Lecture 2: Finite Differences II

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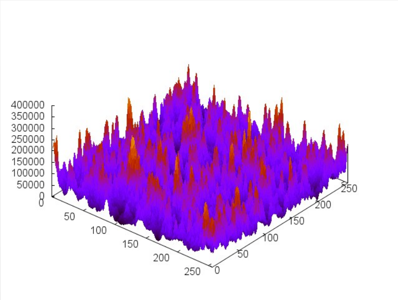
We cover three further basic topics



Dispersion Relation:
Very general and insightful tool to analyse the properties of the FD scheme

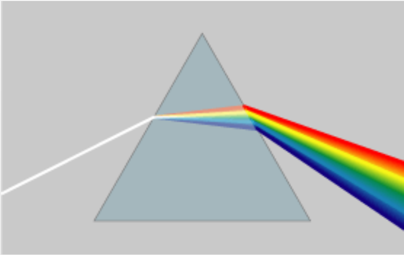
Boundary Conditions:
Essential to the quality of practical implementations

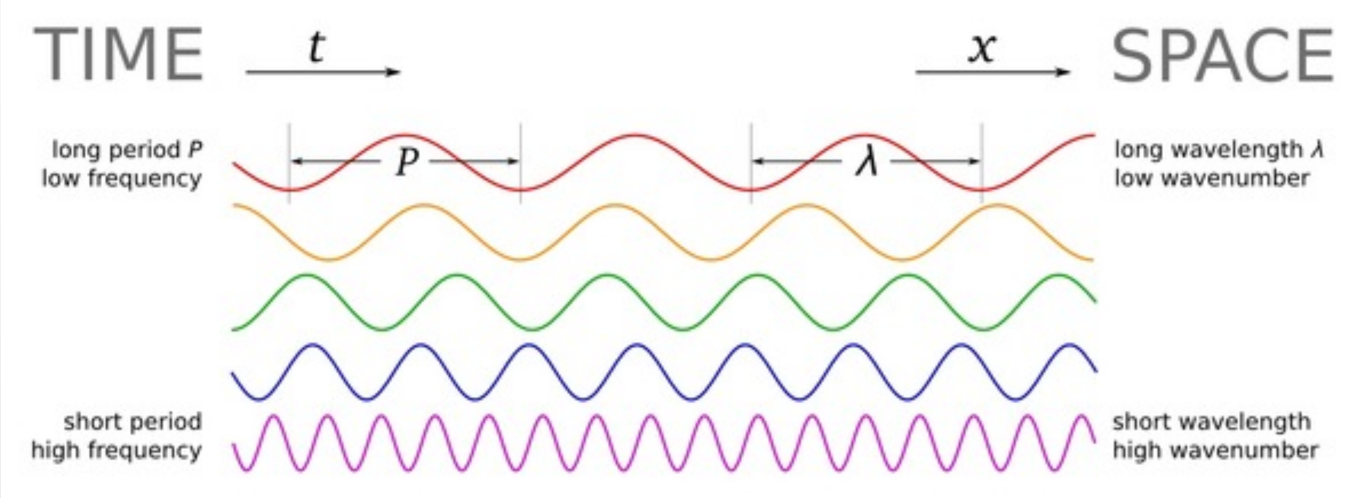
Validation
How to validate the correctness and accuracy of your FD scheme in practice

Dispersion Relation Formalism

Fourier decomposition

$$\varphi(x,t) = \sum_{n=1}^{N} A_n e^{i(k_n x - \omega_n t)}$$





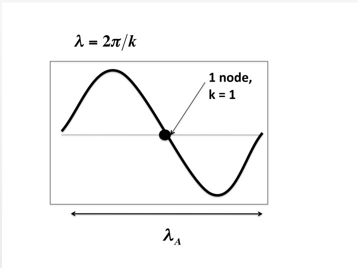
Low k

High k

Dispersion Relation

$$\boxed{\omega_n = \Omega(k_n)}$$

Discrete range and continuum limit



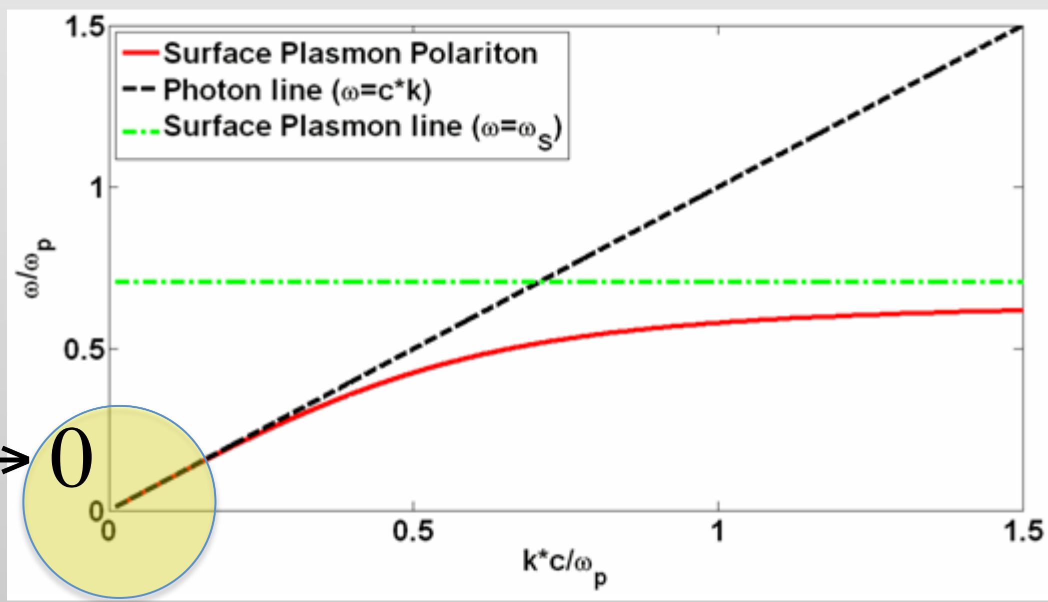
$$k_{\max} = 2\pi / d = N$$

$$k_{\min} = 2\pi / L = 1$$

$$k_n = 2\pi n / L = n$$

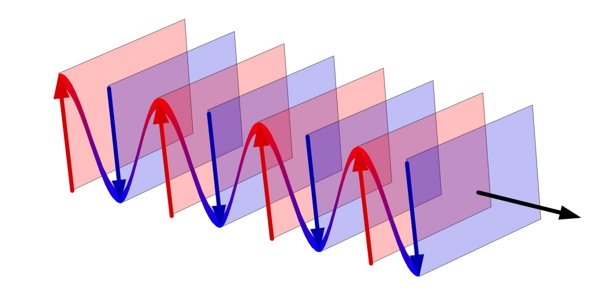
In the limit kd ->0 thewave does not “see” discreteness anymore

$$kd \rightarrow 0$$



Dispersion Relation

The ***Dispersion Relation***
tells how different wavelengths propagate in space.
It says ALL about linear homogeneous systems.
The solution is expressed as a superposition of plane-waves (exponential). Since the problem is linear we can focus on a single plane wave:



$$\varphi(x;t) = Ae^{i(kx-\omega t)} = Ae^{\gamma t}e^{ik(x-Vt)}$$

$$\omega(k) = \omega_r(k) + i\gamma(k)$$

The **real** part tells the **propagation speed** of the signal: $V_{phys} = \frac{d\omega_r}{dk}$

$$\omega_r = \omega_r(k)$$

The **imaginary** part tells the **growth/decay** rate

$$\gamma = \gamma(k)$$

$\gamma < 0$ **Stable**

$\gamma > 0$ **Unstable**

Discrete vs Continuum DR

Two main sources of discretization error:

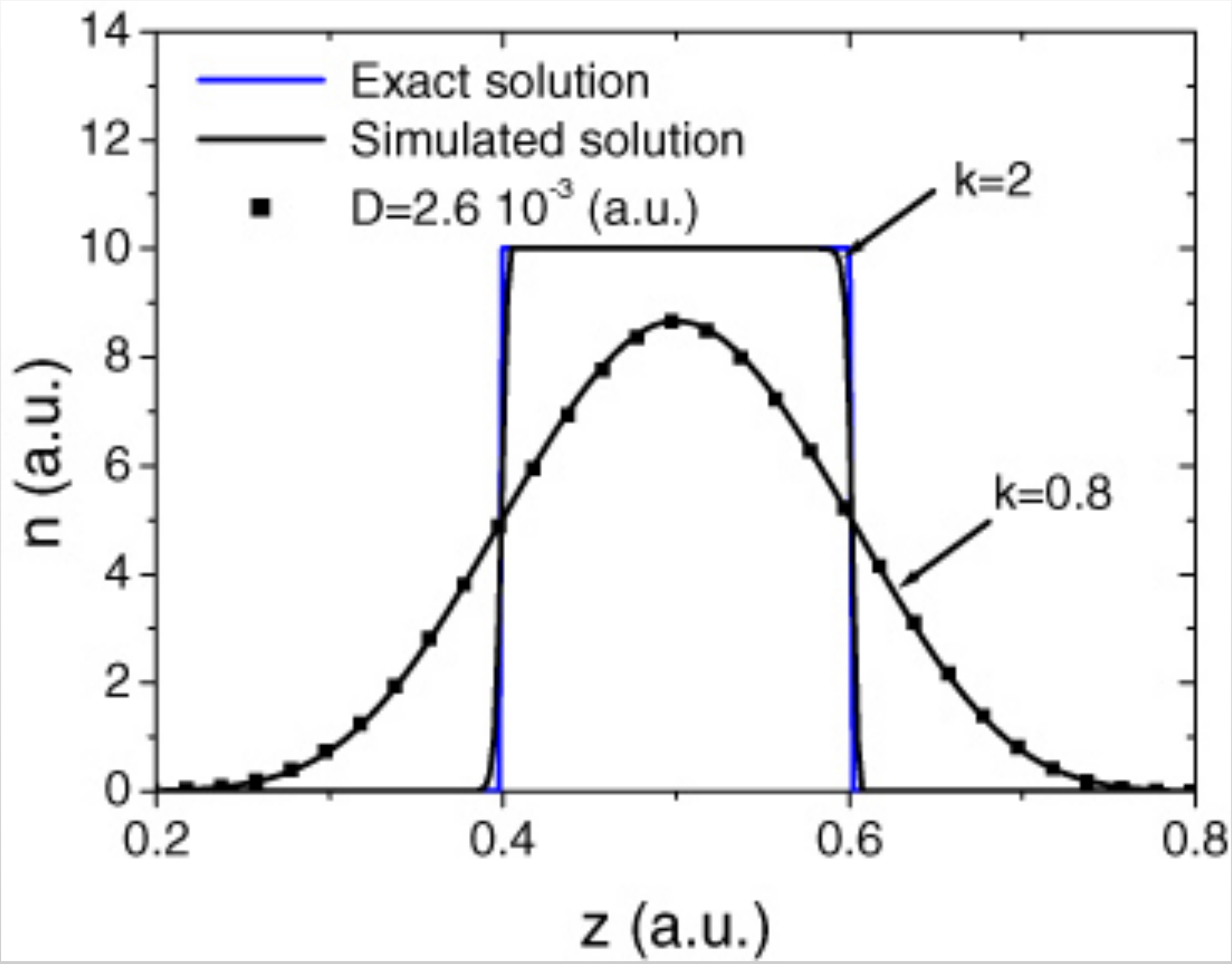
Real(omega), Phase Errors: Numerical **Dispersion**

Imag(omega), Amplitude Errors: **Numerical Diffusion**

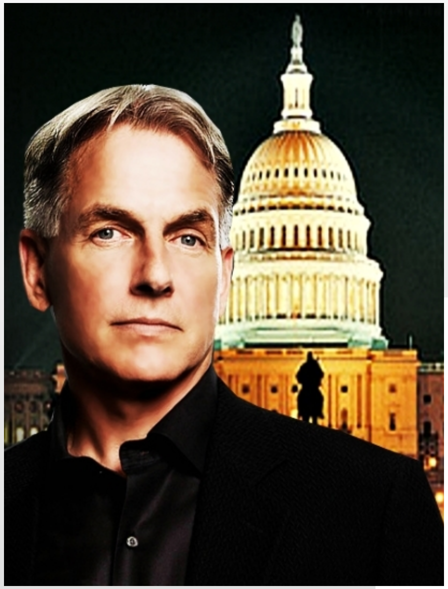
Dispersion means that the plane wave propagates at a different speed than continuum one, thus leading to distorsions in the profile and eventually unphysical oscillations (Gibbs oscillations). Carried by odd-order operators

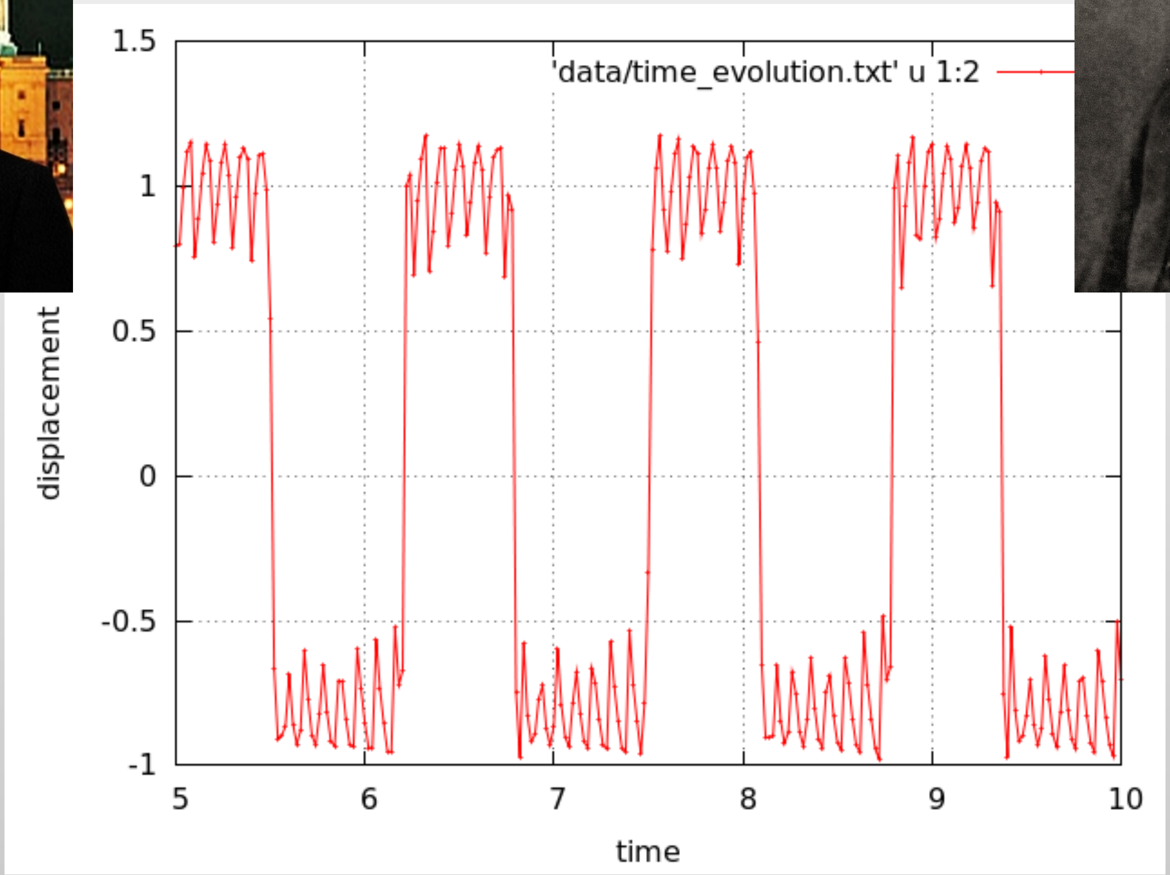
Carried by even-order operators (Diffusion/Dissipation)
Positive numerical diffusion leads to excessive damping.
Negative numerical diffusion leads to artificial growth:
Numerical instability

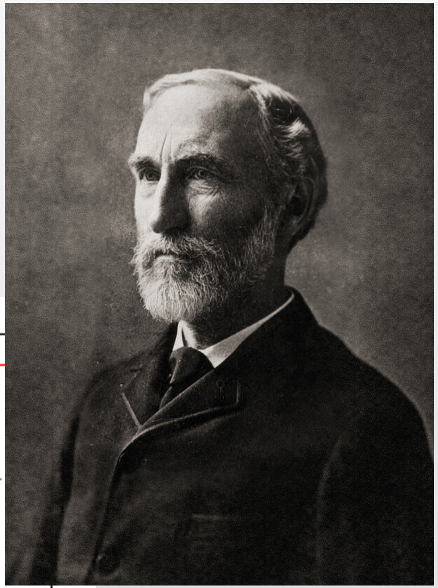
Numerical Diffusion: positive = overdamping



Numerical dispersion: Gibbs phenomena







Practical Example:
The sweetiest cookie: 1d Diffusion

Diffusion Equation d=1

$$\partial_t \varphi = D \partial_{xx} \varphi$$

$$\varphi(x;0) = \delta(x)$$

Analytical solution:

$$\varphi(x;t) = \frac{1}{\sqrt{2Dt}} e^{-x^2/2Dt}$$

Dispersion Relation: Frequency vs Wavenumber (see later)

$$\omega_r = 0$$
$$\gamma = -Dk^2$$

DE: continuum DR

For plane waves the following handy replacement rules hold:

$$\partial_t = -i\omega \qquad \partial_x = ik$$

One-line algebra delivers: $-i\omega = -Dk^2$

Namely:

$$\omega_r = 0 \qquad V_{phys} = 0$$

No propagation

$$\gamma(k) = -Dk^2$$

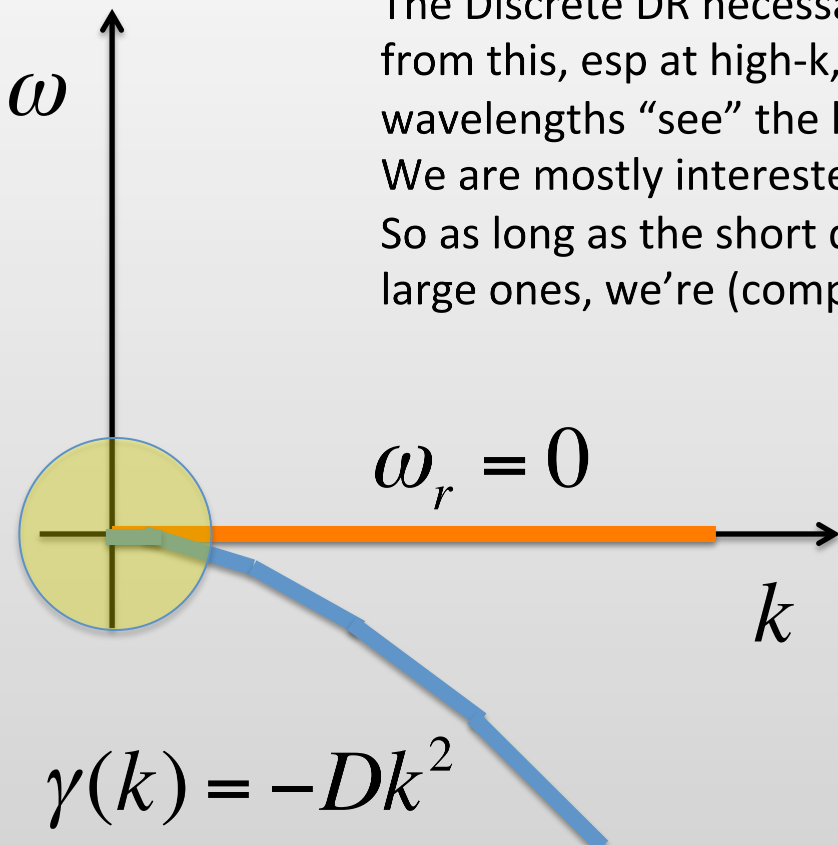
All wavelengths decay (absolute stability)
the shortest decay quadratically fast

Any consistent discretization must reproduce the above relations in
The **Continuum Limit: Note that small scales "see" discreteness…**

$$kd \to 0 \qquad \omega h \to 0$$

Discrete vs Continuum DR

The Discrete DR necessarily deviates from this, esp at high-k, since short wavelengths "see" the lattice.
We are mostly interested in long wavelengths.
So as long as the short do not mess up the large ones, we're (comparatively) fine



DE: Centered-Euler

$$\frac{\varphi_j^{n+1} - \varphi_j^n}{h} = D\left[\frac{\varphi_{j+1}^n - 2\varphi_j^n + \varphi_{j-1}^n}{d^2}\right]$$

$$\boxed{\delta \equiv Dh / d^2 \equiv D / D_{lat}}$$

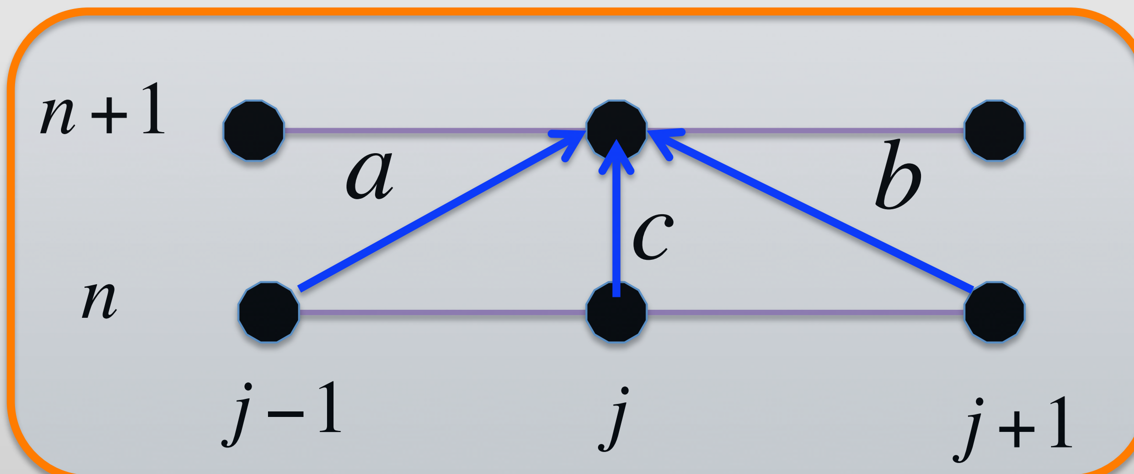
This is known as diffusive Courant-Friedrich-Levy (CFL) number. Key to stability.

$$a = b = \delta$$

$$c = 1 - 2\delta$$

Transfer matrix:

$$T_{jk} = \{\delta, 1-2\delta, \delta\}$$



Note that a+b+c=1 by mass conservation.

General DDR

$$e^{-i\omega h} = ae^{-ikd} + (1-a-b) + be^{+ikd}$$

$$\begin{cases} e^{\gamma h}\cos(\omega_r h) = 1 + (a+b)[\cos(k\,d) - 1] \\ e^{\gamma h}\sin(\omega_r h) = (b-a)\sin(k\,d) = 0 \end{cases}$$

DE: $a = b = \delta$

$\omega_r = 0$ Exact at any k

By squaring both sides and summing up:

$e^{2\gamma h} = (1 + 2\delta C)^2$ with $C \equiv \cos(kd) - 1$

Diffusion DDR: Stability

Diffusion: $a = b = \delta$

$$\boxed{e^{\gamma h} = |1 + 2\delta C|}$$

$$C \equiv \cos(k\,d) - 1$$

The discrete stability condition reads: $-2 < C < 0$

$$-1 < 1 + 2\delta C < 1$$

$$2\delta C < 0 \Rightarrow \delta > 0$$

(Since C<0)

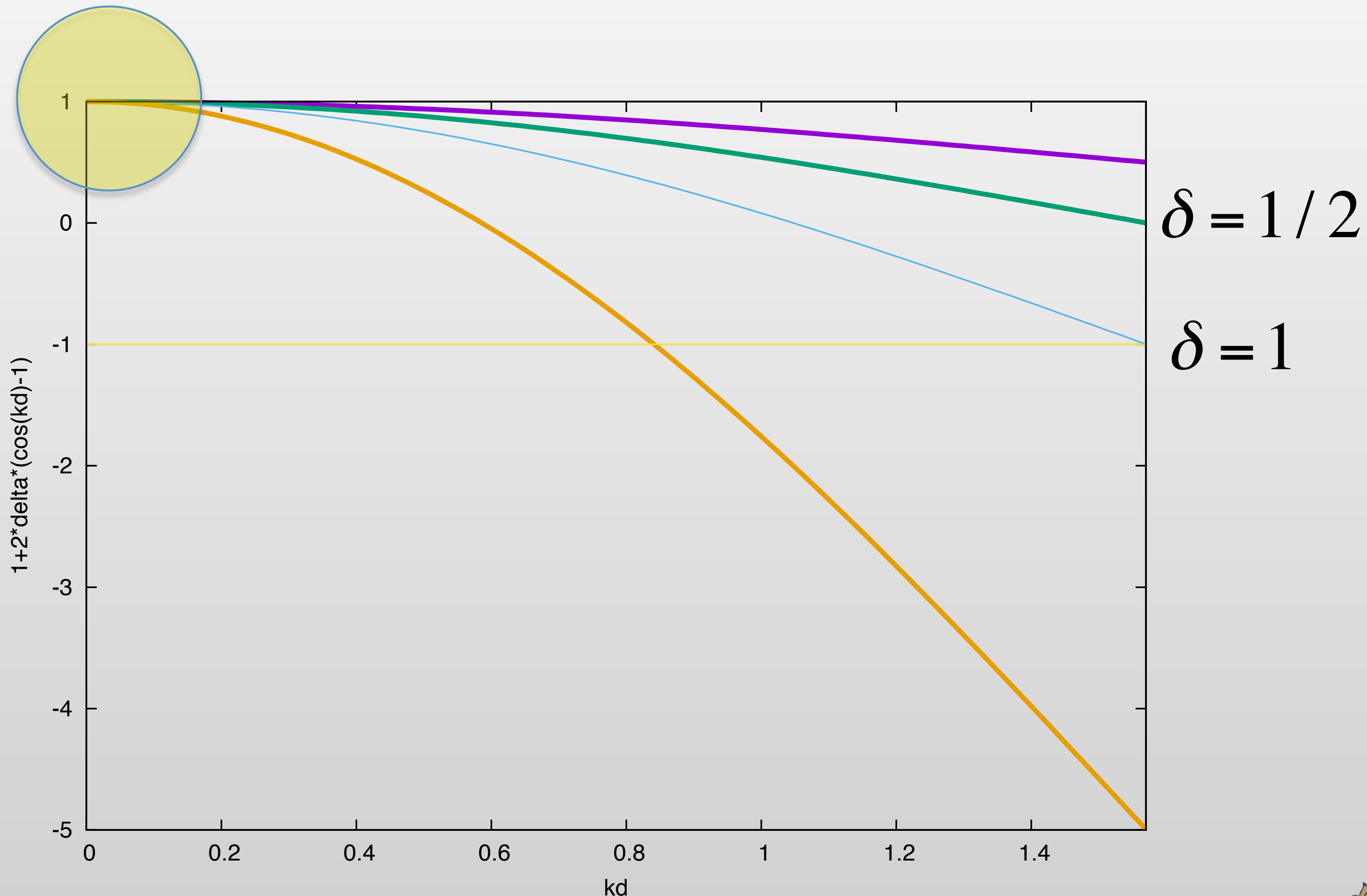
$$\delta \equiv Dh / d^2$$

$$2\delta |C| < 2 \Rightarrow \delta < 1/2$$

(Since |C|<2)

This is the Diffusive CFL condition

Graphical analysis



DDR: continuum limit

$$\omega_r = 0$$ **Exact at any k**

Continuum limit:

$$C \to -k^2 d^2 / 2$$

$$1 + \gamma h \approx 1 - 2\delta k^2 d^2 / 2$$

$$\gamma \to -\delta k^2 d^2 / h = -k^2 (\frac{Dh}{d^2}) \frac{d^2}{h} = -Dk^2 + O(k^2)$$

The Continuum Limit is recovered: accurate to 2° order.
The stability analysis shows that discretization errors canNOT trigger instability at any wavenumber as long as CFL is secured!

Lax Theorem

For a well-posed linear PDE:

If the numerical scheme is stable is also convergent and viceversa

Why is it important?
Because convergence is hard to prove, usually much harder than stability

Stability/Realizability

Probabilistic/Social interpretation

$$\varphi_j^{n+1} = a\varphi_{j-1}^n + c\varphi_j^n + b\varphi_{j+1}^n$$

(a+b+c=1)

a Probability of moving up in time from left

b Probability of moving up in time from right

c Probability of moving up in time from center

Much swifter: **Realizability** (all coeffs must be non-negative):

$$c > 0 \Rightarrow \qquad \delta < 1/2$$

$$c = 1 - 2\delta$$

$$a = b > 0 \Rightarrow \quad \delta > 0$$

Boundary Conditions

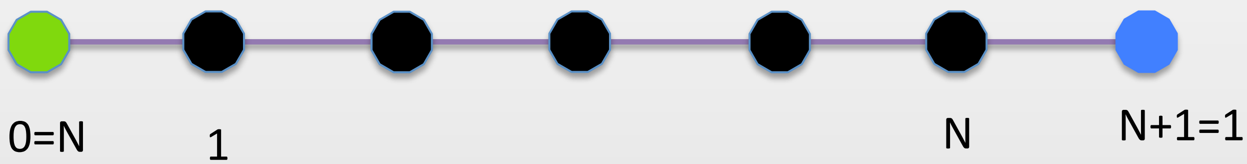
Boundary Conditions

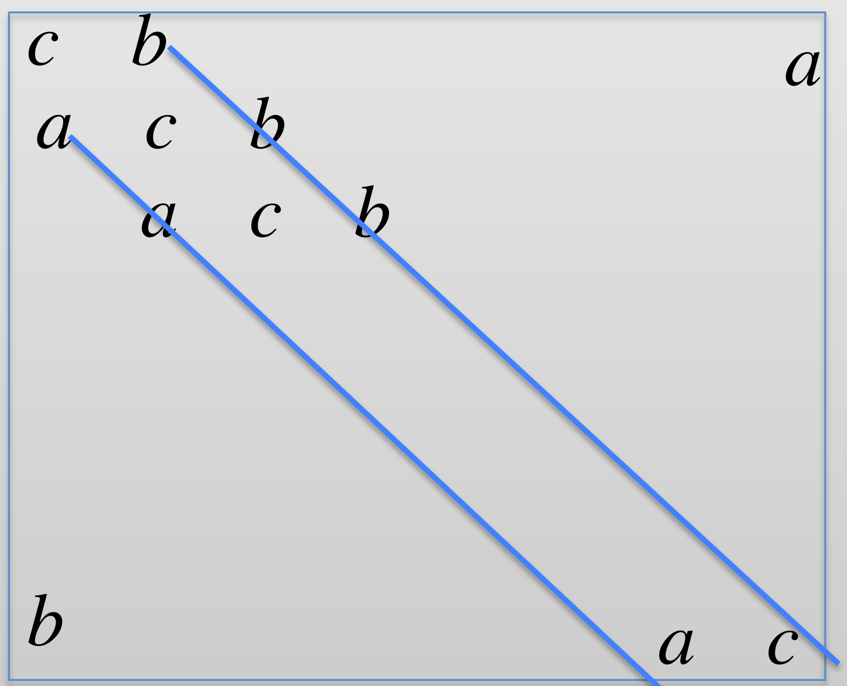
Strongly affect the solutions: BC select the bulk solutions compatible with the **environmental constraints**.

Correct implementation of BC is **the** Key factor for the quality of the numerical scheme

Boundary Conditions: periodic

Periodic: $\varphi_{N+1}^{n} = \varphi_{1}^{n}$ $\qquad \varphi_{0}^{n} = \Phi_{N}$





Boundary Conditions: Dirichlet

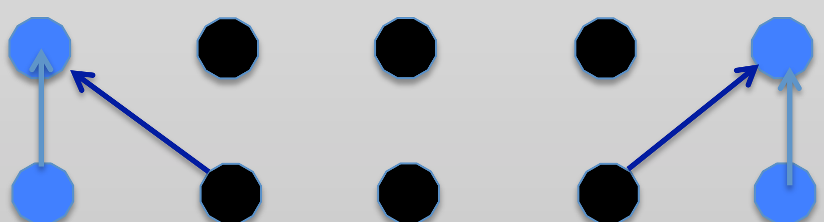
Dirichlet: $\boxed{\varphi\,|_B = \Phi_B}$

FD: $\varphi_1^n = \Phi_1 \qquad \varphi_N^n = \Phi_N$

Bulk: j=1,N $\quad \varphi_j^{n+1} = a\varphi_{j-1}^n + c\varphi_j^n + b\varphi_{j+1}^n$

Boundaries**:** **j=1, j=N** are given on-site by the BC specification:
Thus we update only the bulk **j=2,N-1**

$$\varphi_2^{n+1} = a\Phi_1 + c\varphi_2^n + b\varphi_3^n$$
$$\varphi_{N-1}^{n+1} = a\varphi_{N-2}^n + c\varphi_{N-1}^n + b\Phi_N$$



1 N

Boundary Conditions: von Neumann

Von Neumann BC: $\boxed{\partial_x \varphi \,|_B = 0}$

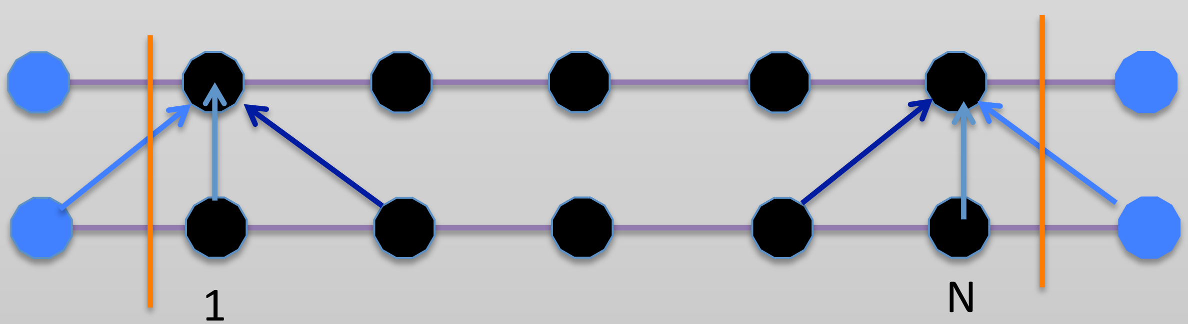
FD: $\varphi_1^n = \varphi_2^n \qquad \varphi_N^n = \varphi_{N-1}^n$

Bulk: j=2,N-1 $\qquad \varphi_j^{n+1} = a\varphi_{j-1}^n + c\varphi_j^n + b\varphi_{j+1}^n$

Boundaries: j=1, j=N are taken from extrapolation:
Thus we have **j=1,N** updates

$$\varphi_1^{n+1} = a\varphi_1^n + c\varphi_1^n + b\varphi_2^n = (a+c)\varphi_1^n + b\varphi_2^n$$
$$\varphi_N^{n+1} = a\varphi_{N-1}^n + c\varphi_N^n + b\varphi_N^n = a\varphi_{N-1}^n + (c+b)\varphi_N^n$$

Note that the Effective boundary is at j=1/2 and j=N+1/2



Full stability analysis (incl. BC's)

Find the numerical eigenvalues of the Transfer matrix

$$\varphi_j^{n+1} = T_{jk}\varphi_k^n$$

$$e^{i\omega_j h} = \lambda_j; \quad j = 1, N$$

For tridiagonal systems the eigenvalues are known analytically. For instance Diffusion Matrix {1,-2,1} gives

$$\lambda_j = 2[\cos(\frac{j\pi}{N+1}) - 1]; \quad j = 1, N$$

In general, however, they must be found via numerical Eigenvalue solvers.

Validation

Strong/Weak Convergence

Define the Local Error

Analytical solution

$$e_j^n = |\varphi_j^n - \varphi(x_j, t^n)|$$

Strong convergence (everywhere)

$$e^n = Max_j \{e_j^n\} < \varepsilon$$

Every grid point must get close the exact solution
If just one does not, convergence is broken!

Weak convergence (global)

$$e^n = \sqrt{\frac{1}{N}\sum_{j=1}^{N}(e_j^n)^2} < \varepsilon$$

Some points can deviate more than others provide the global sum is “small enough” .
More tolerant…

Richardson's extrapolation

How about **no analytical solution is available**?

$$\varphi_{2N} - \varphi_N = (\varphi_{2N} - \varphi_E) - (\varphi_N - \varphi_E)$$

If the space of functions is metric, the departure (measurable!) obeys:

$$d_{N,2N} \equiv \| \varphi_{2N} - \varphi_N \| <= \| \varphi_{2N} - \varphi_E | + \| \varphi_N - \varphi_E \| = e_{2N} + e_N$$

If the method converges at order p:

$$d_{N.2N} = const.*[(1/(2N)^p + 1/N^p] = const*[1/2^p + 1]/N^p$$

Hence, by log-plotting d_{N,2N} versus N for many N, say N/4,N/2,N,N/2,N/4
we should a negative slope –p. **Job done!**

Richardson's Extrapolation

The extrapolation is performed on the lattice sites shared by all different grids

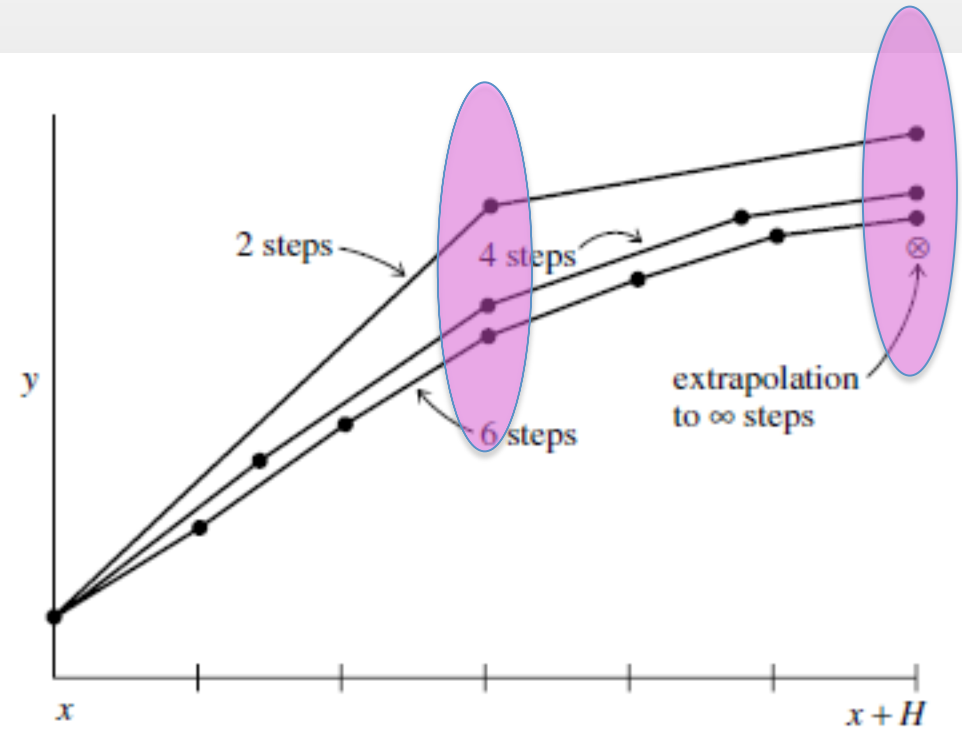


Figure 17.3.1. Richardson extrapolation as used in the Bulirsch-Stoer method. A large interval H is spanned by different sequences of finer and finer substeps. Their results are extrapolated to an answer that is supposed to correspond to infinitely fine substeps. In the Bulirsch-Stoer method, the integrations are done by the modified midpoint method, and the extrapolation technique is polynomial extrapolation.

Assignements

1. Derive the discrete DR for the 1d AD equation and analyze its CASE properties

2. Solve the 1d Diffusion equation with Dirichlet BC's

3. Same as 2. in two dimensions

End of the lecture