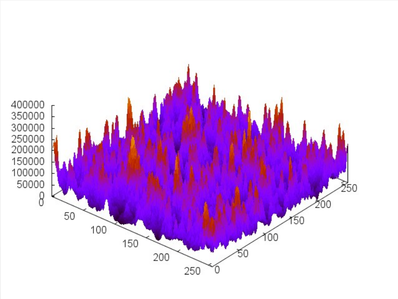
Lecture 1: Finite Differences

Sauro Succi

We shall cover three broad classes of PDE's:



Transport: Advection-Diffusion-Reaction equations
Porous media, environment, you_name_it

Linear Conservation Laws:
Continuity equations, Fokker-Planck, …

Nonlinear Conservation Laws:
Fluids, Burgers equation, shocks and solitons
Cosmological fluids, Growth phenomena …

Lecture 1: Plan

1. ***General notions on grid discretization***
2. ***Main properties of finite-difference schemes***
3. ***Dispersion Relation Formalism***
4. ***Examples (Diffusion equation in d=1 and d=2)***

The Four Levels


MACRO

Continuum Fields

$$\partial_t u + (u \cdot \nabla) u = -\frac{\nabla P}{\rho} + \nu \Delta u$$

MESO

Probability distributions

$$\partial_t f + (v \cdot \nabla) f = -\frac{1}{\tau}(f - f^{(eq)})$$

MICRO

Particles (atoms/molecules

$$\frac{d^2 r_i}{dt^2} = -\sum_{j>i} \nabla V_{ij}$$

QUANTUM

Complex Fields

$$i\hbar\partial_t \Psi = H\psi$$

Wash out Irrelevant details (tube/baby problem)

Finite Differences for Transport PDE's

Evolutionary PDE:
(Liouville)

$$\partial_t \varphi = L\varphi$$

Scalar field in (1+1) dim: $\varphi \equiv \varphi(x;t)$

Homogeneous Linear Transport (Advection-Diffusion-Reaction):

$$\boxed{L = -U\partial_x + D\partial_{xx} + R}$$

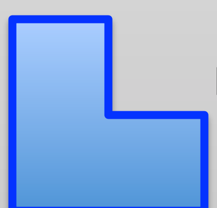
Formal solution: $\varphi_t = e^{Lt}\varphi_0$

Time Propagator

$$\boxed{T_t \equiv e^{Lt}}$$

Initial+Boundary Conditions:

$$\varphi_t(B) = 0$$



B is a boundary region around the bulk volume **V**

What do we do with the propagator?

$$T_t \equiv e^{Lt}$$

How do we compute it, in practice?

Functional Calculus

Series approximants of the Propagator:

$$e^{Lt} = 1 + Lt + \frac{1}{2}L^2t^2 + hot$$

Taylor, Explicit, Causal

$$e^{Lt} = \frac{1 + Lt/2}{1 - Lt/2} + hot$$

Pade', Implicit, Non-causal

$$e^{Lt} = (1 + Lt/n)^n$$

Recursive, Explicit, Causal

For linear-homogeneous this resums exactly: analytical solutions, reflecting basic symmetries:

Translations, Rotations, Scaling, Inflation

Analytic solutions

Linear homogeneous: similarity solutions

$$\varphi(x,0) \rightarrow \varphi(x,t) = \varphi(x - Ut)$$ **Advection**

$$\varphi(x,0) \rightarrow \varphi(x,t) = \varphi(x^2 / Dt)$$ **Diffusion**

$$\varphi(x,0) \rightarrow \varphi(x,t) = e^{Rt}\varphi(x,0)$$ **Growth/Decay**

BUT: Inhomogenous, non-linear; broken syms?

$$U = U(x,\varphi) \qquad D(x,\varphi) \qquad R = R(x,\varphi)$$

This is where numerics takes over analytics!

Functional Calculus

Series approximants of the Propagator:

$$e^{Lt} = 1 + Lt + \frac{1}{2}L^2t^2 + hot$$ Taylor, Explicit, Causal

$$e^{Lt} = \frac{1 + Lt/2}{1 - Lt/2} + hot$$ Pade', Implicit, Non-causal

$$e^{Lt} = (1 + Lt/n)^n$$ Recursive, Explicit, Causal

Inhomogenous, non-linear: broken sym

Still applies, but only to "small" timesteps so that L~const

$$\boxed{|L|\Delta t << 1}$$

And similarly in space: ---> **DISCRETE SPACE TIME**

Functional Calculus

Series approximants of the Propagator:

$$e^{Lt} = 1 + Lt + \frac{1}{2}L^2t^2 + hot$$ Taylor, Explicit, Causal

$$e^{Lt} = \frac{1 + Lt/2}{1 - Lt/2} + hot$$ Pade', Implicit, Non-causal

$$e^{Lt} = (1 + Lt/n)^n$$ Recursive, Explicit, Causal

Inhomogenous, non-linear: broken sym

Still applies, but only to "small" timesteps so that L~const

$$\boxed{|L|\Delta t << 1}$$

And similarly in space: ---> **DISCRETE SPACE TIME**

Spacetime crystal

$$\varphi(x;t) \longrightarrow \varphi_j^n = \varphi(x_j;t_n) + e_j^n$$

Local Error

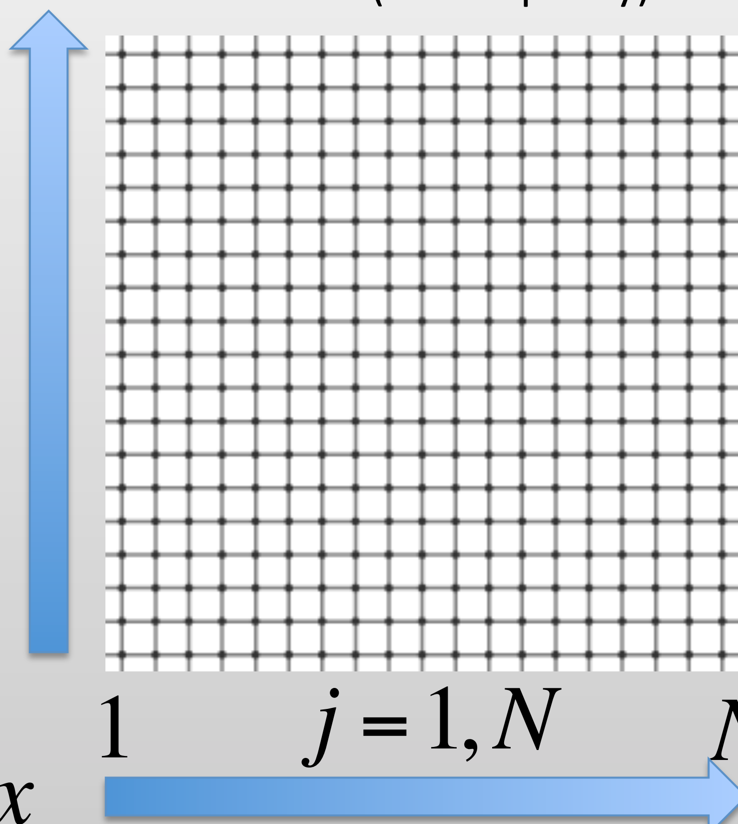
Uniform (for simplicity)

M

$$t \longrightarrow t^n = n\Delta t$$

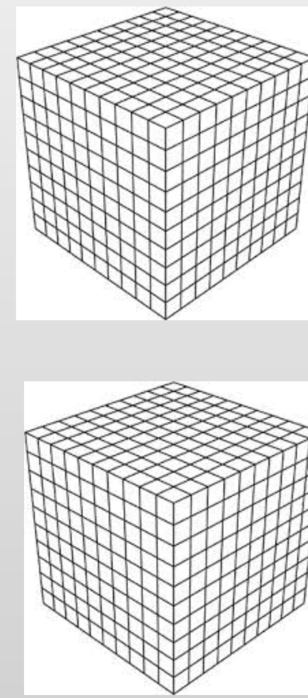
$$n = 1, M$$

1



1 $\quad j = 1, N \quad$ N

$$x \longrightarrow x_j = j\Delta x$$



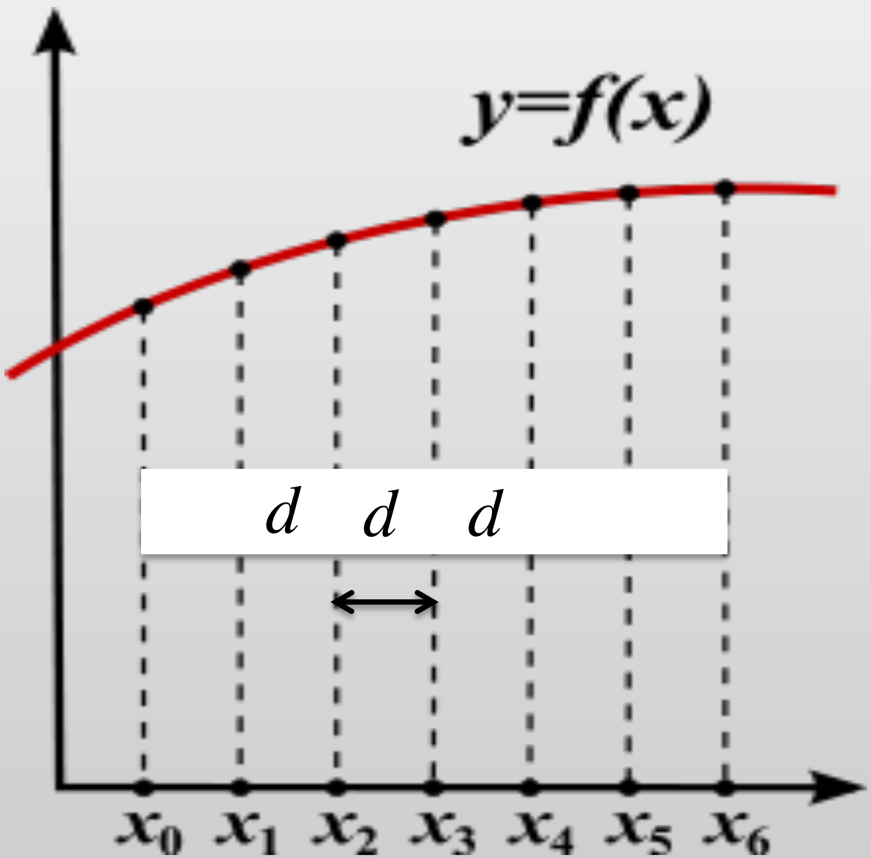
$n+1$

n

Finite-Difference Schemes

From kindergarten:

$$\partial_x f(x) \to \Delta_x^+ f = \frac{f(x+d) - f(x)}{d} \qquad (d \equiv \Delta x)$$



The Discrete Derivative
is by no means unique!
Higher accuracy is obtained
by using larger sets of discrete
points = **STENCIL**

$$\Delta_x^0 f = \frac{f(x+d) - f(x-d)}{2d}$$

Computational molecules (stencils)

Differential operators become SPARSE MATRICES

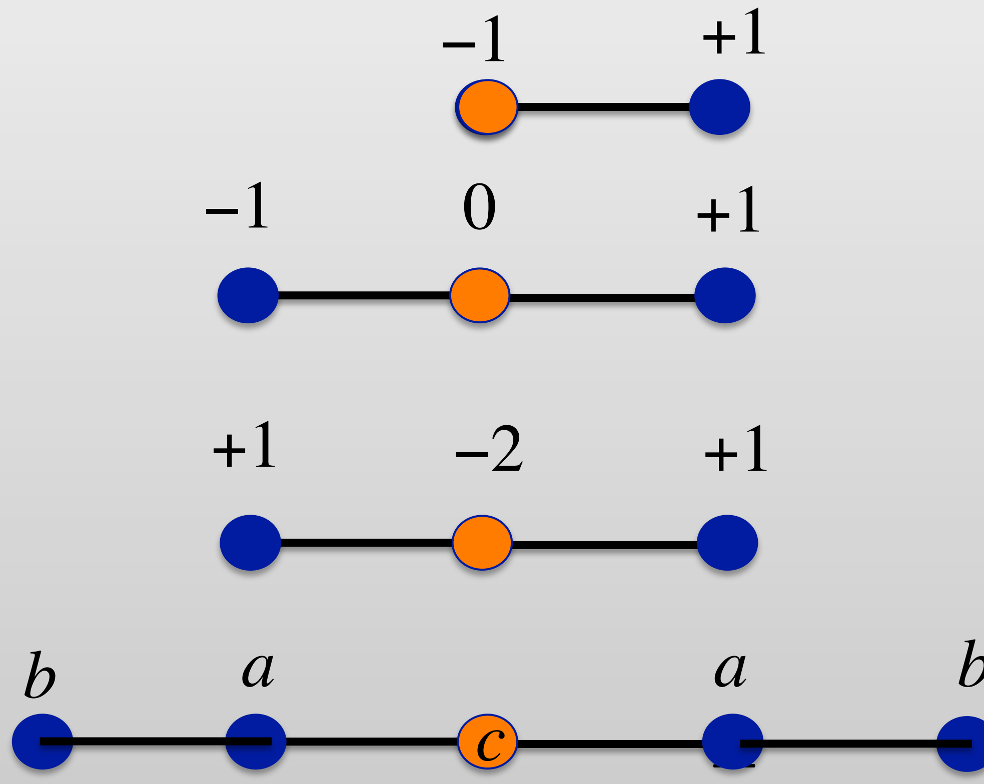
$$f(\varphi)|_j \to \delta_{jk} f(\varphi_k) \qquad \frac{d\varphi}{dx}|_j \to \frac{1}{d} A_{jk}\varphi_k \qquad \frac{d^2\varphi}{dx^2}|_j \to \frac{1}{d^2} D_{jk}\varphi_k$$

$$\frac{d}{dx} \Leftrightarrow \frac{1}{d}\{0,-1,1\}$$

$$\frac{d}{dx} \Leftrightarrow \frac{1}{2d}\{-1,0,1\}$$

$$\frac{d^2}{dx^2} \Leftrightarrow \frac{1}{d^2}\{1,-2,1\}$$

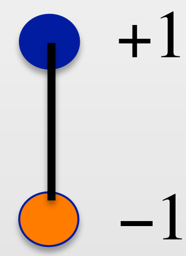
$$\frac{d^2}{dx^2} \Leftrightarrow \frac{1}{d^2}\{b,a,c,b,a\}$$



Computational molecules

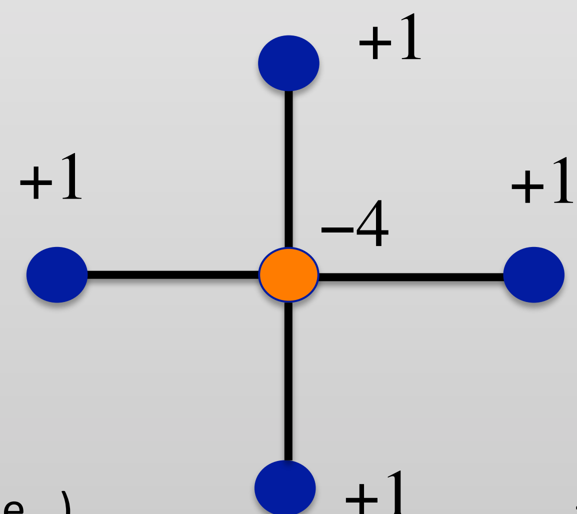
$$\frac{\partial}{\partial x} \Leftrightarrow \frac{1}{d_x}\{-1,1\}$$

$$\frac{\partial}{\partial y} \Leftrightarrow \frac{1}{d_y}\{-1,1\}$$



$$\frac{\partial^2}{\partial x^2} \Leftrightarrow \frac{1}{d_x^2}\{1,-2,1\}$$

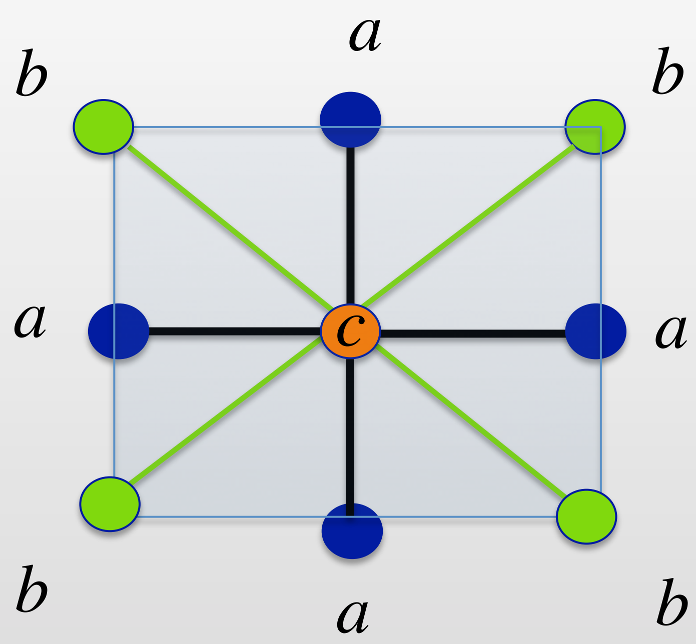
$$\frac{\partial^2}{\partial y^2} \Leftrightarrow \frac{1}{d_y^2}\{1,-2,1\}$$

$\Delta =$ 

(Charges around a neutral molecule…)

2D stencils: isotropy

$$\Delta = \frac{1}{2}[(\partial_x + \partial_y)^2 + (\partial_x - \partial_y)^2]$$

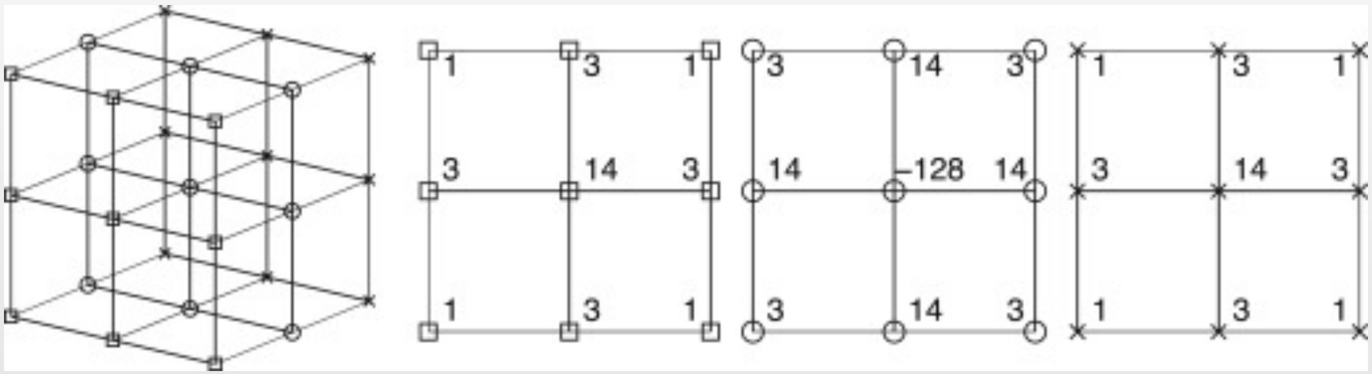


Diagonal links must eliminate mixed derivatives: $\partial_x \partial_y$

$a = 4/36 \qquad b = 1/36 \qquad c = -20/36$

$(4a + 4b + c = 0)$

3D stencils



Very elegant and powerful formalism: weighted sums

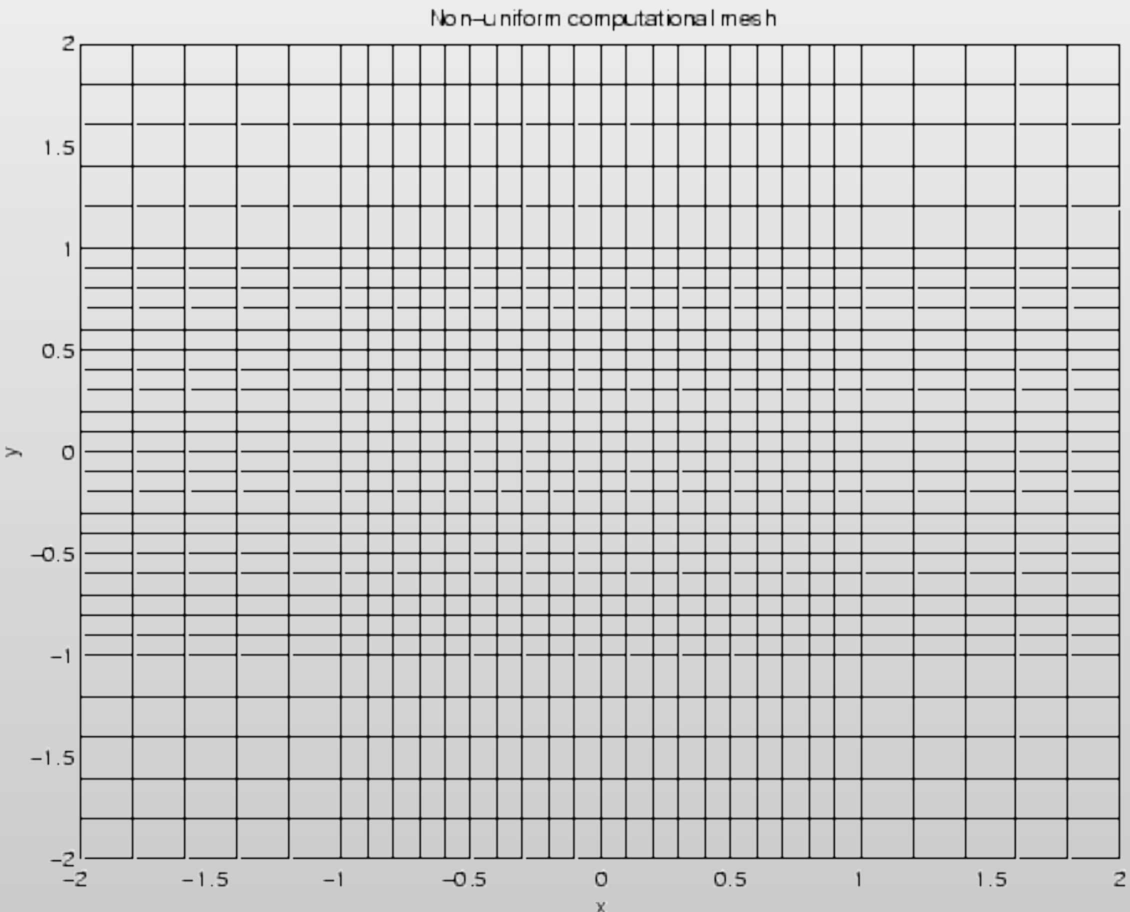
$$\vec{\nabla}\varphi = \sum_{i=0}^{b} w_i \vec{d}_i \varphi(\vec{x} + \vec{d}_i)$$

$$\vec{\nabla}\cdot\vec{V} = \sum_{i=0}^{b} w_i \vec{d}_i \cdot \vec{V}(\vec{x} + \vec{d}_i)$$

Weights? Taylor expand and match coefficients term by term
All coeffs should be 0 except one, which must be = 1.

Non uniform lattices

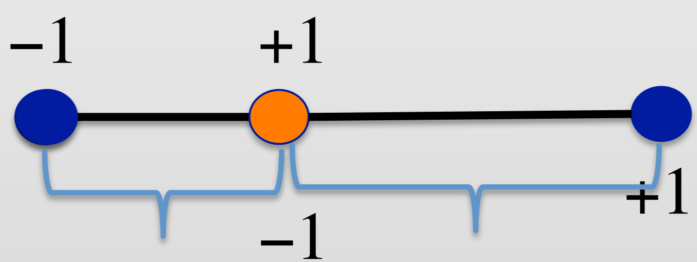
The coefficients **a,b,c,** pick-up a dependence on the position {**a_j,c_j,b_j**}, but the
The matrix structure stays the same because **LOCALITY** is what matters.
Accuracy is affected though, unless the weights are suitably adjusted
Let us see how:



Non uniform lattices

$$\frac{\partial}{\partial x} \Leftrightarrow \Delta_j^+ = \frac{1}{d_{j+}}\{0,-1,1\} \qquad d_{j+} = x_{j+1} - x_j$$

$$\frac{\partial}{\partial x} \Leftrightarrow \Delta_j^- = \frac{1}{d_{j-}}\{-1,1,0\} \qquad d_{j-} = x_j - x_{j-1}$$

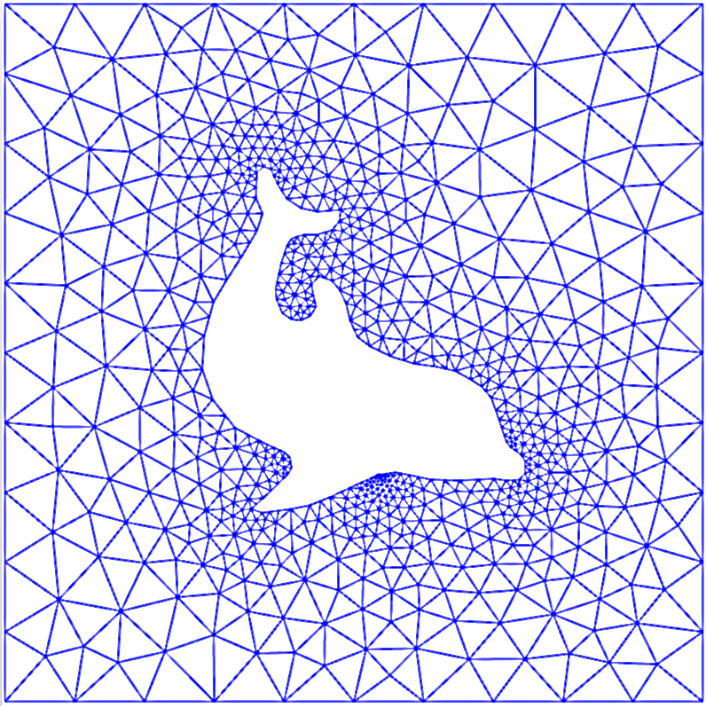


$$\frac{\partial}{\partial x} \Leftrightarrow \frac{1}{2}(\Delta_j^- + \Delta_j^+) = \frac{1}{2}\{-\frac{1}{d_-}, \frac{1}{d_-} - \frac{1}{d_+}, +\frac{1}{d_+}\} \rightarrow \frac{1}{2d}\{-1,0,1\}$$ Uniform limit

a+b+c =0 still, but the diagonal is non-zero.
What does this mean? The left and right Finite Differences must weighted to absorb the nonuniformity.

Finite Volumes take over…

Unstructured lattices



FD unviable: Finite Volumes / Elements

Discrete Time: Forward Euler

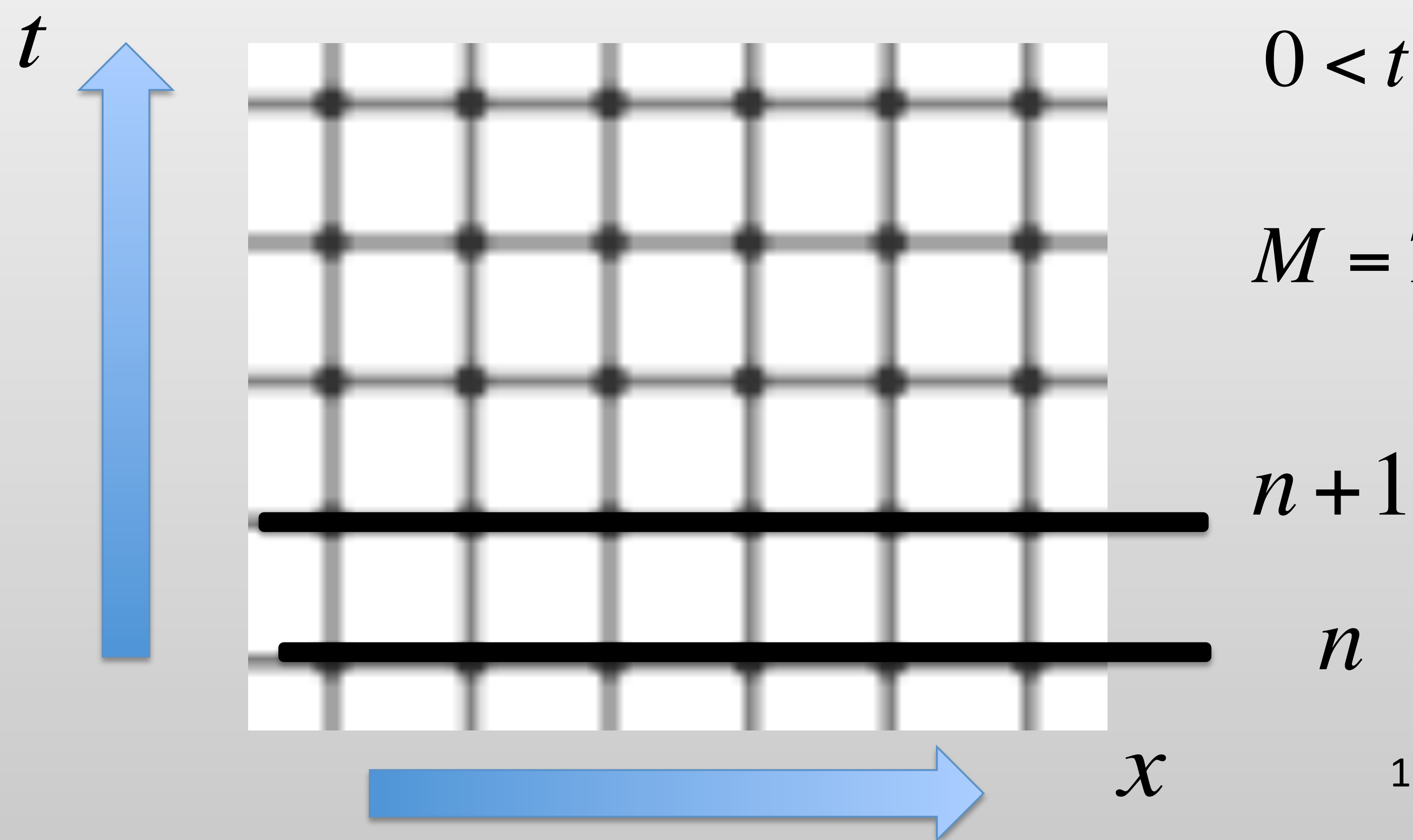
$$\partial_t \varphi = \frac{\varphi_j^{n+1} - \varphi_j^{n}}{h} + Error$$

$(h \equiv \Delta t)$

Timespan:

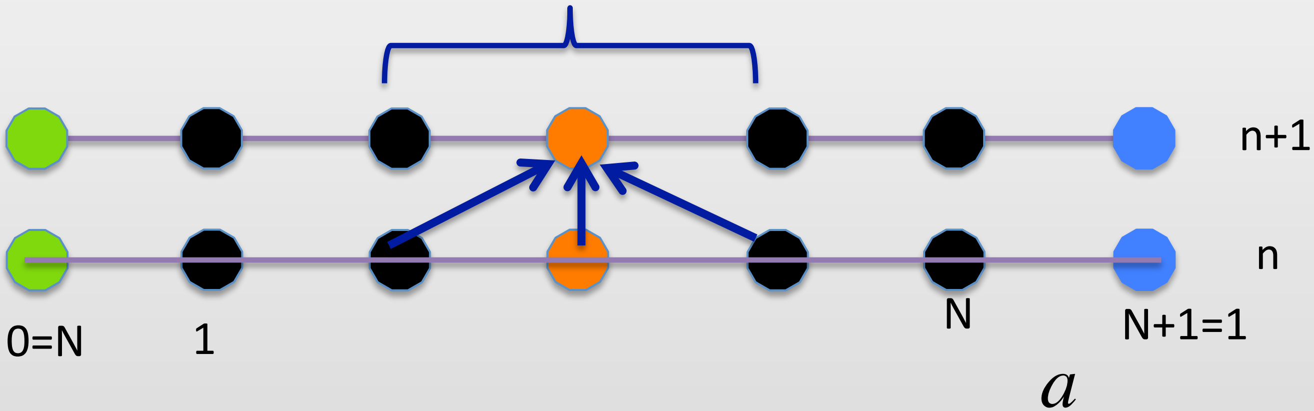
$$0 < t < T$$

$$M = T / h$$



ADR Transfer Matrix

$$\frac{\varphi_j^{n+1}-\varphi_j^{n}}{h} = \{\frac{U}{d}A_{jk} + \frac{D}{d^2}D_{jk} + R\delta_{jk}\}\varphi_k^{n}$$



$$\varphi_j^{n+1} = \{\frac{Uh}{d}A_{jk} + \frac{Dh}{d^2}D_{jk} + (1+Rh)\delta_{jk}\}\varphi_k^{n} \equiv T_{jk}\varphi_k^{n}$$

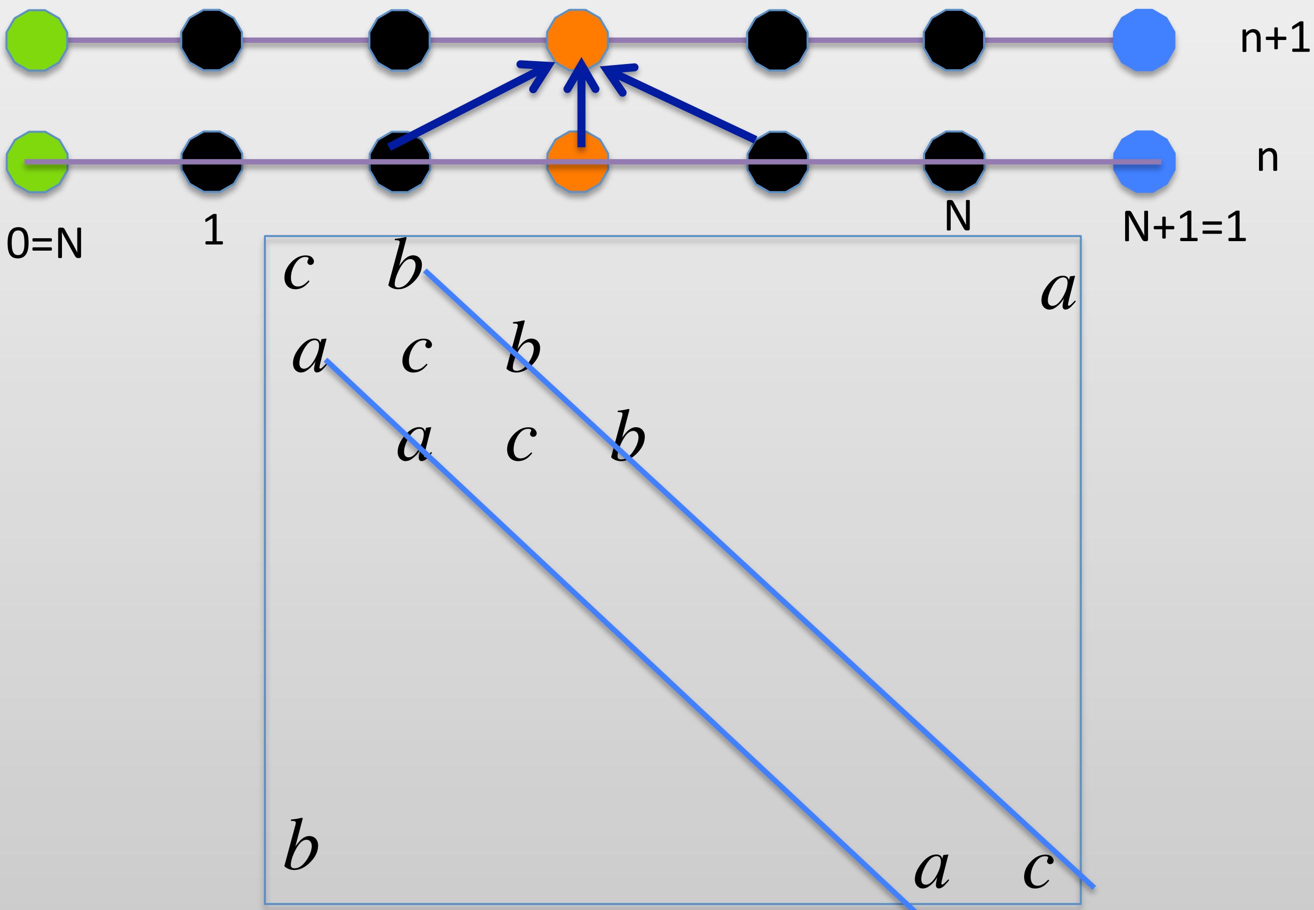
Transfer Matrix T_jk

Tridiagonal form (1+1 dimensions)

$$T = \alpha A + \delta D + (1+\kappa)I$$

Transfer Matrix in (1+1)d: Tridiagonal

$$\varphi_j^{n+1} = a_j \varphi_{j-1}^n + c_j \varphi_j^n + b_j \varphi_{j+1}^n$$



Diffusion Equation

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

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

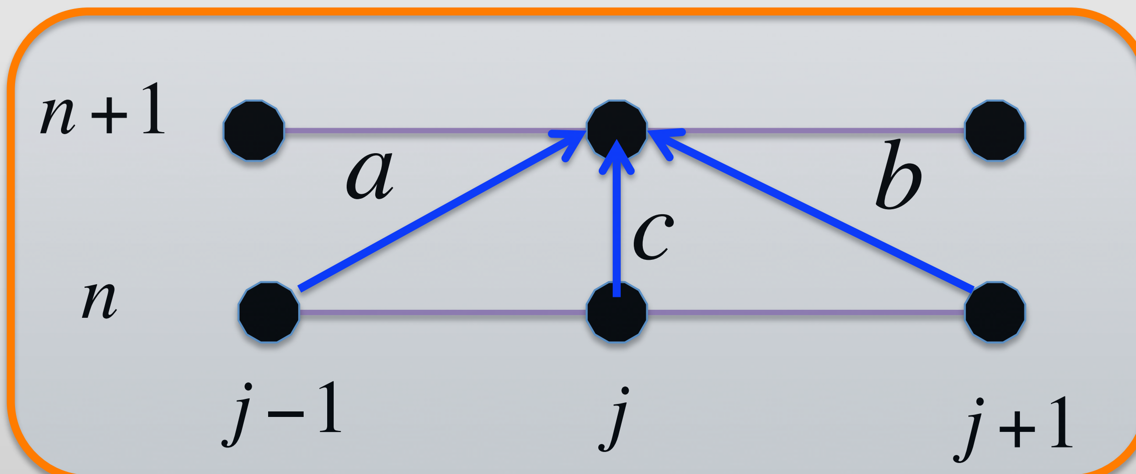
This is known as diffusive **Courant-Friedrich-Levy (CFL)** number. Key to stability.

$$a = b = \delta$$

$$c = 1 - 2\delta$$

Transfer matrix:

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



Note that a+b+c=1   by mass conservation.
We shall discuss it at length later …

General properties of FD schemes

A good FD scheme should be ***Mimetic***: erase the lattice!

Consistency/Convergence

The scheme should reproduce the continuum PDE
in the Continuum Limit of zero mesh spacing (space and time)

Accuracy

The numerical error should decay as fast as
possible with grid resolution

Stability

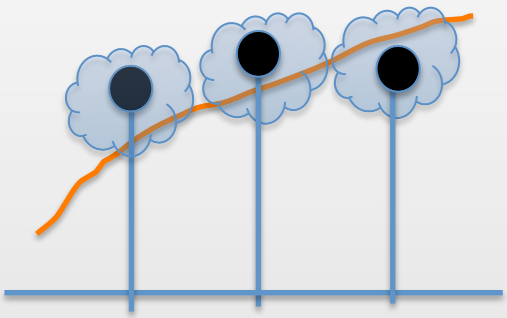
The numerical solutions should not display growing
modes (instabilities), unless the continuum PDE does

Efficiency

The numerical solution should converge with
the least number of operations (incl data access).

Consistency/Convergence

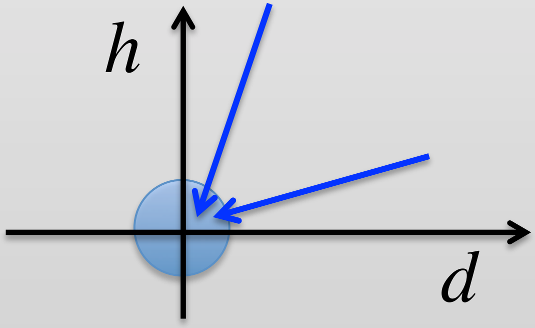
Continuum Limit: $d \equiv \Delta x \to 0; h \equiv \Delta t \to 0$



$$N \to \infty; d \to 0; Nd = L \to L$$

$$\varphi_j^n \to \varphi(x_j; t_n)$$

The discrete operators must reduce to their continuum form: **smoothly.**



$$L_d(d \to 0) \to L$$

$$T_h(d \to 0; h \to 0) \to e^{Lh}$$

Accuracy: smooth errors

Local Error (Strong convergence: everywhere)

$d \to 0$

$h \to 0$

$$e_j^n = |\varphi(x_j; t_n) - \varphi_j^n|$$

The local error should vanish smoothly at increasing resolution:

$$\varepsilon = A * d^p + B * h^q + h.o.t$$

A method of order **p** is EXACT once applied to p-th order polynomials

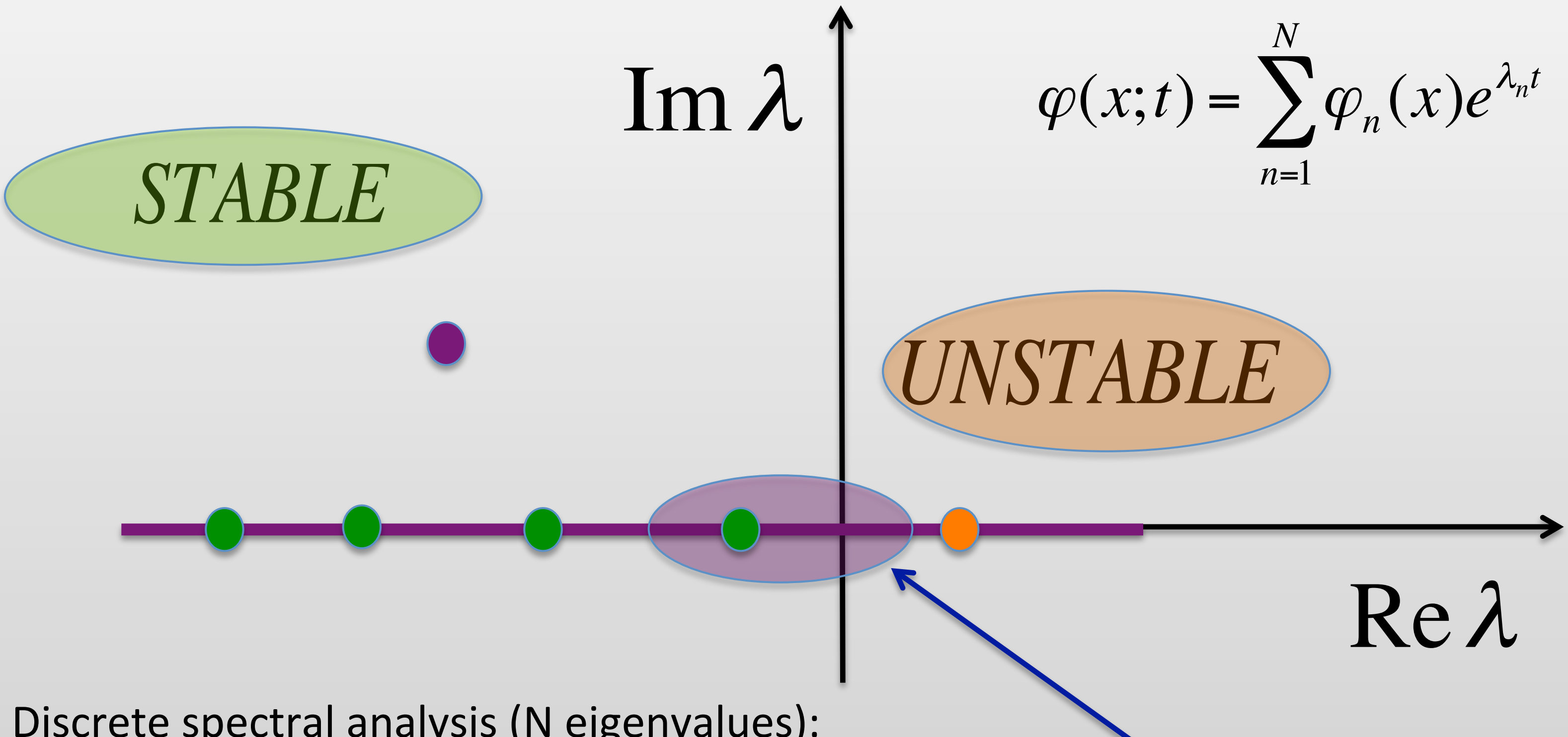
$$P(x) = p_0 + p_1 x + p_2 x^2 + \ldots$$

Higher orders save a lot of work (in principle):
In principle, 2° order achieve the same error with sqrt(N) grid points!
Since the work scales like N^3 in three dimensions this becomes
N^{3/2} instead of N^3, a MAJOR saving with N~100,1000…

Stability

Stability is KEY: best assessed via spectral analysis: $L\varphi = \lambda\varphi$

$$\varphi(x;t) = \sum_{n=1}^{N} \varphi_n(x) e^{\lambda_n t}$$



Discrete spectral analysis (N eigenvalues):

$$L_h \tilde{\varphi}_n = \tilde{\lambda}_n \tilde{\varphi}_n$$

Spectral pollution: discrete lambda's jump over the stability region!

Spectral Deformations: $\lambda_n \neq \tilde{\lambda}_n$

Discrete Stability

If all eigenvalues are real and negative, the solution must decay.
The same must be true for the FD system!

$$|\varphi(x_j;t_{n+1})| <= |\varphi(x_j;t_n)|$$

As a result, the norm of the propagator must be bounded to 1:

$$\| T_h \| < 1$$

This reflects directly into the CFL conditions: physical information cannot propagate faster than permitted by the discrete mesh

CFL (Courant-Friedrichs-Levy): $C_{A,D,R} < 1$

Courant Numbers

$$d \equiv \Delta x \rightarrow 0; \quad h \equiv \Delta t \rightarrow 0$$

Faster than light?

$$L = U\partial_x \qquad C_A = \frac{Uh}{d} \equiv \frac{U}{U_{lat}}$$

$$L = D\partial_x^2 \qquad C_D \equiv Dh / d^2 = D / D_{lat}$$

$$L = R \qquad C_R \equiv hR = R / R_{lat}$$

Physical Information cannot travel faster than "light"
Max allowed by the discrete Lattice!

Peclet and Damkohler numbers:

$$Pe = C_A / C_D \equiv Ud / D$$ Advection/Diffusion

$$Da = C_R / C_D \equiv Rd^2 / D$$ Chemistry/Diffusion

Efficiency

Computational density CD: # Flops/site/step

Memory density: Bytes/site/step

Computational workload: # Flops/run

Memory demand: Bytes/run

With **V=N^D** grid sites in **D** dimensions and **T** timesteps

Computational Complexity:

$$CC = CD * V * T$$

Note: For non-local algorithms CD grows with V (gravity, electrostatics)

Actual numbers

With N=1000, D=3, CD=2D=6, T=1000

CC = 6*10^{9+3}   = 6 ExaFlops

Your laptop = 1 Gflops/s

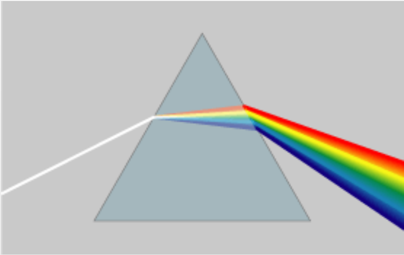
Wall **C**lock **T**ime = 6000 s ~ 2h

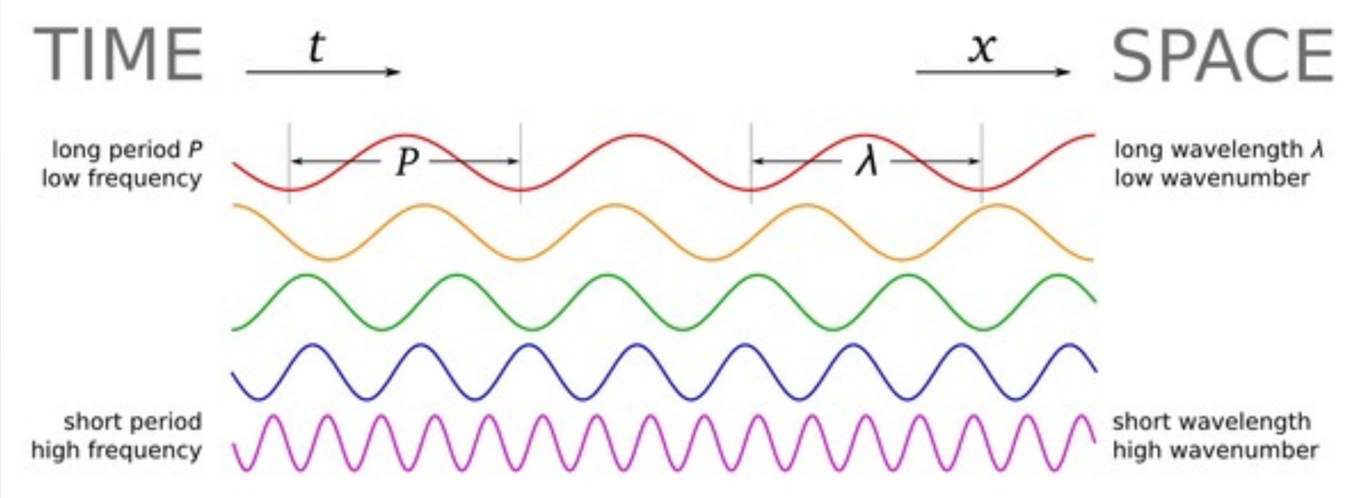
Always get a feel for the WCT of your problem !

Dispersion Relation Formalism

Fourier decomposition

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





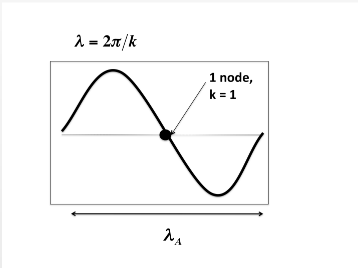
Low k

High k

Dispersion Relation

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

Discrete range and continuum limit

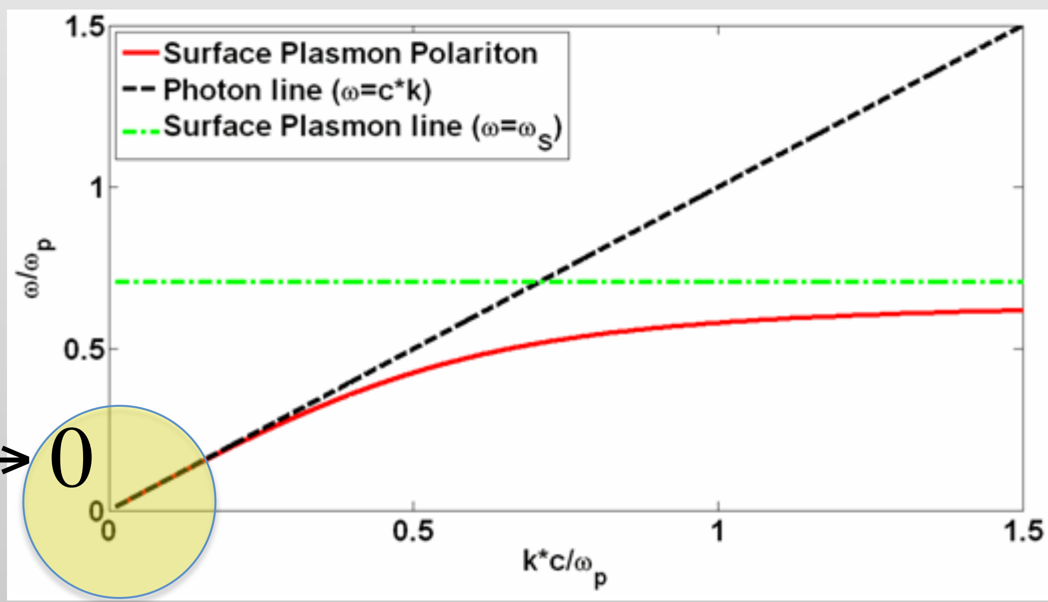


$$k_{\max} = 2\pi / d = N$$

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

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

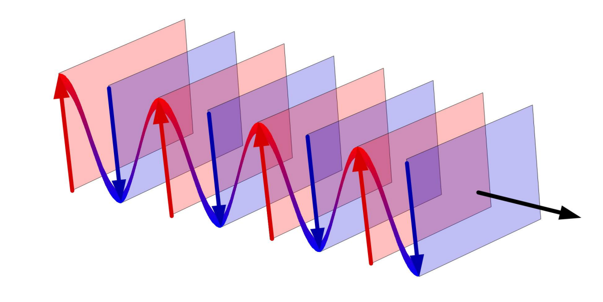
In the limit kd ->0 thewave does not “see” discreteness anymore



$$kd \rightarrow 0$$

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:

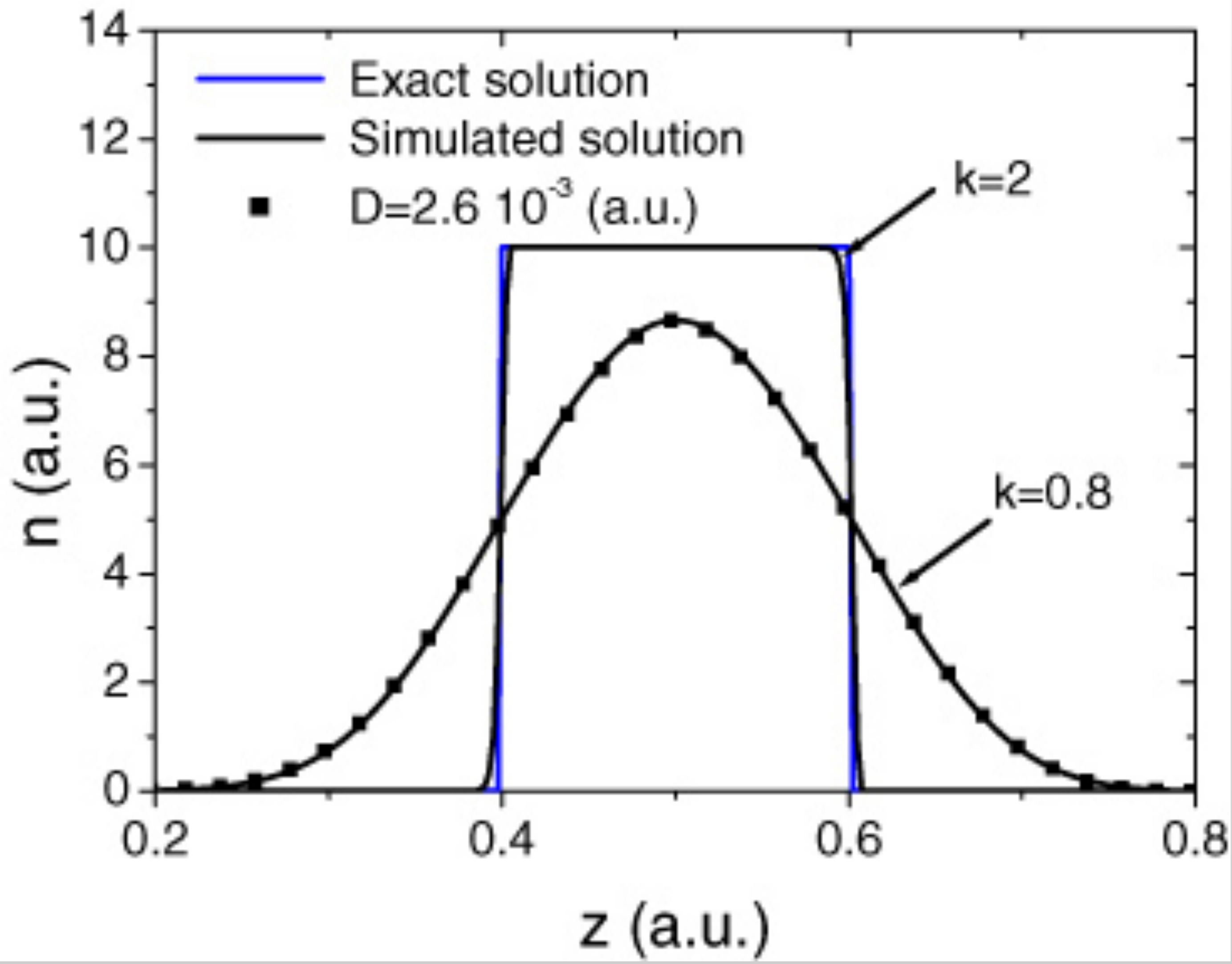
Real(omega), Phase Errors: Numerical **Dispersion**

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

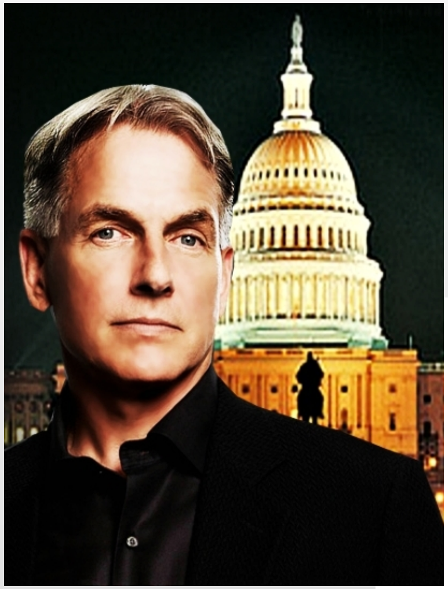
Dispersion means that the plane wave propagates at a different speed than continuum one, thus leading to distorsions in the profile and eventually unphysical oscillations (Gibbs oscillations). Carried by odd-order operators

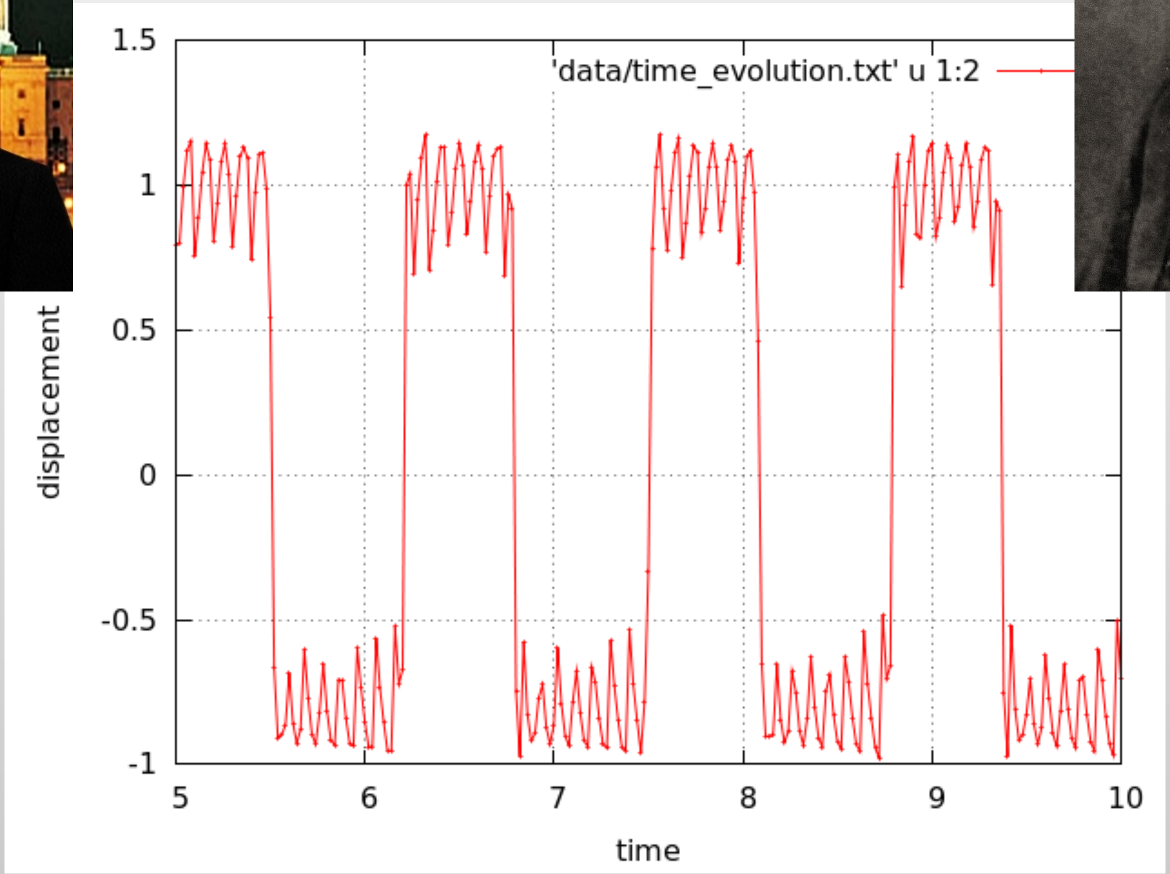
Carried by even-order operators (Diffusion/Dissipation)
Positive numerical diffusion leads to excessive damping.
Negative numerical diffusion leads to artificial growth:
Numerical instability

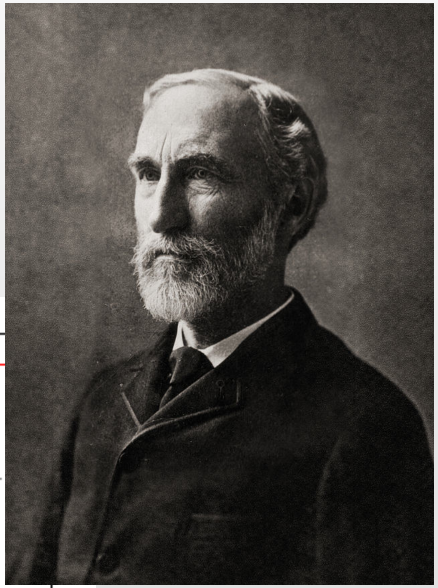
Numerical Diffusion: positive = overdamping



Numerical dispersion: Gibbs phenomena







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

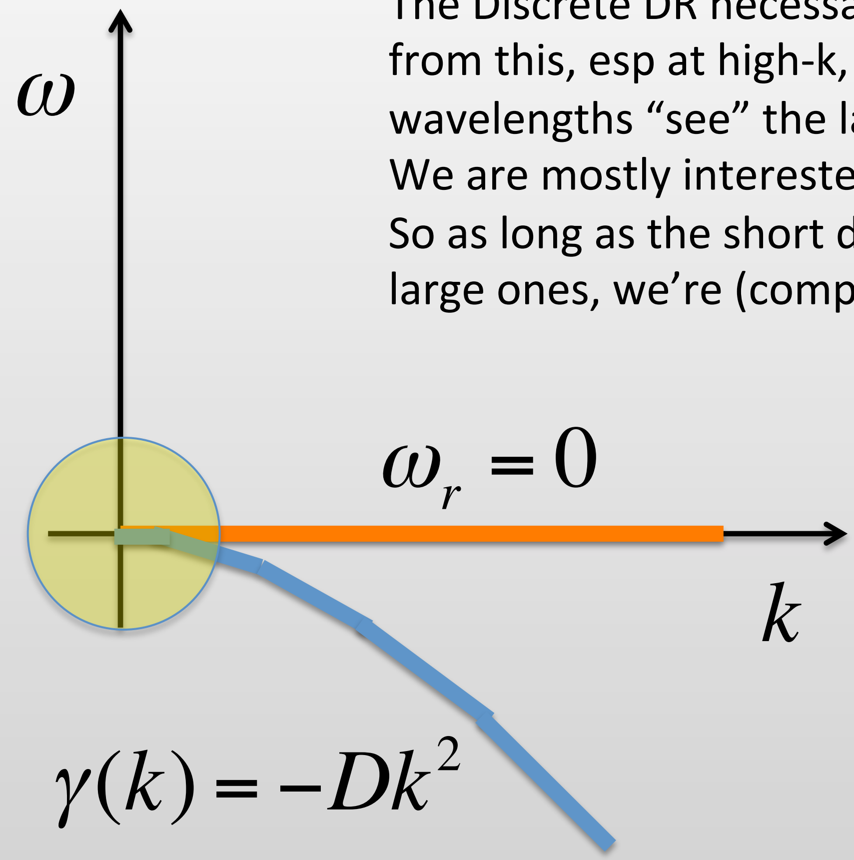
$$\gamma(k) = -Dk^2$$

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

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

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

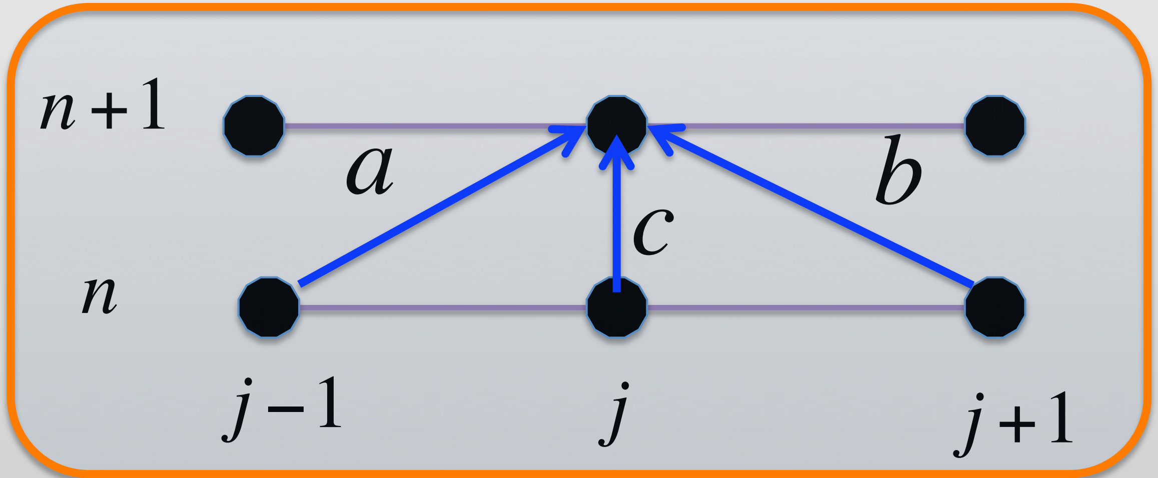
This is known as diffusive Courant-Friedrich-Levy (CFL) number. Key to stability.

$$a = b = \delta$$

$$c = 1 - 2\delta$$

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: $a = b = \delta$

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

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

(-2<X<0)

The discrete stability condition reads:

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

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

(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

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!

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):

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

$$c = 1 - 2\delta$$

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

Assignements

1. **Solve numerically the diffusion equation in d=1 (periodic boundary conditions), playing with CFL numbers**

2. **Compare against analytical solution at different grid resolutions and check the order of accuracy**

3. **Estimate&verify computational complexity by reporting your WCT**

4. Optional: same in d=2

Codelets: ad1.f

End of the lecture