Lecture 1

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Numerical Methods for PDEs

Outline of Lecture 1

- organization of the course
- wellposedness: Hadamard, 1902
- classification & method of characteristics, *canonical form
- time-dependent PDEs and application areas
- Fourier series method
- Fourier transform method
- outlook to lecture 2

Organization of the course

- webpage
- "location" and "hours"
- communication
- *final exam* (70%) $\leftrightarrow$ exercises in lectures (check the webpage!)
- *assignments* (5% C1A, 10% C1B, 15% C2)
- programming: Matlab, Python

Well-posed vs ill-posed [1]

Before analyzing **ill-posed** problems, we must define what makes a partial differential equation (along with its boundary and initial conditions) mathematically sound.

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Hadamard's Definition (1902)

A mathematical problem is called **well-posed** if it satisfies the following three fundamental criteria:

1. **Existence:** There exists at least one solution $u(x, t)$.
2. **Uniqueness:** There exists at most one solution (no ambiguity).
3. **Stability:** The solution depends **continuously** on the initial and boundary data.

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The Core Breakdown

If **at least one** of these three conditions is violated, the PDE is classified as **ill-posed**. In physical applications, it is almost always the **stability** criterion that fails.

Well-posed vs ill-posed [2]

- **Physical reality:** In practical experiments, initial conditions can never be measured with 100% precision. There is always an inherent measurement noise $\delta > 0$.
- **Numerical reality:** Computers introduce floating-point round-off errors when discretizing a continuous domain onto a grid.

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Mathematical Definition of Stability

Let u_1 be the solution corresponding to initial data ϕ_1, and u_2 correspond to ϕ_2. Stability in a norm $\|\cdot\|$ implies the existence of a constant $C > 0$ such that:

$$\|u_1(\cdot, t) - u_2(\cdot, t)\| \leq C\|\phi_1 - \phi_2\| \quad \text{for all } t > 0$$

In an ill-posed problem, an infinitely small perturbation in the input ($\|\phi_1 - \phi_2\| \to 0$) can trigger a catastrophic **explosion** in the output ($\|u_1 - u_2\| \to \infty$).

Well-posed vs ill-posed [3]

Consider the classical heat equation on $x \in (0, \pi)$, but we solve it **backward in time** ($t < 0$, or equivalently for $t > 0$ with a reversed sign):

$$\frac{\partial u}{\partial t} = -\frac{\partial^2 u}{\partial x^2}, \quad u(0, t) = u(\pi, t) = 0, \quad u(x, 0) = \phi(x)$$

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We test this system using two different initial conditions via Fourier modes:

- **Case 1:** $\phi_1(x) = 0 \implies u_1(x, t) = 0$
- **Case 2:** $\phi_2(x) = \frac{1}{n} \sin(nx) \implies u_2(x, t) = \frac{1}{n} e^{n^2 t} \sin(nx)$

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The Catastrophic Blow-up

Observe the discrepancy between the initial conditions as $n \to \infty$:

$$\|\phi_1 - \phi_2\|_\infty = \frac{1}{n} \longrightarrow 0$$

However, for the solution at any fixed time $t > 0$, the exponential factor dominates:

$$\|u_1(\cdot,t) - u_2(\cdot,t)\|_\infty = \frac{1}{n}e^{n^2 t} \longrightarrow \infty \quad (\text{as } n \to \infty)$$

Conclusion: Infinitely small high-frequency noise completely destroys the solution.

Well-posed vs ill-posed [4]

For the standard wave equation ($u_{tt} = u_{xx}$), time-reversal is perfectly well-behaved because the equation is symmetric under $t \to -t$.

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$$\frac{\partial^2 u}{\partial t^2} = -\frac{\partial^2 u}{\partial x^2} \quad \text{(instead of } +\text{)}$$

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Modal Analysis

Applying separation of variables here transforms the stable trigonometric time oscillations ($\cos(\omega t)$) into **hyperbolic functions**:

$$u_n(x,t) = \frac{1}{n^2}\cosh(nt)\sin(nx)$$

Once again, the initial high-frequency amplitude $\frac{1}{n^2}$ suppresses the noise at $t = 0$, but for any $t > 0$, the $\cosh(nt)$ blows up at a rate of e^{nt}. The system is severely **ill-posed**.

Well-posed vs ill-posed [5]

Ill-posed problems are not mathematical errors; they appear frequently in physics and engineering as **Inverse Problems**:

- **Geophysics:** Reconstructing the historical temperature profile of the Earth's core based on current surface readings (Backward Heat).
- **Medical Imaging:** Tomography processes like CT and MRI scans (back-calculating captured signals into internal anatomical density maps).

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How do we solve them numerically?

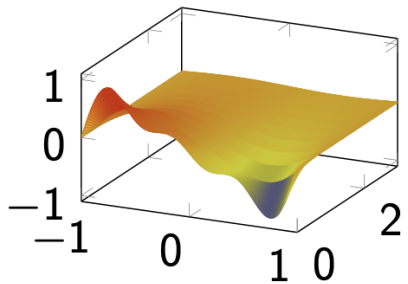
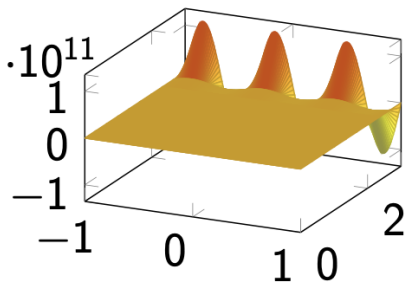
Standard numerical schemes (like FTCS or Crank-Nicolson) crash instantly on ill-posed PDEs due to round-off amplification. We must modify the math:

- **Regularization:** Artificially adding a tiny dampening term (e.g., Tikhonov regularization or a higher-order derivative ϵu_{xxxx}) to suppress and truncate high frequencies.
- **Restricting the solution space:** Forcing the solution to live inside a compact subset where the amplitudes of high Fourier modes are strictly bounded a priori.

Well-posed vs ill-posed [6]

Parabolic PDEs: well-posed vs. ill-posed - cont.

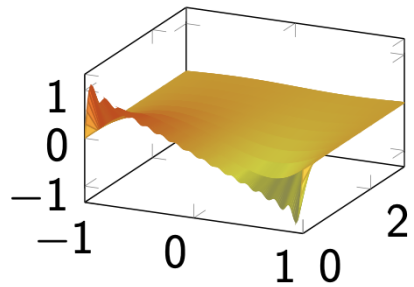
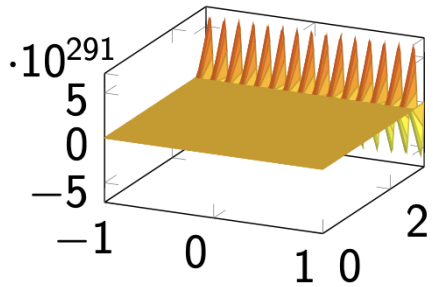
Given the Fourier series we found for $f(x) = -x, [-1, 1]$ at $k = 3$, here's what the graph of $u(x, t)$ looks like:

Heat equation	(Reversed time)
$u_t - u_{xx} = 0$	$u_t + u_{xx} = 0$
	
A reasonable approximation	Huh...?

Well-posed vs ill-posed [7]

Why heat equation with reverse time is ill-posed

As we increase k, one graph becomes more accurate, while the other becomes more and more chaotic. $k = 15$:

Heat equation	(Reversed time)
$u_t - u_{xx} = 0$	$u_t + u_{xx} = 0$
	
More accurate	Chaos!

Well-posed vs ill-posed [8]

Well-posed problems	Ill-posed problems
Arithmetic	
Multiplication by a small number A $Aq = f$	Division by a small number $q = A^{-1}f \quad (A \ll 1)$
Algebra	
Multiplication by a matrix $Aq = f$	$q = A^{-1}f$, A is an ill-conditioned, degenerate or rectangular $m \times n$-matrix
Calculus	
Integration $f(x) = f(0) + \int_0^x q(\xi)\, d\xi$	Differentiation $q(x) = f'(x)$
Differential equations	
The Sturm–Liouville problem $u''(x) - q(x)u(x) = \lambda u(x)$, $u(0) - hu'(0) = 0$, $u(1) - Hu'(1) = 0$	The inverse Sturm–Liouville problem. Find $q(x)$ using spectral data $\{\lambda_n, \|u_n\|\}$

FDs versus FEs

- **Finite differences** **&** **finite volumes**





conservation laws

based on:
– Taylor expansions, eigenvalues, time-integration methods

- **parabolic and hyperbolic PDEs (time-dependent)**

[* **finite elements** $\rightsquigarrow$ **based on variational formulations**
(*functional analysis plays an important role*)

– **elliptic PDEs** (time-independent; stationary)]

- **Stationary PDEs**

Notation and definitions

Partial Differential Equations : P D Es

notation: $u_x = \dfrac{\partial u}{\partial x} = \partial_x u$, $u_{xx} = \dfrac{\partial^2 u}{\partial x^2} = \partial_{xx} u = \partial_x^2 u = \ldots$, $u_{4x} = u_{xxxx} = \dfrac{\partial^4 u}{\partial x^4} = \ldots$

general form of PDE: $F\left(x, y, z, t, u, u_x, u_y, u_t, u_{xx}, \ldots\right) = 0$

↖ *a given "operator" (function)*

Independent variables: $x, y, z, t, \ldots$

Dependent variables: $u, v, P, T, \rho, \ldots$

Linear PDE: $Lu(\vec{x}) = f(\vec{x})$ with $L(a \cdot u + b \cdot v) = a \cdot L(u) + b \cdot L(v)$

f not linear, then: quasilinear . . . nonlinear

$f = 0 \implies$ homogeneous PDE, else: inhomogeneous

Example: $u_{xy} = 0$ $\implies$ [integrating twice] $u(x, y) = g(y) + f(x)$ arbitrary functions!

Boundary conditions

a) **Dirichlet BC** (on $\partial\Omega$): $u\Big|_{\partial\Omega} = \text{given}$

↖ boundary of spatial domain

b) **Neumann BC:** $\dfrac{\partial u}{\partial n}\Big|_{\partial\Omega} = \text{given}$

c) **Robin BC:** $\left(\dfrac{\partial u}{\partial n} + a \cdot u\right)\Big|_{\partial\Omega} = \text{given}$

d) **periodic BC:** $u(0,t) = u(1,t)$ (example), if $\Omega = [0,1]$

e) **absorbing BC**, **flux BC**, **transport BC**, **etcetera ...**

In general: "count the number of derivatives in PDE" $\longleftrightarrow$ "how many conditions needed"

($\approx$ "highest" derivative)

Time-dependent PDEs:
$$\begin{cases} \longrightarrow \text{boundary conditions (BCs)} \\ \longrightarrow \text{initial condition(s) (IC(s))} \end{cases}$$

Basic (linear) examples [1]

1) **Laplace equation** (stationary): $\Delta u = 0$
2) **Poisson equation** (stationary): $\Delta u = f$
3) **Helmholtz equation** (stationary): $\Delta u + k^2 u = 0$
4) **wave equation:** $u_{tt} - c^2 \Delta u = 0$
5) **heat or diffusion equation:** $u_t - \kappa \Delta u = 0$
6) **advection equation:** $u_t + a u_x = 0$
7) **telegraph equation** (*transmission lines*):
   $u_{tt} + a u_t + b u = u_{xx}$

Basic (linear) examples [1]

8) Klein–Gordon equation (*relativistic electrons*):
$\Box u + \gamma u = 0$

$$\Box = \frac{\partial^2}{\partial t^2} - c^2\Delta \quad (\text{“d'Alembert operator”})$$

9) Boussinesq equation (*hydrodynamics*):
$u_{tt} - \alpha^2 \Delta u - \beta^2 \Delta u_{tt} = 0$

mixed derivatives!

10) Bi-harmonic wave equation (*elasticity*): $u_{tt} + c^2\Delta^2 u = 0$

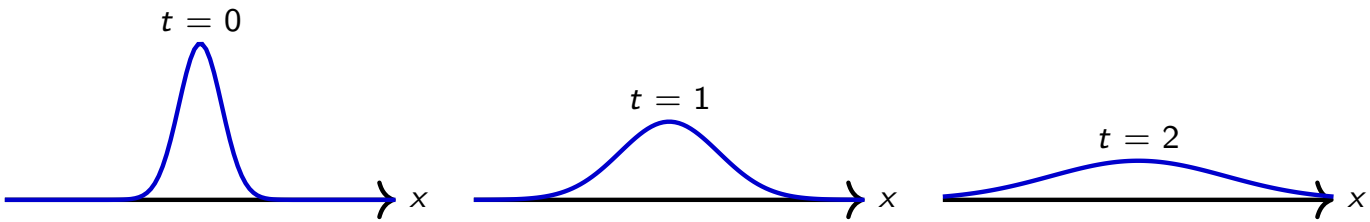
fourth-derivatives!

Basic (linear) examples [3]

Heat equation (*"diffusion equation"*)

Classification: linear, first/second order, parabolic

$$\begin{cases} u_t = k \cdot u_{xx} \\ u(x,0) = u_0(x) \qquad \text{(IC – Initial Condition)} \end{cases}$$



the initial solution damps out ("diffuses")

Example of a solution:

$$u(x,t) = \frac{e^{-\frac{x^2}{1+4kt}}}{\sqrt{1+4kt}}$$

"backward" heat equation: $u_t = -u_{xx}$ **ill-posed**

Basic (linear) examples [4]

Advection equation

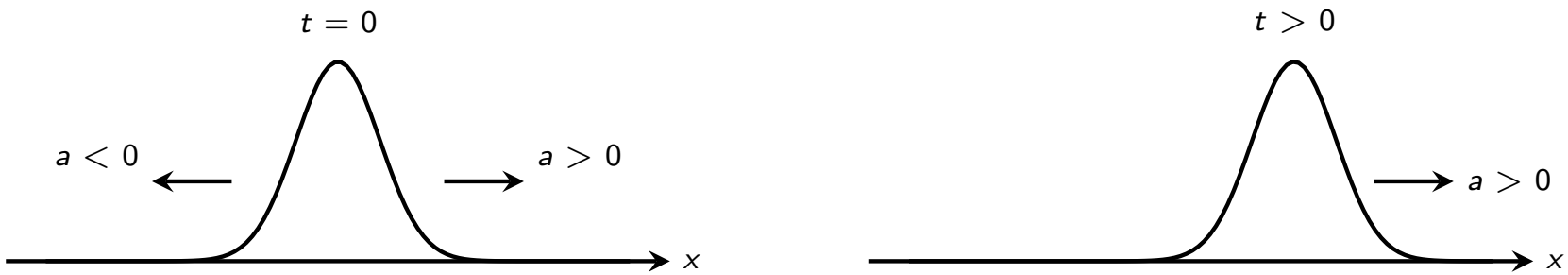
("transport equation", "one-way wave equation")

linear, first-order, "hyperbolic"

$$\begin{cases} u_t + a u_x = 0 \\ u(x,0) = u_0(x) \qquad \text{IC (Initial Condition)} \end{cases}$$

Solution:

$$u(x,t) = u_0(x - at)$$



wave moves with velocity a, without changing its shape

Basic (linear) examples [5]

Wave equation

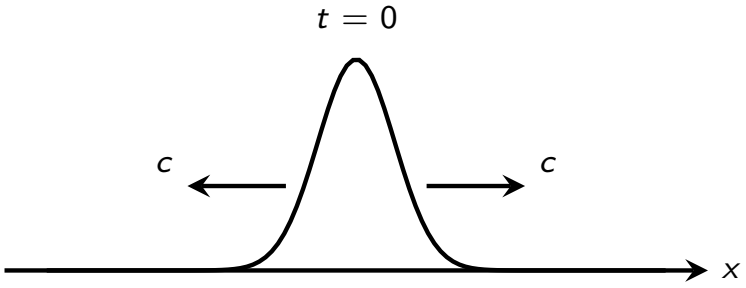
("two-way" wave equation)

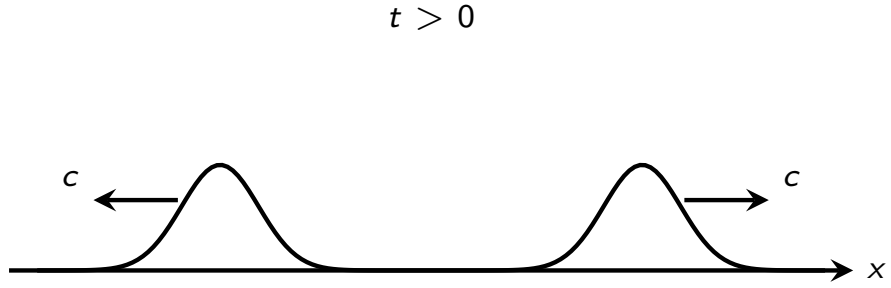
linear, second-order, hyperbolic

$$\begin{cases} u_{tt} = c^2 u_{xx} \\ u(x,0) = g(x) \\ u_t(x,0) = h(x) \end{cases} \quad \text{ICs} \quad \Longrightarrow$$

d'Alembert solution:

$$u(x,t) = \frac{1}{2}\left[g(x-ct) + g(x+ct)\right] + \frac{1}{2c}\int_{x-ct}^{x+ct} h(\xi)\, d\xi$$





"backward" wave equation: $u_{tt} + u_{xx} = 0$ ill-posed as an initial-value problem

however: $u_{xx} + u_{yy} = 0$ + BCs (elliptic) is well-posed

Some nonlinear examples [1a]

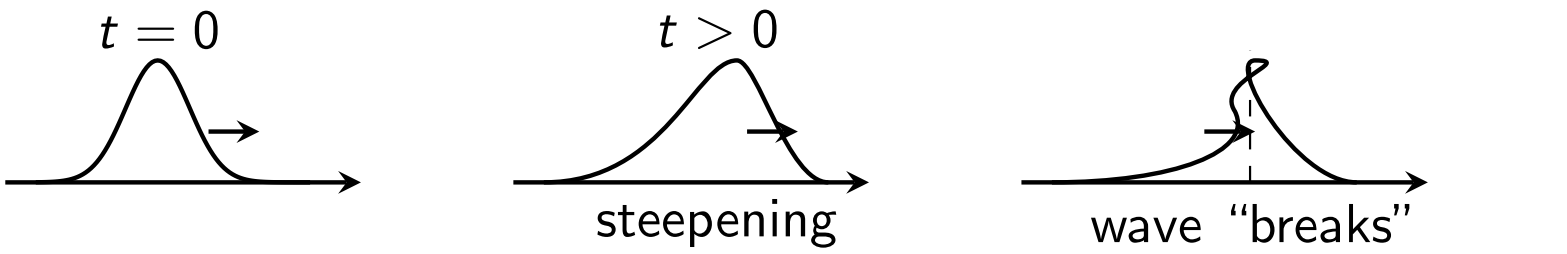
Burgers' equation non-linear, second/first-order, parabolic/hyperbolic

$$u_t = \varepsilon u_{xx} - u u_x$$

$\varepsilon = 0$: inviscid Burgers' equation

$\varepsilon > 0$: viscous Burgers' equation

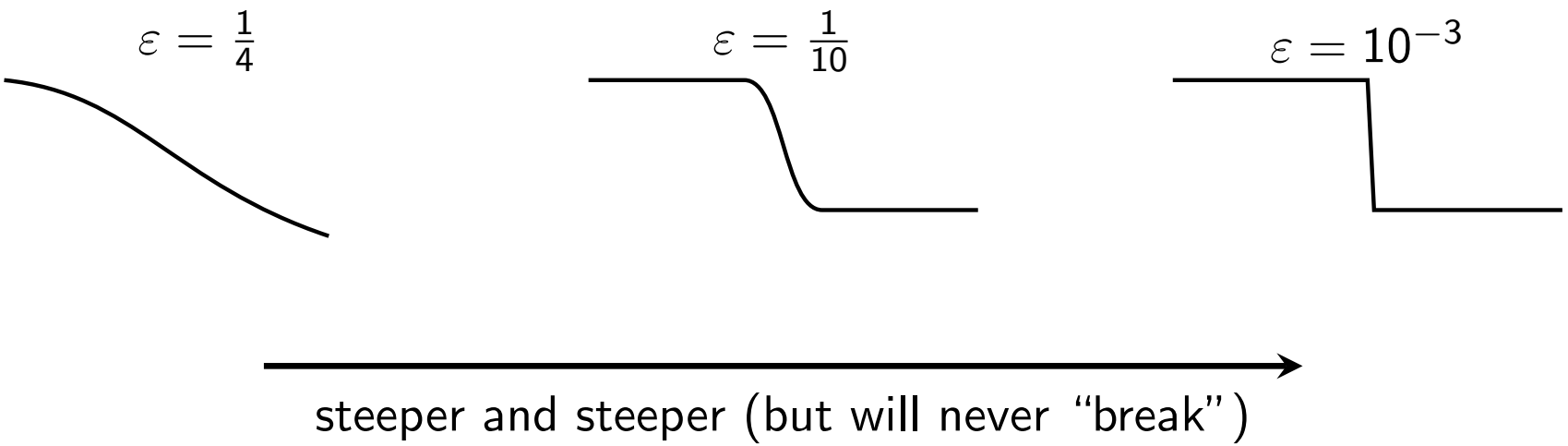
$\varepsilon = 0$ (hyperbolic) : **shock waves** are possible (depending on IC)



Some nonlinear examples [1b]

$\varepsilon > 0$

(parabolic) for $t > 0$:



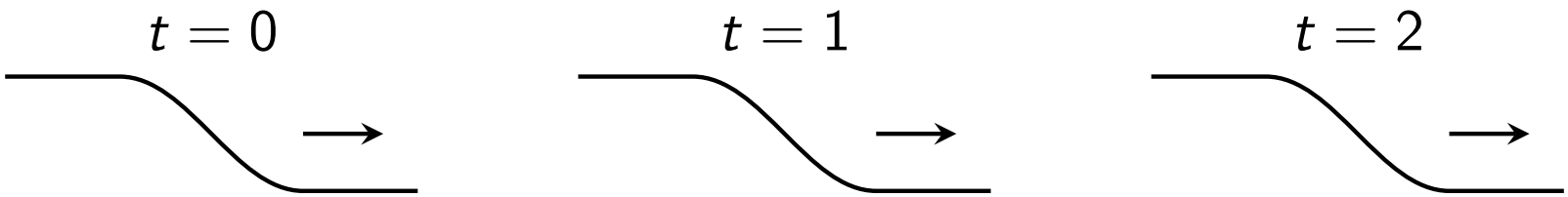
Some nonlinear examples [2]

Fisher equation

$$u_t = u_{xx} + u(1-u)$$

Travelling wave solutions are possible:

$$\text{(example)} \quad u(x,t) = \frac{1}{\left(1 + e^{\frac{x-ct}{\sqrt{6}}}\right)^2}, \quad c = \frac{5}{\sqrt{6}}$$



constant velocity c

waves do not change shape (see advection equation) note that this is a **nonlinear** PDE! $\left(\text{advection equation is linear}\right)$

Some nonlinear examples [3]

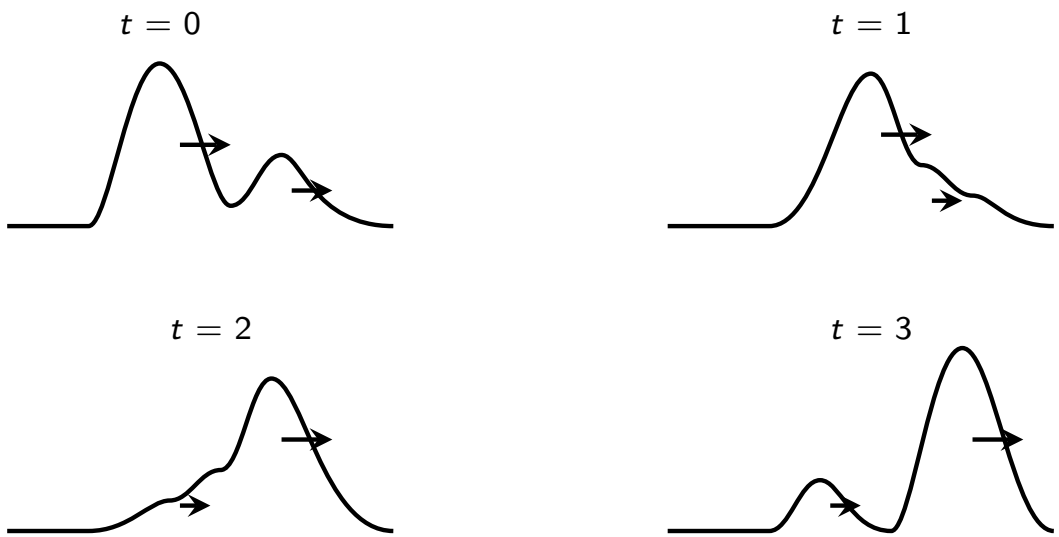
Korteweg – deVries equation "KdV"

$$u_t + 6 \underbrace{uu_x}_{\text{nonlinear}} + \underbrace{u_{xxx}}_{\text{third order}} = 0 \qquad \text{type} = ?$$

Soliton solutions:

$$u(x,t) = \frac{c}{2}\operatorname{sech}^2\left(\frac{\sqrt{c}}{2}(x - ct - x_0)\right) \qquad \left(\operatorname{sech} = \frac{1}{\cosh}\right)$$

Nonlinear superposition of waves!



Classification [1]

Two independent variables

2nd order linear PDE:

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu + G = 0$$

Suppose first: $A, B, C, \ldots$ *are constants* **Remember** 2nd order algebraic equation:

$$ax^2 + bxy + cy^2 + dx + ey + f = 0$$

These are curves in the x-y plane.

"Principal part":

- If $b^2 - 4ac > 0$, then the curve is a **hyperbola**
- If $b^2 - 4ac = 0$, then the curve is a **parabola**
- If $b^2 - 4ac < 0$, then the curve is an **ellipse**

Applying a suitable transformation of variables $\rightarrow$ **"normal form"**:

$$\begin{cases} \frac{\xi^2}{a^2} - \frac{\eta^2}{b^2} = 1 \\ \eta^2 = 4a\xi \\ \frac{\xi^2}{a^2} + \frac{\eta^2}{b^2} = 1 \end{cases}$$

Classification [2]

"Principal part" of PDE: $Au_{xx} + Bu_{xy} + Cu_{yy}$

- If $B^2 - 4AC > 0$, then the PDE is **hyperbolic**
- If $B^2 - 4AC = 0$, then the PDE is **parabolic**
- If $B^2 - 4AC < 0$, then the PDE is **elliptic**

Linear PDE with variable coefficients: $A, B, C, \ldots$ depend on x and y

(Check $B^2(x, y) - 4A(x, y)C(x, y)$*)*

- If $B^2(x, y) - 4A(x, y)C(x, y) > 0$ at (x, y), then the PDE is **hyperbolic** at (x, y)
- If $B^2(x, y) - 4A(x, y)C(x, y) = 0$ at (x, y), then the PDE is **parabolic** at (x, y)
- If $B^2(x, y) - 4A(x, y)C(x, y) < 0$ at (x, y), then the PDE is **elliptic** at (x, y)

Note: First-order derivatives and the inhomogeneous term in this PDE do not play a role in this classification!

Classification [3]

1. $u_{xx} + u_{yy} = 0$

$$A = 1, \quad B = 0, \quad C = 1 \implies B^2 - 4AC = -4 < 0 \implies \textbf{elliptic PDE}$$

2. $u_y = u_{xx} \quad (\text{of } u_{xx} - u_y = 0)$

$$A = 1, \quad B = 0, \quad C = 0 \implies B^2 - 4AC = 0 \implies \textbf{parabolic PDE}$$

3. $u_{xx} + xu_{yy} = 0 \quad (x \neq 0)$

$$A = 1, \quad B = 0, \quad C = x \implies B^2 - 4AC = -4x$$

$$\text{PDE is } \begin{cases} \textbf{hyperbolic} & \text{for } x < 0 \\ \textbf{elliptic} & \text{for } x > 0 \end{cases}$$

Classification based on eigenvalues λ_i of the principal part matrix:

4. $\Delta u = u_{xx} + u_{yy} + u_{zz} = 0$

$$\lambda_1 = \lambda_2 = \lambda_3 = 1 > 0 \quad (\text{all eigenvalues have the same sign}) \implies \textbf{elliptic PDE}$$

5. $u_z = u_{xx} + u_{yy}$

$$\lambda_1 = \lambda_2 = 1 > 0, \quad \lambda_3 = 0 \implies \textbf{parabolic PDE}$$

6. $u_{zz} = u_{xx} + u_{yy} \quad (\text{or } u_{xx} + u_{yy} - u_{zz} = 0)$

$$\lambda_1 = \lambda_2 = 1 > 0, \quad \lambda_3 = -1 < 0 \implies \textbf{hyperbolic PDE}$$

Method of characteristics [1]

Linear First-Order) PDEs
Consider (define $z(x, y)$):

$$a(x, y)z_x + b(x, y)z_y + c(x, y)z = d(x, y)$$

where a, b, c, d are given functions.

Re-write:

$$a(x, y)z_x + b(x, y)z_y = -c(x, y)z + d(x, y)$$

Observe:

$$a(x, y)z_x + b(x, y)z_y = \nabla z \cdot \begin{pmatrix} a \\ b \end{pmatrix} = D_{\begin{pmatrix} a \\ b \end{pmatrix}} z$$

(directional derivative along the vector $\begin{pmatrix} a \\ b \end{pmatrix}$*).*

ODE system (note that t in the following discussion does not represent "time"):

$$\begin{cases} \dfrac{dx}{dt} = a(x, y) \\ \dfrac{dy}{dt} = b(x, y) \end{cases}$$

Tangent vector to these curves:

$$\frac{d}{dt}\begin{pmatrix} x(t) \\ y(t) \end{pmatrix} = \begin{pmatrix} a(x, y) \\ b(x, y) \end{pmatrix}$$

Note: This gives a family of characteristic curves $x(t), y(t)$ whose tangent vector is in the direction of $\begin{pmatrix} a \\ b \end{pmatrix}$.

Method of characteristics [2]

Take the "time" derivative of z along these curves:

$$\frac{dz}{dt} = \frac{d}{dt} z(x(t), y(t)) \underset{\text{chain rule}}{=} \frac{\partial z}{\partial x}\frac{dx}{dt} + \frac{\partial z}{\partial y}\frac{dy}{dt} = z_x \cdot a(x,y) + z_y \cdot b(x,y)$$

$$\underset{\text{PDE}}{\longrightarrow} \quad = -c(x,y)z + d(x,y) \underset{\text{re-write}}{=} -c(t)z(t) + d(t)$$

Solving this ODE using an **"integrating factor"**:

$$z(t) = e^{-\int_0^t c(\tau)\,d\tau}\left[\int_0^t e^{\int_0^\tau c(\tilde{\tau})\,d\tilde{\tau}} d(\tau)\,d\tau + z(0)\right]$$

$\rightsquigarrow$ **"Method of Characteristics"** (*characteristic curves* $x(t), y(t)$)

Initial Conditions & Parameterization
Family of characteristic curves connected to the points of curve C:

$$\begin{cases} x(s,t) = \dots \\ y(s,t) = \dots \\ z(s,t) = \dots \end{cases}$$

At "time" $t = 0$ ('initial' condition for PDE on curve C):

$$\begin{cases} x(s,0) = x(s) \\ y(s,0) = y(s) \\ z(s,0) = z(s) \end{cases}$$

where s is the parameter along the initial curve C.

Method of characteristics [3]

Inversion using the Jacobian:
If the Jacobian $J = x_s y_t - x_t y_s \neq 0$ for all (s, t), then we can invert

$$x = x(s, t), \quad y = y(s, t)$$

to express s and t as functions of x and y:

$$s = s(x, y), \quad t = t(x, y)$$

$\implies z = z(x, y) = z(s(x, y), t(x, y))$ solves the original PDE and satisfies the initial condition!

Unique solution formula:

$$z(s, t) = \frac{1}{\mu(s, t)} \left[\int_0^t \mu(s, \tau) d(s, \tau) \, d\tau + g(s) \right]$$

where the integrating factor is given by $\mu(s, t) = \exp\left(\int_0^t c(s, \tau) \, d\tau \right)$.

Method of characteristics [4]

Example
(note: real time t is represented by y)

$$\begin{cases} \dfrac{\partial z}{\partial y} + \gamma \dfrac{\partial z}{\partial x} = 0 \\ z(x,0) = u_0(x) \quad \text{(given IC)} \end{cases}$$

1) Find characteristic curves:

- Parameterize initial curve C at $t = 0$: $x(s,0) = s, \quad y(s,0) = 0, \quad z(s,0) = u_0(s)$.
- Family of characteristic curves satisfy:

$$\begin{cases} \dfrac{dx}{dt}(s,t) = \gamma \\ \dfrac{dy}{dt}(s,t) = 1 \end{cases}$$

Solve (integrate):

$$\begin{cases} x(s,t) = \gamma t + c_1(s) \\ y(s,t) = t + c_2(s) \end{cases}$$

Method of characteristics [5]

Example (Continued)

2) Apply initial conditions:

$$\begin{cases} x(s,0) = s \\ y(s,0) = 0 \end{cases} \Rightarrow \begin{cases} c_1(s) = s \\ c_2(s) = 0 \end{cases} \Rightarrow \begin{cases} x(s,t) = \gamma t + s \\ y(s,t) = t \end{cases}$$

3) Here, we have $c(x,y) = 0$ and $d(x,y) = 0$:

$$\Rightarrow d(s,t) = 0, \quad \mu(s,t) = 1 \quad (\text{see } \exp(\dots))$$

Note:

$$z(x(s,0), y(s,0)) \underset{\substack{\uparrow \\ t=0}}{=} z(s,0) \underset{\substack{\uparrow \\ t=0}}{=} u_0(s) \Rightarrow \begin{cases} x(s,t) = \gamma t + s \\ y(s,t) = t \\ z(s,t) = u_0(s) \end{cases}$$

4) Transform $z(s,t) \to z(x,y)$:

$$\begin{cases} s = x - \gamma t = x - \gamma y \\ t = y \end{cases}$$

$$\Rightarrow z(x,y) = z\big(s(x,y), t(x,y)\big) = u_0(x - \gamma y)$$

*Canonical form [1]

$$A u_{xx} + B u_{xy} + C u_{yy} + D u_x + E u_y + F u + G = 0$$

transform $(x,y) \longmapsto (\xi,\eta)$: $\begin{cases} \xi = \xi(x,y) \\ \eta = \eta(x,y) \end{cases}$

Jacobian $J = \det \begin{pmatrix} \xi_x & \xi_y \\ \eta_x & \eta_y \end{pmatrix} \neq 0$ ← assume

chainrule

$$\Rightarrow \quad u_x = u_\xi \xi_x + u_\eta \eta_x \qquad u_{xx} = u_{\xi\xi}\xi_x^2 + 2u_{\xi\eta}\xi_x\eta_x + u_{\eta\eta}\eta_x^2 + u_\xi \xi_{xx} + u_\eta \eta_{xx}$$

$$u_y = u_\xi \xi_y + u_\eta \eta_y \qquad u_{yy} = u_{\xi\xi}\xi_y^2 + 2u_{\xi\eta}\xi_y\eta_y + u_{\eta\eta}\eta_y^2 + u_\xi \xi_{yy} + u_\eta \eta_{yy}$$

$$u_{xy} = u_{\xi\xi}\xi_y\xi_x + u_{\xi\eta}(\xi_x\eta_y + \xi_y\eta_x) + u_{\eta\eta}\eta_x\eta_y + u_\xi \xi_{xy} + u_\eta \eta_{xy}$$

substitute

$$\Rightarrow \begin{cases} \tilde{A}(\xi_x,\xi_y)u_{\xi\xi} + \tilde{B}(\xi_x,\xi_y,\eta_x,\eta_y)u_{\xi\eta} + \tilde{C}(\eta_x,\eta_y)u_{\eta\eta} = F(\xi,\eta,u,u_\xi,u_\eta) \\ \tilde{A} = A\xi_x^2 + B\xi_x\xi_y + C\xi_y^2 \\ \tilde{B} = 2A\xi_x\eta_x + B\cdot(\xi_x\eta_y + \xi_y\eta_x) + 2C\xi_y\eta_y \\ \tilde{C} = A\eta_x^2 + B\eta_x\eta_y + C\eta_y^2 \end{cases} \Rightarrow \tilde{B}^2 - 4\tilde{A}\tilde{C} = \underbrace{(\xi_x\eta_y - \xi_y\eta_x)^2}_{>0}(B^2 - 4AC)$$

$\Rightarrow$ same classification as before transformation !

*Canonical form [2]

Determine "special" ξ and η such that we obtain the simplest possible form

case 1 : $B^2 - 4AC > 0$ (hyperbolic) $\Rightarrow$ equation $A\alpha^2 + B\alpha + C = 0$ has two real and distinct roots

say: $\alpha = \lambda_1$ and $\alpha = \lambda_2$

choose ξ and η such that $\xi_x = \lambda_1 \xi_y$ and $\eta_x = \lambda_2 \eta_y$ (*)

$$\Rightarrow \begin{cases} \tilde{A} = A\cdot\lambda_1^2\xi_y^2 + B\lambda_1^2\xi_y^2 + C\xi_y^2 \\ \quad = \xi_y^2 \underbrace{(A\lambda_1^2 + B\lambda_1 + C)}_{=0} = 0 \\ \text{similarly: } \tilde{C} = 0 \end{cases}$$

$$\tilde{B}^2 = (B^2 - 4AC)(\xi_x\eta_y - \xi_y\eta_x)^2 > 0$$

Note: (*)'s are first-order linear PDEs in ξ and η

MofCh $\Rightarrow$ $\begin{cases} x_t = 1 \\ y_t = -\lambda_1 \end{cases}$ and $\begin{cases} x_t = 1 \\ y_t = -\lambda_2 \end{cases}$ $\Rightarrow$ $\begin{cases} \frac{dy}{dx} + \lambda_1 = 0 \\ \frac{dy}{dx} + \lambda_2 = 0 \end{cases}$

characteristic curves are: $f_1(x,y) = c_1$ and $f_2(x,y) = c_2$

divide transformed PDE (previous page) by $\tilde{B} > 0$ $\Rightarrow$ canonical form (case 1) $\boxed{u_{\xi\eta} = \varphi(\xi, \eta, u, u_\xi, u_\eta)}$

*Canonical form [3]

Case 2: $B^2 - 4AC = 0 \Rightarrow \tilde{A} = \tilde{B} = 0, \tilde{C} \neq 0$

canonical form (case2)

$$\Rightarrow \boxed{u_{\eta\eta} = \varphi(\xi, \eta, u, u_\xi, u_\eta)}$$

Case 3: $B^2 - 4AC < 0 \Rightarrow$ (complex roots)

$$\boxed{u_{\alpha\alpha} + u_{\beta\beta} = \psi(\alpha, \beta, u, u_\alpha, u_\beta)}$$

with $\begin{cases} \alpha = \frac{1}{2}(\xi + \eta) \\ \beta = \frac{1}{2i}(\xi - \eta) \end{cases}$

canonical form (case3)

Example: $u_{xx} = x^2 u_{yy}$

$A = 1, B = 0, C = -x^2 \Rightarrow \begin{cases} y + \frac{1}{2}x^2 = c_1 \\ y - \frac{1}{2}x^2 = c_2 \end{cases}$, choose $\begin{cases} \xi = y + \frac{1}{2}x^2 \\ \eta = y - \frac{1}{2}x^2 \end{cases}$

$$\Longrightarrow 4x^2 u_{\xi\eta} = u_\xi - u_\eta$$

$$\Leftrightarrow 4(\xi - \eta) u_{\xi\eta} = u_\xi - u_\eta$$

$$\Leftrightarrow \boxed{u_{\xi\eta} = \frac{1}{4(\xi - \eta)}(u_\xi - u_\eta)}$$

PDE examples [1]: Fourier and linear PDEs [1]

The most basic of all problems involving partial differential equations are linear PDEs with constant coefficients posed on unbounded domains. Such problems are translation-invariant, and as a result, their solutions can be found by the Fourier transform.

For example, here are three linear constant-coefficient equations in one space variable:

$$u_t = u_x, \qquad u_t = -u_{xx} - u_{xxxx}, \qquad u_t = u_{xxxx}. \tag{1}$$

Inserting the ansatz $u(x,t) = \exp(\mathrm{i}kx + f(k)t)$ gives a relation between k and $f(k)$—the *dispersion relation*,

$$f(k) = \mathrm{i}k, \qquad f(k) = k^2 - k^4, \qquad f(k) = k^4.$$

The corresponding solutions for real k are

$$u(x,t) = e^{\mathrm{i}kx + \mathrm{i}kt}, \qquad u(x,t) = e^{\mathrm{i}kx + (k^2 - k^4)t}, \qquad u(x,t) = e^{\mathrm{i}kx + k^4 t}. \tag{2}$$

Fourier analysis tells us that in the space L^2 defined by the norm $\|u\| = (\int_{-\infty}^{\infty} |u(x)|^2 \, \mathrm{d}x)^{1/2}$, all solutions to (1) can be obtained as superpositions of the solutions (2):

$$u(x,t) \;=\; \int_{-\infty}^{\infty} \hat{u}(k,t) e^{\mathrm{i}kx} \, \mathrm{d}k \;=\; \int_{-\infty}^{\infty} \hat{u}(k,0) e^{\mathrm{i}kx + f(k)t} \, \mathrm{d}k, \tag{3}$$

where $\hat{u}(k,t)$ denotes the Fourier transform of $u(x,t)$ with respect to x. In other words, $\hat{u}(k,t)$ evolves for each k according to the trivial ordinary differential equation $\hat{u}_t = f(k)\hat{u}$ with solution $\hat{u}(k,t) = \exp(f(k)t)\hat{u}(k,0)$. Thus we see that for linear equations with constant coefficients on unbounded domains, when we take the Fourier transform,

- *Differential operators become polynomials in k*, and
- *The PDE becomes an uncoupled system of ODEs, one ODE for each k.*

[1] © Nick Trefethen, Oxford University

PDE examples [2]: forward heat equation

$$u_t = \Delta u.$$

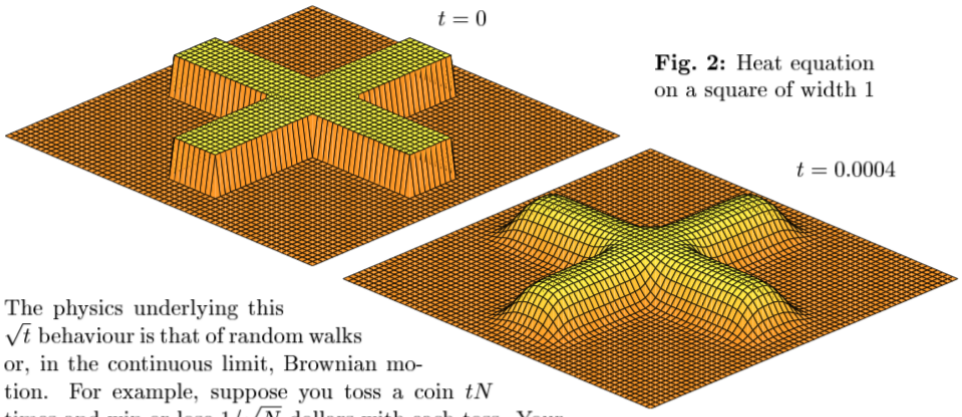


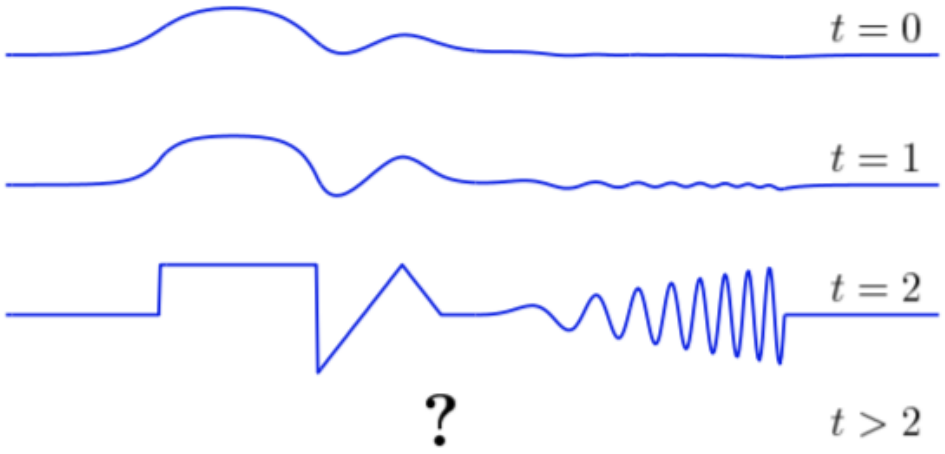
Fig. 2: Heat equation on a square of width 1

The physics underlying this $\sqrt{t}$ behaviour is that of random walks or, in the continuous limit, Brownian motion. For example, suppose you toss a coin tN times and win or lose $1/\sqrt{N}$ dollars with each toss. Your profit follows a binomial distribution that converges to the Gaussian $e^{-x^2/4t}/\sqrt{4\pi t}$ in the limit $N \to \infty$. Arbitrarily large profits are possible, but anything much bigger than $\sqrt{t}$ is very unlikely. This $\sqrt{t}$ effect is at the root of much of the field of statistics, and it was the basis of Einstein's epochal paper on Brownian motion in his *annus mirabilis* 1905.

PDE examples [3]: backward heat equation

$$u_t = -\Delta u.$$

Fig. 1: Loss of smoothness



PDE examples [4]: wave equation

$$u_{tt} = \Delta u,$$

The wave equation describes linear, nondispersive wave propagation. For example, Figure 1 presents a pair of images that show the outward spread of a circular pulse in 2D. At $t = 0$ we begin with a cone of radius 0.1 with $u_t(0) = 0$. At $t = 2$, the cone has spread to a concentric ring of outer radius exactly 2.1.

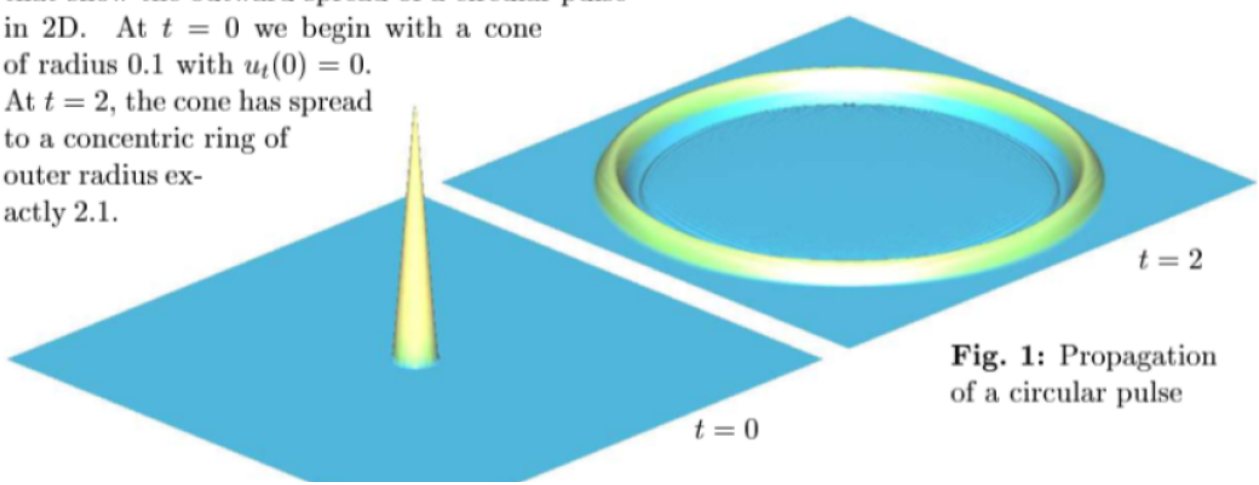


Fig. 1: Propagation of a circular pulse

PDE examples [5]: beam equation

$$u_{tt} = -u_{xxxx}.$$

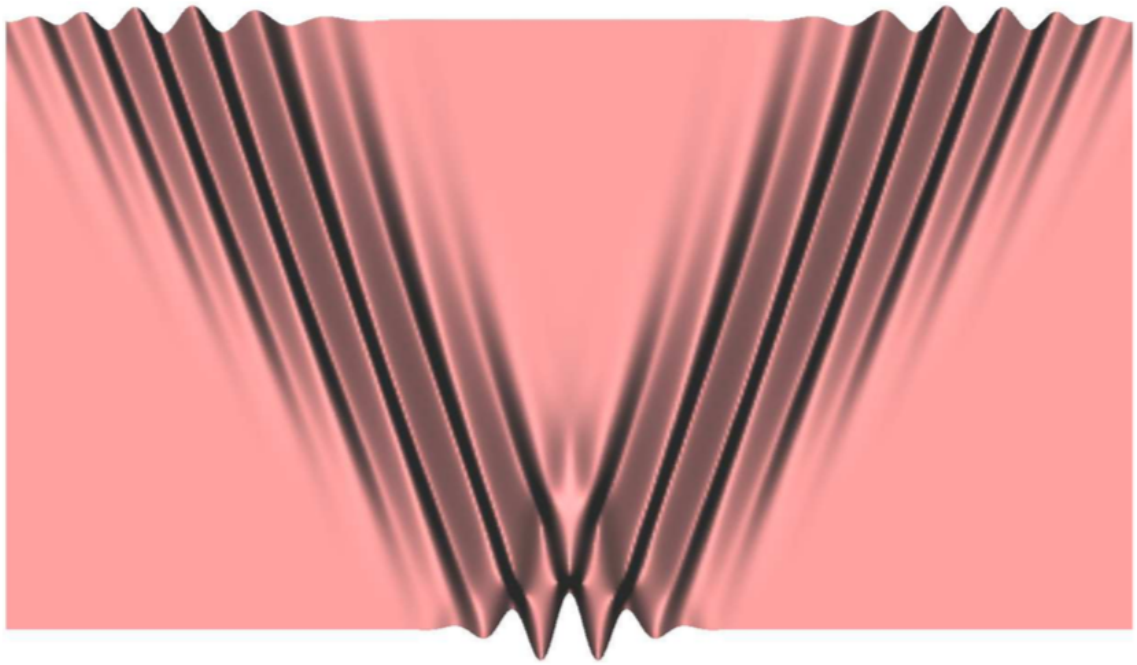


Fig. 1: Wave propagation with $c = \pm 4$, $c_g = \pm 8$

PDE examples [6]: Schrödinger equation

The Schrödinger equation, the basis of quantum mechanics, was discovered by Erwin Schrödinger during his skiing holiday at the end of 1925 and analyzed by him in a series of papers published in *Annalen der Physik* in 1926. By the end of that year, the face of physics had changed. Schrödinger won the Nobel Prize in Physics in 1933.

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar}{2m}\Delta + V(\mathbf{r})\right]\Psi(\mathbf{r},t) \tag{1}$$

where $\mathrm{i} = \sqrt{-1}$, Ψ is called the *wave function* and $\hbar$ is Planck's constant divided by 2π. Since our convention in this book is to take u as the dependent variable and strip away constants, we shall take the *time-dependent Schrödinger equation* instead to be

$$\boxed{\mathrm{i}u_t = [-\Delta + V(\mathbf{r})]u.} \tag{2}$$

PDE examples [7]: Gray-Scott model

The *Gray–Scott equations* were formulated originally by Gray and Scott in 1983; we shall not discuss their original chemical motivation:

$$u_t = \epsilon_1 \Delta u - uv^2 + F(1-u), \qquad v_t = \epsilon_2 \Delta v + uv^2 - (k+F)v. \tag{1}$$

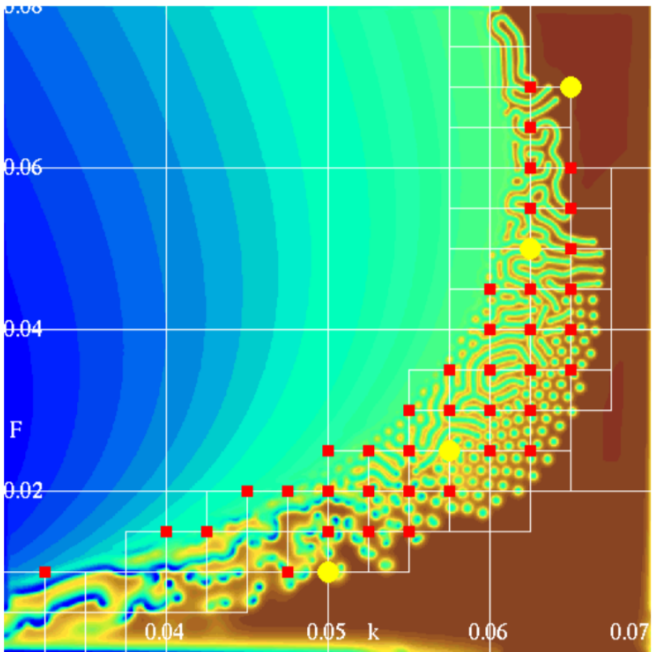


Fig. 2. Dependence on k and F.

PDE examples [8]: Korteweg-de Vries equation

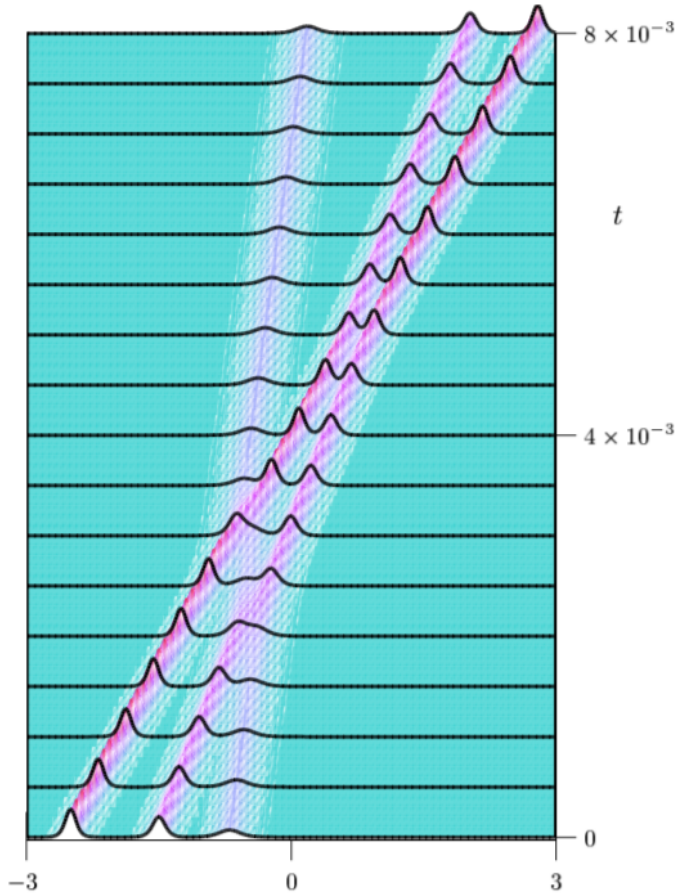


Fig. 1: Soliton interactions

$$u_t + uu_x + u_{xxx} = 0.$$

PDE examples [9]: sine-Gordon model

$$u_{tt} - u_{xx} = \sin u.$$

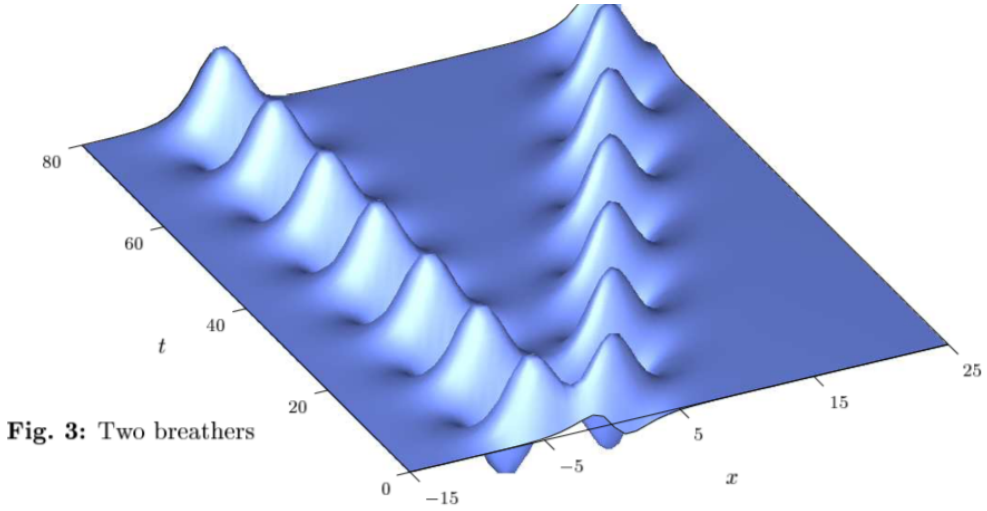


Fig. 3: Two breathers

PDE examples [10]: compacton equations

$$u_t + (u^m)_x + (u^n)_{xxx} = 0.$$

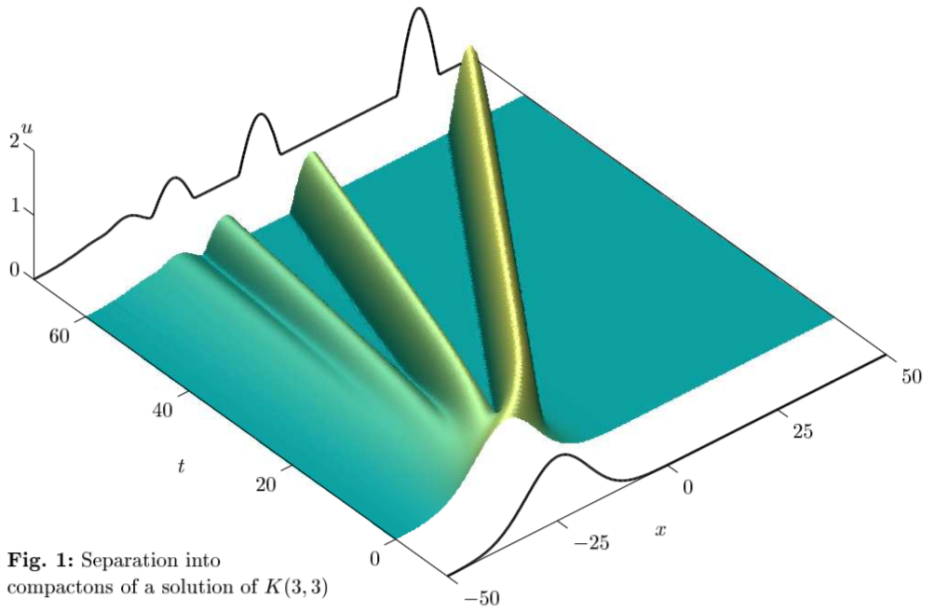


Fig. 1: Separation into compactons of a solution of $K(3,3)$

PDE examples [11]: Boussinesq equation

$$u_{tt} - u_{xx} = u_{xxxx} + (u^2)_{xx},$$

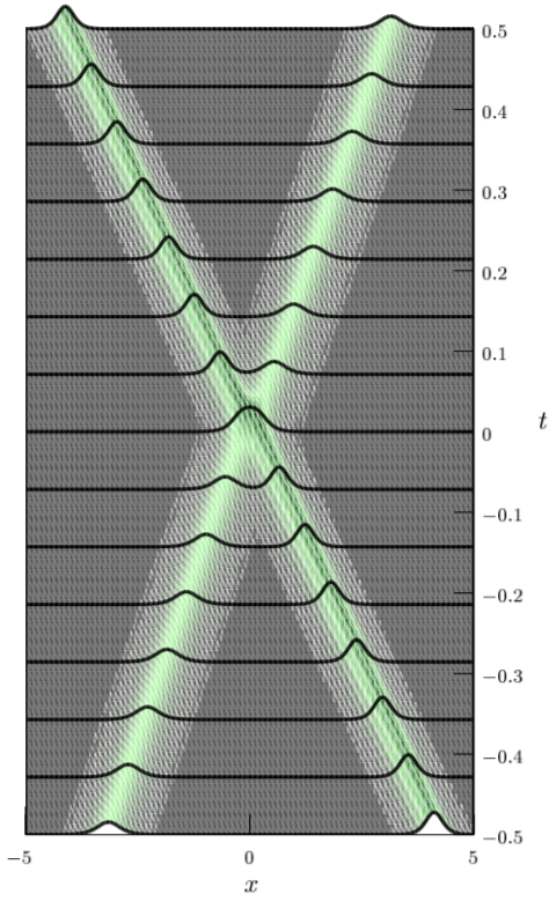


Fig. 2: soliton interactions

PDE examples [12]: blow-up with u^p nonlinearity

$$u_t = u_{xx} + u^p$$

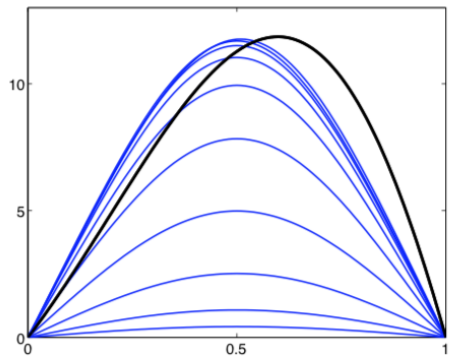


Fig. 2: $\alpha = 6.84$: decay to 0
($t = 0, 0.1, 0.2, \ldots, 1$ from top to bottom)

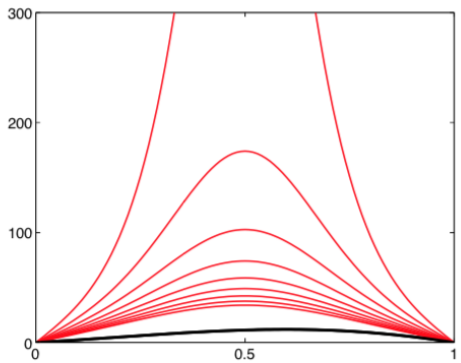


Fig. 3: $\alpha = 6.85$: blow-up
($t = 0, 0.8, 0.805, 0.810, \ldots, 0.840$ from bottom to top)

PDE examples [13]: blow-up with e^u nonlinearity

$$u_t = u_{xx} + \lambda e^u$$

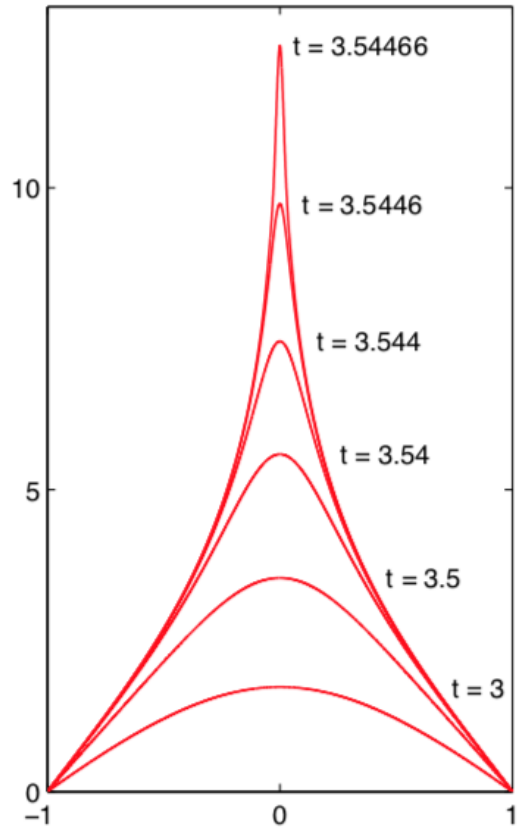


Fig. 1: blowup at $t \approx 3.54466$ with $\lambda = 1$ and zero initial data.

PDE examples [14]: advection-diffusion

$$u_t + \mathbf{a} \cdot \nabla u = \varepsilon \Delta u.$$

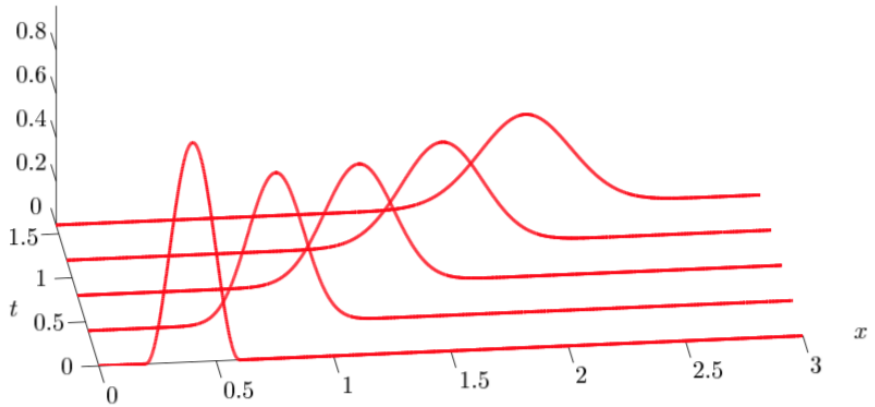


Fig. 1: Solution with $a(x,t) = 1$, $\varepsilon = 10^{-2}$

PDE examples [15]: porous media

$$u_t = \Delta(u^m).$$

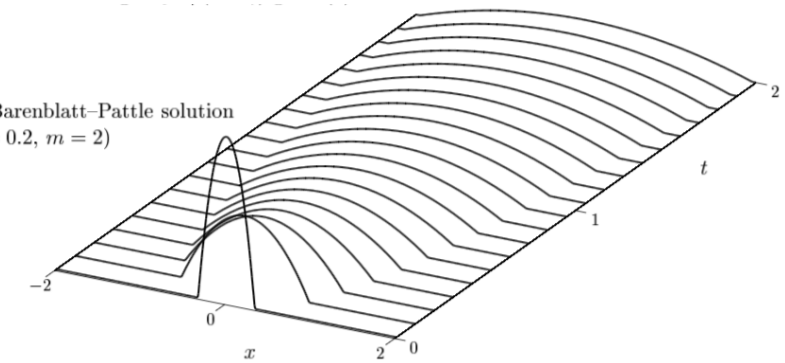


Fig. 1: 1D Barenblatt–Pattle solution ($\Gamma = 0.2$, $m = 2$)

PDE examples [16]: Allen-Cahn equation

$$u_t = u_{xx} + u - u^3.$$

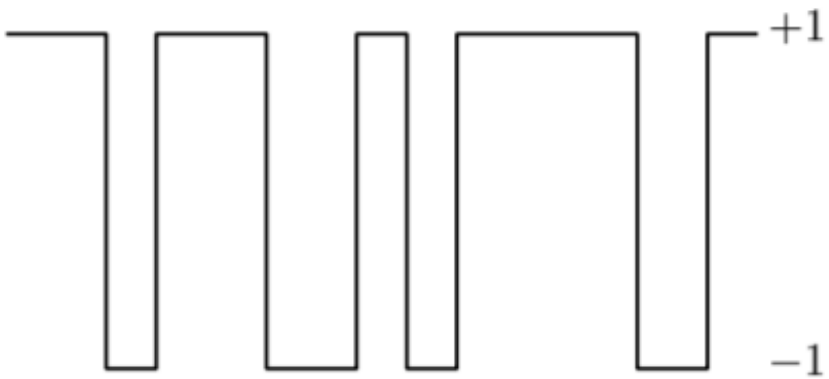


Fig. 1: Metastable fronts (schematic)

PDE examples [17]: Cahn-Hilliard equation

$$u_t = \Delta(u^3 - u) - \varepsilon \Delta^2 u.$$

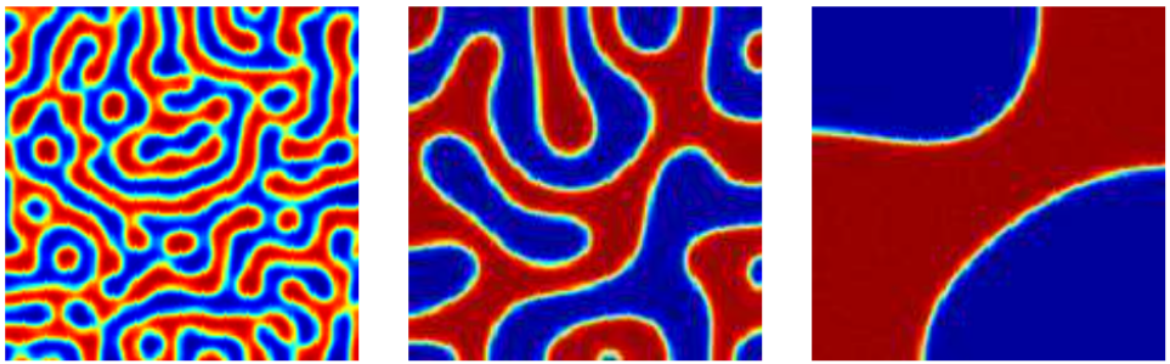


Fig. 1: Solutions in 2D for small, medium, and large t

PDE examples [18]: Perona-Malik model

$$u_t = \nabla \cdot \left(g(|\nabla u|) \, \nabla u \right),$$

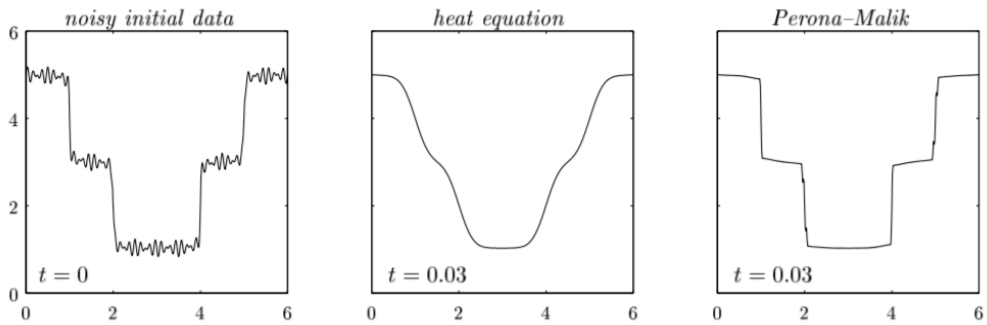
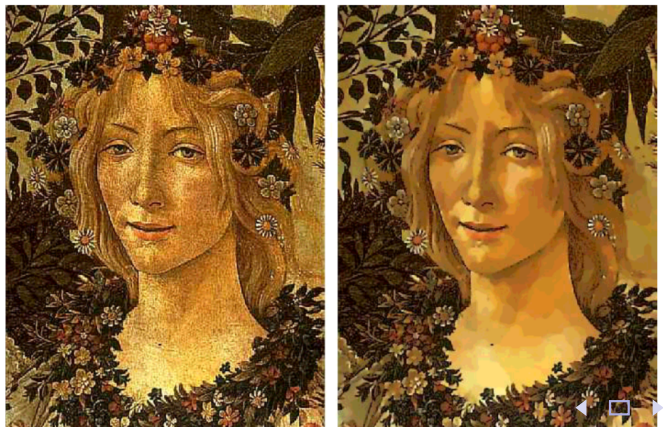


Fig. 1: Edge enhancement in 1D



PDE examples [19]: Kuramoto-Sivashinsky model

$$u_t + uu_x = -u_{xx} - u_{xxxx}.$$

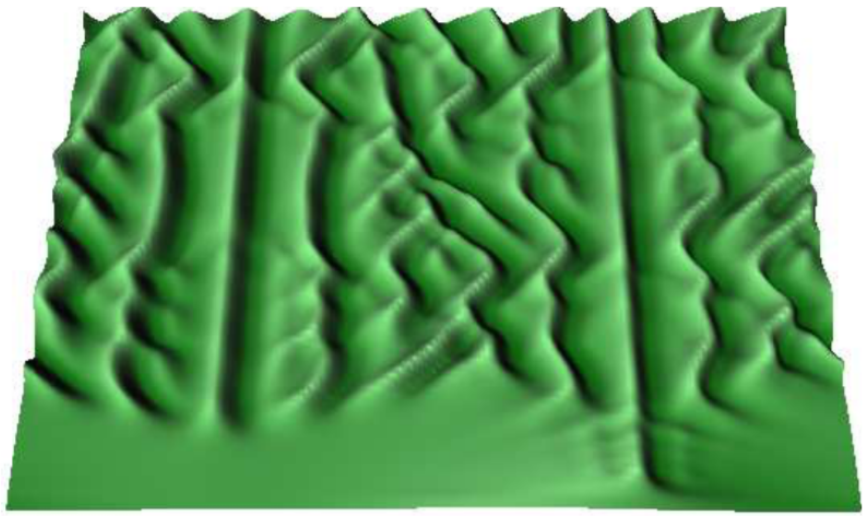


Fig. 2: Chaotic structure emerging from smooth initial data

PDE examples [20]: Ginzburg-Landau equations

$$u_t = (1 + \mathrm{i}\nu)u_{xx} + u - (1 + \mathrm{i}\mu)u|u|^2, \qquad u \in \mathbb{C}$$

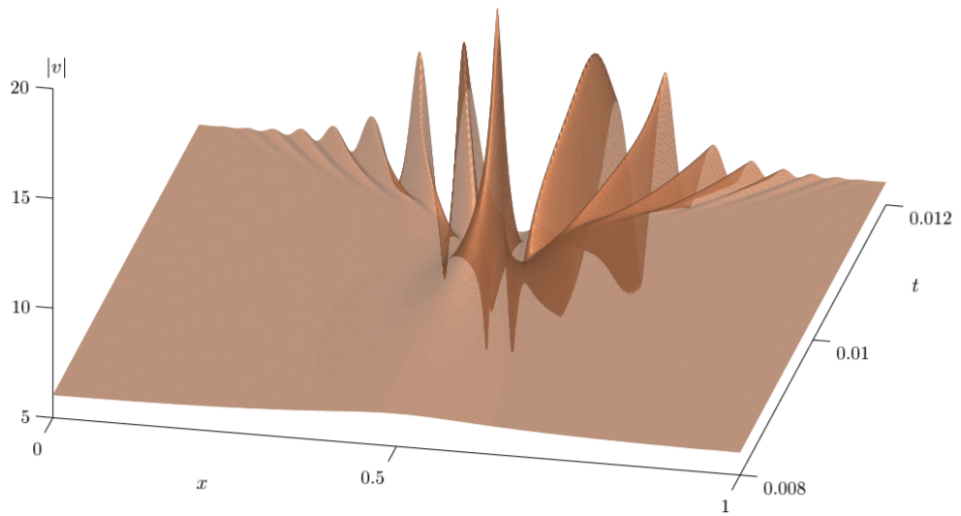


Fig. 2: Burst and collapse for a quintic complex Ginzburg–Landau equation

PDE examples [21]: Klein-Gordon model

$$u_{tt} = \nabla^2 u - u,$$

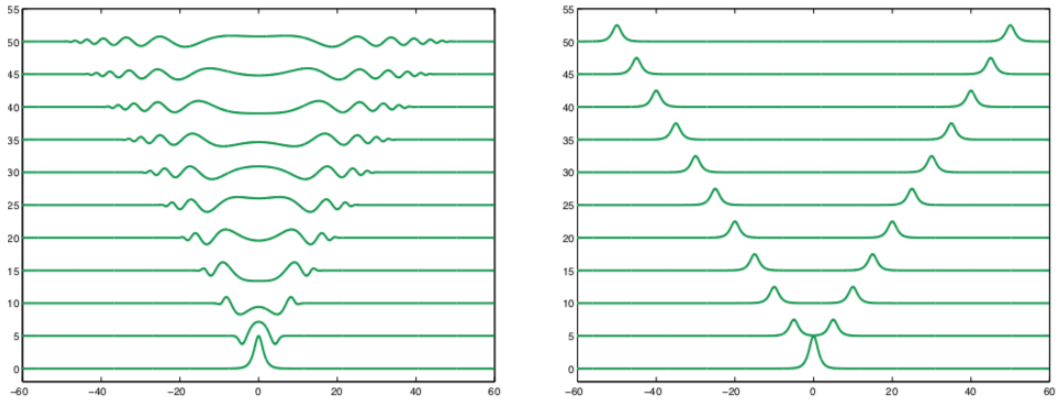


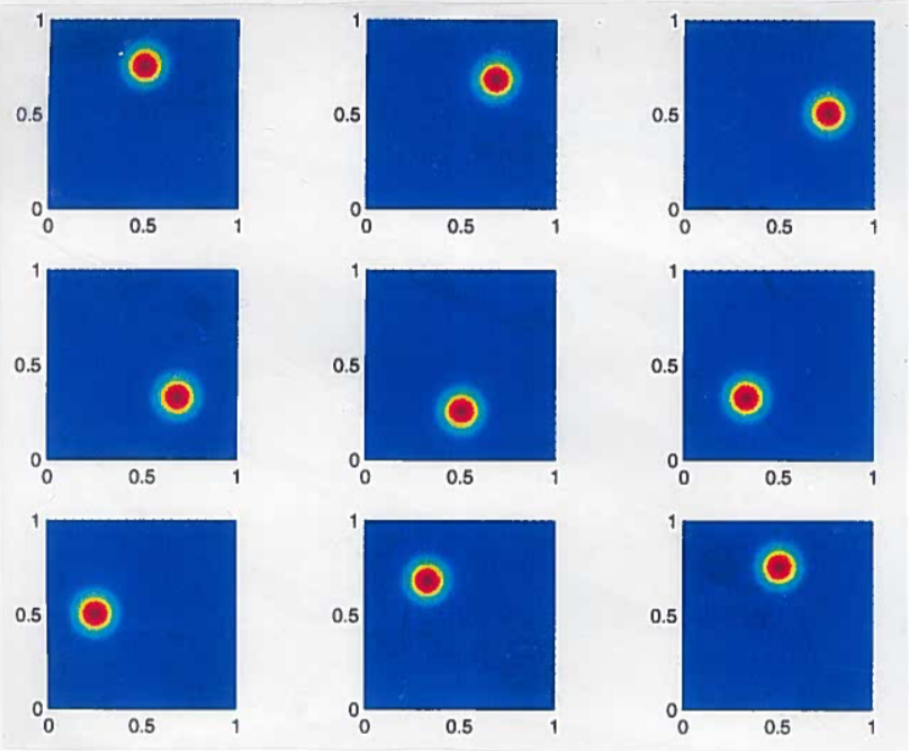
Fig. 1: Klein–Gordon (left) and wave equations (right)

PDEs in two space dimensions [1]

- solution = rotating cone (non-changing shape $\forall t \geq 0$)

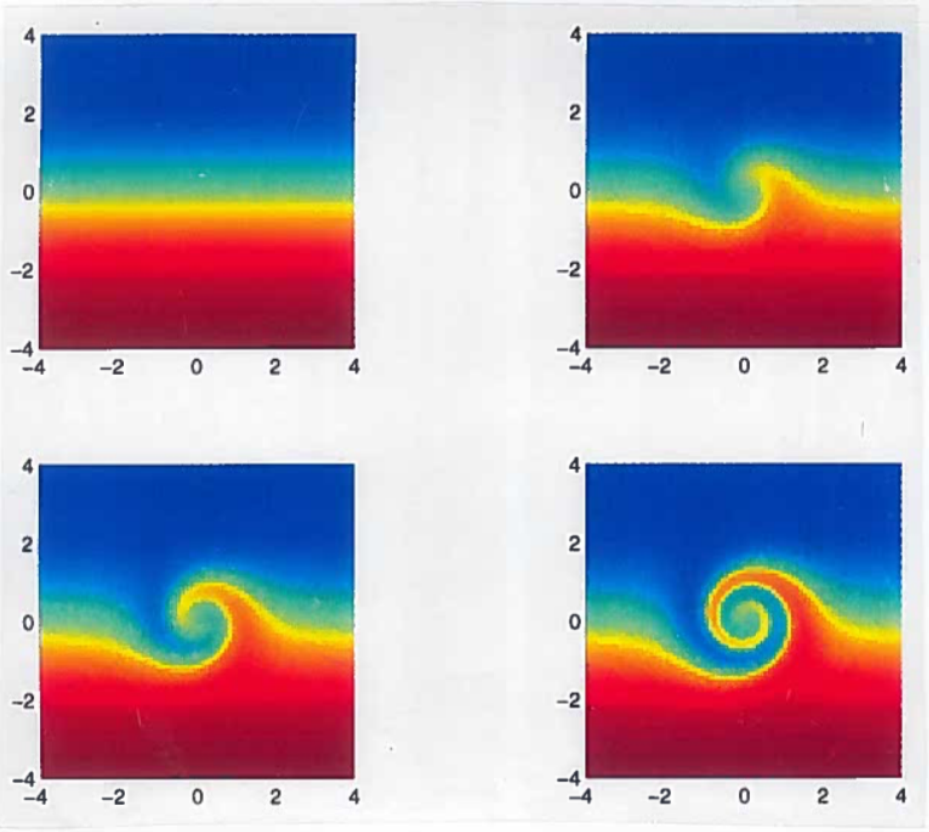
∇ !

$$\begin{cases} \text{heat equation with source (parabolic)} : u_t = \Delta u + f \\ \text{transport equation (hyperbolic)} : u_t + \beta_1 u_x + \beta_2 u_y = 0 \end{cases}$$



PDEs in two space dimensions [2]

- hyperbolic PDE
- hurricane model from meteorology
- developing 'whirlpool'

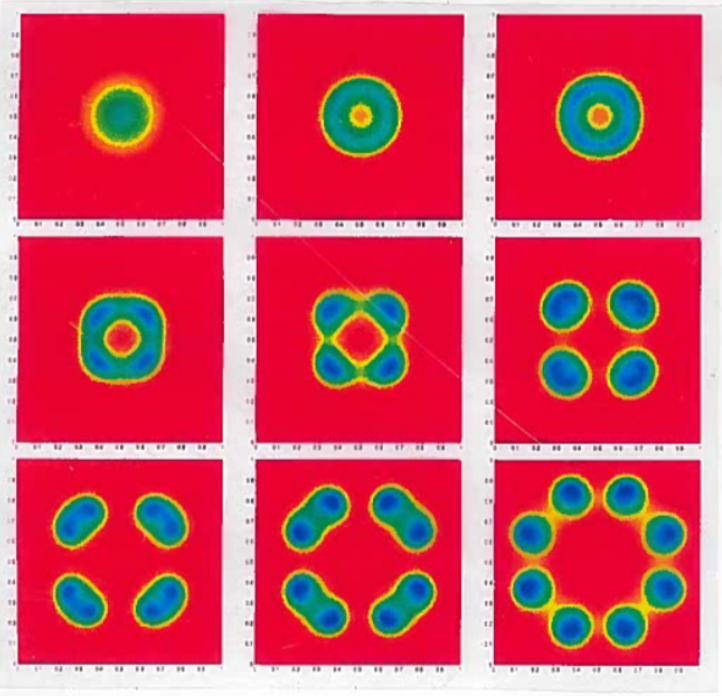


$$\frac{\partial u}{\partial t} + r_1 \frac{\partial u}{\partial x} + r_2 \frac{\partial u}{\partial y} = 0$$

$$\nabla \cdot \begin{pmatrix} r_1 \\ r_2 \end{pmatrix} = 0$$

PDEs in two space dimensions [3]

$$\frac{\partial u}{\partial t} = D_1 \Delta u + f_1(u,v)$$
$$\frac{\partial v}{\partial t} = D_2 \Delta v + f_2(u,v)$$



- parabolic PDE (s)
- reaction-diffusion system from chemistry
- splitting pulses

Application areas



- weather prediction & climate models
- chemical reactions
- ecology, biology, ...
- traffic flow
- financial models
- geology, hydrology, ...
- languages, archaeology
- fluid flow, MHD
- water flows, rivers, oceans, ...
- image processing, visualization
- ETCETERA...!!!

Fourier series method [1]

Method of separation of variables

Seek a solution of the form:

$$u(x,t) = X(x)T(t) \qquad (\star) \quad \Leftrightarrow \quad \text{find } X(x) \text{ and } T(t)$$

Example: Heat equation in 1D

$$u_t = \alpha^2 u_{xx}, \qquad x \in [0, L], \ t > 0$$

$$u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \qquad \text{(BCs)}$$

$$u(x,0) = u_0(x), \qquad x \in [0, L] \qquad \text{(IC)}$$

$u \sim$ temperature
$L \sim$ length of bar
$u_0 \sim$ initial temperature

1) From $(\star)$:

$$u_t = X(x)\dot{T}(t), \qquad u_{xx} = X''(x)T(t)$$

Substitute:

$$\Rightarrow \quad \underbrace{\frac{\dot{T}(t)}{\alpha^2 T(t)}}_{\text{function of } t} = \underbrace{\frac{X''(x)}{X(x)}}_{\text{function of } x}$$

(this must hold for all t and x under consideration!) $\Rightarrow$

Fourier series method [2]

$$\implies \frac{\dot{T}(t)}{\alpha^2 T(t)} = \frac{X''(x)}{X(x)} = c \quad \text{(constant)} \implies \begin{cases} \dot{T}(t) - \alpha^2 c T(t) = 0 \\ X''(x) - cX(x) = 0 \end{cases}$$

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2) Apply BCs:

$$u(0,t) = X(0)T(t) = 0 \quad \& \quad u(L,t) = X(L)T(t) = 0 \qquad \forall t > 0$$

- If $T(t) = 0 \ \ \forall t > 0 \implies u(x,t) = 0$ **(trivial solution)** $\times$
- Or, if $X(0) = X(L) = 0$ **(nontrivial solutions)**

$$\implies \begin{cases} X''(x) - cX(x) = 0 \\ X(0) = X(L) = 0 \end{cases}$$

Three cases:

1. **Case $c > 0$ ($c = \lambda^2$):**

$$X(x) = C_1 e^{\lambda x} + C_2 e^{-\lambda x} \xrightarrow{\text{BCs}} C_1 = C_2 = 0 \implies X = 0 \implies u = 0 \quad \times$$

2. **Case $c = 0$:**

$$X(x) = C_3 + C_4 x \xrightarrow{\text{BCs}} C_3 = C_4 = 0 \implies X = 0 \implies u = 0 \quad \times$$

3. **Case $c < 0$ ($c = -\lambda^2$):**

$$X(x) = C_5 \cos(\lambda x) + C_6 \sin(\lambda x)$$

$$\xrightarrow{\text{BCs}} \begin{cases} X(0) = C_5 = 0 \\ X(L) = C_5 \cos(\lambda L) + C_6 \sin(\lambda L) = 0 \implies C_6 \sin(\lambda L) = 0 \end{cases}$$

Fourier series method [3]

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Since $C_6 \neq 0$ for non-trivial solutions:

$$\sin(\lambda L) = 0 \implies \lambda L = n\pi, \quad n = 0, \pm 1, \pm 2, \ldots$$

$$\implies \lambda_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots \qquad (n = 0 \implies u = 0 \times, \quad n = -1, -2, \cdots \implies \text{no extra info})$$

Eigenfunctions:

$$X_n(x) = a_n \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \ldots \qquad (a_n \leftrightarrow C_6)$$

Fourier series method [4]

3) Apply IC:

$$c = -\lambda_n^2 = -\left(\frac{n\pi}{L}\right)^2 \implies T_n(t) = b_n e^{-\alpha^2\left(\frac{n\pi}{L}\right)^2 t}, \qquad n = 1, 2, 3, \ldots$$

(from $\dot{T}(t) - \alpha^2 c T(t) = 0$*)*

$$\implies u_n(x,t) = X_n(x)T_n(t) = a_n \sin\left(\frac{n\pi x}{L}\right) \cdot b_n e^{-\alpha^2\left(\frac{n\pi}{L}\right)^2 t}$$

$$= c_n e^{-\alpha^2\left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi x}{L}\right), \qquad n = 1, 2, 3, \ldots \quad (c_n = a_n b_n)$$

Fourier series method [5]

Linear, homogeneous PDE $\Longrightarrow$ "Superposition principle":

$$u(x,t) = \sum_{n=1}^{\infty} u_n(x,t) = \sum_{n=1}^{\infty} c_n e^{-\alpha^2 \left(\frac{n\pi}{L}\right)^2 t} \sin\left(\frac{n\pi x}{L}\right)$$

Apply IC at $t = 0$:

$$u(x,0) = \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right) = u_0(x), \qquad x \in [0, L]$$

(Fourier sine series expansion $= \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi x}{L}\right)$*)*

$$\Longrightarrow \quad c_n = \frac{2}{L} \int_0^L u_0(x) \sin\left(\frac{n\pi x}{L}\right) dx$$

We have solved the PDE!

$$u(x,t) \approx \sum_{n=1}^{N} c_n \sin\left(\frac{n\pi x}{L}\right) \ldots\ldots\ldots\ldots \text{(what are the } c_n\text{'s?)}$$

Fourier transform method [1]

Heat Equation on an Infinite Domain
Consider:

$$\begin{cases} u_t = \alpha^2 u_{xx}, & x \in (-\infty, \infty),\ t > 0 \\ u(x,0) = u_0(x), & x \in (-\infty, \infty) \end{cases}$$

This holds when $u_0(x)$ is continuous, $u \to 0$ and $u_x \to 0$ as $x \to \pm\infty$ for $t > 0$, and $\int_{-\infty}^{\infty} |u_0(x)|\, dx < \infty$.

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1) Transform PDE to ODE:

Apply Fourier transform to the PDE and initial condition (IC):

$$\mathcal{F}[u] = \hat{u}(\omega, t), \qquad \mathcal{F}[u_0(x)] = \hat{u}_0(\omega)$$

Using the derivative property of the Fourier transform ($\mathcal{F}[u_{xx}] = -\omega^2 \hat{u}$):

$$\begin{cases} \mathcal{F}[u_t] = \mathcal{F}[\alpha^2 u_{xx}] \implies \dfrac{d}{dt}\hat{u}(\omega, t) = -\alpha^2 \omega^2 \hat{u}(\omega, t) \\ \mathcal{F}[u(x,0)] = \mathcal{F}[u_0(x)] \implies \hat{u}(\omega, 0) = \hat{u}_0(\omega) \end{cases}$$

2) Solve ODE (for fixed ω):

$$\hat{u}(\omega, t) = \hat{u}_0(\omega) e^{-\alpha^2 \omega^2 t}$$

3) Apply inverse transform:

$$u(x,t) = \mathcal{F}^{-1}[\hat{u}(\omega, t)] = \mathcal{F}^{-1}\left[\hat{u}_0(\omega) e^{-\alpha^2 \omega^2 t}\right]$$

Fourier transform method [2]

3) Apply inverse transform:

$$u(x,t) = \mathcal{F}^{-1}[\hat{u}(\omega,t)] = \mathcal{F}^{-1}\left[\hat{u}_0(\omega)e^{-\alpha^2\omega^2 t}\right]$$

4) Use convolution property:

$$u(x,t) = \mathcal{F}^{-1}[\hat{u}_0(\omega)] * \mathcal{F}^{-1}\left[e^{-\alpha^2\omega^2 t}\right]$$

$$= u_0(x) * \left[\frac{1}{\sqrt{2\alpha^2 t}}e^{-\frac{x^2}{4\alpha^2 t}}\right]$$

$$= \frac{1}{2\sqrt{\alpha^2\pi t}}\int_{-\infty}^{\infty} u_0(\bar{x})e^{-\frac{(x-\bar{x})^2}{4\alpha^2 t}}\,d\bar{x}$$

Numerical approximation:

$$u(x,t) \approx \frac{1}{2\sqrt{\alpha^2\pi t}}\int_{-M}^{M} u_0(\bar{x})e^{-\frac{(x-\bar{x})^2}{4\alpha^2 t}}\,d\bar{x} \approx \ldots \qquad (M = ?)$$

(using numerical quadrature)

Fourier transform method [3]

Another example:

$$u_t + \gamma u_x = 0 \qquad (\star), \qquad u(x,0) = u_0(x)$$

Fourier transform definitions:

$$\mathcal{F}[u] = \hat{u}(\omega, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x,t) e^{-i\omega x}\, dx$$

$$\mathcal{F}^{-1}[\hat{u}] = u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(\omega,t) e^{i\omega x}\, d\omega$$

Apply to $(\star)$:

$$\Rightarrow \begin{cases} \frac{d}{dt}\hat{u}(\omega,t) + \gamma i\omega \hat{u}(\omega,t) = 0 & \text{(ODE)} \\ \hat{u}(\omega,0) = \hat{u}_0(\omega) \end{cases}$$

Fourier transform method [4]

Solve ODE:

$$\implies \hat{u}(\omega, t) = \hat{u}_0(\omega) e^{-i\omega\gamma t}$$

Inverse Fourier transform:

$$\implies u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\omega\gamma t} \hat{u}_0(\omega) e^{i\omega x} \, d\omega$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}_0(\omega) e^{i\omega(x-\gamma t)} \, d\omega$$

$$= u_0(x - \gamma t)$$

Note:

$$|\hat{u}(\omega, t)| = |\hat{u}_0(\omega)| \qquad \forall\, t \geq 0$$

"Each Fourier component maintains its original amplitude and is modified only in phase"
*(***travelling wave** *behaviour)*

Outlook to Lecture 2

- exercises for Lecture 1 (see webpage!)
- finite difference approximations of derivatives
- method of undetermined coefficients
- finite difference *matrices* and their *eigenvalues*
- treatment of boundary conditions
- non-uniform grids & transformations
- boundary-value models (stationary)