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Numerical Methods for Partial Differential Equations

Introduction to PDEs

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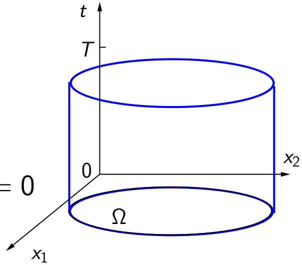
Partial Differential Equation

$\Omega \subset \mathbb{R}^d$ (with $d = 1, 2, 3$) open and bounded domain (space domain)
$(t_0, T) \subset \mathbb{R}$ an open interval (time domain)
$u : \Omega \times (t_0, T) \to \mathbb{R}$ a function.



A Partial Differential Equation (PDE)

$$F\left(\mathbf{x}, t, u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \ldots, g\right) = 0$$

is a relation between:
– two independent variables t and $\mathbf{x}$,
– a function $u = u(\mathbf{x}, t)$ and its partial derivatives,
- the data g

g	$\longrightarrow$	PDE	$\longrightarrow$	u
(data)		(model)		(solution)

The PDE $F(\mathbf{x}, t, u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \ldots, g) = 0$ can also be written as

$$L(\mathbf{x}, t, u) = f$$

L is called **partial differential operator**, while f is the right hand side.

Definition. If L is linear in u, i.e.

$$L(\mathbf{x}, t, \alpha_1 u_1 + \alpha_2 u_2) = \alpha_1 L(\mathbf{x}, t, u_1) + \alpha_2 L(\mathbf{x}, t, u_2),$$

for any $\alpha_1,\ \alpha_2 \in \mathbb{R}$ (or $\mathbb{C}$), then, the **PDE** is called **linear**, otherwise non-linear.

Elementary differential operators

Let $u = u(\mathbf{x})$ a scalar function and $\mathbf{b} = [b_1(\mathbf{x}), \ldots, b_d(\mathbf{x})]$ a vector function.

- gradient of u: $\nabla u = \begin{bmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_d} \end{bmatrix}$
- divergence of $\mathbf{b}$: $\text{div}\, \mathbf{b} = \nabla \cdot \mathbf{b} = \dfrac{\partial b_1}{\partial x_1} + \cdots + \dfrac{\partial b_d}{\partial x_d}$
- Laplacian of u: $\Delta u = \nabla \cdot (\nabla u) = \dfrac{\partial^2 u}{\partial x_1^2} + \cdots + \dfrac{\partial^2 u}{\partial x_d^2}$
- curl of $\mathbf{b} \in \mathbb{R}^3$: $\text{curl}\, \mathbf{b} = \nabla \times \mathbf{b} = \det \begin{bmatrix} i & j & k \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ b_1 & b_2 & b_3 \end{bmatrix}$

Poisson and Laplace equations

Given $f : \Omega \to \mathbb{R}$, look for $u : \Omega \to \mathbb{R}$ such that

$$-\Delta u = f \qquad \text{in } \Omega$$

[Laplace when $f \equiv 0$]

Some applications:

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steady state of the diffusion of a drop of soluble substance in a liquid

u = ink concentration

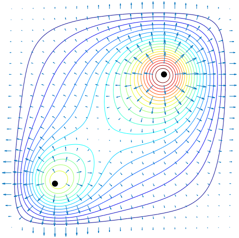
f = source of ink

Photo by Edith Lüthi from Pixabay

an elastic membrane subject to an external force (steady case)

u = vertical displacement

f = external force



electric potential generated by two ideal charges

u = electric potential

$f = \rho/\epsilon$ (density over dielectric constant)

Heat equation

Given $f : \Omega \times (t_0, T) \to \mathbb{R}$, look for $u : \Omega \times (t_0, T) \to \mathbb{R}$ such that

$$\frac{\partial u}{\partial t} - \mu \Delta u = f \qquad \text{in } \Omega \times (t_0, T)$$

- u = temperature of a body occupying the space Ω
- f = heat source
- μ = thermal diffusivity

The larger μ, the faster the heat diffusion

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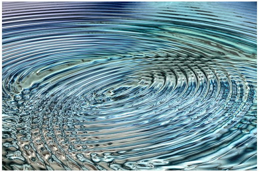
Wave equation

Given $f : \Omega \times (t_0, T) \to \mathbb{R}$, look for $u : \Omega \times (t_0, T) \to \mathbb{R}$ such that

$$\frac{\partial^2 u}{\partial t^2} - c\Delta u = f \qquad \text{in } \Omega \times (t_0, T)$$

- u = wave form
- f = source
- c = speed of propagation ($c > 0$)

plane wave



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incident circular waves on water surface

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Convection-diffusion-reaction equation

Given $f : \Omega \times (t_0, T) \to \mathbb{R}$, $\mu = \mu(\mathbf{x}) > 0$, $\mathbf{b}(\mathbf{x})$, and $\gamma(\mathbf{x}) > 0$, look for $u : \Omega \times (t_0, T) \to \mathbb{R}$ such that

$$\frac{\partial u}{\partial t} - \underbrace{\nabla \cdot (\mu \nabla u)}_{\textit{diffusion}} + \underbrace{\nabla \cdot (\mathbf{b} u)}_{\textit{convection}} + \underbrace{\gamma u}_{\textit{absorption (or reaction)}} = f$$

Photo by Nikola Belopitov from Pixabay

pollution diffusion due to industrial chimneys in the presence of wind **b**

Florida Division of Plant Industry, Florida Department of Agriculture and Consumer Services, Bugwood.org. CC3.0

evolution of population abundance, $\mathbf{b} =$ growth rate, $\gamma =$mortality rate, $\mu =$ stochastic dispersion

Other PDEs

Helmholtz equation:	$-\Delta u - \omega^2 u = 0$ with $\omega \neq 0$
Plate equation:	$u_{tt} + \Delta^2 u = f$
Telegraph equation:	$u_{tt} - \tau^2 u_{xx} + \alpha u_t + \beta u = 0$
Burgers equation:	$u_t + u u_x = \varepsilon u_{xx}$ (viscous $\varepsilon > 0$; inviscid $\varepsilon = 0$)
Korteg-de Vries equation:	$u_t + c u u_x + u_{xxx} = 0$ (with $c \neq 0$)
Vahn-Hilliard equation:	$u_t + \nu \Delta^2 u - \Delta(\beta u^3 - \alpha u) = 0$ (with $\nu > 0,\ \alpha > 0,\ \beta > 0$)
Monge-Ampere equation:	$\det(Hu) = f(\mathbf{x}, u, \nabla u)$ (where H is the Hessian matrix).

Classification of PDEs

Based on:

- **order of a PDE**: the maximum derivation order,
- **linear / non–linear** PDE: when L is linear (or non–linear) w.r.t. u.

Examples:

- $-\Delta u = f$, linear 2nd-order pde,
- $\Delta^2 u + u = f$, linear 4th-order pde,
- $-\Delta u + u^2 = f$, non-linear 2nd-order pde,
- $u_t + uu_x = 0$ non-linear 1st-order pde

Classification of 2nd-order linear PDEs

Let us start from the case $d = 2$, with $u = u(\mathbf{x})$ (indep. of time):

$$-\frac{\partial^2 u}{\partial x_1^2} - \frac{\partial^2 u}{\partial x_2^2} + 0\frac{\partial^2 u}{\partial x_1 \partial x_2} + \underbrace{\cdots\cdots\cdots}_{lower\ \ order\ \ terms} = f$$

and set

$$a_{ij} = coefficient\ \ of\ \ \frac{\partial^2 u}{\partial x_i \partial x_j}$$

and

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}.$$

The eigenvalues of A are $\lambda_{1,2}(A) = -1 < 0$.

Definition. A 2nd order–linear PDE is named **elliptic** when the eigenvalues of A are either **all positive** or **all negative**.

Thus, the Poisson equation $-\Delta u = f$ is a linear 2nd-order elliptic pde.

Classification of 2nd-order PDEs (cont'd)

The heat equation (with $\mu > 0$)

$$\frac{\partial u}{\partial t} - \mu \Delta u = f$$

The time variable plays the same role as the space variables, $\frac{\partial^2 u}{\partial t^2}$ is missing, then (if $d = 2$) we have

$$\begin{array}{cc} & \begin{array}{ccc} t & x_1 & x_2 \end{array} \\ A = & \begin{bmatrix} 0 & 0 & 0 \\ 0 & -\mu & 0 \\ 0 & 0 & -\mu \end{bmatrix} \begin{array}{c} t \\ x_1 \\ x_2 \end{array} \end{array}$$

The eigenvalues of A are $\lambda_1 = 0$, $\lambda_{2,3} = -\mu < 0$.

Def. When A has a unique null eigenvalue, while the others are either **all positive** or **all negative**, then the PDE is named parabolic.

The heat equation is a linear 2nd-order parabolic pde.

Classification of 2nd-order PDEs (cont'd)

The wave equation

$$\frac{\partial^2 u}{\partial t^2} - c\Delta u = f$$

with $c > 0$. If $d = 2$ we have

$$\begin{array}{cc} & \begin{array}{ccc} t & x_1 & x_2 \end{array} \\ A = & \begin{bmatrix} 1 & 0 & 0 \\ 0 & -c & 0 \\ 0 & 0 & -c \end{bmatrix} \begin{array}{c} t \\ x_1 \\ x_2 \end{array} \end{array}$$

The eigenvalues of A are $\lambda_1 = 1$, $\lambda_{2,3} = -c < 0$.
Def. When there exists a unique positive (resp. negative) eigenvalue, while the others are **all negative** (resp., **all positive**), then the PDE is named hyperbolic.

Boundary and initial conditions

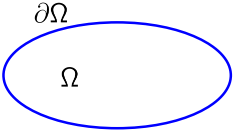
A PDE, like an ODE, can have infinite solutions.

If a PDE admits solutions, to **guarantee** that the **solution is unique**, the **PDE** needs to be **supplemented** by boundary conditions and initial conditions (the latter are only required if the solution is time dependent).

Boundary conditions for 2nd order elliptic PDEs

Dirichlet condition: you know the solution on the boundary, where it equals a known function g_D.

Dirichlet boundary conditions guarantee the uniqueness of the solution of a PDE.



Given f and g_d, look for u such that

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = g_D & \text{on } \partial\Omega \end{cases} \longleftarrow \textbf{Dirichlet condition}$$

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Example: If u is the displacement of a membrane, $u = 0$ ($g_D = 0$) on the boundary means "the bubble sticks to the floor"

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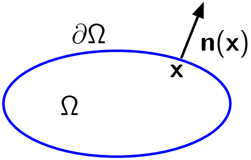
Boundary conditions for 2nd order elliptic PDEs (2)

Let $\mathbf{n}(\mathbf{x}) = [n_1(\mathbf{x}), n_2(\mathbf{x})]$ be the outward unit normal vector on $\partial\Omega$.
Neumann condition: you know the flux $\frac{\partial u}{\partial \mathbf{n}} = \nabla u \cdot \mathbf{n}$ through the boundary, where it equals the known function g_N.
Given f and g_N, look for u such that:



$$(N) \qquad \begin{cases} -\Delta u = f & \text{in } \Omega \\ \frac{\partial u}{\partial \mathbf{n}} = g_N & \text{on } \partial\Omega \end{cases} \longleftarrow \textbf{Neumann condition}$$

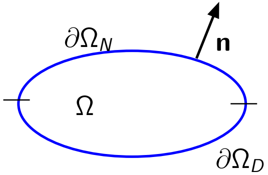
Remark 1: to guarantee existence of solution, a **compatibility condition** on f and g_N is required: $-\int_{\partial\Omega} g_N = \int_\Omega f$

Remark 2: Problem (N) still has infinite solutions, while problem $(N1)$ has a unique solution

$$(N1) \qquad \begin{cases} -\Delta u + u = f & \text{in } \Omega \\ \frac{\partial u}{\partial \mathbf{n}} = g_N & \text{on } \partial\Omega \end{cases}$$

Boundary conditions for 2nd order elliptic PDEs (3)

$\partial\Omega_N,\ \partial\Omega_D \subset \partial\Omega$, with:
$\partial\Omega_N \cap \partial\Omega_D = \emptyset$ and $\overline{\partial\Omega_N \cup \partial\Omega_D} = \partial\Omega$



Mixed boundary conditions:

$$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = g_D & \text{on } \partial\Omega_D \\ \frac{\partial u}{\partial \mathbf{n}} = g_N & \text{on } \partial\Omega_N \end{cases}$$

Robin condition:

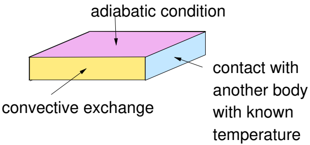
$$\alpha u + \beta \frac{\partial u}{\partial \mathbf{n}} = g_R \quad \text{on } \partial\Omega_R \subseteq \partial\Omega$$

where $\alpha, \beta \in \mathbb{R}$ are given

BC and initial conditions

For **time dependent PDEs**, initial conditions at time $t = t_0$ are required to guarantee the uniqueness of solution.
Given f, g_D, u_{ext}, and u_0, look for u solution of

$$\begin{cases} \dfrac{\partial u}{\partial t} - \mu\Delta u = f & \text{in } \Omega \times (t_0, T) \\ \mu\dfrac{\partial u}{\partial \mathbf{n}} + \alpha u = \alpha u_{ext} & \text{on } \partial\Omega_R \times (t_0, T) \quad \longleftarrow \quad \textbf{convection thermal exchange} \\ u = g_D & \text{on } \partial\Omega_D \times (t_0, T) \quad \longleftarrow \quad \textbf{fixed temperature} \\ \mu\frac{\partial u}{\partial \mathbf{n}} = 0 & \text{on } \partial\Omega_N \times (t_0, T) \quad \longleftarrow \quad \textbf{adiabatic condition} \\ u = u_0 & \Omega \times \{t_0\} \quad \longleftarrow \quad \textbf{initial condition} \end{cases}$$



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How to solve PDEs?

Mathematical Analysis studies the well posedness of the continuous problem

$$\mathcal{P}(u,g) = 0$$

$$\text{(e.g. } \mathcal{P}(u,g) = F(\mathbf{x}, t, u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}, \frac{\partial^2 u}{\partial x_1^2}, \ldots, g) = 0,)$$

i.e., it proves

- the existence of solutions
- the uniqueness of a solution
- the continuous dependence on the data

but almost always a **closed formula** to find the solution **does not exist**.

Help is given by **Numerical Analysis** and, more in general, by **Scientific Computing**.

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Numerical approximation

Instead of looking for the solution u of $\mathcal{P}(u, g) = 0$, we look for an approximation u_N of u, i.e. u_N solution of

$$\mathcal{P}_N(u_N, g_N) = 0$$

(the numerical model)

N is a **discretization parameter**.
We require our method to provide **numerical solutions that converge to the continuous one when N increases**, i.e., that $u_N \to u$ when $N \to \infty$.

Def. A numerical method is said **convergent** if:

$$\forall \varepsilon > 0 \; \exists N_0 = N_0(\varepsilon), \; \exists \delta = \delta(N_0, \varepsilon) : \; \forall N > N_0$$

$$\forall g_N : \|g_N - g\| < \delta \; \Rightarrow \; \|u_N - u\| < \varepsilon$$

Tipically, the larger N, the more accurate the approximation, but the heavier the computational cost.

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