14. Partial differential equations

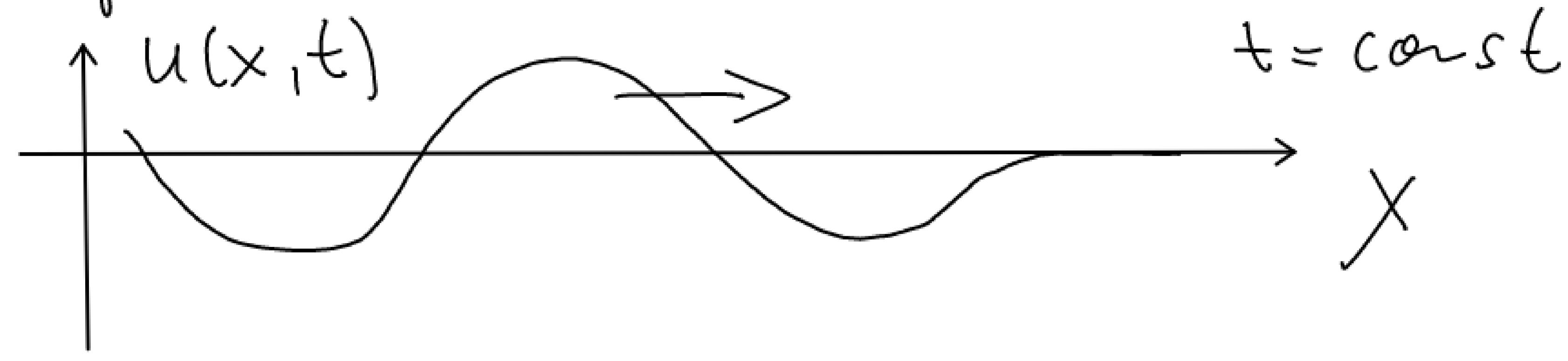
examples: 1) poisson equation (elliptic)

$$\Delta \phi = -\rho(\vec{r})$$ for the potential $\phi(\vec{r})$ sourced

→ boundary conditions (BCs) by a charge distribution $\rho(\vec{r})$

2) wave equation (hyperbolic)

$\frac{\partial}{\partial t}$ $\partial_t^2 u = v^2 \partial_x^2 u$ for a wave on a rope



→ BCs and initial
and initial condition

3a) diffusion equation (parabolic)

$$\partial_t c = D \partial_x c^2$$ for a concentration $c(x,t)$

3b) Schrödinger equation ✓ (:-))

$$i\hbar \partial_t \psi = \hat{H} \psi$$ for the wave function $\psi(x,t)$ of a particle

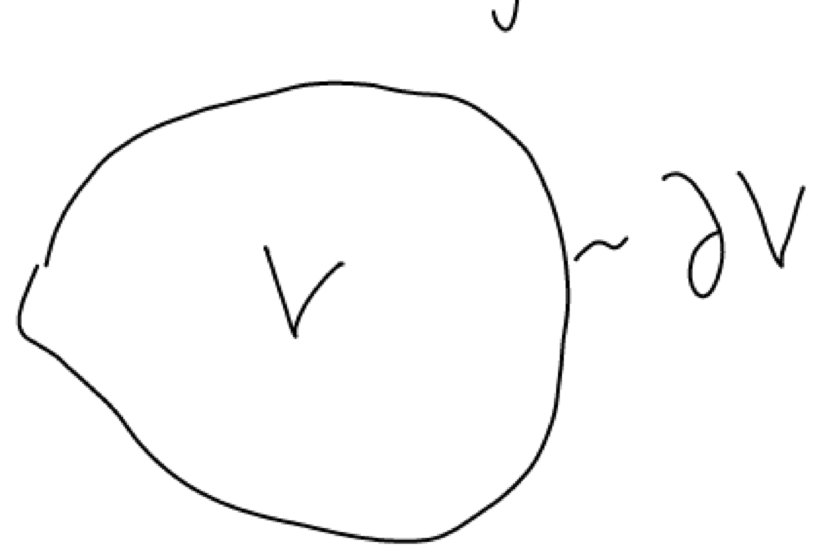
complex diffusion coefficient

General trick: Discretize time and space points on multi dimensional lattice!

6.1. Poisson equation

example in 2 dimensions: $\boxed{\Delta \phi = \partial_x^2 \phi + \partial_y^2 \phi = -\rho(x,y)}$

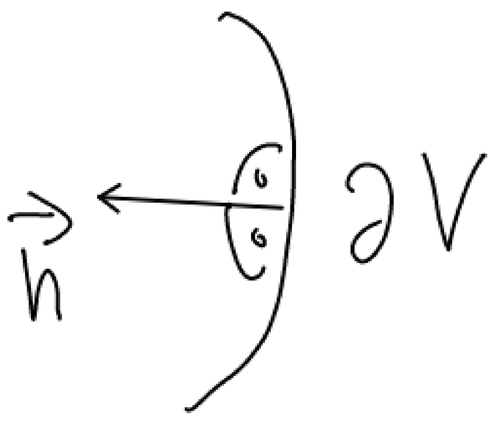
boundary conditions:



$\phi|_{\partial V} = \phi_D$ Dirichlet bc

$\nabla_{\vec{n}} \phi|_{\partial V} = \phi_N$ Neumann bc

$\nabla_{\vec{n}}$ = directional derivative orthogonal to boundary

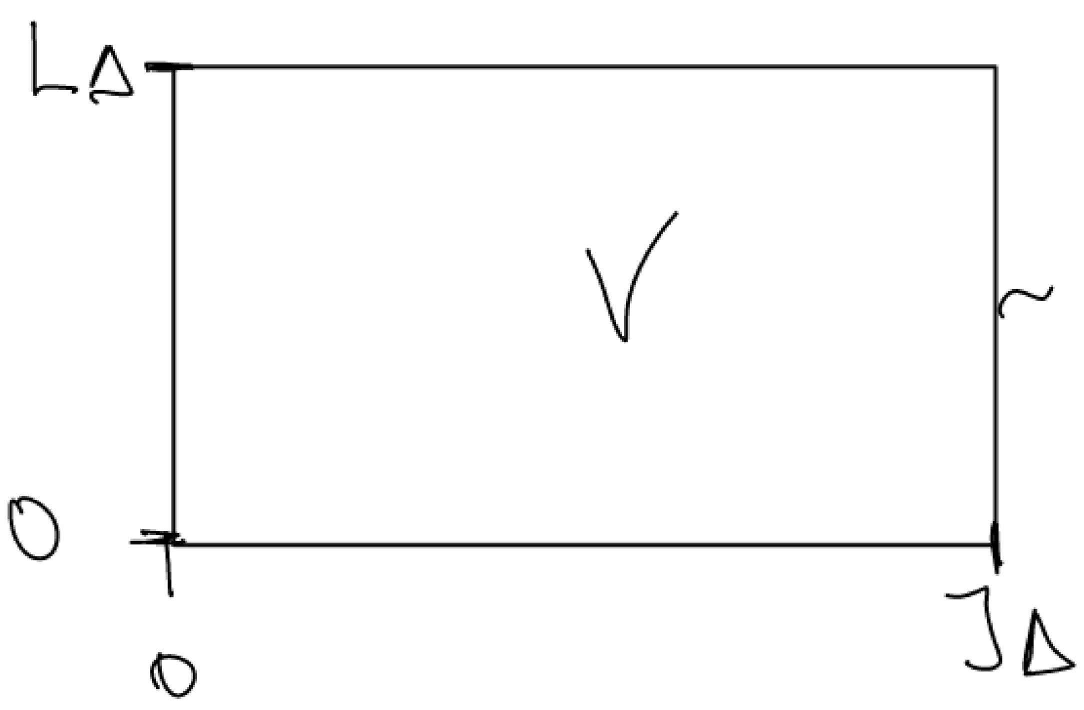


for $|\vec{n}| = 1$ $\quad \nabla_{\vec{n}} = \vec{n} \cdot \vec{\nabla}$

discretization like before $\phi(x,y) \to \phi_{j,\ell} = \phi(j\Delta, \ell\Delta)$

$\varrho(x,y) \to \varrho_{j,\ell} = \varrho(\; -\text{''}- \;)$

simple V is a rectangle $\rightsquigarrow$ V has $j = 1, \dots, J-1$ and $\ell = 1, \dots, L-1$



$\sim \partial V$ while ∂V is given by $j = 0,\; j = J,\; \ell = 0,$ or $\ell = L$

with Dirichlet bc $\phi|_{\partial V} = 0$

$$\partial_x^2 \phi + \partial_y^2 \phi \approx \frac{\phi_{j+1,\ell} - 2\phi_{j,\ell} + \phi_{j-1,\ell}}{\Delta^2} + \frac{\phi_{j,\ell+1} - 2\phi_{j,\ell} + \phi_{j,\ell-1}}{\Delta^2}$$

$$= -\varrho_{j,\ell}$$

Linear system! How to solve?

⊙ 1-dim version $\quad \dfrac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta^2} = -\rho_i \qquad (1)$

with b.c. $\phi_0 = \phi_\ell$ and $\phi_N = \phi_r \quad i = 0, \dots, N$

$$\boxed{A \cdot \vec{\phi} = \vec{r}} \quad \text{for} \quad A = \frac{1}{\Delta^2}\begin{pmatrix} -2 & 1 & & 0 \\ 1 & -2 & 1 & \\ 0 & 1 & \ddots & \ddots \\ & & \ddots & \ddots \end{pmatrix} \quad \text{and}$$

$$\vec{\phi}^T = (\phi_1, \dots, \phi_{N-1})$$

$$\vec{r} = \underbrace{-\begin{pmatrix} \varrho_1 \\ \vdots \\ \varrho_{N-1} \end{pmatrix}}_{\text{source}} \underbrace{- \frac{1}{\Delta^2}\begin{pmatrix} \phi_\ell \\ \vdots \\ \phi_r \end{pmatrix}}_{\text{b.c.}}$$

solved by QR-iteration ($\nearrow$ 8.3) or Jacobi-Iteration

1) Write (1) as fixed point equation,

$$\vec{\phi} = F(\vec{\phi}), \qquad \boxed{\phi_i = \frac{1}{2}(\phi_{i-1} + \phi_{i+1}) + \frac{1}{2}\Delta^2 \rho_i}$$

2) Guess initial value $\vec{\phi}^{(0)}$ and iterate

$$\vec{\phi}^{(i+1)} = F(\vec{\phi}^{(i)})$$

remember Banach fixed point theorem, F is contraction
$\rightsquigarrow$ always converges :-) $\rightsquigarrow$ check

$$|\vec{\phi}^{(i+1)} - \vec{\phi}^{(i)}| < \varepsilon \qquad \text{the stop iteration}$$

remark: similar work Gauß-Seidel iteration and relaxation method.

In 2-dim.
$$\boxed{\phi_{j,l}^{(n+1)} = \frac{1}{4}\left(\phi_{j+1,l}^{(n)} + \phi_{j-1,l}^{(n)} + \phi_{j,l+1}^{(n)} + \phi_{j,l-1}^{(n)}\right) + \frac{1}{4}\Delta^2 \rho_{j,l}}$$

6.2. Wave equation

is a special form of the continuity equation

$$\boxed{\partial_t \vec{u} = -\partial_x \vec{j}(\vec{u})} \quad \text{with the current (density) } \vec{j}(\vec{u})$$

take now $\vec{u} = \begin{pmatrix} E \\ B \end{pmatrix}$ and $\vec{j} = -v\begin{pmatrix} B \\ E \end{pmatrix}$ to get

$$\left.\begin{aligned} \partial_t E &= -v\,\partial_x B \\ \partial_t^2 E &= -v\,\partial_x \partial_t B = v^2 \partial_x^2 E \end{aligned}\right\} \text{1+1-dim. ED}$$

⇝ we rather solve $\boxed{\partial_t u = - v \, \partial_x u}$

for

remember 2^{nd} order -> $2\times$ 1^{st} order

$u_j^n = u(j\Delta x, n\Delta t)$

after discretization:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = - \frac{j(u_{j+1}^n) - j(u_{j-1}^n)}{2\Delta x} = - v \, \frac{u_{j+1}^n - u_{j-1}^n}{2\Delta x}$$

$$\leadsto \boxed{u_j^{n+1} = u_j^n - \frac{v\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right)}$$

forward in time, centered in space (FTCS-scheme)

explicit method, similar to Eulers method

BUT instable, errors magnify over time

Better is the Lax scheme

$$\boxed{u_j^{n+1} = \frac{1}{2}\left(u_{j+1}^n + u_{j-1}^n\right) - \frac{v\Delta t}{2\Delta x}\left(u_{j+1}^n - u_{j-1}^n\right)}$$

which is stable for $\frac{v \cdot \Delta t}{\Delta x} < 1$

6.3. Diffusion equation

Continuity equation with $j(u) = -D \, \partial_x u$ diffusion const.

For $\frac{2D\Delta t}{\Delta x^2} < 1$, already FTCS-scheme is stable.