# Partial Differential Equations

Most common form in which the static and dynamic properties of particles and fields are encoded. Some examples are

Non-relativistic quantum particles: $i\partial_t \psi(t,x) = \left(-\frac{\nabla^2}{2m} + V(x,t)\right)\psi(t,x) + g|\psi|^2\psi$
(Non-linear) Schrödinger equation — deterministic or stochastic

Heavy-quarkonium in heavy-ion collisions, Bose-Einstein condensation (Gross-Pitaevskii)

Classical fields: $\partial_t^2 \phi = \left(+\nabla^2 + m^2\right)\phi + \frac{\lambda}{4!}\phi^3$ inflation dynamics, reheating in the early universe

Multi-particle systems formulated in terms of distribution functions $f(t,x,v)$

Boltzmann eq.: $\partial_t f + \vec{v}\vec{\nabla}_x f + \frac{\partial \vec{p}}{\partial t}\vec{\nabla}_v f = C[f] \leftarrow$ collision term

Vlasov eq.: without B-field $\partial_t f + \vec{v}\vec{\nabla}_x f + \frac{q\vec{E}}{m}\vec{\nabla}_v f = 0$ & $\Delta\phi = \rho(f)$ poisson eq.

Three general categories: - Hyperbolic: wave equation $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$
- Parabolic: diffusion equation $\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial u}{\partial x}\right)$
- Elliptic: poisson equation $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \rho(x,y)$

Solution of any PDE requires input to fix "integration constants"

Initial value problem vs. Boundary value problem

function and derivatives given at one specific point $f(a), f'(a)$ $\xleftrightarrow{\text{often combination}}$ input given at different point $f(a), f(b)$

Homogeneous BC: Dirichlet $f(a) = c$
Neumann $\frac{\partial f}{\partial x}\big|_{x=a} = c$ OR $q$-periodic $f(L) = q\cdot f(0)$

Solved via finite difference or spectral methods. The former reduces differential to algebraic relations.

(in low dimensions reverted to initial value problem + minimization via shooting method)

When attempting solution of PDE numerically, STABILITY and EFFICIENCY of solver need to be ascertained.

Deterministic vs. Stochastic: PDE's including e.g. Gaussian noise need to be treated with particular care, due to modified chain rule (Ito's lemma): $df(X_t) = f'(X_t)\,dX_t + \frac{1}{2}f''(X_t)\sigma_t^2\,dt$
where $X_t$ is a random process with variance $\sigma$. In practice one needs to expand functions to higher orders in $dt$. (see also Stratonovich)

# Boundary value problems   Example: generalized Poisson in 2d

$$a(x,y)\frac{\partial^2 u}{\partial x^2} + b(x,y)\frac{\partial u}{\partial x} + c(x,y)\frac{\partial^2 u}{\partial y^2} + d(x,y)\frac{\partial u}{\partial y} + e(x,y)\frac{\partial^2 u}{\partial x \partial y} = \rho(x,y)$$

$u(x,y)$ given at boundary $\Rightarrow$ what is $u(x,y)$ in the interior?

Discretize evenly in a 2-d grid. $x_j = x_0 + ja \quad y_i = y_0 + ia \quad j = 0 \dots N_x - 1$, $i = 0 \dots N_y - 1$

**Finite differences:**

1st derivative

$$\frac{\partial u}{\partial x} \to \frac{1}{a}\left(u(x+a,y) - u(x,y)\right) = \nabla_x^F u \quad O(a) \text{ forward}$$

$$\to \frac{1}{a}\left(u(x,y) - u(x-a,y)\right) = \nabla_x^B u \quad O(a) \text{ backward}$$

$$\to \frac{1}{2a}\left(u(x+a,y) - u(x-a,y)\right) = \nabla_x^C u \quad O(a^2) \text{ central}$$

$$\nabla_x^F u = \frac{1}{a}\left(u(x,y) + a\,\partial_x u(x,y) + O(a^2) - u(x,y)\right) = \partial_x u(x,y) + O(a)$$

2nd derivative $\quad \frac{\partial^2 u}{\partial x^2} \to \nabla_x^F \nabla_x^B u = \frac{1}{a^2}\left(u(x+a,y) - 2u(x,y) + u(x-a,y)\right)$

$$\nabla_x^F \nabla_x^B u = \frac{1}{a^2}\left(u(x,y) + a\,\partial_x u + \frac{a^2}{2}\partial_x^2 u + O(a^3) - 2u(x,y) + u(x,y) - a\,\partial_x u + \frac{a^2}{2}\partial_x^2 u + O(a^3)\right)$$

$$= \partial_x^2 u + O(a^2)$$

Systematically improve discretization (increasingly non-local)

$$\frac{\partial^2 u}{\partial x^2} \to \frac{1}{a^2}\left(c_1 u(x+2a,y) + c_2 u(x+a,y) + c_3 u(x,y) + c_4 u(x-a,y) + c_5 u(x-2a,y)\right)$$

$$= \Delta_x^I u = \partial_x^2 u + O(a^3) \quad \text{if} \quad c_1 = c_5 = -\tfrac{1}{2} \quad c_2 = c_4 = 4/3 \quad c_3 = -5/3$$

$\Rightarrow$ original PDE discretized as linear system of equations.


$A \cdot \vec{u} = \vec{\rho}$

$\vec{u}$ 2d vector of unknown function $u$ on grid points

$\vec{\rho}$ 2d vector of known values

$A$ 2d×2d matrix <u>including BC</u> $\quad N_x = 100 \quad A \in \mathbb{R}^{10^4 \times 10^4}$

Note that $A$ is sparse, only certain bands are populated. Use this fact for efficient solution. Gauss-elimination does NOT profit $O(N^3)$. Instead use <u>conjugate gradient</u> or <u>relaxation</u> methods:

Jakobi Iteration: approach the correct solution along intermediate steps

$$\sum_{j=1}^{N} a_{ij} u_j = b_i \to a_{ii} u_i + \sum_{j \neq i} a_{ij} u_j = b_i \Rightarrow u_i = \frac{1}{a_{ii}}\Big(b_i - \underbrace{\sum_{j \neq i} a_{ij} u_j}_{\text{small \# for sparse matrices}}\Big)$$

take $a = b = 1 \quad c = d = e = 0 \qquad 4u^{n+1}(x,y) = \left[u(x+a,y) + u(x-a,y) + u(x,y-a) + u(x,y+a) - a^2 \rho(x,y)\right]$

Can be accelerated via over-relaxation

$$u^{n+1}(x,y) = \Big(\frac{1}{4}\sum_{\text{stencil}} u^n(x') - u^n(x,y)\Big)\gamma + u^n(x)$$

$C = 1$ relaxation

$C > 1$ faster

$C > 2$ instable?

## Hyperbolic Initial Value Problem: $\frac{\partial^2 u}{\partial t^2} = v^2 \frac{\partial^2 u}{\partial x^2}$ rewrite to 1st order

$q = \binom{r}{s}$ $\quad \frac{\partial r}{\partial t} = v \frac{\partial s}{\partial x}$ $\quad \frac{\partial s}{\partial t} = v \frac{\partial r}{\partial x}$ $\quad s = \frac{\partial u}{\partial t}$ $\; r = v \frac{\partial u}{\partial x}$ $\qquad$ discretize space and time

$\Rightarrow \partial_t q = - \partial_x F \qquad F(q) = \begin{pmatrix} 0 & -v \\ -v & 0 \end{pmatrix} q$ so called flux. $\qquad x_j = x_0 + j \cdot a$, $\; t_n = t_0 + n \cdot \Delta t$

consider $\partial_t q = - v \partial_x q \qquad q(x_j, t_{n+1}) - q(x_j, t_n) = - \frac{v \Delta t}{2a} \left( q(x_{j-1}, t_n) - q(x_{j+1}, t_n) \right)$

<u>explicit (Euler)</u> scheme since $q(t_{n+1})$ explicitly given i.t.o. $q(t_n)$, <u>not</u> recommended due to <u>STABILITY</u>:

Since PDE is linear, the error $u = u^{\text{exact}} + \varepsilon$ fulfills the same equation.
parametrize $\varepsilon_j^n = \sum_k c_j^n e^{ijka}$ as plane wave and insert single mode

$$c_j^{n+1} - c_j^n = - \frac{v \Delta t}{2a} c_j^n \left( e^{ika} - e^{-ika} \right) \Rightarrow G_j^n = \frac{c_j^{n+1}}{c_j^n} = 1 - i \frac{v \Delta t}{a} \sin(ka)$$

stable if $|G| \leq 1$ but $|G|^2 = 1 + \left(\frac{v \Delta t}{a}\right)^2 \sin^2(ka) > 1$ (always instable)

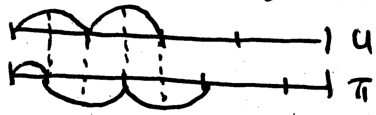
Instead if one uses lower order discretization in space

$v \partial_x u^n \approx \frac{v}{a} (u_i^n - u_{i-1}^n) \Rightarrow |G|^2 \leq 1$ for $\frac{v \Delta t}{a} < 1$ (conditional stability)

Courant-Friedrichs-Lewy condition shows stability threshold.

Quick reminder: <u>leap-frog</u> discretization (for 2nd order PDE)

$\frac{\partial^2 u}{\partial t^2} = v \frac{\partial^2 u}{\partial x^2} \Rightarrow \frac{\partial u}{\partial t} = \pi, \; \frac{\partial \pi}{\partial t} = v \frac{\partial^2 u}{\partial x^2} \qquad \pi @ t_0 + n \cdot \Delta t + \frac{\Delta t}{2}$




conditionally stable if $v \frac{\Delta t}{a} < \frac{1}{2}$ and $\mathcal{O}(dt^2)$

## Parabolic Initial Value Problem $\quad \frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2} = F(u, x, t)$

① <u>Forward Euler</u>: $u(x_j, t_{n+1}) - u(x_j, t_n) = \frac{\Delta t D}{a^2} \left( u(x_{j+1}, t_n) - 2u(x_j, t_n) + u(x_{j-1}, t_n) \right)$
conditionally stable if $\frac{D \Delta t}{a^2} < \frac{1}{2} \Leftrightarrow \Delta t \leq \frac{1}{2} \left( \frac{\Delta x^2}{D} \right)$ and $\mathcal{O}(\Delta t)$

② <u>Backward Euler</u>: $u(x_j, t_{n+1}) - u(x_j, t_n) = \frac{\Delta t D}{a^2} \left( u(x_{j+1}, t_{n+1}) - 2u(x_j, t_{n+1}) + u(x_{j-1}, t_{n+1}) \right)$
still order $\mathcal{O}(\Delta t)$, need to solve linear system of eq. in each step BUT <u>unconditionally</u> stable.

③ <u>Crank-Nicolson</u>: $u(x_j, t_{n+1}) - u(x_j, t_n) = \frac{\Delta t}{2} \left[ F(u^{n+1}) + F(u^n) \right]$
again implicit method BUT $\mathcal{O}(\Delta t^2)$ and also unconditionally stable.

<u>Explicit examples for Schrödinger equation</u>

$i\partial_t \psi = \left(-\frac{\vec\nabla^2}{2m} + U\right)\psi = H\psi$

① $\frac{1}{\Delta t}(\psi(t+1) - \psi(t)) = -iH\psi(t) \Rightarrow \psi(t+1) = \underbrace{(1 - H\Delta t)}_{|\ldots|>1 \text{ unbounded growth in } |\psi|}\psi(t) = e^{i\tilde H_{eff}\Delta t}\psi(t)$

② $\frac{1}{\Delta t}(\psi(t+1) - \psi(t)) = -iH\psi(t+1) \Rightarrow \psi(t+1) = \frac{1}{\underbrace{1 + iH\Delta t}_{|\ldots|<1 \text{ shrinkage in } |\psi|}}\psi(t) = e^{iH'_{eff}\Delta t}\psi(t)$

In both cases the discretized time evolution operator is NOT unitary

③ $\frac{1}{\Delta t}(\psi(t+1) - \psi(t)) = -\frac{i}{2}H(\psi(t) + \psi(t+1))$

$(1 + \frac{1}{2}iH\Delta t)\psi(t+1) = (1 - \frac{1}{2}iH\Delta t)\psi(t) \Rightarrow \psi(t+1) = \overbrace{\frac{1 - \frac{1}{2}iH\Delta t}{1 + \frac{1}{2}iH\Delta t}}^{|\ldots|=1 \text{ unitary}}\psi(t)$

Need to make sure that the solver preserves vital physical properties of the system. (Energy, probability etc)

(see MacNamara, Strang)

Operator splitting: Often $\dot u = (\mathcal{L}_1 + \mathcal{L}_2)u$ exact $u(t) = e^{\mathcal{L}_1 + \mathcal{L}_2}u(0)$

e.g. different directions in the Laplace operator. $\mathcal{L}_1, \mathcal{L}_2$ after discretization are non-commuting matrices $L_1, L_2$. Use Campbell-Baker-Hausdorff

$e^{b_2\Delta t L_2} e^{a_2\Delta t L_1} e^{b_1\Delta t L_2} e^{a_1\Delta t L_1} = e^{\Delta t[(a_1+a_2)L_1 + (b_1+b_2)L_2 - \frac{1}{2}\Delta t(a_1(b_1+b_2) + a_2(b_2-b_1))(A,B)] + O(\Delta t^3)]}$

Strang scheme: $b_2 = b_1 = \frac{1}{2}$ $a_2 = 1$ $a_1 = 0$ $\psi(t+\Delta t) = e^{\frac{1}{2}\Delta t L_1} e^{\Delta t L_2} e^{\frac{1}{2}\Delta t L_1}$

Once splitted, significant reduction in numerical cost possible

A. Ordinary Schrödinger equation: One-dimensional CN scheme

$\underbrace{\left(1 - \frac{i}{2}\frac{\partial_x^2}{2m}\Delta t\right)}_{\text{tridiagonal matrix}}\psi(t+1) = \underbrace{\left(1 + \frac{i}{2}\frac{\partial_x^2}{2m}\Delta t\right)\psi(t)}_{\text{vector}}$ solver for tridiag. matrix has cost $O(N_x)$ instead of $O(N_x^3)$

If periodic BC used in space, need to solve two subsequent systems of linear equations, so called Thomas algorithm. (PBC NOT required)

B. Non-linear Schrödinger equation (Gross-Pitaevskii)

$i\partial_t\psi = \left(-\frac{\nabla^2}{2m} + V(x,t) + g|\psi|^2\right)\psi$ split in linear-non linear parts

1. Non-linear part solved exactly $i\partial_t\psi = g|\psi|^2\psi$ by $\psi(x,t) = \exp(-2i|\psi(x,0)|^2 t)\psi(x,0)$

2. Kinetic part via Fourier transform (Needs PBC) $f(x+L) = f(x)$

$\Rightarrow p = p_n = \frac{2\pi n}{L}$ $n \in [-\frac{N}{2}, \frac{N}{2}]$ $n$ $\boxed{0|1|2|-1}$ $\ell$ $\boxed{0|1|2|3}$

$\hat f_n = \frac{1}{\sqrt N}\sum_{\ell=0}^{N-1} e^{-i2\pi\frac{n\ell}{N}} f_\ell$ $f_\ell = \frac{1}{\sqrt N}\sum_{n} e^{i2\pi\frac{\ell n}{N}}\hat f_n$ correct to $O(\Delta x^2)$ since $\hat f_{-N/2} = \hat f_{N/2}$

Unitarity: $U_{mn} = \frac{1}{\sqrt{N}} e^{i 2\pi \frac{mn}{N}}$

$$\sum_k U^\dagger_{mk} U_{nk} = \frac{1}{N} \sum_{k=0}^{N-1} e^{i \frac{2\pi}{N}(n-m)k} = \frac{1}{N} \sum_{k=0}^{N-1} r^k = \frac{1}{N} \frac{1-r^N}{1-r} = \delta_{mn}$$

Convolution: $h(y) = \int dx\, f(x)\, g(y-x) \Rightarrow \hat{h}(p) = \hat{f}(p)\, \hat{g}(p)$

discrete $h = \mathrm{IFT}[\mathrm{FT}[f]\, \mathrm{FT}[g]]$ in practice via Fast Fourier Transform with $O(\mathrm{Vol} \log(\mathrm{Vol}))$ cost.

FT diagonalizes finite difference operators but dispersion changes: $\Delta u = \frac{1}{a^2}\left(u(x+a) - 2u(x) + u(x-a)\right)$

$$\Rightarrow \hat{p}^2 \hat{u}(p) = \frac{1}{a^2}\left[e^{-i 2\pi \frac{k}{N}} - 2 + e^{i 2\pi \frac{k}{N}}\right] u(p)$$

$$= \frac{1}{a^2}\left[-2 + 2\cos\left(\frac{2\pi k}{N}\right)\right] u(p) = \frac{1}{a^2}\left(-4 \sin^2\left(\frac{\pi k}{N}\right)\right) u(p)$$