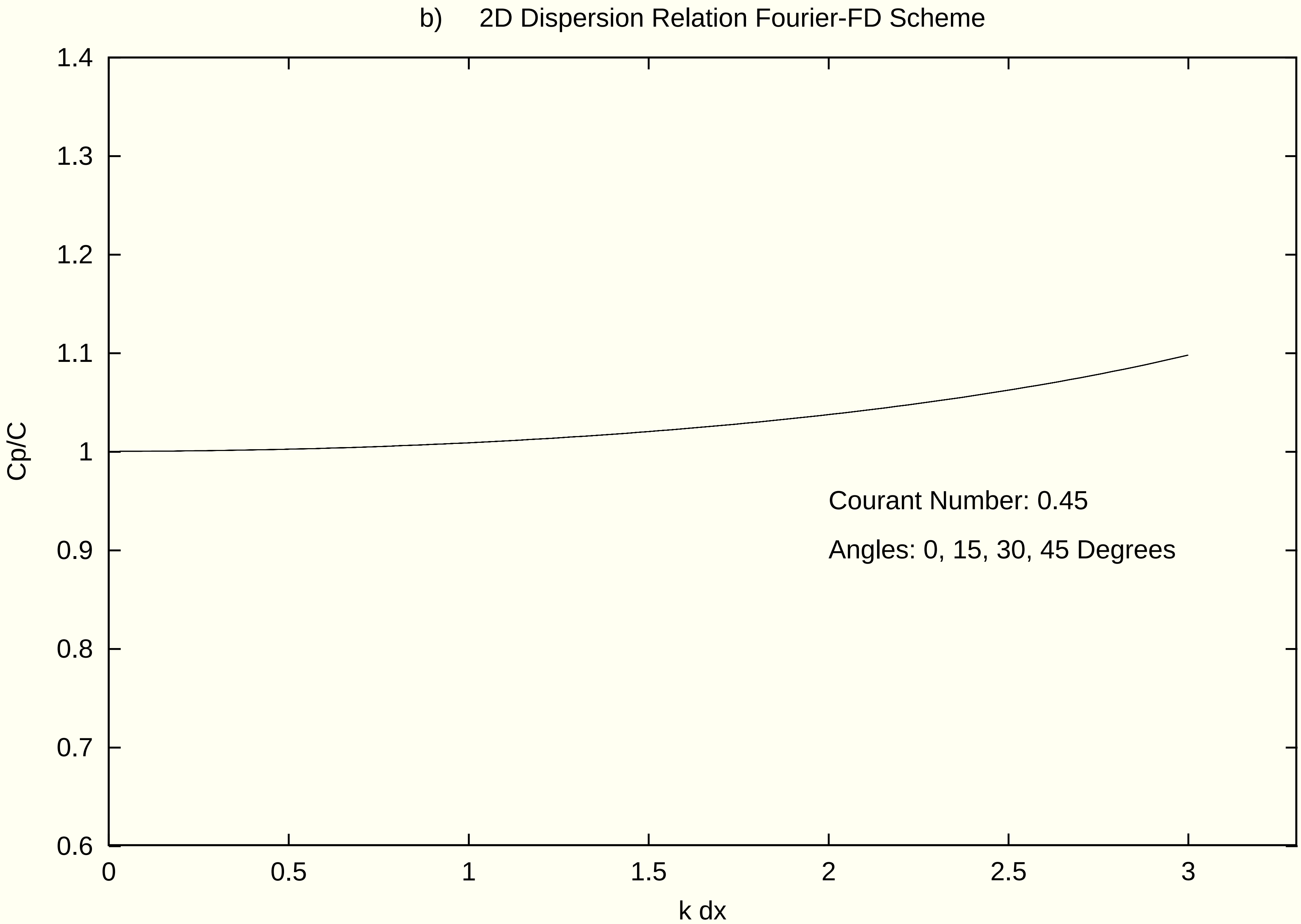
With $k_{max} = \frac{\pi}{\Delta}\,(\Delta = \Delta x = \Delta z)$ stability is maintained, if $\frac{\pi}{\sqrt{2}}\frac{c\Delta t}{\Delta} \leq 1$.

n-dimensional case: $\frac{\sqrt{n}\pi}{2}\frac{c\Delta t}{\Delta} \leq 1$.

Dispersion and stability (cont'd): 2D dispersion



Dispersion and stability (cont'd): 2D dispersion



Time integration

Starting from the 1D wave equation

$$\frac{\partial^2 p}{\partial t^2} = c^2 \frac{\partial^2 p}{\partial x^2} + S$$

we need to perform time integration to solve for p.

Discretizing in time, i.e. $p^n = p(n \cdot \Delta t)$ with the abbreviation

$$R^n = \frac{\partial^2 p^n}{\partial x^2}$$

the wave equation reads:

$$\frac{\partial^2 p^n}{\partial t^2} = c^2 R^n + S^n$$

Time integration (cont'd): FD

Using finite differences for the left hand side:

$$\frac{p^{n+1} - 2p^n + p^{n-1}}{(\Delta t)^2} = c^2 R^n + S^n$$

This can be solved for p^{n+1}:

$$p^{n+1} = 2p^n - p^{n-1} + (\Delta t)^2 [c^2 R^n + S^n]$$

The solution can thus be extrapolated in time by a so called time stepping scheme with time steps of size Δt until the maximum propagation time is reached.

Time integration (cont'd): Formal solution

Consider the 1D wave equation (second order PDE):

$$\frac{\partial^2 p}{\partial t^2} = c^2 \frac{\partial^2 p}{\partial x^2} + S$$

This can be rewritten as a system of first order PDEs:

$$\frac{\partial}{\partial t} \begin{pmatrix} p \\ \dot{p} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ c^2 \frac{\partial^2}{\partial x^2} & 0 \end{pmatrix} \begin{pmatrix} p \\ \dot{p} \end{pmatrix} + \begin{pmatrix} 0 \\ S \end{pmatrix}$$

System of $2N$ coupled PDEs, if number of grid points is N.

Time integration (cont'd): Formal solution

With

$$\mathbf{V}(t) = \begin{pmatrix} p \\ \\ \dot{p} \end{pmatrix}, \qquad \mathbf{A} = \begin{pmatrix} 0 & 1 \\ \\ c^2 \dfrac{\partial^2}{\partial x^2} & 0 \end{pmatrix} \quad \text{and} \quad \mathbf{f}(t) = \begin{pmatrix} 0 \\ \\ S \end{pmatrix}$$

the wave equation can be rewritten:

$$\frac{\partial}{\partial t}\mathbf{V}(t) = \mathbf{A} \cdot \mathbf{V}(t) + \mathbf{f}(t)$$

The formal solution is:

$$\mathbf{V}(t) = e^{t\mathbf{A}}\mathbf{V}(0) + \int_0^t e^{\tau \mathbf{A}}\, \mathbf{f}(t - \tau)\, d\tau$$

Time integration (cont'd): Taylor expansion

To represent operators of the form $e^{t\mathbf{A}}$ we use the Taylor expansion:

$$e^{t\mathbf{A}} = \mathbf{I} + t\mathbf{A} + \frac{t^2\mathbf{A}^2}{2!} + \frac{t^3\mathbf{A}^3}{3!} + \frac{t^4\mathbf{A}^4}{4!} + \cdots$$

Then

$$e^{t\mathbf{A}}\mathbf{V}(0) = \mathbf{V}(0) + t\mathbf{A}\mathbf{V}(0) + \frac{t^2}{2!}\mathbf{A}(\mathbf{A}\mathbf{V}(0)) + \frac{t^3}{3!}\mathbf{A}(\mathbf{A}(\mathbf{A}\mathbf{V}(0))) + \cdots$$

Time integration (cont'd): Taylor expansion

If we assume that $\mathbf{f}(t)$ is constant during the time period t

$$\mathbf{V}(t) = e^{t\mathbf{A}}\mathbf{V}(0) + \int_0^t e^{\tau\mathbf{A}}\,\mathbf{f}(t-\tau)\,d\tau$$

can be simplified:

$$\mathbf{V}(t) = e^{t\mathbf{A}}\mathbf{V}(0) + (e^{t\mathbf{A}} - \mathbf{I})/\mathbf{A}\;\mathbf{f}(t)$$

This can be rearranged:

$$\mathbf{V}(t) = \mathbf{V}(0) + \frac{(e^{t\mathbf{A}} - \mathbf{I})}{\mathbf{A}}\,(\mathbf{A}\mathbf{V}(0) + \mathbf{f}(t))$$

Time integration (cont'd): Taylor expansion

The Taylor expansion of $\left(e^{t\mathbf{A}} - \mathbf{I}\right) / \mathbf{A}$ is:

$$\frac{\left(e^{t\mathbf{A}} - \mathbf{I}\right)}{\mathbf{A}} = t\,\mathbf{I} + \frac{t^2}{2!}\mathbf{A} + \frac{t^3}{3!}\mathbf{A}^2 + \frac{t^4}{4!}\mathbf{A}^3 + \cdots$$

A useful approximation can be obtained, if truncated after fourth term. This is then equivalent to a fourth order Runge-Kutta scheme.

As always, truncation means an error, which in general leads to dispersion. The Taylor expansion converges relative slowly. Therefore dispersion is difficult to avoid.

Time integration (cont'd): Chebyshev exp.

More effective is the Chebyshev expansion:

$$e^z = \sum_{k=0}^{\infty} c_k \; J_k(tR) \; Q_k\left(\frac{z}{tR}\right)$$

where $c_0 = 1$ and $c_k = 2$ if $k \neq 0$, and $|z| < tR$

J_k are Bessel functions.
Q_k are modified Chebyshev polynomials. Relation to ordinary Chebyshev polynomials $T_k(x)$:

$$Q_k(x) := i^k \; T_k(-ix)$$

$Q_0(x) = 1, \; Q_1(x) = x, \; Q_2(x) = 2x^2 + 1$ etc.

Time integration (cont'd): Chebyshev exp.

Recurrence relation:

$$Q_{n+1}(x) = 2x\,Q_n(x) + Q_{n-1}(x)$$

The exponential matrix operator then reads:

$$e^{t\mathbf{A}} = \sum_{k=0}^{M} c_k\; J_k(tR)\; Q_k\left(\frac{\mathbf{A}}{R}\right)$$

Converges fast with machine accuracy, if $M > tR$. R is the largest eigenvalue of $\mathbf{A}$.

Modified Chebyshev polynomials can be calculated recursively. Argument x is replaced by $\frac{\mathbf{A}}{R}$. Then:

$Q_0(\frac{\mathbf{A}}{R}) = \mathbf{I}$, $\quad Q_1(\frac{\mathbf{A}}{R}) = \frac{\mathbf{A}}{R}$, $\quad Q_2(\frac{\mathbf{A}}{R}) = \frac{\mathbf{A}^2}{R^2} + \mathbf{I}$, etc.

Time integration (cont'd): Tal-Ezer method

Formal solution (again):

$$\mathbf{V}(t) = e^{t\mathbf{A}}\mathbf{V}(0) + \int_0^t e^{\tau\mathbf{A}}\,\mathbf{f}(t-\tau)\,d\tau$$

Solution without source term:

$$\mathbf{V}(t) = \sum_{k=0}^{M} c_k\; J_k(tR)\; Q_k(\frac{\mathbf{A}}{R})\;\mathbf{V}(0)$$

We start the recurrence by

$$Q_0(\frac{\mathbf{A}}{R})\mathbf{V}(0) = \mathbf{V}(0)\;, \qquad Q_1(\frac{\mathbf{A}}{R})\mathbf{V}(0) = \frac{\mathbf{A}}{R}\mathbf{V}(0)$$

Time integration (cont'd): Tal-Ezer method

Formal solution with source term (zero initial conds.):

$$\mathbf{V}(t) = \left[\int_0^t e^{\tau \mathbf{A}} \, h(t-\tau) \, d\tau \right] \mathbf{g}(\mathbf{x})$$

$\mathbf{f}(\mathbf{x}, t) = \mathbf{g}(\mathbf{x}) \cdot h(t)$, i.e. assumed separable.

Solution using Chebyshev expansion:

$$\mathbf{V}(t) = \sum_{k=0}^{M} \left[\int_0^t c_k \, J_k(\tau R) \, h(t-\tau) \, d\tau \right] Q_k(\frac{\mathbf{A}}{R}) \, \mathbf{g}(\mathbf{x})$$

Time integration (cont'd): Tal-Ezer method

Using the abbreviation

$$b_k = \int_0^t c_k \, J_k(\tau R) \, h(t - \tau) \, d\tau$$

the solution is:

$$\mathbf{V}(t) = \sum_{k=0}^{M} b_k \, Q_k(\frac{\mathbf{A}}{R}) \, \mathbf{g}(\mathbf{x})$$

Only b_k is time dependent. Therefore, the solution for different times t require only different sets of b_k.
The Chebyshev polynomials, need not to be calculated again.

Time integration (cont'd): REM

We start with the second order PDE in operator notation:

$$\frac{\partial^2 \mathbf{p}}{\partial t^2} = -\mathbf{L}^2 \mathbf{p}$$

We define the operator $-\mathbf{L}^2 = c^2 \dfrac{\partial^2}{\partial x^2}$

The formal solution is

$$\mathbf{p}(t) = \cos \mathbf{L}t \; \mathbf{p}(0) + \frac{\sin \mathbf{L}t}{\mathbf{L}} \; \dot{\mathbf{p}}(0)$$

Adding the solution at time $-t$ yields

$$\mathbf{p}(t) = -\mathbf{p}(-t) + 2 \cos \mathbf{L}t \; \mathbf{p}(0)$$

Time integration (cont'd): REM

Excursus:

Expansion of the operator $\cos \mathbf{L}t$ into a Taylor series and inserting into the last equation yields:

$$\mathbf{p}(t) = -\mathbf{p}(-t) + 2\,\mathbf{p}(0) - \mathbf{L}^2 t^2 \mathbf{p}(0) + \frac{1}{12}\mathbf{L}^4 t^4 \mathbf{p}(0) - \ldots$$

Truncating after the second order term and replacing $\mathbf{p}(t)$ by $\mathbf{p}^{n+1}$, $\mathbf{p}(0)$ by $\mathbf{p}^n$ and $\mathbf{p}(-t)$ by $\mathbf{p}^{n-1}$ results in the well known second order FD time integration scheme:

$$\mathbf{p}^{n+1} = -\mathbf{p}^{n-1} + 2\,\mathbf{p}^n + c^2\,(\Delta t)^2\,\frac{\partial^2 \mathbf{p}^n}{\partial x^2}$$

Time integration (cont'd): REM

Expansion of $\cos \mathbf{L}t$ for modified Chebyshev polynomials reads:

$$\cos \mathbf{L}t = \sum_{k=0}^{\infty} c_{2k}\ J_{2k}(tR)\ Q_{2k}\left(\frac{i\mathbf{L}}{R}\right)$$

Only modified Chebyshev polynomials of even order are present. Therefore, the solution is:

$$\mathbf{p}(t) = -\mathbf{p}(-t) + 2\sum_{k=0}^{M/2} c_{2k}\ J_{2k}(tR)\ Q_{2k}(\frac{i\mathbf{L}}{R})\ \mathbf{p}(0)$$

Since the indices of the modified Chebyshev polynomials $Q_{2k}(\frac{i\mathbf{L}}{R})$ are even numbered, only powers of $-\mathbf{L}^2/R^2$ occur.

Time integration (cont'd): REM

Here a recurrence relation with index steps of two are required:

$$Q_{n+2}(x) = (4x^2 + 2)\, Q_n(x) - Q_{n-2}(x)$$

The recurrence is initiated by

$$Q_0(\frac{i\mathbf{L}}{R})\, \mathbf{p}(0) = \mathbf{p}(0)$$

and

$$Q_2(\frac{i\mathbf{L}}{R})\, \mathbf{p}(0) = (2 \cdot \frac{-\mathbf{L}^2}{R^2} + \mathbf{I})\, \mathbf{p}(0)$$

Time integration (cont'd): REM

Formal solution with source term (zero initial conds.):

$$\mathbf{p}(t) = \left[\int_0^t \frac{\sin \mathbf{L}\tau}{\mathbf{L}} \, h(t-\tau) \, d\tau \right] \mathbf{g}(\mathbf{x})$$

Expansion of the sine-function for modified Chebyshev polynomials:

$$i \sin \mathbf{L}t = \sum_{k=0}^{\infty} c_{2k+1} \; J_{2k+1}(tR) \; Q_{2k+1}(\frac{i\mathbf{L}}{R})$$

and therefore

$$\frac{\sin \mathbf{L}t}{\mathbf{L}} = \sum_{k=0}^{\infty} c_{2k+1} \; \frac{J_{2k+1}(tR)}{R} \; \frac{R}{i\mathbf{L}} \; Q_{2k+1}(\frac{i\mathbf{L}}{R})$$

Time integration (cont'd): REM

Solution with Chebyshev expansion:

$$\mathbf{p}(t) = \left[\sum_{k=0}^{M/2} \int_0^t c_{2k+1} \, \frac{J_{2k+1}(\tau R)}{R} \, h(t-\tau) \, d\tau \, \frac{R}{i\mathbf{L}} \, Q_{2k+1}\left(\frac{i\mathbf{L}}{R}\right) \right] \mathbf{g}(\mathbf{x})$$

Using the abbreviation

$$b_k = \int_0^t c_k \frac{J_k(\tau R)}{R} \, h(t-\tau) \, d\tau$$

the solution is:

$$\mathbf{p}(t) = \left[\sum_{k=0}^{M/2} b_{2k+1} \, \frac{R}{i\mathbf{L}} \, Q_{2k+1}\left(\frac{i\mathbf{L}}{R}\right) \right] \mathbf{g}(\mathbf{x})$$

Time integration (cont'd): REM

The recurrence is initiated by

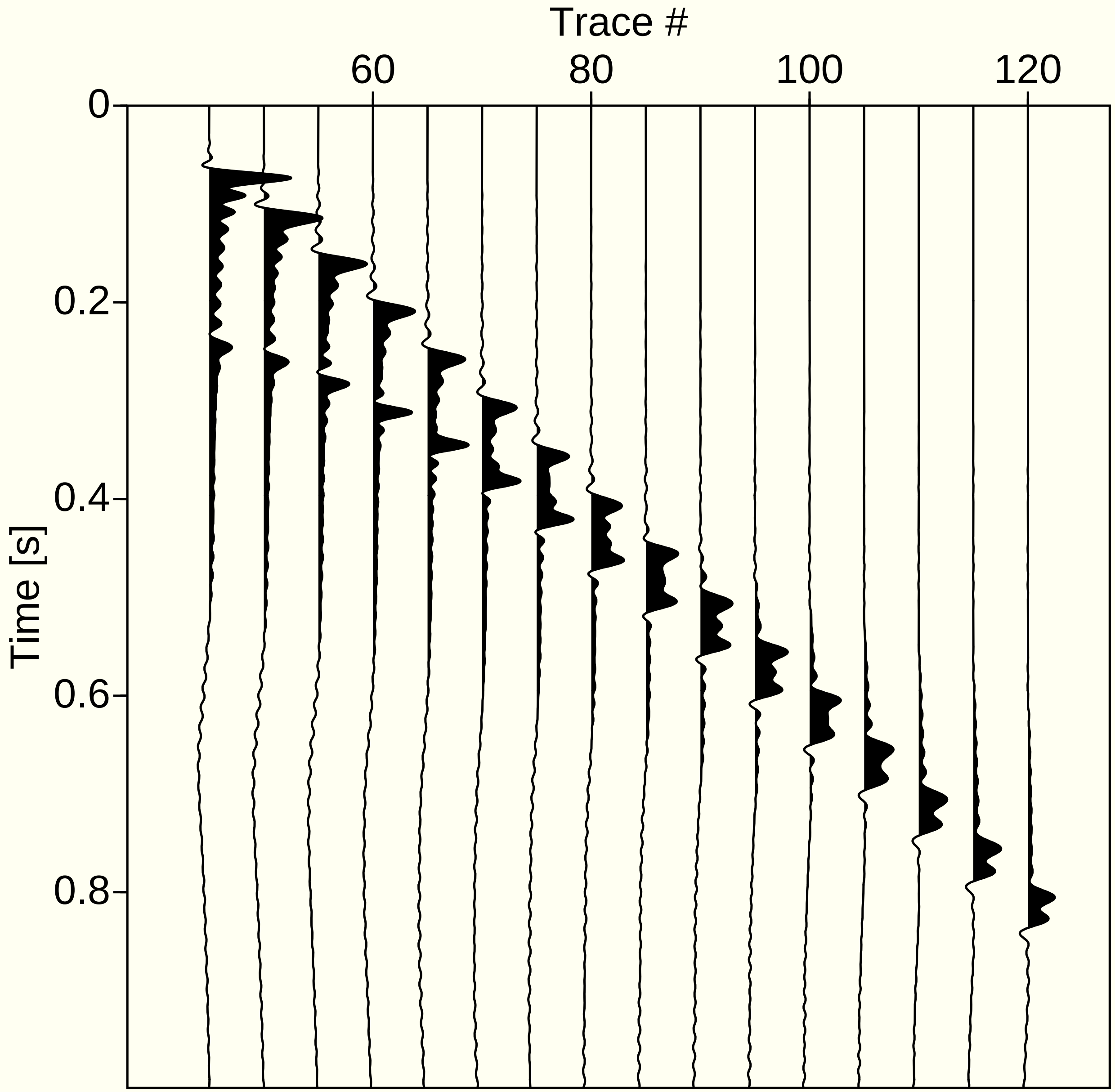
$$\frac{R}{i\mathbf{L}}\, Q_1\left(\frac{i\mathbf{L}}{R}\right)\mathbf{g}(\mathbf{x}) = \mathbf{g}(\mathbf{x})$$

and

$$\frac{R}{i\mathbf{L}}\, Q_3\left(\frac{i\mathbf{L}}{R}\right)\mathbf{g}(\mathbf{x}) = \left(4\cdot\frac{-\mathbf{L}^2}{R^2} + 3\cdot\mathbf{I}\right)\mathbf{g}(\mathbf{x})$$

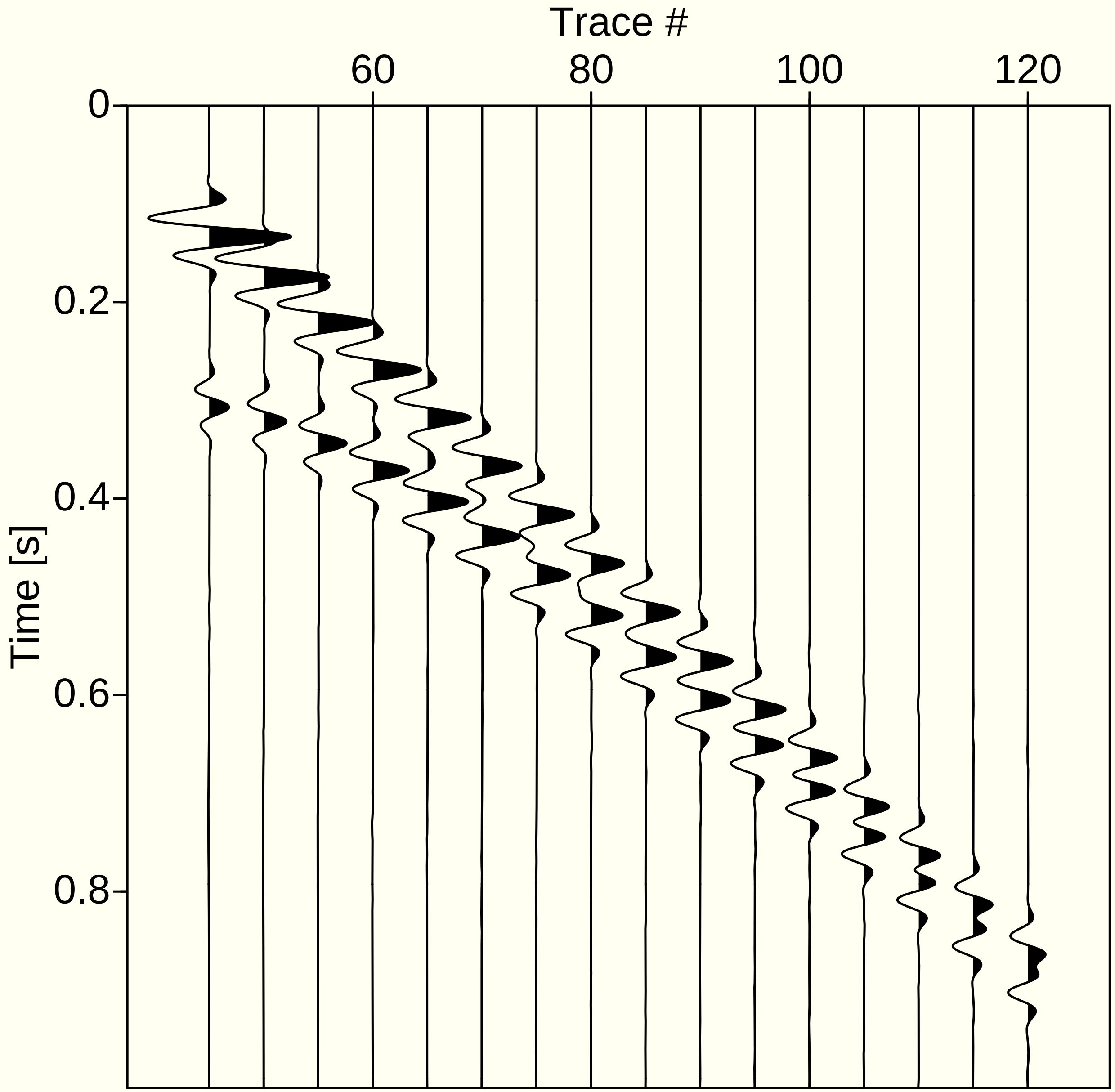
Only terms of odd order are present. Because of the factor $R/i\mathbf{L}$ one obtains also here only powers of $-\mathbf{L}^2/R^2$

Time integration (cont'd): REM



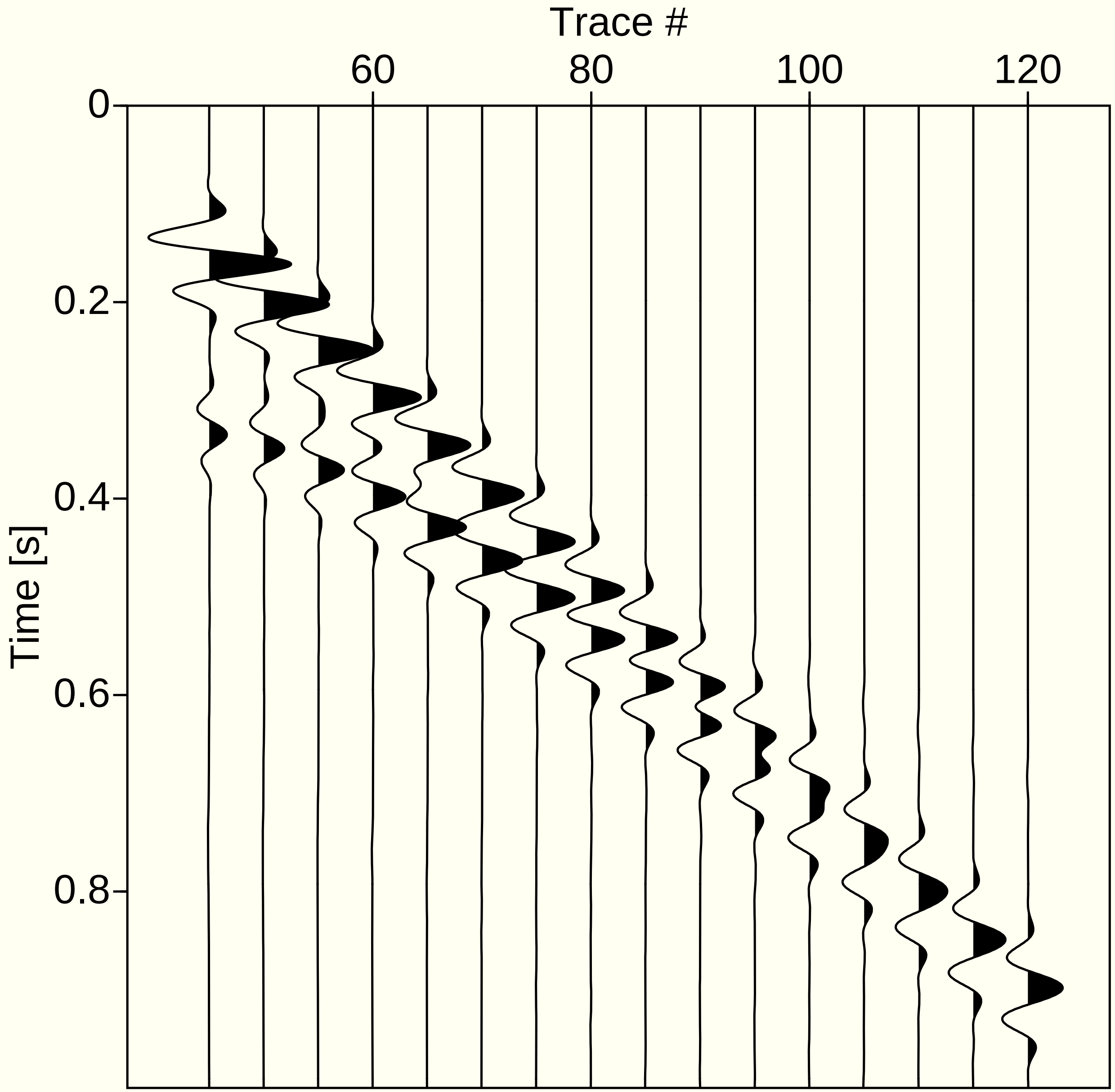
a) Spike

Time integration (cont'd): REM



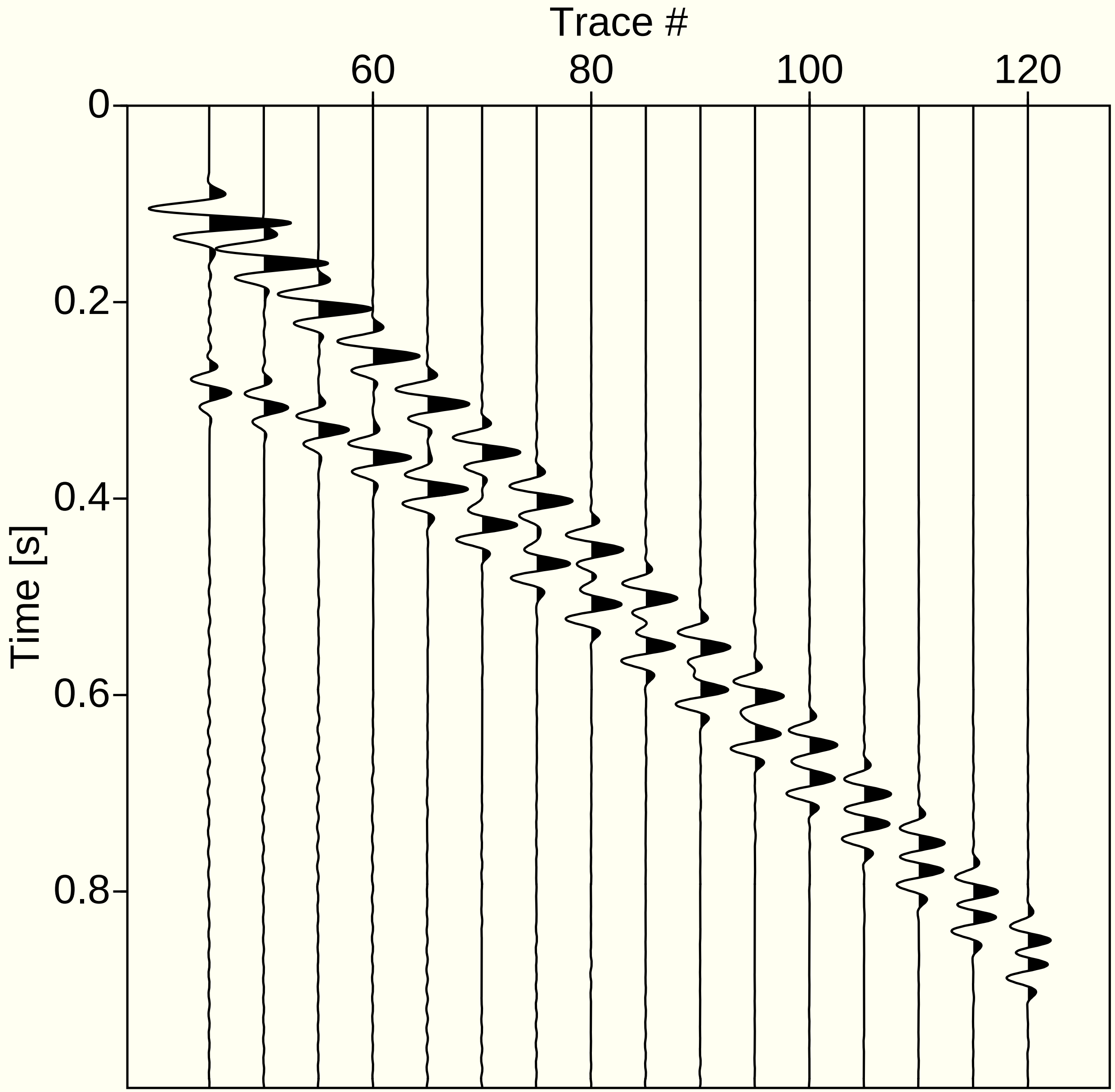
b) 50 Hz

Time integration (cont'd): REM



c) 35 Hz

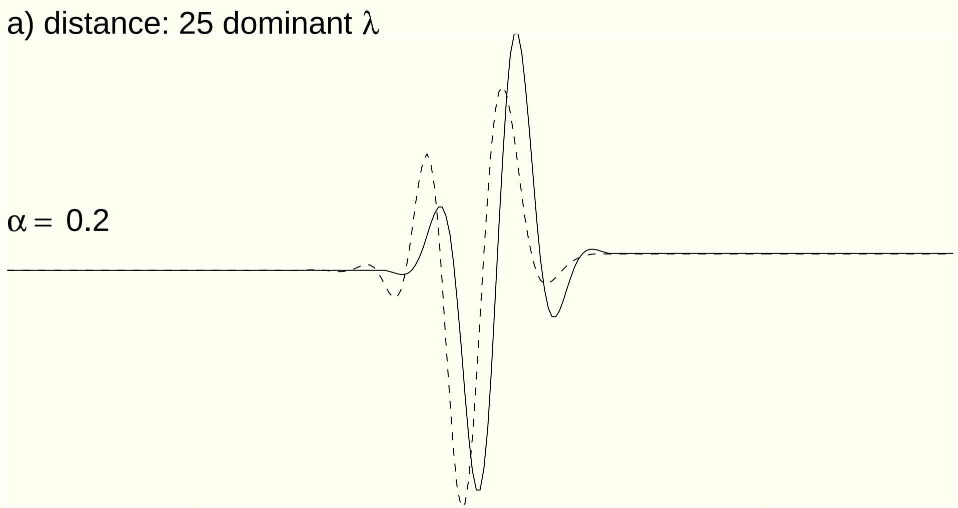
Time integration (cont'd): REM

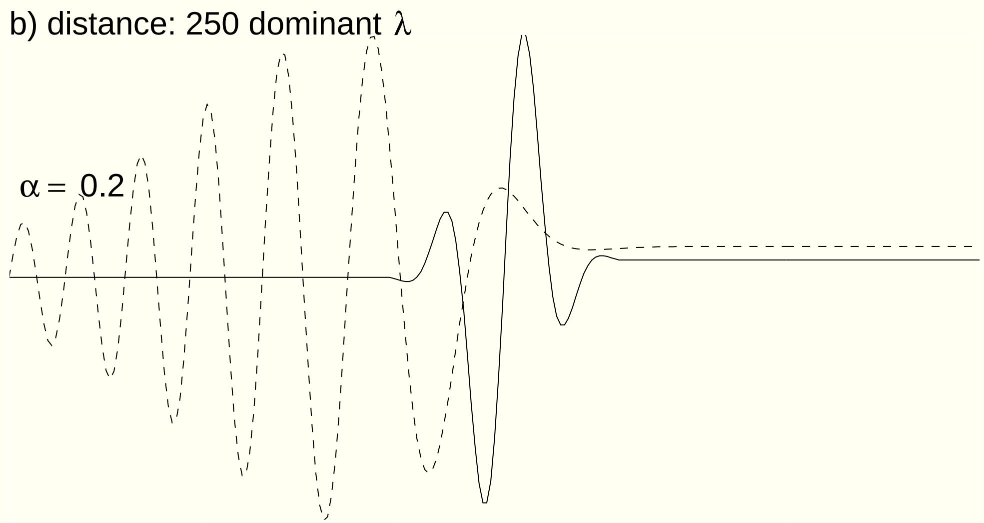


d) 65 Hz

Time integration (cont'd): REM

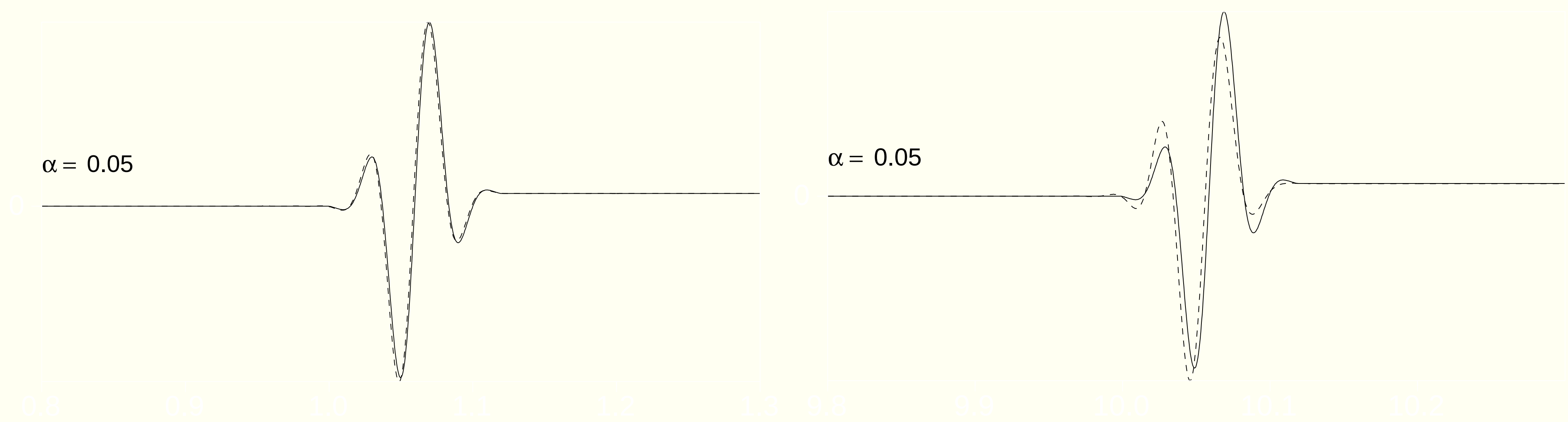
1D test: comparison of FD against analytic solution ($\alpha = 0.2$)
25 versus 250 dominant wavelengths





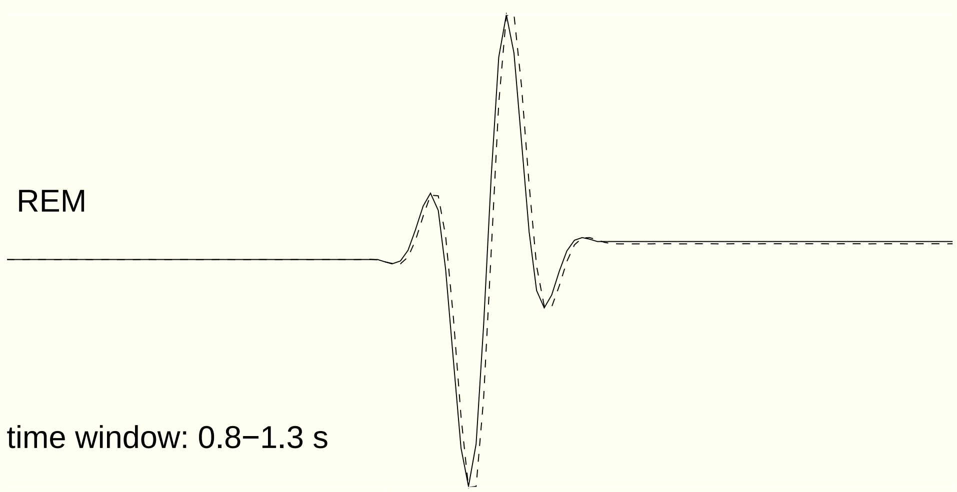
Time integration (cont'd): REM

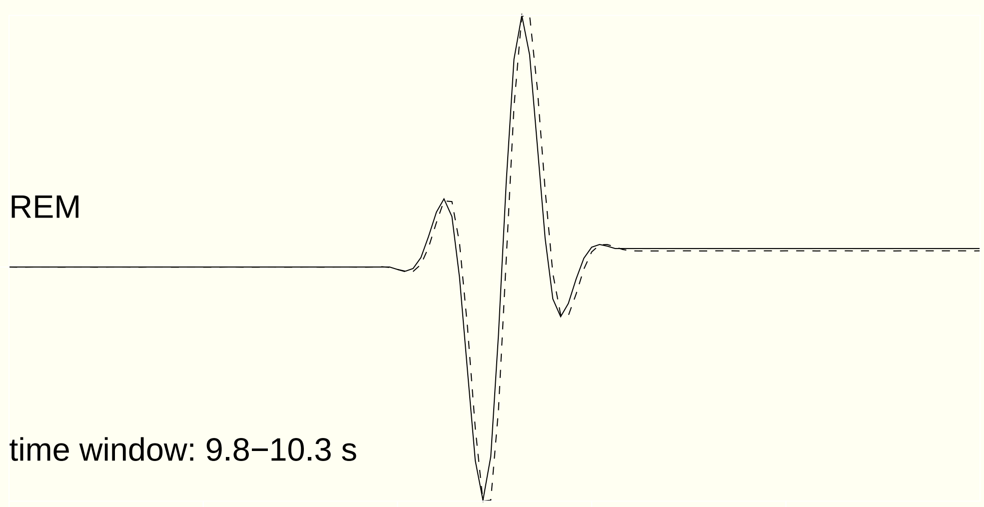
1D test: comparison of FD against analytic solution ($\alpha = 0.05$)
25 versus 250 dominant wavelengths



Time integration (cont'd): REM

1D test: comparison of REM against analytic solution
25 versus 250 dominant wavelengths





Implementation Details: Sources

Single force:

$$\varrho \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial \sigma_{ij}}{\partial x_j} + f_i$$

where often is assumed separable:

$$\mathbf{f}(\mathbf{x}, t) = \mathbf{S}(\mathbf{x}) \cdot h(t)$$

$\mathbf{S}(\mathbf{x})$ is a function of the position vector $\mathbf{x}$

$h(t)$ is the time history of the excitation function

Point force:

$$\mathbf{S}(\mathbf{x}) = \mathbf{S}_0 \cdot \delta(\mathbf{x} - \mathbf{x}_0),$$

Implementation Details (cont'd): Sources

Explosive source:

$$\mathbf{f}(\mathbf{x}, t) = \left(\frac{\partial \Phi}{\partial x}, \frac{\partial \Phi}{\partial y}, \frac{\partial \Phi}{\partial z} \right)^T$$

with scalar potential

$$\Phi(\mathbf{x}, t) = a(\mathbf{x}) \cdot h(t)$$

For the Fourier method and higher order FD methods $a(\mathbf{x})$ must be smooth, e.g. may have Gaussian shape:

$$a(\mathbf{x}) = \exp(-\alpha(\mathbf{x} - \mathbf{x}_0)^2)$$

Implementation Details (cont'd): Sources

Shear source:

$$\mathbf{f}(\mathbf{x},t) = \nabla \times \mathbf{\Psi}(\mathbf{x},t)$$

with the vector potential:

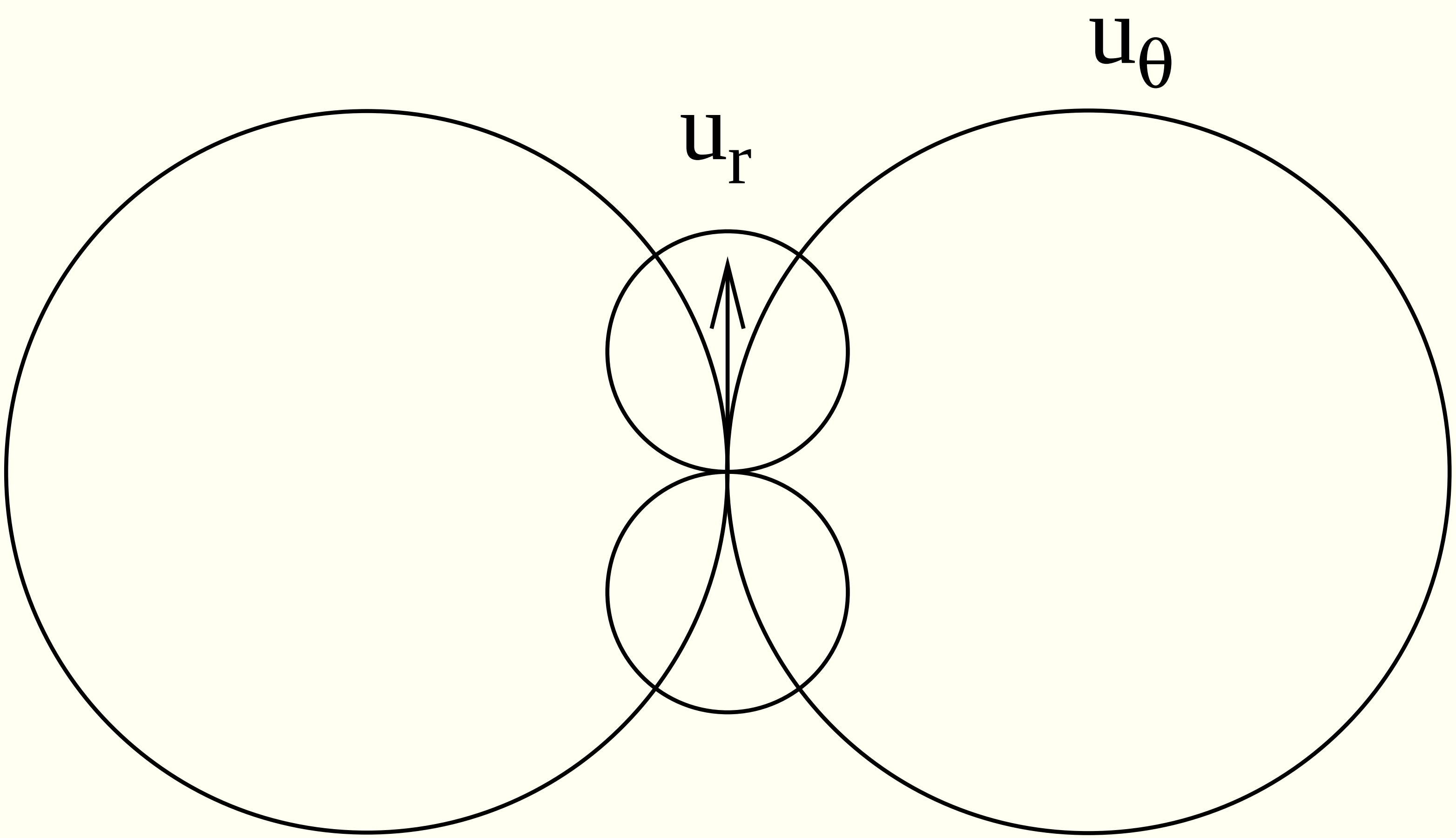
$$\mathbf{\Psi}(\mathbf{x},t) = (a_x, a_y, a_z)^T \cdot h(t)$$

In general explosive, shear and moment sources can be implemented via altering components of the stress tensor.

Other types of sources can be combined by the above mentioned ones.

Implementation Details (cont'd): Sources

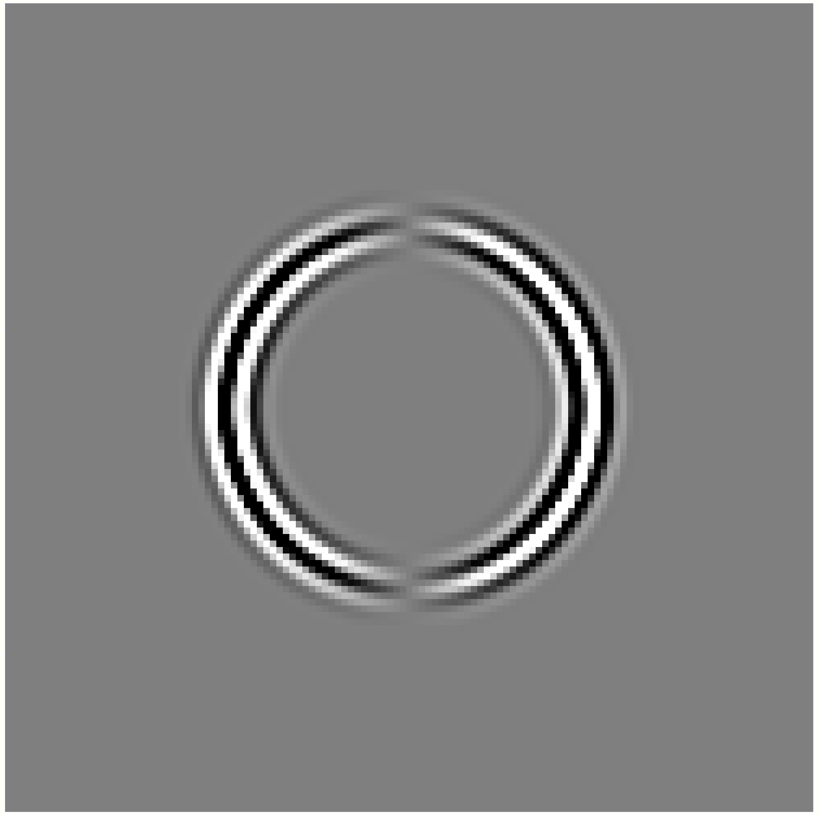
Vertical point force:



Implementation Details (cont'd): Sources

Vertical point force:

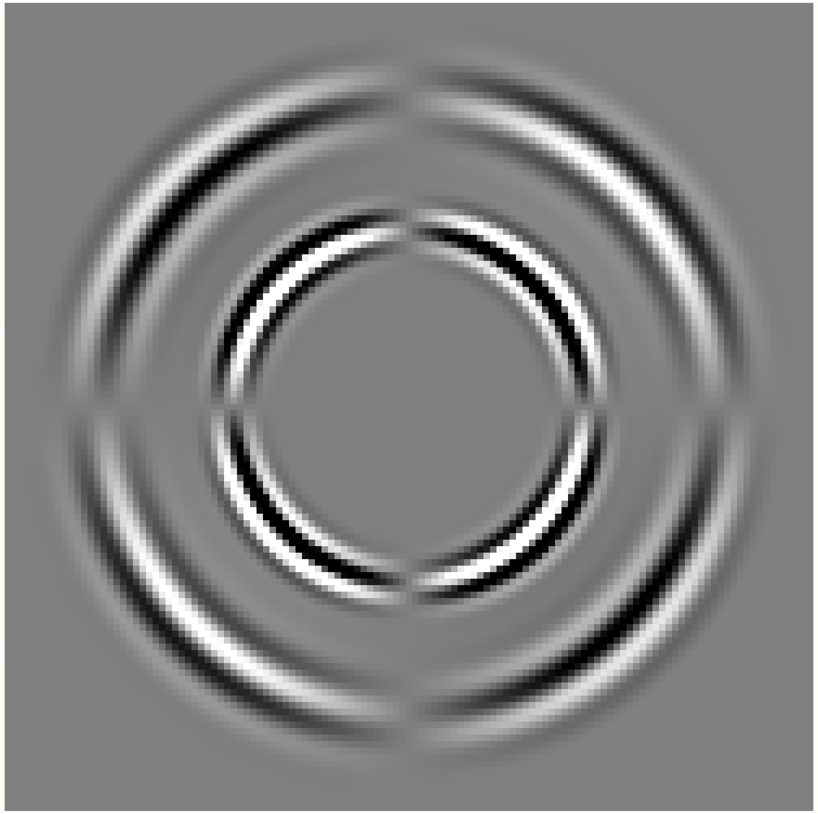
Pressure t=300 ms



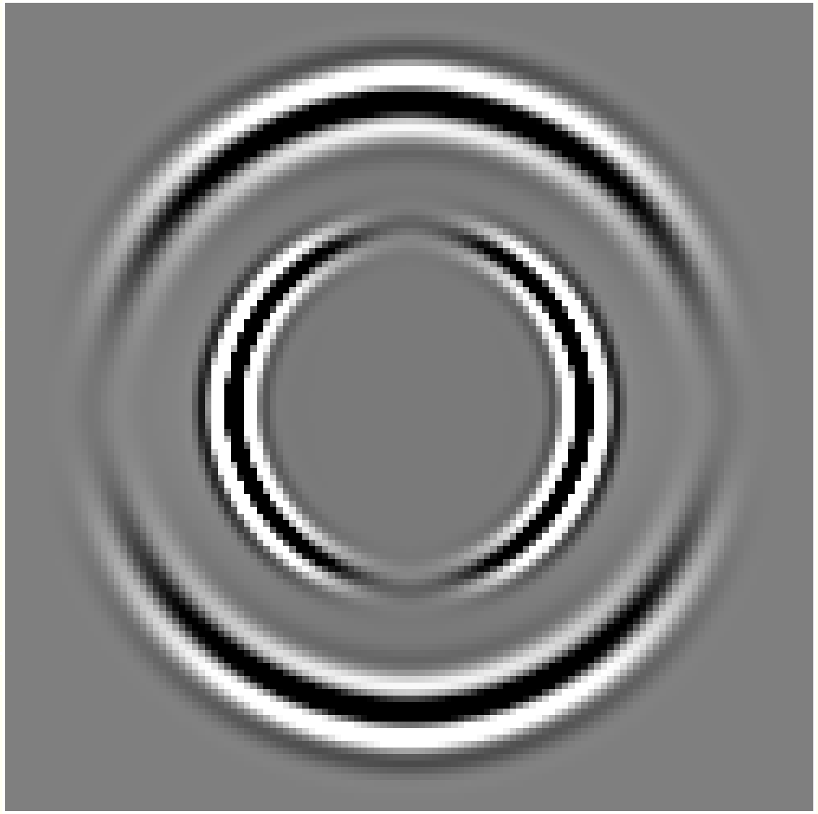
Shear t=300 ms

Implementation Details (cont'd): Sources

Vertical point force:



x-Displacement   t=300 ms

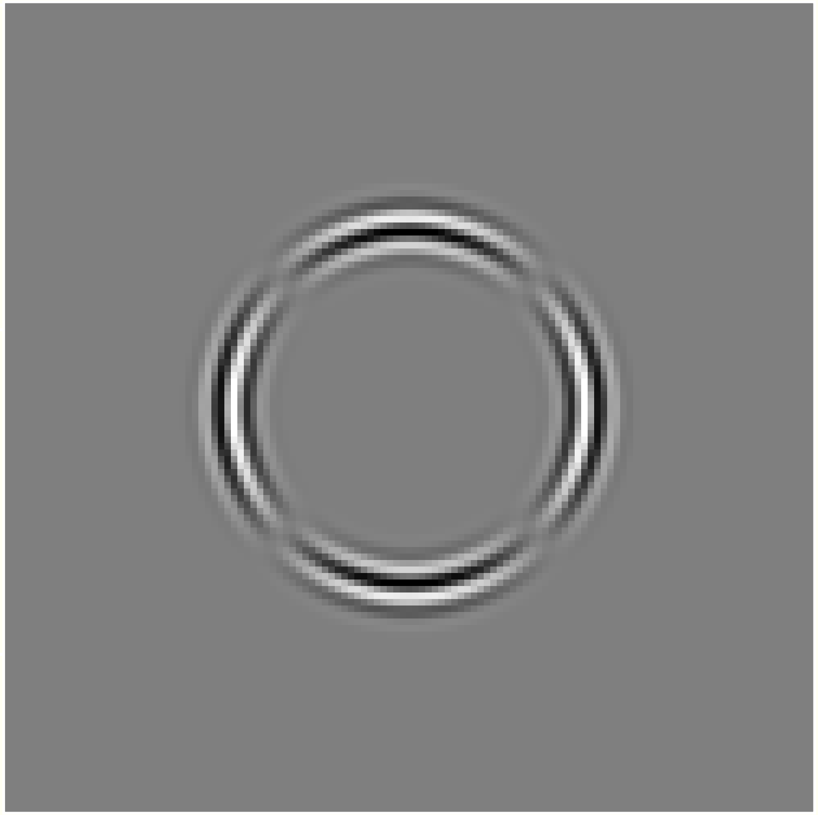


z-Displacement   t=300 ms

Implementation Details (cont'd): Sources

Double couple:

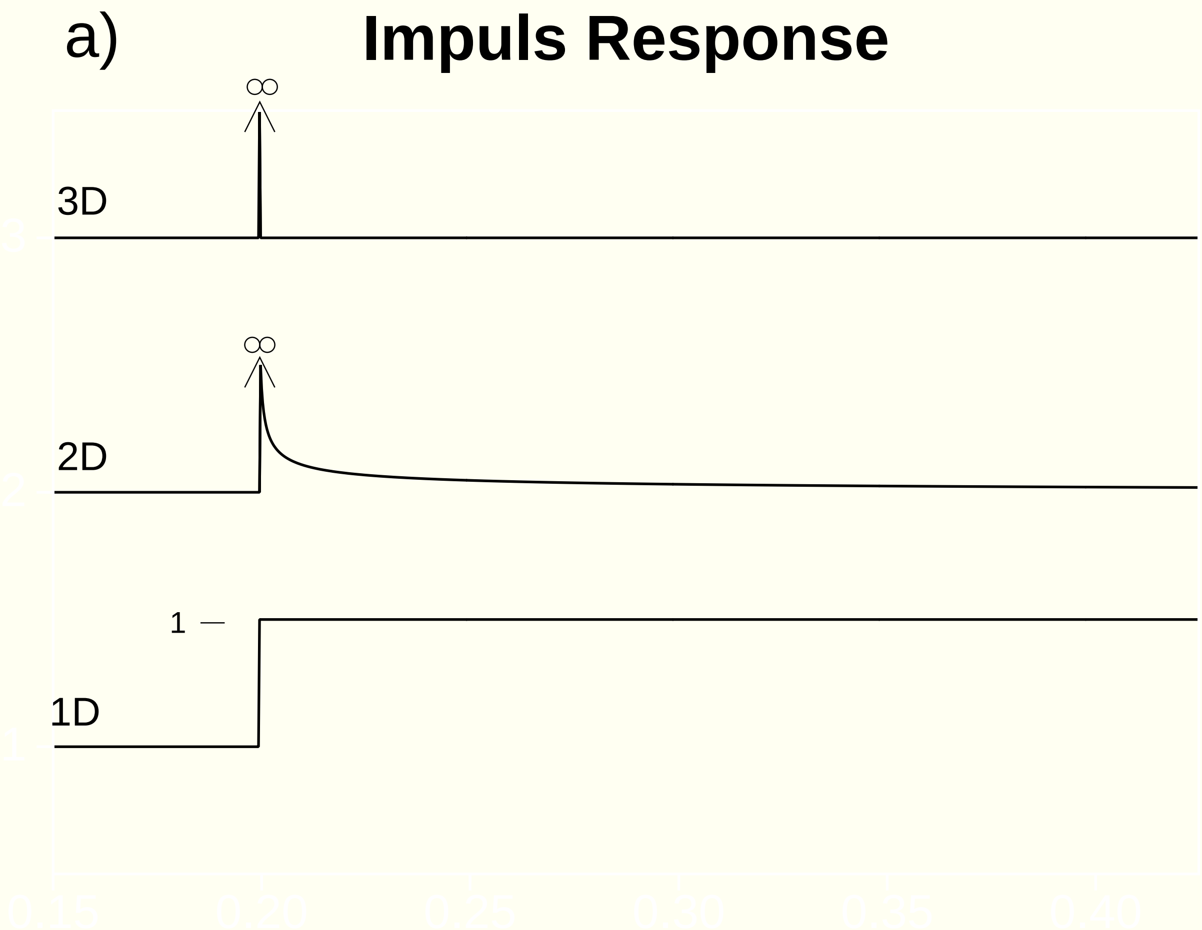
Pressure   t=300 ms



Shear   t=300 ms

Implementation Details: Response functions

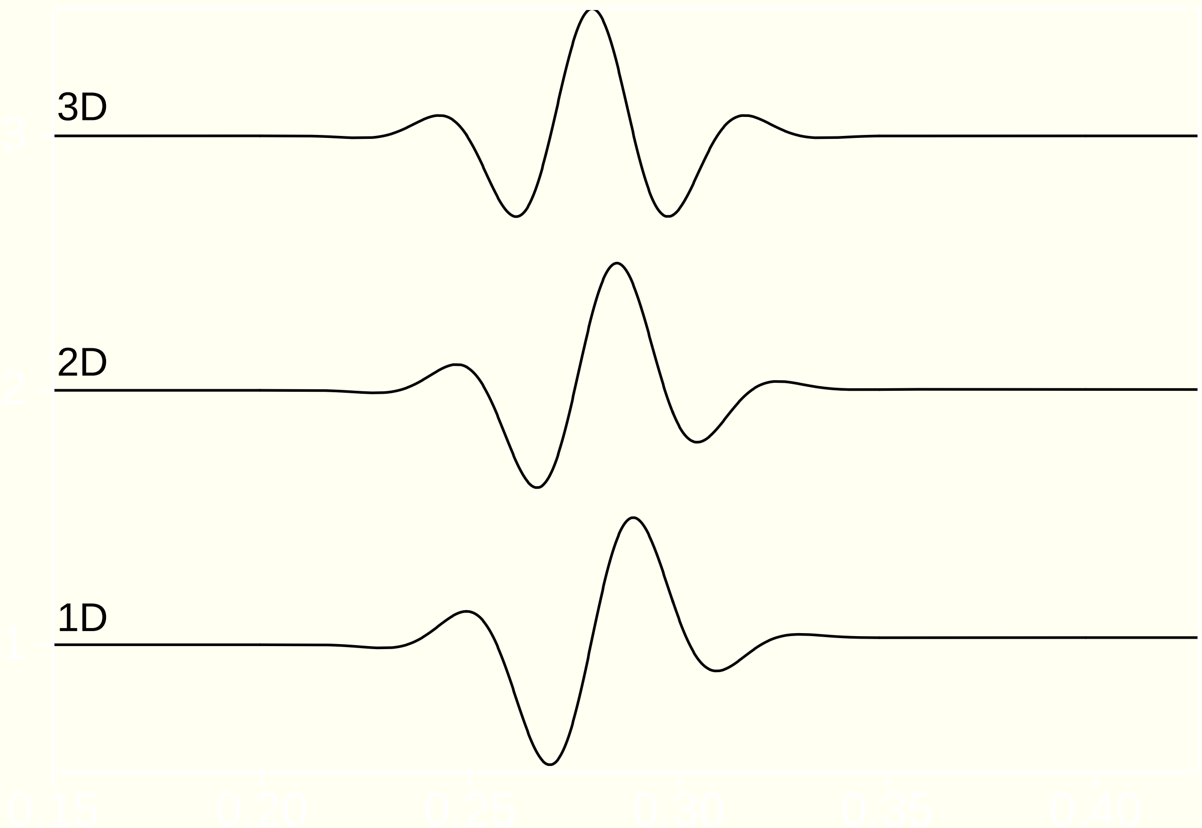
Excursus:



Implementation Details: Response functions

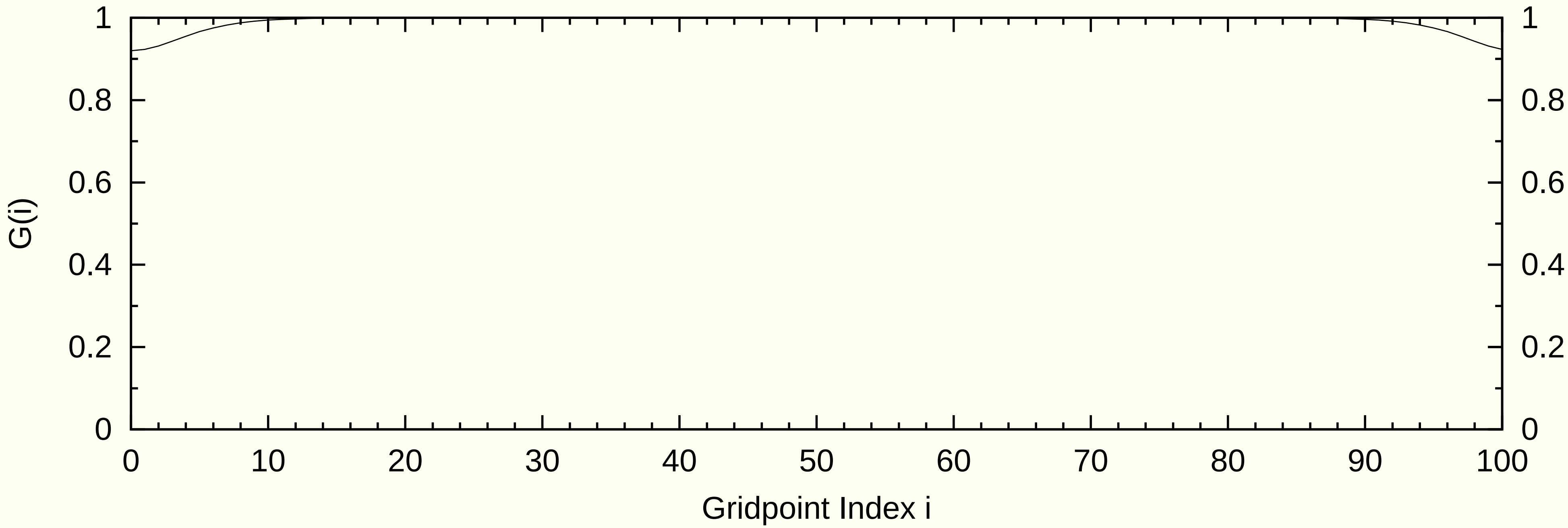
Excursus:

b) **Convolved Impuls Response**



Implementation Details: Absorbing boundaries

Periodicity of the Fourier method makes it difficult to implement absorbing boundaries. Usually tapering is used in a stripe surrounding the computational area.



Free Surface

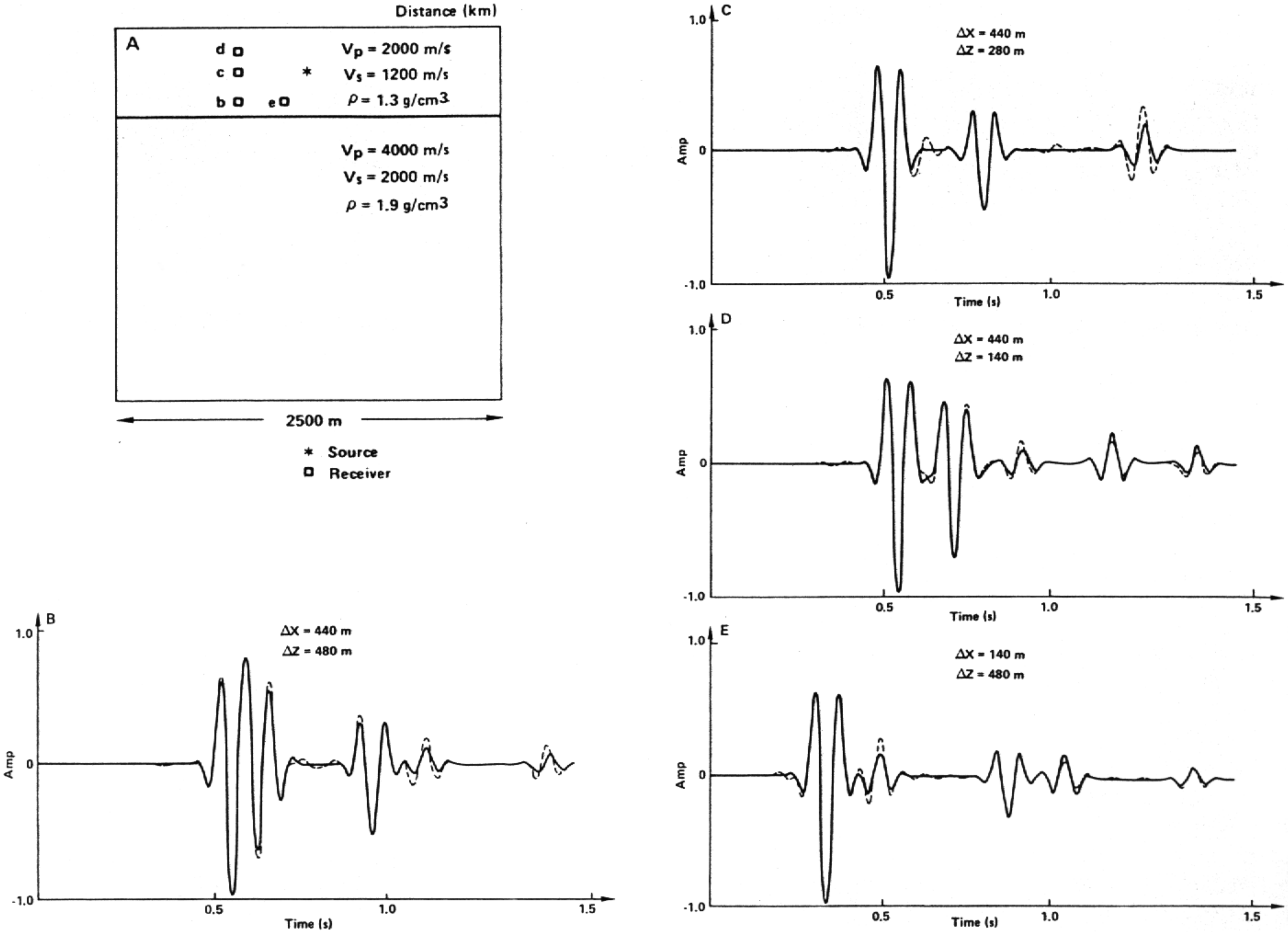
For realistic simulations the free surface of an elastic halfspace is important, since surface waves are generated and guided there.

A clean implementation of the boundary conditions is essential to obtain accurate numerical results.

Due to periodicity these boundary conditions cannot cleanly be introduced to the Fourier method. An approximation can be achieved by zero padding.

However, results are sufficiently accurate only if source and receivers are far away from the free surface.

Free Surface (cont'd)



Free Surface (cont'd): Chebyshev method

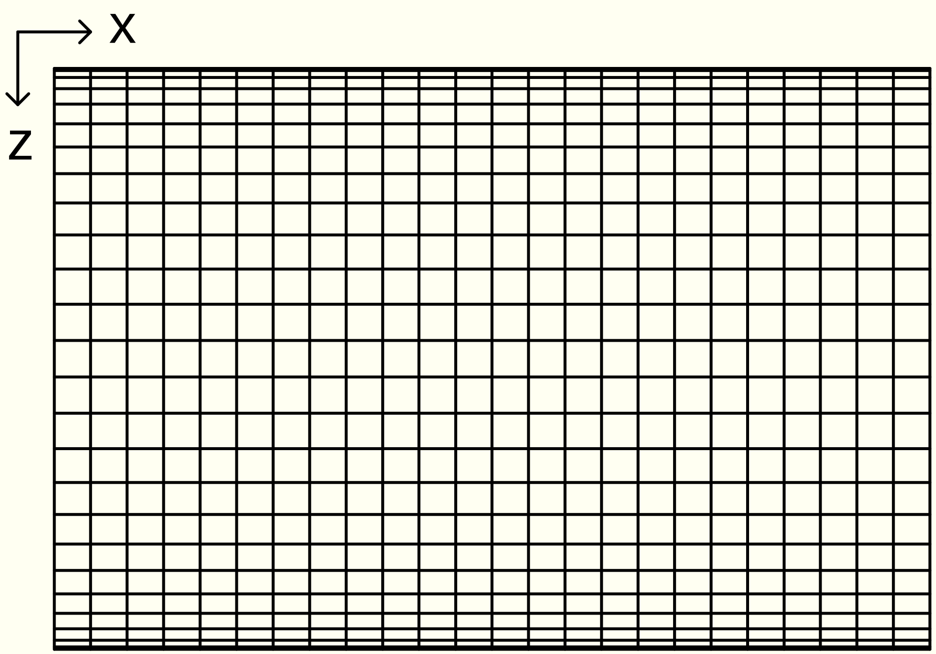
A very accurate implementation of free surface boundary conditions into spectral methods can be obtained when using the Chebyshev method.

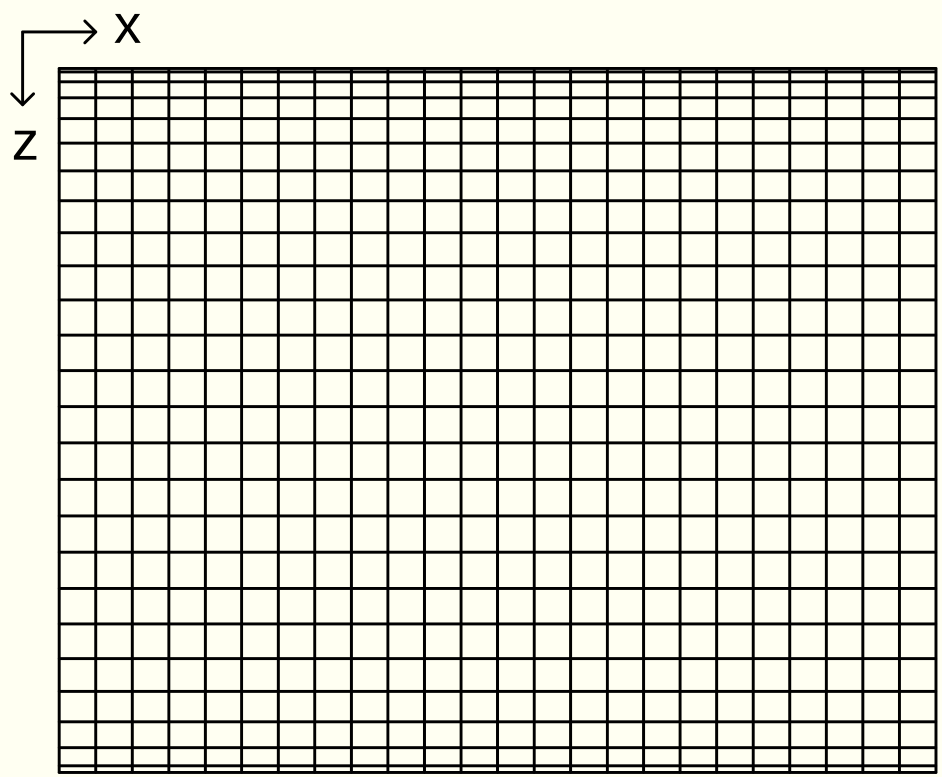
In the vertical direction Chebyshev derivative operators are used, whereas the Fourier derivative is used in the horizontal directions. The grid is equidistant in the horizontal directions but non-equidistant in the vertical direction.

For the implementation of boundary conditions the elasto-dynamic equations of motion are rewritten as the velocity-stress formulation.

Free Surface (cont'd): Chebyshev method

Unstretched and stretched Chebyshev grids:





Free Surface (cont'd): Chebyshev method

The 2D isotropic elastic equations of motion in Cartesian co-ordinates reads:

$$\varrho \ddot{u}_x = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} + f_x$$
$$\varrho \ddot{u}_z = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} + f_z$$

Stress-strain relation:

$$\sigma_{xx} = (\lambda + 2\mu)\,\varepsilon_{xx} + \lambda\,\varepsilon_{zz}$$
$$\sigma_{zz} = \lambda\,\varepsilon_{xx} + (\lambda + 2\mu)\,\varepsilon_{zz}$$
$$\sigma_{xz} = 2\mu\,\varepsilon_{xz}$$

Strains:

$$\varepsilon_{xx} = \frac{\partial u_x}{\partial x}$$
$$\varepsilon_{zz} = \frac{\partial u_z}{\partial z}$$
$$\varepsilon_{xz} = \frac{1}{2}\left(\frac{\partial u_x}{\partial z} + \frac{\partial u_z}{\partial x}\right)$$

Free Surface (cont'd): Chebyshev method

Velocity-stress formulation:

$$\varrho \dot{v}_x = \frac{\partial \sigma_{xx}}{\partial x} + \frac{\partial \sigma_{xz}}{\partial z} + f_x$$

$$\varrho \dot{v}_z = \frac{\partial \sigma_{xz}}{\partial x} + \frac{\partial \sigma_{zz}}{\partial z} + f_z$$

$$\dot{\sigma}_{xx} = (\lambda + 2\mu) \frac{\partial v_x}{\partial x} + \lambda \frac{\partial v_z}{\partial z}$$

$$\dot{\sigma}_{zz} = \lambda \frac{\partial v_x}{\partial x} + (\lambda + 2\mu) \frac{\partial v_z}{\partial z}$$

$$\dot{\sigma}_{xz} = \mu \left(\frac{\partial v_z}{\partial x} + \frac{\partial v_x}{\partial z} \right)$$

v_i is the particle velocity $\dot{u}_i$.

Free Surface (cont'd): Chebyshev method

The velocity-stress equations can be rewritten in vector form:

$$\frac{\partial \mathbf{W}}{\partial t} = \mathbf{A}\,\frac{\partial \mathbf{W}}{\partial x} + \mathbf{B}\,\frac{\partial \mathbf{W}}{\partial z}$$

$\mathbf{W}$ contains particle velocities and stresses:

$$\mathbf{W} = (v_x, v_z, \sigma_{xx}, \sigma_{zz}, \sigma_{xz})^T$$

$\mathbf{A}$ and $\mathbf{B}$ are 5×5 matrices.

Free Surface (cont'd): Chebyshev method

Using $\varrho v_s^2 = \mu$ and $\varrho v_p^2 = \lambda + 2\mu$:

$$\mathbf{A} = \begin{pmatrix} 0 & 0 & \varrho^{-1} & 0 & 0 \\ 0 & 0 & 0 & 0 & \varrho^{-1} \\ \varrho v_p^2 & 0 & 0 & 0 & 0 \\ \varrho(v_p^2 - 2v_s^2) & 0 & 0 & 0 & 0 \\ 0 & \varrho v_s^2 & 0 & 0 & 0 \end{pmatrix}$$

and

$$\mathbf{B} = \begin{pmatrix} 0 & 0 & 0 & 0 & \varrho^{-1} \\ 0 & 0 & 0 & \varrho^{-1} & 0 \\ 0 & \varrho(v_p^2 - 2v_s^2) & 0 & 0 & 0 \\ 0 & \varrho v_p^2 & 0 & 0 & 0 \\ \varrho v_s^2 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Free Surface (cont'd): Chebyshev method

Free surface boundary conditions:

$$\sigma_{xz} = 0 \qquad \text{and} \qquad \sigma_{zz} = 0$$

These boundary conditions need to be enforced, since they are not automatically satisfied.

This requires also to change the remaining variables to maintain a stable numerical scheme.

Q: How to change other variables?

A: Use of characteristic variables, which relate stresses and particle velocities.

Free Surface (cont'd): Chebyshev method

One-dimensional analysis in vertical direction only:

$$\frac{\partial \mathbf{W}}{\partial t} = \mathbf{B}\,\frac{\partial \mathbf{W}}{\partial z}$$

Diagonalizing the system to find the characteristic variables:

$$\frac{\partial \mathbf{S}}{\partial t} = \mathbf{\Lambda}\,\frac{\partial \mathbf{S}}{\partial z}$$

With the diagonal matrix $\mathbf{\Lambda}$:

$$\mathbf{\Lambda} = \mathbf{Q}^{-1}\mathbf{B}\mathbf{Q}$$

the vector of the characteristic variables reads:

$$\mathbf{S} = \mathbf{Q}^{-1}\mathbf{W}$$

Free Surface (cont'd): Chebyshev method

So we need to calculate $\mathbf{Q}^{-1}$ or $\mathbf{Q}$, respectively.
The eigenvectors of B form the columns of $\mathbf{Q}$.

First we find the eigenvalues of B, i.e. solve

$$|\mathbf{B} - \lambda\mathbf{I}| = 0$$

which leads to fifth order polynomial:

$$-\lambda^5 + \lambda^3 \left(v_p^2 + v_s^2\right) - \lambda v_p^2 v_s^2 = 0$$

We find: $\lambda_0 = 0$, $\lambda_1 = \pm\, v_p$ and $\lambda_2 = \pm\, v_s$

Free Surface (cont'd): Chebyshev method

Calculating the eigenvectors of B, i.e. solve

$$\mathbf{B}\mathbf{x} = \lambda \mathbf{x}$$

we obtain:

$$\mathbf{x} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \pm\varrho v_s \end{pmatrix} \qquad \mathbf{x} = \begin{pmatrix} 0 \\ 1 \\ \pm\varrho(v_p^2 - 2v_s^2)/v_p \\ \pm\varrho v_p \\ 0 \end{pmatrix} \qquad \mathbf{x} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Free Surface (cont'd): Chebyshev method

From the eigenvectors:

$$\mathbf{Q} = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & \frac{\varrho(v_p^2 - 2v_s^2)}{v_p} & \frac{-\varrho(v_p^2 - 2v_s^2)}{v_p} \\ 0 & 0 & 0 & \varrho v_p & -\varrho v_p \\ \varrho v_s & -\varrho v_s & 0 & 0 & 0 \end{pmatrix}$$

Free Surface (cont'd): Chebyshev method

Its inverse is:

$$\mathbf{Q}^{-1} = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & 0 & \frac{1}{\varrho v_s} \\ 1 & 0 & 0 & 0 & \frac{-1}{\varrho v_s} \\ 0 & 0 & 2 & 4\frac{v_s^2}{v_p^2} - 2 & 0 \\ 0 & 1 & 0 & \frac{1}{\varrho v_p} & 0 \\ 0 & 1 & 0 & \frac{-1}{\varrho v_p} & 0 \end{pmatrix}$$

Free Surface (cont'd): Chebyshev method

We finally have the characteristic variables:

$$\mathbf{S} = \mathbf{Q}^{-1}\mathbf{W} = \frac{1}{2}\begin{pmatrix} v_x + \dfrac{\sigma_{xz}}{\varrho v_s} \\ \\ v_x - \dfrac{\sigma_{xz}}{\varrho v_s} \\ \\ 2\sigma_{xx} - 2(1 - 2\dfrac{v_s^2}{v_p^2})\sigma_{zz} \\ \\ v_z + \dfrac{\sigma_{zz}}{\varrho v_p} \\ \\ v_z - \dfrac{\sigma_{zz}}{\varrho v_p} \end{pmatrix}$$

Free Surface (cont'd): Chebyshev method

Quantities superscripted by N are obtained after applying boundary conditions.For the numerical treatment of the boundary conditions only outgoing, i.e. propagation towards the boundary, characteristic variables are used.

At the free surface, because of $\sigma_{xz}^N = 0$ and $\sigma_{zz}^N = 0$, we obtain:

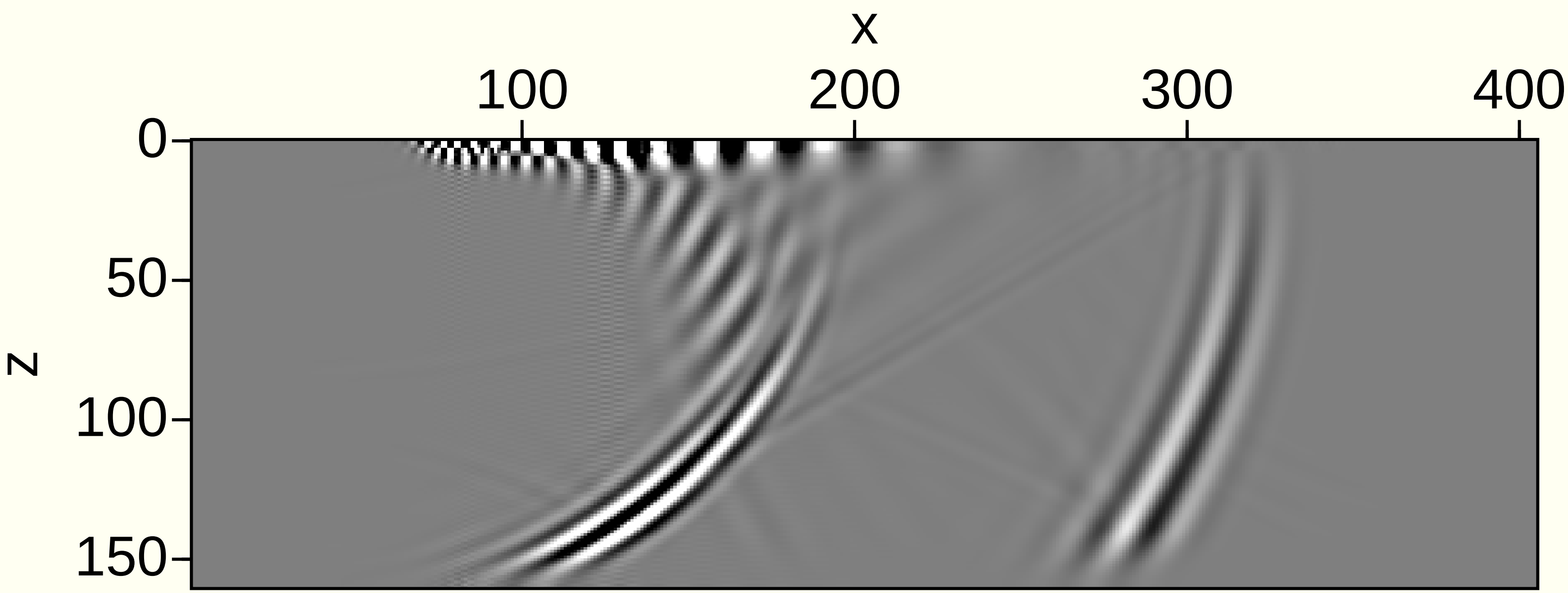
$$v_x^N = v_x + \frac{\sigma_{xz}}{\varrho v_s}$$

$$v_z^N = v_z + \frac{\sigma_{zz}}{\varrho v_p}$$

$$\sigma_{xx}^N = \sigma_{xx} - \frac{\lambda}{(\lambda + 2\mu)}\,\sigma_{zz}$$

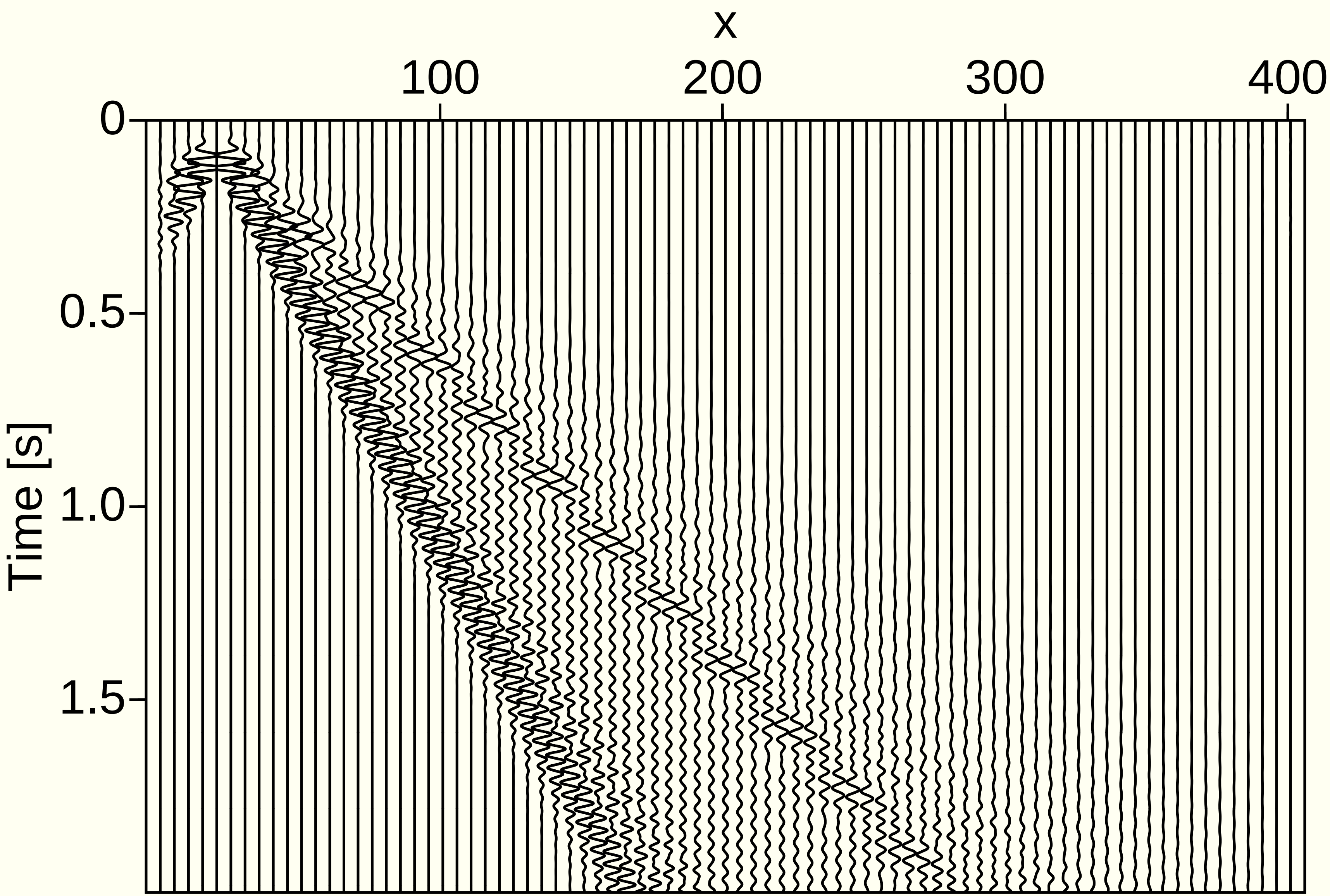
Free Surface (cont'd): Chebyshev method

Thin layer over halfspace:



v_x Snapshot t = 800 ms

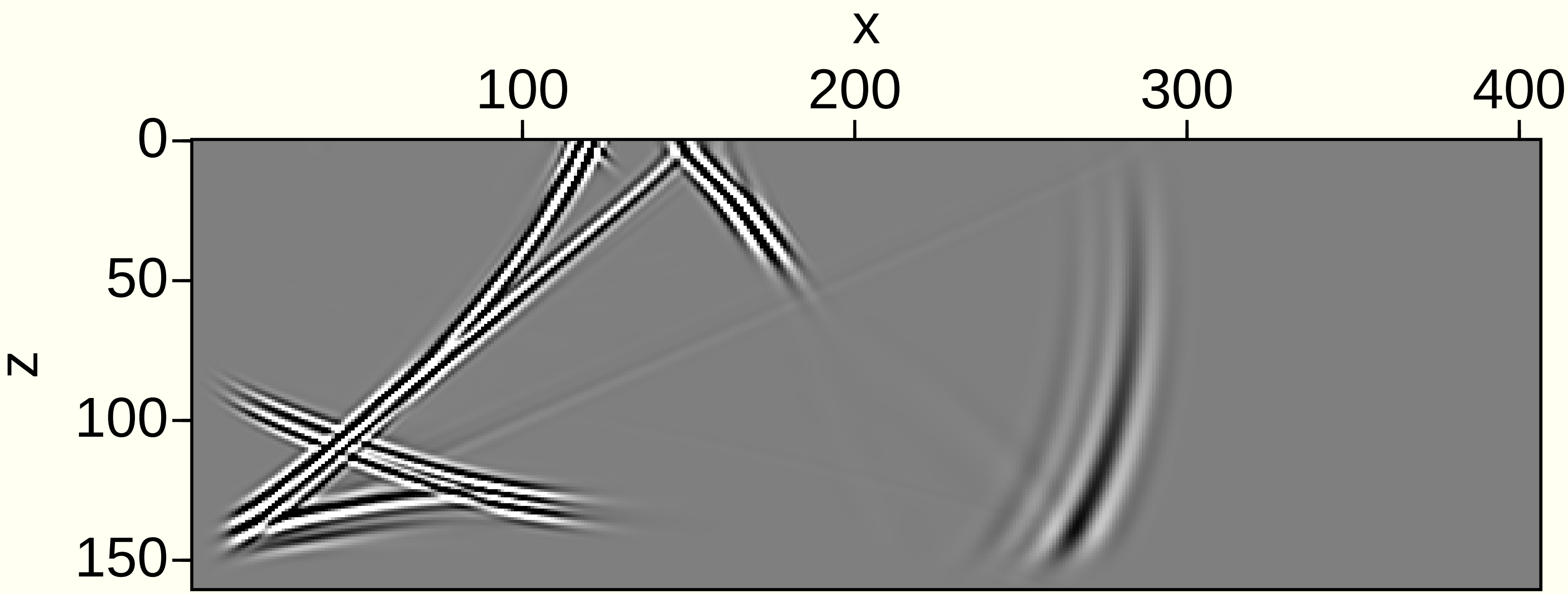
Free Surface (cont'd): Chebyshev method



Time Section

Free Surface (cont'd): Chebyshev method

Transversely isotropic halfspace:



v_x Snapshot t = 800 ms