Numerical Methods for Partial Differential Equations (PDE) (1)

Partial Differential Equations - PDE

Relationship (mathematical equation):

$$F\left(t, x, y, \ldots, u, u_t, u_x, u_y, u_{xx}, u_{xy}, u_{yy}, \ldots, g\right) = 0$$

between two or more *independent variables t, x, y, …,* an *unknown function u(t, x, y, …)* of those variables and some *partial derivatives* of the unknown function:

$$u_x = \partial u\left(t, x, y, \ldots\right) / \partial x, \quad u_y = \partial u\left(t, x, y\right) / \partial y, \quad u_t = \partial u\left(t, x, y, \ldots\right) / \partial t$$

$$u_{xx} = \partial^2 u\left(t, x, y, \ldots\right) / \partial x^2, \quad u_{xy} = \partial^2 u\left(t, x, y, \ldots\right) / \left(\partial x \partial y\right) \; \ldots..$$

Order of the PDE:

highest order of the (partial) derivatives involved in the PDE

PDE of order m solution - Definitions

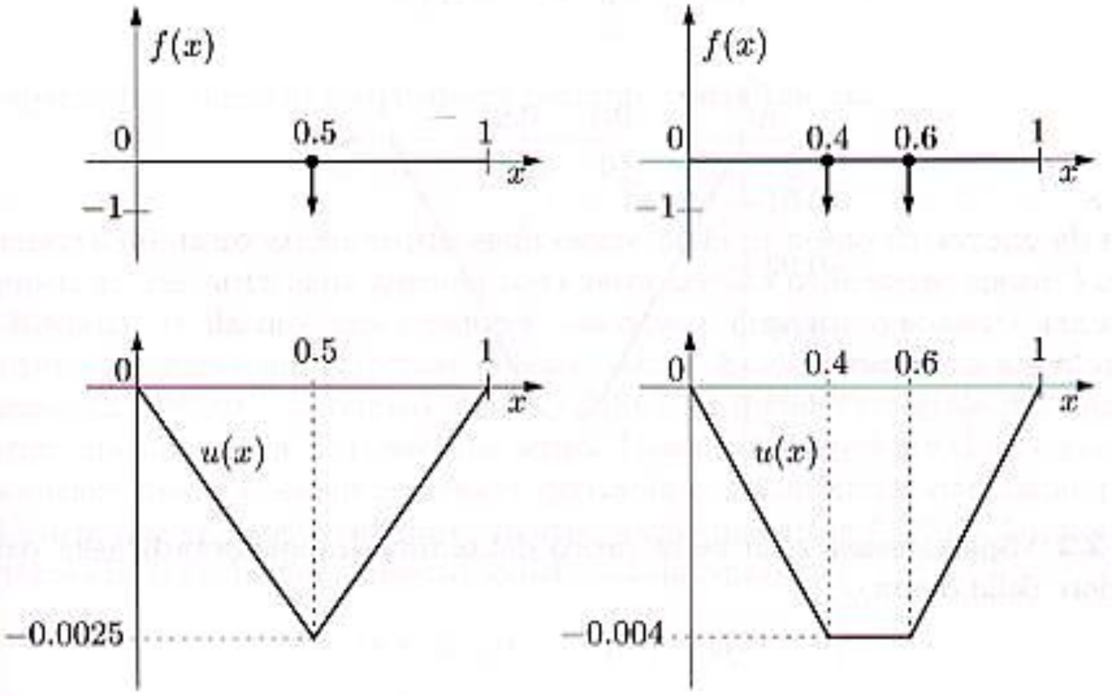
Strong (classical) solutions: functions *u(t,x,y,…)* that are continuously differentiable of order m at each point of the domain of the PDE (are $C^m(D)$) and that satisfy the PDE at each point of D.

Weak solutions: less regular functions u(t,x,y,...) (that is, are not $C^m(D)$) that do not satisfy the PDE everywhere in D. They are characterized by an integral formulation (called variational formulation), associated with the original PDE, that involves partial derivatives of order less than m defined in the sense of distributions.

PDE solution- Definitions

Equilibrium of an elastic cord

$$\begin{cases} -u''(x) = f(x), & 0 < x < 1, \\ u(0) = 0, & u(1) = 0 \end{cases}$$



f concentrated loads

u transversal displacement

Strong formulation is not adequate

PDE - Definitions

$$F\left(t, x, y, \ldots, u, u_t, u_x, u_y, u_{xx}, u_{xy}, u_{yy}, \ldots\right) = 0$$ order m

Linear *F* is linear in the unknown *u* and in its partial derivatives, with coefficients depending only on the independent variables t,x,y,….

$$\boldsymbol{u_t = d(x,t)u_{xx} - v(x,t)u_x + a(x,t)u + f(x,t)}$$ Linear 2nd order

Quasi-linear: *F* is linear in the partial derivatives of highest order m, with coefficients depending on t,x,y,…., on the unknown u and on its derivatives of order less than m

$$\boldsymbol{u_y u_{xx} - u_x^2 - u_y^2 + u = 1}$$ Quasi-linear 2nd order

Non-linear $$(u_{xx})^2 + (u_{yy})^2 = f$$ Non linear 2nd order

Exercise

- Classify the following PDE
  (order, linear/nonlinear)

$$(a) \quad \left[1+\left(\frac{\partial u}{\partial x_1}\right)^2\right]\frac{\partial^2 u}{\partial x_2^2} - 2\frac{\partial u}{\partial x_1}\frac{\partial u}{\partial x_2}\frac{\partial^2 u}{\partial x_1 \partial x_2} + \left[1+\left(\frac{\partial u}{\partial x_2}\right)^2\right]\frac{\partial^2 u}{\partial x_1^2} = 0,$$

$$(b) \quad \rho\frac{\partial^2 u}{\partial t^2} + K\frac{\partial^4 u}{\partial x_1^4} = f,$$

$$(c) \quad \left(\frac{\partial u}{\partial x_1}\right)^2 + \left(\frac{\partial u}{\partial x_2}\right)^2 = f.$$

Classification of PDEs

General form of linear second-order PDEs with two independent variables

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu + g = 0$$

- linear PDEs: a, b, c,….,g = f(x,y) only

Type of the PDE:

$$\begin{cases} b^2 - 4ac > 0, & Hyperbolic\ (2\ \ real\ \ roots) \\ b^2 - 4ac = 0, & Parabolic\ \ (1\ \ double\ \ root) \\ b^2 - 4ac < 0, & Elliptic\ \ \ \ (2\ \ complex\ \ roots) \end{cases}$$

PDE types

Hyperbolic PDEs: model a conservative physical process, such as convection, that evolves toward a stationary state (energy is preserved).

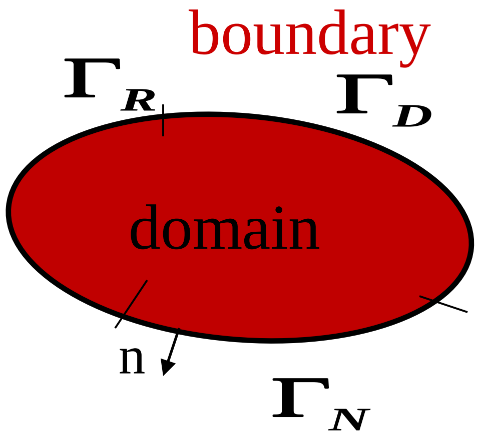
The hyperbolic category, also deals with propagation problems.

Parabolic PDEs: model a dissipative physical process, such as heat conduction, that evolves toward a stationary state (energy decreases in time)

Elliptic PDEs: model stationary (equilibrium) states (nothing changes in time)

Boundary and Initial conditions

- **Boundary Conditions** on $\Gamma = \Gamma_D \cup \Gamma_N \cup \Gamma_R$.
  - **Dirichlet:** $u = g \quad \text{on } \Gamma_D$
  - **Neumann:** $u_n = \dfrac{\partial u}{\partial n} = \nabla u \cdot n = g \quad \text{on } \Gamma_N$
  - **Robin :** $au + bu_n = g$ ***on*** Γ_R.



- **Initial Conditions** (for t = 0).

$$u(t=0,x,y,\ldots) = u_0(x,y,\ldots).$$

- **PDE problem: well-posed** (Hadamard) if and only if:
  - **A solution exists**
  - **The solution is unique**
  - **The solution depends on the data but it is not sensitive to (reasonably small) changes in the data**
- Otherwise **ill-posed**.

Boundary conditions

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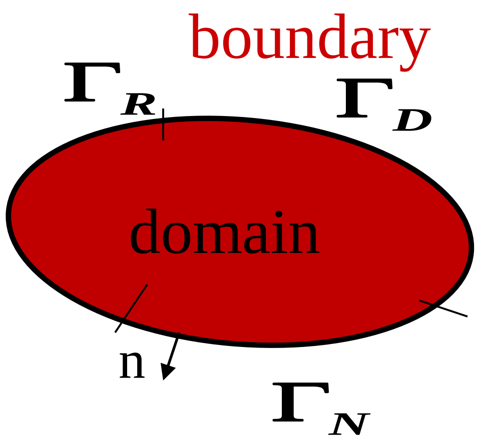
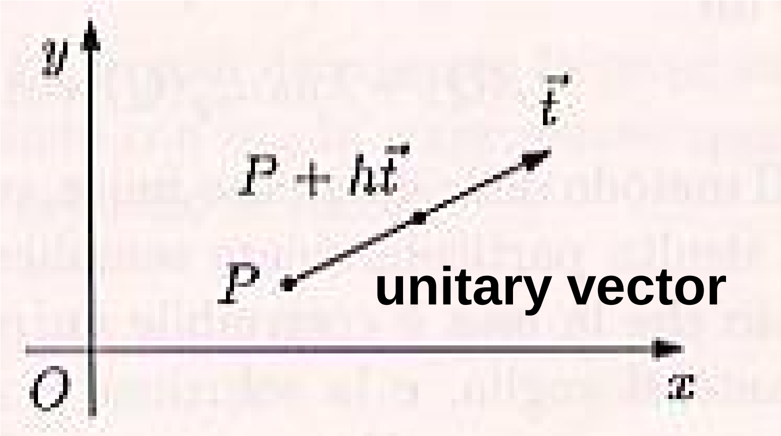


$u = g_D$	on Γ	Dirichlet boundary conditions
$\nabla u \cdot n = g_N$	on Γ	Neumann boundary conditions (n = outward normal vector to Γ)
$\nabla u \cdot n + cu = g_R$	on Γ	Robin boundary conditions
$u = g_D$ $\nabla u \cdot n = g_N$	on Γ_D on Γ_N	Mixed boundary conditions $\overline{\Gamma}_D \cup \overline{\Gamma}_N = \partial\Omega$ $\mathring{\Gamma}_D \cap \mathring{\Gamma}_N = \phi$ (no overlap)

Boundary conditions

Directional derivative of a function u(x,y)=u(P) at a point P

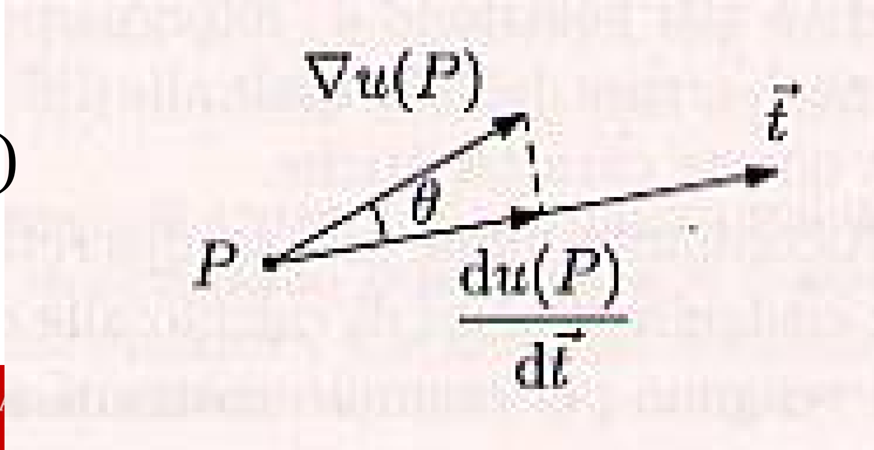
$$\frac{du(P)}{d\vec{t}} = \lim_{h \to 0} \frac{u(P + h\vec{t}\,) - u(P)}{h}$$



$\dfrac{du(P)}{d\vec{t}}$ is the component of the gradient $\nabla u(P)$

along vector direction $\vec{t}$

$$\frac{du(P)}{d\vec{t}} = \nabla u(P) \cdot \vec{t} = \left\| \nabla u(P) \right\|_2 \cos(\vartheta)$$



PDEs – models in one (space) dimension

- **Heat** Equation (linear, 2nd order): PARABOLIC

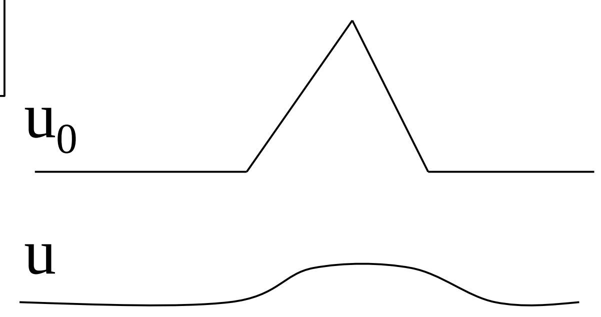
$$u_t = u_{xx} \qquad u(0,x) = u_0(x)$$

$$\text{solution: } u(t,x) = \frac{1}{\sqrt{4\pi t}} \int_{-\infty}^{+\infty} e^{-(x-s)^2/4t} u_0(s)\,ds$$

Diffusion of a "quantity" in time (ex. Heat)

Source term:
IN +f OUT -f

$$u_t = a u_{xx} + f(x,t)$$
$$u(0,x) = u_0(x)$$
$$u(t,0) = g_0(t) \quad u(t,1) = g_1(t)$$



a>0, if a<0 then the PDE would be a backward heat eq. (ill-posed problem)

PDEs – models in one (space) dimension

- **Transport (Convection)** Equation (linear, 1st order): HYPERBOLIC

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

$$\text{solution: } u(t,x) = u_0(x+t)$$

The initial function u_0 is propagated to the left with velocity -1.

$$u_t = cu_x \quad c \text{ non-zero constant}$$

$$\text{solution: } u(t,x) = u_0(x+ct)$$

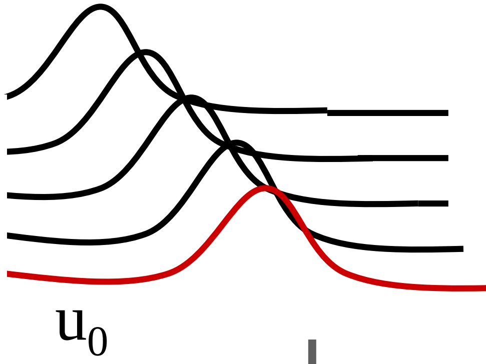
The initial function u_0 is propagated to the right (if c<0) or to the left (if c>0) with velocity c.

- **Wave** Equation (linear, 2nd order):

$$u_{tt} = c^2 u_{xx}$$

$$IC: \; u(0,x) = f(x) \quad u'(0,x) = g(x)$$

$$\text{solution: } u(t,x) = u_0(x+ct) + u_0(x-ct)$$



PDEs – multiple (space) dimensions…

Transport linear equation (2D)

$$u(x,y), \quad v=[a \quad b];$$

$$u_t + a u_x + b u_y = f(x,t) \qquad u(x,y,0) = u_0(x,y)$$

In general: $u_t + v \cdot \nabla u = f$

is the convection or transport term.

- Example: model of the motion of a pollutant in suspension in another liquid. In this context, x in R^3, u is the density of the pollutant, v(x, t) is the speed of the pollutant in the point x at the instant t and f represents the production of pollution per unit of time at the point x .

PDEs – Laplacian : 2nd order

Laplace Operator (Laplacian)

$$\Delta u \equiv \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}$$

Laplace-Poisson Equation (elliptic):

$$-\Delta u = f(x, y) \qquad \begin{cases} f = 0 & Laplace \\ f \neq 0 & Poisson \end{cases}$$

Heat (or Diffusion) Equation (parabolic):

$$u_t - \Delta u = 0$$

Wave Equation (hyperbolic): models the propagation of a wave travelling through a given medium at a constant speed c.

$$u_{tt} - \Delta u = 0$$

Helmholtz
(second-order linear)

$$\Delta u + c^2 u = 0$$

PDE – quasi linear/nonlinear

Eikonal equation

$$\|\nabla u\| = 1 \quad \|\nabla u\| = \left(\sum_{i=1}^{n} \left| \frac{\partial u}{\partial x_i} \right|^2 \right)^{1/2}$$

Minimal surface equation

$$div\left(\frac{\nabla u}{\sqrt{1 + \|\nabla u\|^2}} \right) = 0$$

Burgers eq. (order 1 quasi linear)

$$u_t + u\, u_x = 0 \quad u(x,0) = f(x)$$

Physical problems governed by PDE

Propagation problems (or non-stationary)

The propagation problems are initial values problems, also called Cauchy problems, representing a phenomenon (non-stationary) in evolution.
Assigned the initial data (at $t = 0$), we want to determine the behavior of the phenomenon under consideration in successive instants ($t>0$).
The mathematical model consists of:
-one or more PDE defined in a spatial domain (open) D for all $t>0$,
-the equations that describe the initial state, and any boundary conditions assigned on the contour G of D.
The solution $u = u(x, y, ..)$ depends on the variable "time" and one or more spatial variables.

Examples:

propagation of pressure waves in a fluid,
propagation of stresses and displacements in elastic systems,
propagation of heat in a medium.

Physical problems governed by PDE

Steady State Problems (or stationary)

The steady state problems are stationary (i.e., independent on time)
The equilibrium configuration u = u (x, y, ..) in the domain of interest D is described by one or more differential equations, defined in D, and by conditions (u) assigned to the boundaries of D.
They are generally referred to as boundary value problems.
Often these problems arise in the study of final system configuration of an evolutionary phenomena (which depends then on time).

Examples:

stationary viscous flow,
stationary distribution of temperatures in a medium,
balance of tension in elastic structures.

Physical problems governed by PDE

Eigenvalue problems

Extensions of equilibrium problems with no external forces where nontrivial (i.e. not identically zero) steady-state distributions exist only for special values of certain parameters, called eigenvalues. These eigenvalues, denoted λ, are to be determined along with the steady-state distributions themselves. The simplest form of an eigenvalue problem is

$$-\Delta u = \lambda u(x,y) \quad BC(u)=0 \quad on\ \partial\Omega$$

Examples:

deformations and stability of structures,
resonance phenomena in electrical circuits / acoustics,
search of natural frequencies in the vibration problems

Example: Poisson Equation in 2D

Heat conduction on the rectangular domain (no resources of heat f(x, y) = 0

Dirichlet Boundary conditions

$- u_{xx} - u_{yy} = f$ in $(0,1)^2$; $u = 0$ on $\delta(0,1)^2$

$u_n = 0$ on $\delta(0,1)^2$

Neumann BC:
Boundary Insulated
No heat flow

coefficient of thermal conductivity k> 0

$$-\nabla \bullet (k \nabla u) = f(x,y) \quad k(x,y) \text{ varies on } \Omega$$

$$-\nabla \bullet (k \nabla u) = -k \nabla \bullet (\nabla u) = -k \Delta u = f(x,y) \quad k > 0, \quad k \text{ const}$$

Example: Poisson Equation in 2D

Distribution of electric potential due to a density electric charge f

$-u_{xx} - u_{yy} = f$ in $(0,1)^2$;$u = 0$ on $\delta(0,1)^2$

Vertical displacement u of an elastic membrane due to the application of a specific force equal to f,

$-u_{xx} - u_{yy} = f$ in $(0,1)^2$;$u = 0$ su $\delta(0,1)^2$

Boundary conditions
Fixed membrane at the boundary

$u_n = 0$ su $\delta(0,1)^2$
No traction at the boundary

T membrane stress

$$-T\Delta u = f(x,y) \quad T \text{ cost}$$

Advection – Diffusion - Reaction PDE

- The physical processes of diffusion, transport and reaction can be modeled by PDEs involving more than one term

diffusion

Reaction

$$\frac{\partial u}{\partial t} - \nabla \cdot (c \nabla u) + \beta \cdot \nabla u + R(u) = f \quad in\ \Omega$$

$$u = 0 \qquad su\ \partial\Omega$$

Advection/ transport

source

$$c(x) > 0$$

In many practical applications the diffusion term is dominated by the convective term or by the reaction one. In these cases, the solution can give rise to **boundary layers**, i.e. regions, generally in the vicinity of the border, in which the solution varies rapidly (characterized by strong gradients).

Numerical solution of PDEs

Need for the numerical solution: in general it is not possible to derive analytically a solution u to the PDE on the geometry g.

$$\wp(u, g) = 0$$ **Exact PDE**

$$\downarrow$$ **[numerical methods]**

$$\wp_N(u_N, g_N) = 0$$ **Approximate(discretized) PDE**

A numerical method is *convergent* if:

$$\left\| u - u_N \right\| \to 0 \quad \text{for} \quad \mathrm{N} \to \infty$$

in a proper norm.

Numerical solution of PDEs

A numerical method is *stable* if *small* perturbations of data yield *small* perturbations of the solution.

Lax Equivalence Theorem:

consistency + stability ⟺ convergence

The «quality» of a convergent numerical method for solving PDEs depends also on:

- ***speed of convergence***
- ***computational cost***

Numerical methods for PDEs

Numerical methods: determine a finite-dimensional problem whose solution can be computed and which approximates the exact solution

- Three popular methods:
  - **Finite Differences**
  - **Finite Elements**
  - **Finite Volumes**
- Every method has its “optimal” application field, supporters and detractors.
- There exist other methods, such as collocation methods, spectral methods, ….

Basics: FD,FE,FV

Finite Difference (FD)

Divide the domain grid

Replace differential operators with differences operators, this essentially means approximate

$$f'(x) \approx \frac{f(x+h) - f(x)}{h}$$

Finite Volume (FV)

Divide the domain into non-overlapped subdomains

Applying Gauss's theorem to the PDE

The relationship between subdomains through the Flux flow

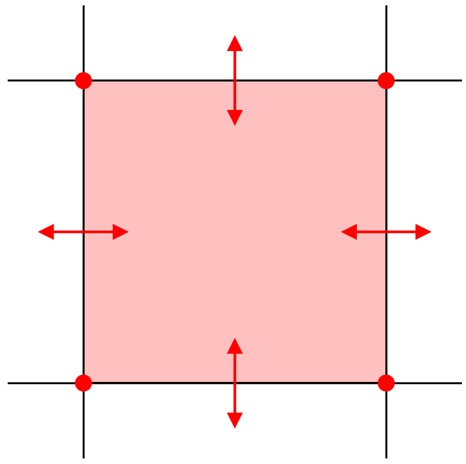
Finite Elements (FE)

Divide the domain into non-overlapped subdomains

Rewrite the PDE into an equivalent variational form

Solving the variational problem

Basics: FD,FE,FV



Ω

• Finite Difference

↔ Finite Volume

Finite Element

Basics: FD,FE,FV

Advantages and Disadvantages

Finite Difference:
+ Easy to program
- No local refinement of the grid
- Only for simple domains

Finite Volume:
+ Local refinement of the grid
+ Is also suitable for geometrically complex spatial domains

Finite Element:
+ Local refinement of the grid
+ Is also suitable for geometrically complex spatial domains

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