Lecture 15

Differencing Schemes for Partial Differential Equations

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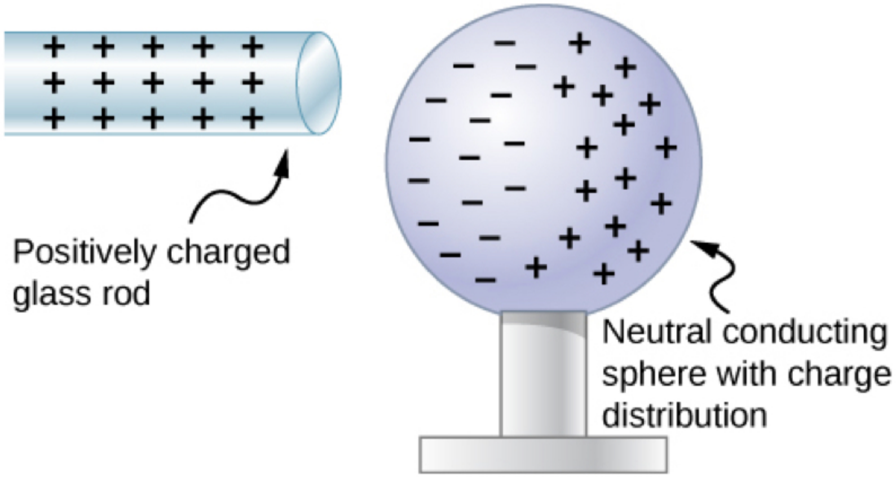
Topics of this lecture:

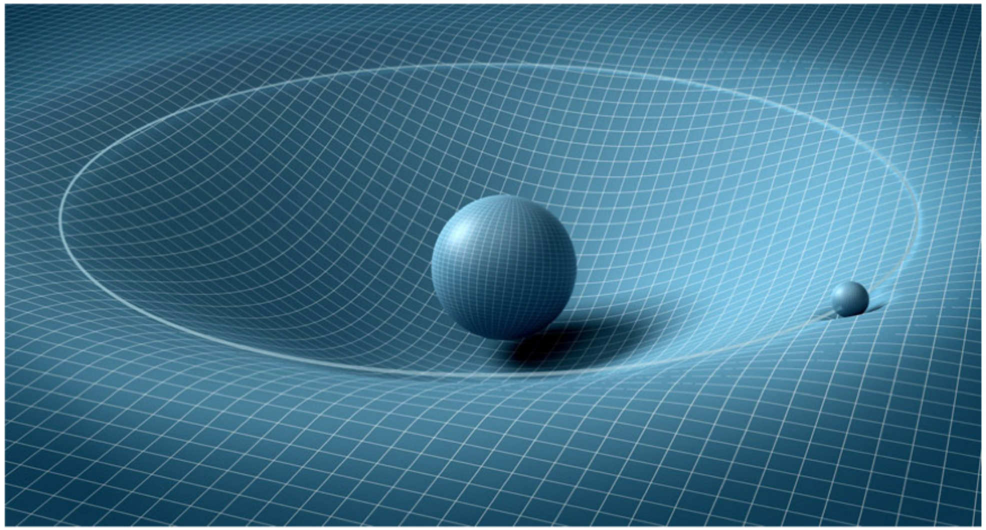
- random walk for Laplace equation $\nabla^2\phi = 0$
- differencing schemes for convection equation $t^n = n\Delta t, x_i = i\Delta x, \phi(x_i, t^n) = \phi_i^n$
- leapfrog design (half-step)
- Courant-Friedrichs-Lewy (CFL) condition $\Delta t \leq \frac{\Delta x}{|u|} \leftrightarrow \frac{\Delta x}{\Delta t} \geq |u|$
- numerical dissipation $\sim D\nabla^2\phi$
- Crank-Nicolson algorithm and absolutely stable

Prelude: Poisson and Laplace equations

$$\nabla^2 \phi = \mathbf{s}(\rho), \ \phi = \phi(\mathbf{x})$$

Ex.: what is the form of Laplace operator in spherical coordinates?



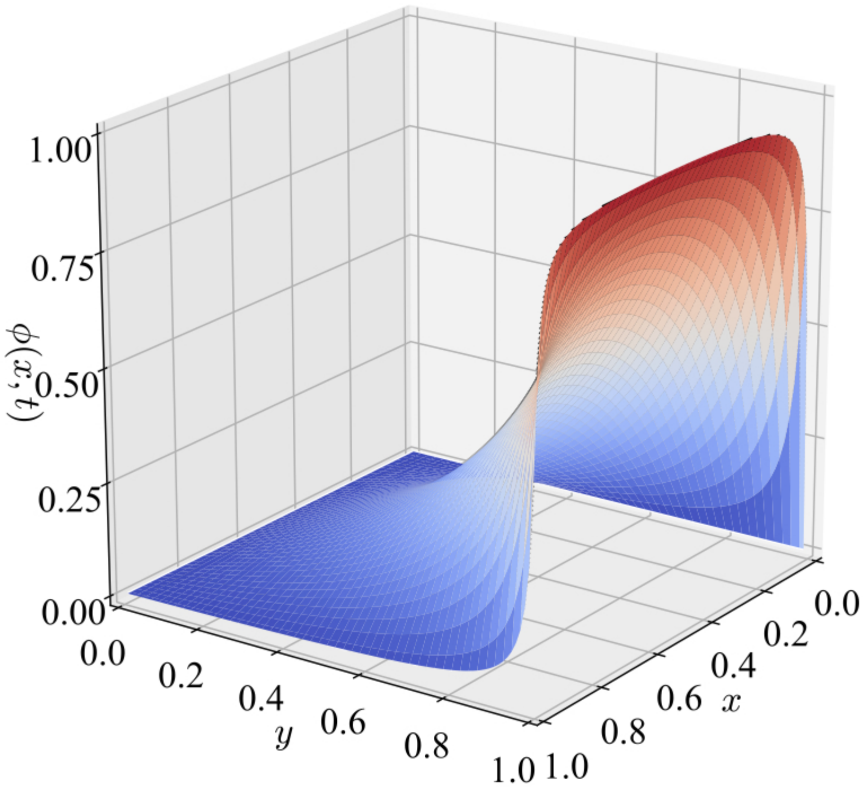


$$s(\rho) = -\rho/\epsilon_0$$

$$s(\rho) = 4\pi G\rho$$

Solution with appropriate boundary conditions

$$\nabla^2\phi = 0,\ \phi(0,y) = \phi(1,y) = \phi(x,0) = 1,\ \phi(x,1) = 1$$



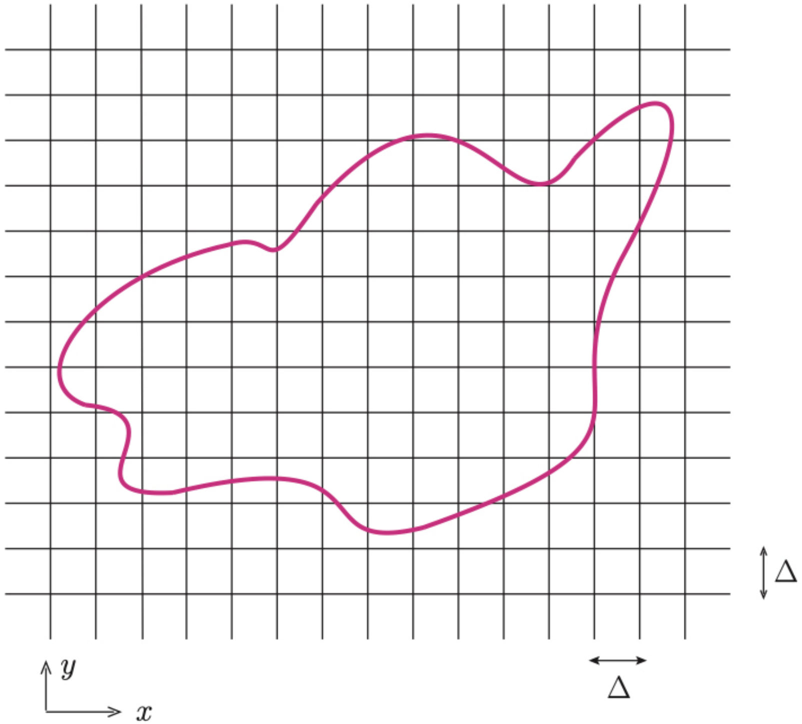
$$\phi(x,y) = \sum_{n=1,3,5,\cdots}^{\infty} \frac{4 \sin n\pi x \sinh n\pi y}{n\pi \sinh n\pi}$$

generally a summation over a few terms makes the approximation good

Can we use the idea of random walk?

$$\nabla^2\phi \approx \frac{1}{\Delta^2}\left[\phi(x+\Delta,y)+\phi(x-\Delta,y)+\phi(x,y+\Delta)+\phi(x,y-\Delta)-4\phi(x,y)\right]$$

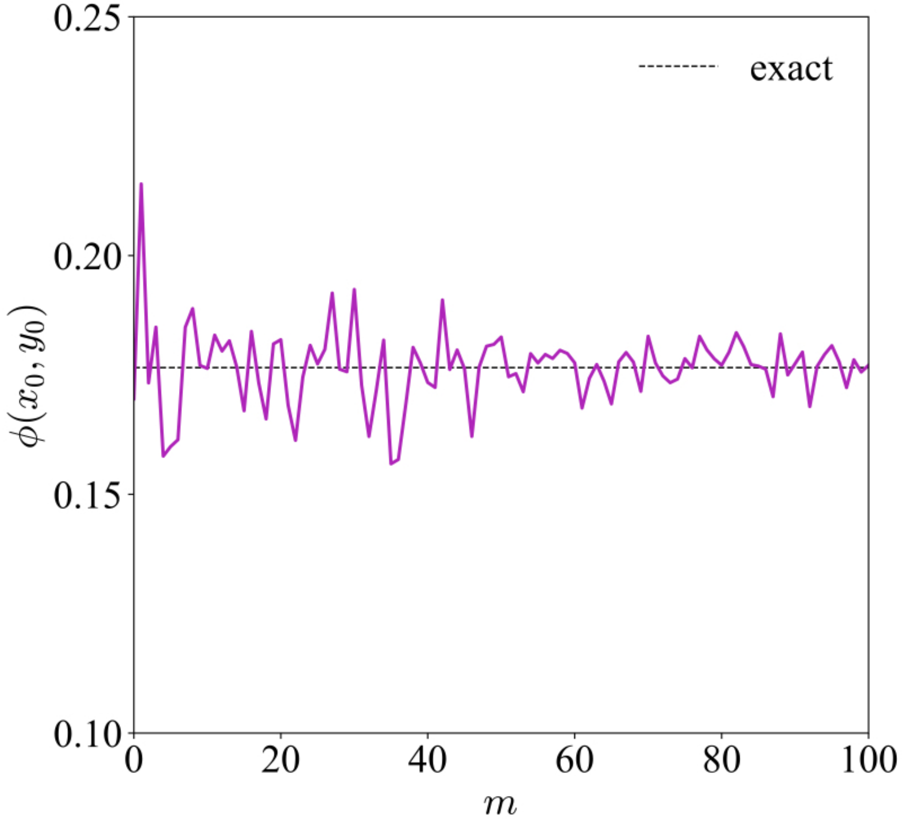
$$\phi(x,y) \approx \frac{1}{4}\left[\phi(x+\Delta,y)+\phi(x-\Delta,y)+\phi(x,y+\Delta)+\phi(x,y-\Delta)\right]$$



1. probability of a random walk returning to the point (x,y) is 1/4
2. a random walk will terminate at a boundary point (x',y') where the function ϕ has the value $\phi(x',y') = f(x',y')$
3. estimate the function ϕ accordingly by taking the walk from (x,y) and evaluating the first boundary point the walk reaches

$$\phi(x,y) \approx \frac{1}{m}\sum_{i=1}^{m} f(x_i',y_i')$$

Simulation example



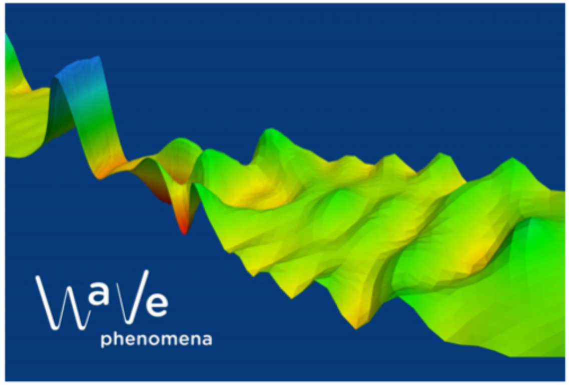
$$\phi(x, y) \approx \frac{1}{m} \sum_{i=1}^{m} f(x_i', y_i')$$

$$\phi(x, y) = \sum_{n=1,3,5,\cdots}^{\infty} \frac{4 \sin n\pi x \sinh n\pi y}{n\pi \sinh n\pi}$$

$$\text{error} \sim \frac{1}{\sqrt{m}}$$

Classification of 2nd-order PDE

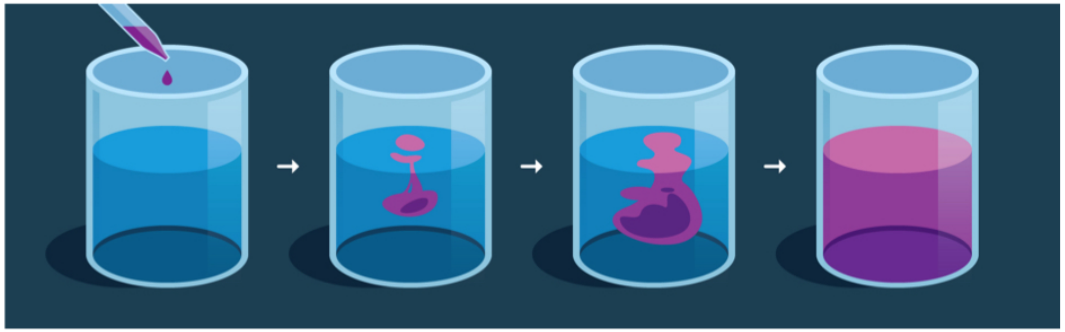
$$A\frac{\partial^2\phi}{\partial x^2} + B\frac{\partial^2\phi}{\partial x\partial y} + C\frac{\partial^2\phi}{\partial y^2} + D\frac{\partial\phi}{\partial x} + E\frac{\partial\phi}{\partial y} = F$$



wave equation: $\frac{\partial^2\phi}{\partial t^2} = u^2\frac{\partial^2\phi}{\partial x^2}$

determinant: $\Delta = B^2 - 4AC$

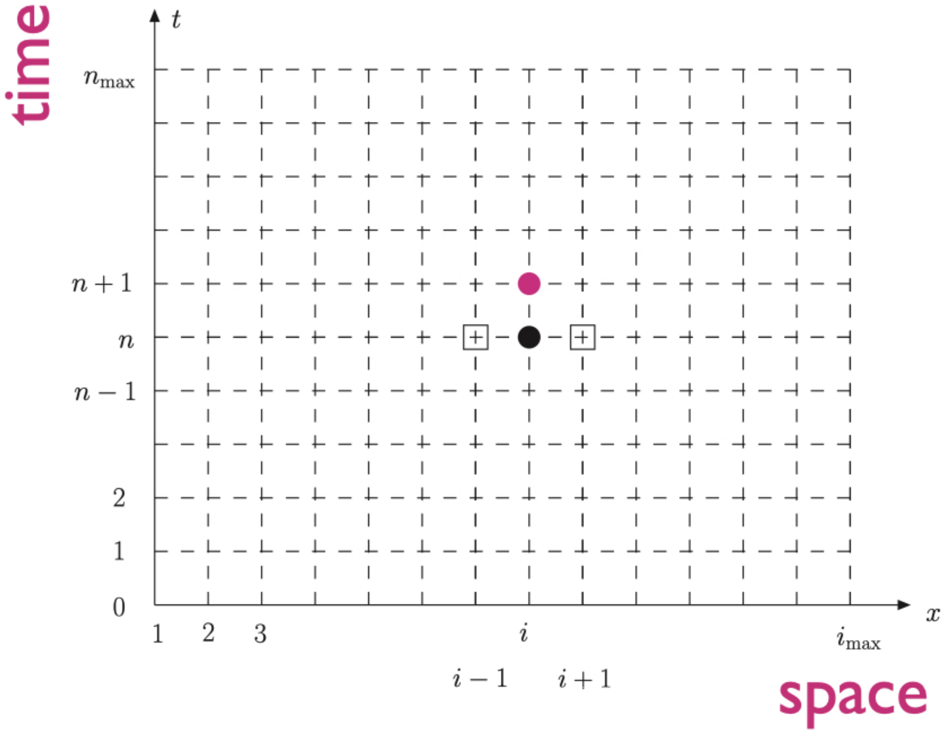
$$\begin{cases} \Delta > 0: & \text{hyperbolic} \\ \Delta = 0: & \text{parabolic} \\ \Delta < 0: & \text{elliptic} \end{cases}$$



diffusion equation: $\frac{\partial\phi}{\partial t} = D\frac{\partial^2\phi}{\partial x^2}$

Convection equation and the FT-CS scheme

$$\frac{\partial \phi}{\partial t} + u\frac{\partial \phi}{\partial x} = 0$$



$$\frac{\partial \phi}{\partial t} \approx \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t}, \quad \frac{\partial \phi}{\partial x} \approx \frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}$$

$$\phi_i^{n+1} = \phi_i^n - \frac{1}{2}\chi\left(\phi_{i+1}^n - \phi_{i-1}^n\right), \; \chi = \frac{u}{\Delta x/\Delta t}$$

$$t^n = n\Delta t, \; x_i = i\Delta x, \; \phi(x_i, t^n) = \phi_i^n$$

Modification/improvement (1st)

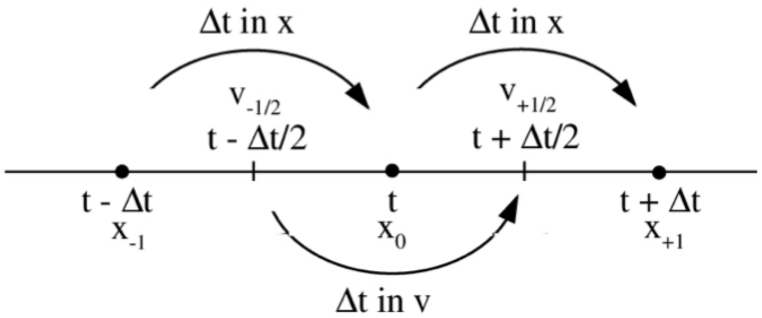
$$\frac{\partial \phi}{\partial t} \approx \frac{\phi_i^{n+1} - \phi_i^{n-1}}{2\Delta t}, \quad \frac{\partial \phi}{\partial x} \approx \frac{\phi_{i+1}^{n} - \phi_{i-1}^{n}}{2\Delta x}$$

$$\phi_i^{n+1} = \phi_i^{n-1} - \chi\left(\phi_{i+1}^{n} - \phi_{i-1}^{n}\right)$$

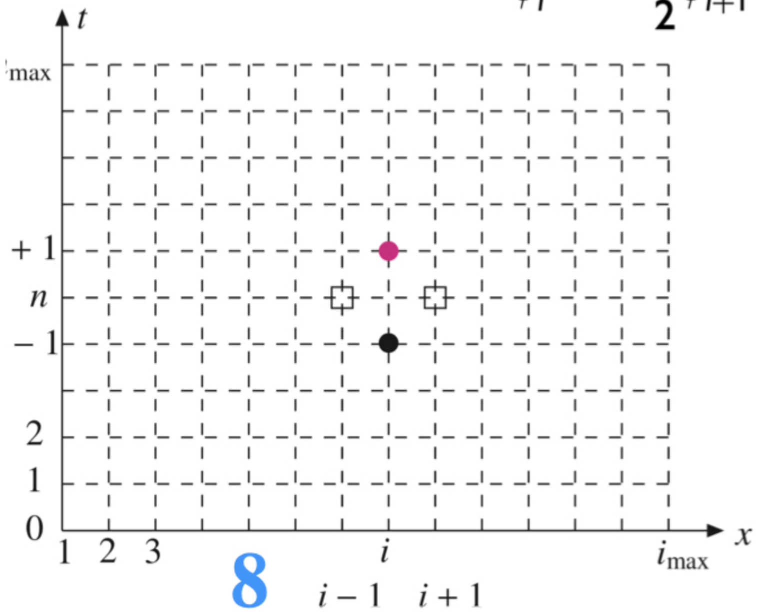
FT-CS $\phi_i^{n+1} = \phi_i^n - \frac{1}{2}\chi\left(\phi_{i+1}^{n} - \phi_{i-1}^{n}\right)$

Lax $\phi_i^{n+1} = \frac{\phi_{i+1}^{n} + \phi_{i-1}^{n}}{2} - \frac{1}{2}\chi\left(\phi_{i+1}^{n} - \phi_{i-1}^{n}\right)$

$$\phi_i^{n+1} = \frac{1}{2}\phi_{i+1}^{n}\left(1-\chi\right) + \frac{1}{2}\phi_{i-1}^{n}\left(1+\chi\right)$$



leapfrog



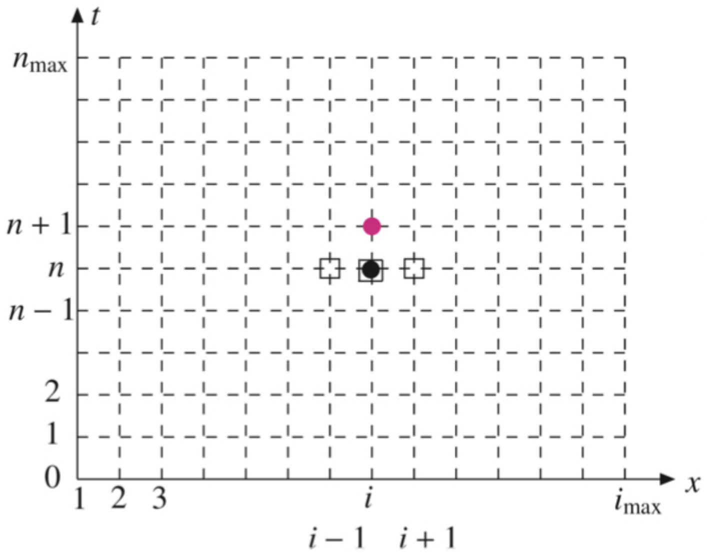
Modification/improvement (2nd)

$$\partial\phi/\partial t = -u\partial\phi/\partial x,\ \partial^2\phi/\partial t^2 = u^2\partial^2\phi/\partial x^2$$

$$\phi_i^{n+1} \approx \phi_i^n + \Delta t \left.\frac{\partial\phi}{\partial t}\right|_i^n + \frac{1}{2}\Delta t^2 \left.\frac{\partial^2\phi}{\partial t^2}\right|_i^n + \mathcal{O}(\Delta t^3)$$

$$\approx \phi_i^{n+1} \approx \phi_i^n - u\Delta t \left.\frac{\partial\phi}{\partial x}\right|_i^n + \frac{1}{2}u^2\Delta t^2 \left.\frac{\partial^2\phi}{\partial x^2}\right|_i^n$$

$$\approx \phi_i^n - u\Delta t\left(\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right) + \frac{1}{2}u^2\Delta t^2\left(\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta x^2}\right)$$



Lax-Wendroff

$$\phi_i^{n+1} \approx \phi_i^n - \frac{1}{2}\chi\left(\phi_{i+1}^n - \phi_{i-1}^n\right) + \frac{1}{2}\chi^2\left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n\right)$$

5-point

$$\left.\frac{\partial\phi}{\partial x}\right|_i^n \approx \frac{\phi_{i-2}^n - 8\phi_{i-1}^n + 8\phi_{i+1}^n - \phi_{i+2}^n}{12\Delta x},\ \left.\frac{\partial^2\phi}{\partial x^2}\right|_i^n \approx \frac{-\phi_{i-2}^n + 16\phi_{i-1}^n - 30\phi_i^n + 16\phi_{i+1}^n - \phi_{i+2}^n}{12\Delta x^2}$$

$$\phi_i^{n+1} \approx \frac{1}{12}\chi\left[\phi_{i+2}^n\left(1 - \frac{1}{2}\chi\right) - \phi_{i-2}^n\left(1 + \frac{1}{2}\chi\right)\right] - \frac{2}{3}\chi\left[\phi_{i+1}^n\left(1-\chi\right) - \phi_{i-1}^n\left(1+\chi\right)\right] + \phi_i^n\left(1 - \frac{5}{4}\chi^2\right)$$

Numerical example: performance comparison

$$\Phi(x) \equiv \phi(x,0) = \begin{cases} -4\Phi_{\mathrm{m}}\left(x^2 - x\right), & 0 \le x \le 1 \\ 0, & \text{otherwise} \end{cases}$$

$\Phi_m = 1.5$

$\Delta t = 0.01$

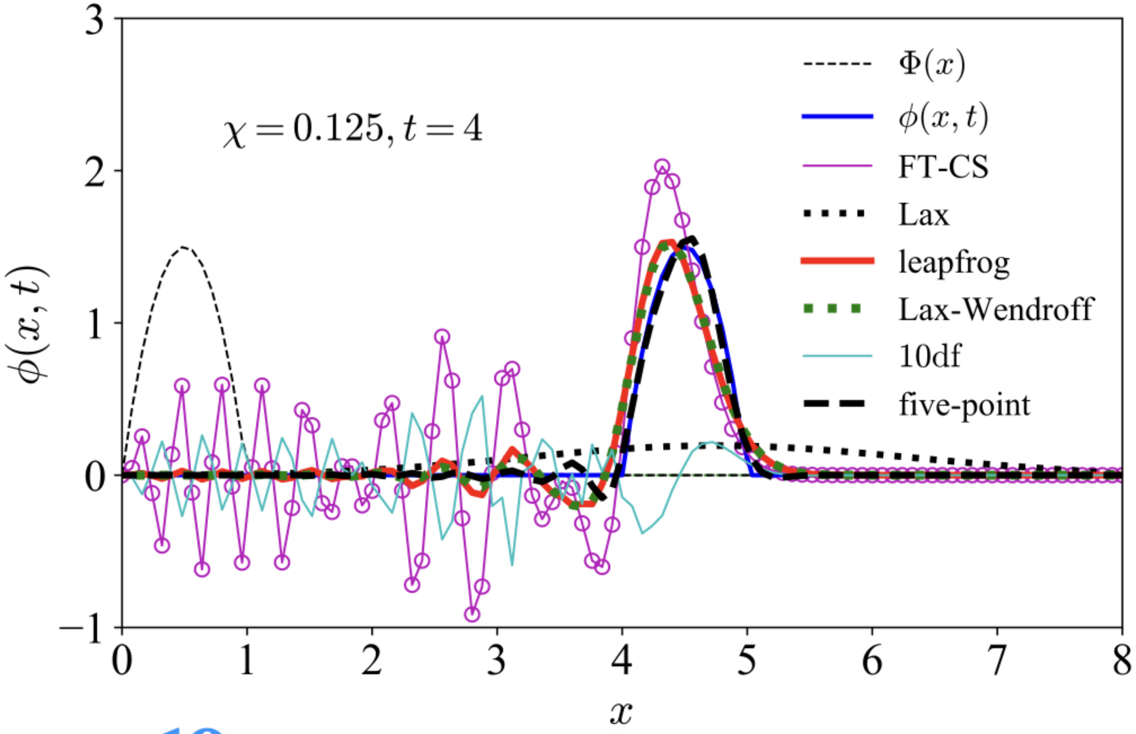
$\Delta x = 0.08$

$u = 1$

$i_{\max} = 101$

$\chi = 0.125$

$$\phi_{\mathrm{exact}}(x,t) = \Phi(x - ut)$$



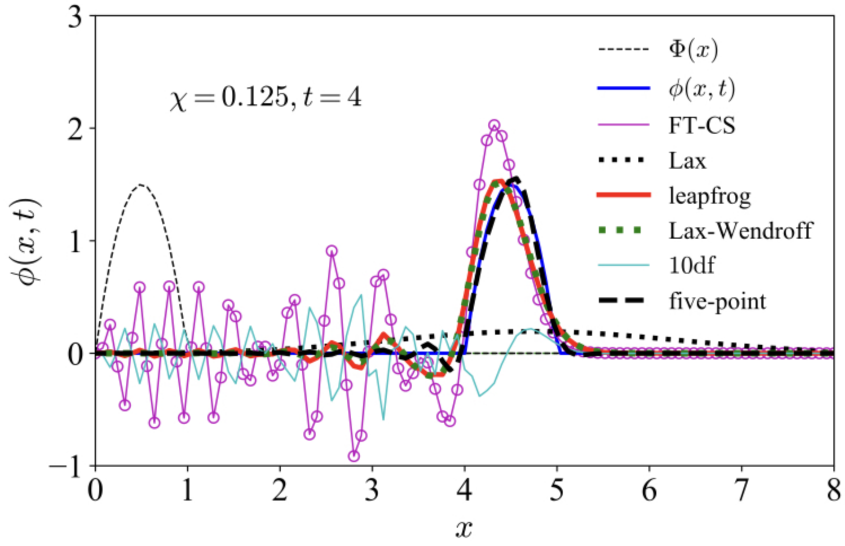
FT-CS is unstable

$$\phi_i^n = \xi^n e^{\sqrt{-1}ik\Delta x}$$

see how the factor $\xi = \xi(k)$ develops?

$$\phi_{i\pm 1}^n = \phi_i^n e^{\pm\sqrt{-1}k\Delta x}, \ \phi_i^{n+1} = \xi\phi_i^n$$

$$\xi = 1 - \sqrt{-1}\left(\frac{u\Delta t}{\Delta x}\right)\sin k\Delta x, \ |\xi| = \sqrt{1 + \left(\frac{u\Delta t}{\Delta x}\right)^2 \sin^2 k\Delta x}$$



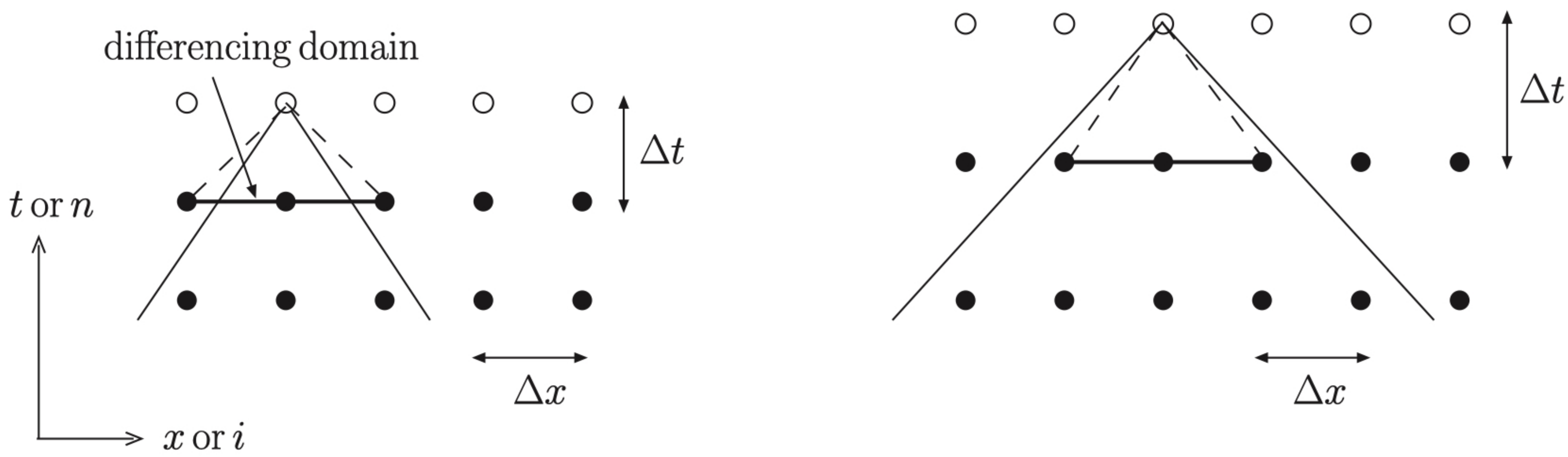
Ex.: show that for the Lax algorithm

$$|\xi|_{\mathrm{Lax}} = \sqrt{1 - \sin^2 k\Delta x\left[1 - \left(\frac{u\Delta t}{\Delta x}\right)^2\right]}$$

Courant-Friedrichs-Lewy (CFL) condition

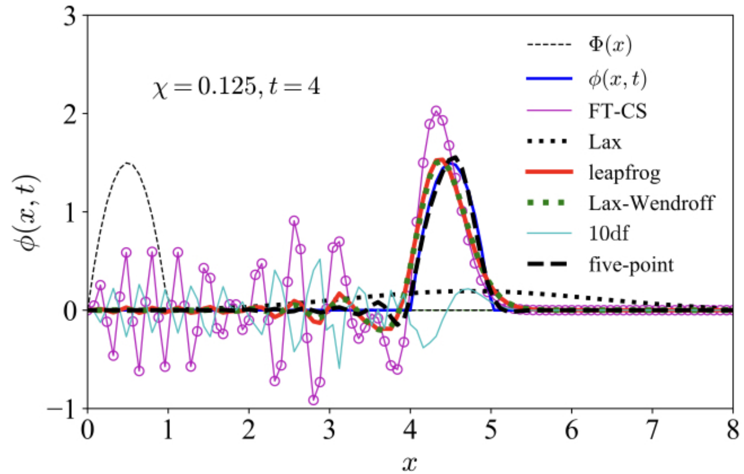
$$\Delta t \le \frac{\Delta x}{|u|} \leftrightarrow \frac{\Delta x}{\Delta t} \ge |u|$$

How to understand the CFL condition?



(a) stable (b) unstable

Numerical dissipation of Lax algorithm



$$\phi_i^{n+1} = \frac{1}{2}\phi_{i+1}^n (1-\chi) + \frac{1}{2}\phi_{i-1}^n (1+\chi)$$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = -u\left(\frac{\phi_{i+1}^n - \phi_{i-1}^n}{2\Delta x}\right) + \frac{1}{2}\left(\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n}{\Delta t}\right)$$

$$\frac{\partial \phi}{\partial t} = -u\frac{\partial \phi}{\partial x} + \frac{(\Delta x)^2}{2\Delta t}\frac{\partial^2 \phi}{\partial x^2}$$

diffusion equation: $\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2}$

effective diffusion/dissipative term

Quiz 5: 6/10/2026

Quiz 5.1:

What is aliasing? What is the Nyquist frequency? Describe or give mathematical definitions.

Quiz 5.2:

For $Q(f) = 2\pi ift/(1 + 2\pi ift)$, it is a (   ) filter.
(a) low-pass; (b) high-pass; (c) low and high-pass; (d) none of them

Quiz 5.3:

Correlation is defined as $c(t) = \int dt' h(t') g(t + t')$, show $C(f) = G(f)H(-f)$.

Quiz 5.4:

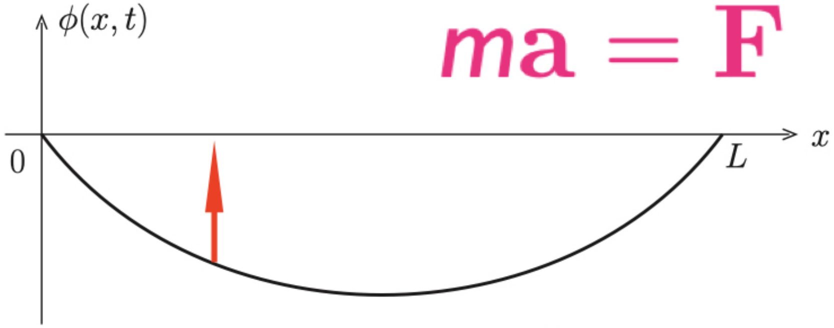
In the FFT, if we denote $H_k^{eeo\cdots oee} = f_n$ and set $n = 0 \sim 7$, write down the circuit path for H_5.

Quiz 5.5:

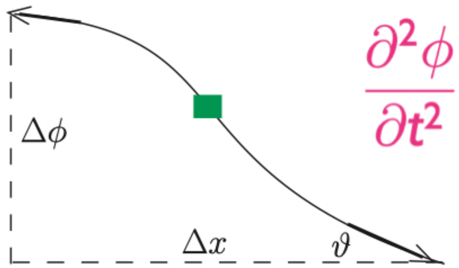
What is the geometrical meaning of $|z - a| + |z - b| = c$ with $a, b, c \in$ R and $c > |a - b|$?

Hyperbolic: from convection to wave

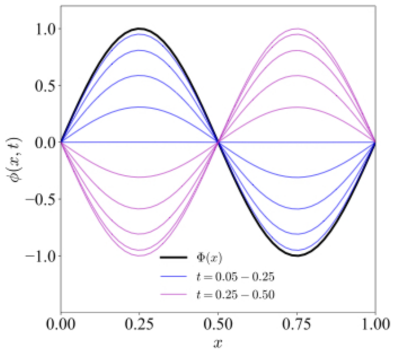
$$\rho\Delta x\frac{\partial^2\phi(x,t)}{\partial t^2} = T\sin[\vartheta(x+\Delta x)] - T\sin\vartheta(x) \approx T\frac{\partial\phi}{\partial x}\Big|_{x+\Delta x} - T\frac{\partial\phi}{\partial x}\Big|_{x} \approx T\frac{\partial^2\phi(x,t)}{\partial x^2}\Delta x$$

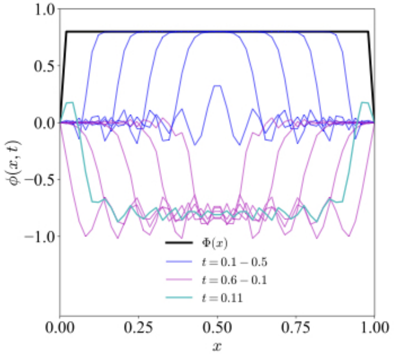


$$\mathbf{ma} = \mathbf{F}$$



$$\frac{\partial^2\phi}{\partial t^2} = u^2\frac{\partial^2\phi}{\partial x^2},\ u = \sqrt{\frac{T}{\rho}}$$





$$\frac{\partial\phi}{\partial t} = u\frac{\partial\phi}{\partial x} \to \frac{\partial^2\phi}{\partial t^2} = u^2\frac{\partial^2\phi}{\partial x^2}$$

$\alpha = u\partial\phi/\partial x,\ \beta = \partial\phi/\partial t$

$$\frac{\partial}{\partial t}\begin{pmatrix}\alpha\\ \beta\end{pmatrix} = \frac{\partial}{\partial x}\begin{pmatrix}u\beta\\ u\alpha\end{pmatrix}$$

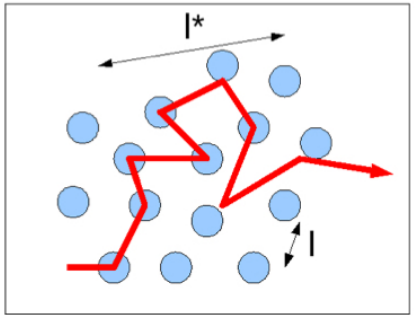
Ex.: Write down an effective algorithm.

Parabolic: diffusion equation

$$\frac{\partial \phi}{\partial t} = D\frac{\partial^2 \phi}{\partial x^2} \xrightarrow{\text{FT-CS}} \phi_i^{n+1} = \phi_i^n + \frac{D\Delta t}{\Delta^2 x}\left(\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n\right), \ \xi = 1 - \frac{4D\Delta t}{\Delta^2 x}\sin^2\left(\frac{k\Delta x}{2}\right)$$

CFL

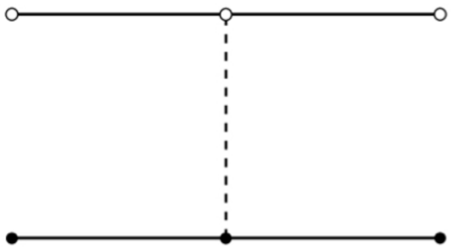
$$\Delta t \lesssim \frac{\Delta^2 x}{2D} \sim \frac{\Delta^2 x}{D}$$



diffusion time $\tau \sim \frac{\ell^2}{D}$ (Einstein theory)

$$\ell \gg \Delta x \rightarrow \#\text{evolution} \sim \frac{\ell^2}{\Delta^2 x} \text{ is large}$$

$$\chi = \frac{D\Delta t}{\Delta^2 x}$$



(c) Crank-Nicolson

Crank-Nicolson

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = \frac{D}{2}\frac{\phi_{i+1}^n - 2\phi_i^n + \phi_{i-1}^n + \phi_{i+1}^{n+1} - 2\phi_i^{n+1} + \phi_{i-1}^{n+1}}{\Delta^2 x}$$

 Ex.: What is the ξ factor for CN algorithm?

Crank-Nicolson is implicit

$$\chi = \frac{D\Delta t}{\Delta^2 x} \qquad a = 2/\chi + 2, \; b = 2/\chi - 2$$

$$\begin{pmatrix} a & -1 & 0 & 0 & 0 \\ -1 & a & -1 & 0 & 0 \\ 0 & -1 & a & -1 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots \\ 0 & 0 & 0 & -1 & a \end{pmatrix} \begin{pmatrix} \phi_1^{n+1} \\ \phi_2^{n+1} \\ \phi_3^{n+1} \\ \vdots \\ \phi_{i_{\max}-1}^{n+1} \end{pmatrix} = \begin{pmatrix} \phi_0^{n+1} + \phi_0^n + b\phi_1^n + \phi_2^n \\ \phi_1^n + b\phi_2^n + \phi_3^n \\ \phi_2^n + b\phi_3^n + \phi_4^n \\ \vdots \\ \phi_{i_{\max}}^{n+1} + \phi_{i_{\max}-2}^n + b\phi_{i_{\max}-1}^n + \phi_{i_{\max}}^n \end{pmatrix}$$