Amirkabir University of Technology
(Tehran Polytechnic)

Special Topics (Numerical Methods for Continuum Mechanics)

Lecture #1

Lecture Notes: Introduction

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Chapter 1

Introduction

We study PDEs because most of mathematical physics can be described by such equations. For instance, we can model

- electrical behavior of an electrochestry system with Poisson-Boltzmann equation.
- charge transport of charge carriers with Boltzmann-transport equation
- model and electronic device with drift-diffusion equation
- the motion of viscous fluid substances with Navier-Stokes
- pattern formation Swift–Hohenberg
- process of phase separation with Cahn-Hilliard equation
- description of waves, (e.g., water, sound, and light waves) with wave equation

Often physical systems are also subject to noise. This noise might be either due to thermal fluctuations, noise in some control parameter, coarse-graining of a high-dimensional deterministic system with random initial conditions, or the stochastic parameterization of small scales. In this case, the fluctuation/variation must be taken into consideration in order to solve the equation.

1.1 Mathematical backgrounds

We consider $f(x, y, z) : \mathbb{R}^3 \to \mathbb{R}$ and $u(x, y, z) : \mathbb{R}^3 \to \mathbb{R}^3$ in three dimensional Cartesian coordinate system $(\mathbf{i}, \mathbf{j}, \mathbf{k})$. Then we can review

- **Partial derivatives:** The differential (or differential form) of a function f of n independent variables, $(x_1, x_2, \ldots, x_n)$, is a linear combination of the basis form

$$\mathrm{d}f = \sum_{i=1}^{n} \frac{\partial f}{\partial x_i} \mathrm{d}x_i = \frac{\partial f}{\partial x_1} \mathrm{d}x_1 + \frac{\partial f}{\partial x_2} \mathrm{d}x_2 + \ldots + \frac{\partial f}{\partial x_n} \mathrm{d}x_n \tag{1.1}$$

- **Gradient:** $\nabla f = \partial_x f \mathbf{i} + \partial_y f \mathbf{j} + \partial_z f \mathbf{k}$

- **Divergence** $\mathrm{div} u = \nabla \cdot u = \partial_x u_x + \partial_y u_y + \partial_z u_z$
- **Laplacian:** $\Delta f = \nabla^2 f = \partial_x^2 f + \partial_y^2 f + \partial_z^2 f$
- **Laplacian of a vector:** $\Delta u = \nabla^2 u = \nabla^2 u_x \mathbf{i} + \nabla^2 u_y \mathbf{j} + \nabla^2 u_z \mathbf{k}$

1.2 Gradient, divergence, trace, Laplace

Well-known in physics, it is convenient to work with the nabla-operator to define derivative expressions.

Gradient

The gradient of a single-valued function $v : \mathbb{R}^n \to \mathbb{R}$ reads:

$$\nabla v = \begin{pmatrix} \partial_1 v \\ \vdots \\ \partial_n v \end{pmatrix}.$$

The gradient of a vector-valued function $\mathbf{v} : \mathbb{R}^n \to \mathbb{R}^m$ is called the Jacobian matrix and reads:

$$\nabla \mathbf{v} = \begin{pmatrix} \partial_1 v_1 & \cdots & \partial_n v_1 \\ \vdots & \ddots & \vdots \\ \partial_1 v_m & \cdots & \partial_n v_m \end{pmatrix}.$$

Divergence

The divergence is defined for vector-valued functions $\mathbf{v} : \mathbb{R}^n \to \mathbb{R}^n$:

$$\mathrm{div}\, \mathbf{v} := \nabla \cdot \mathbf{v} := \nabla \cdot \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} = \sum_{k=1}^{n} \partial_k v_k.$$

The divergence for a tensor $\sigma \in \mathbb{R}^{n\times n}$ is defined as:

$$(\nabla \cdot \sigma)_i = \sum_{j=1}^{n} \frac{\partial \sigma_{ij}}{\partial x_j} \quad \text{for } 1 \le i \le n,$$

or in vector form:

$$\nabla \cdot \sigma = \begin{pmatrix} \displaystyle\sum_{j=1}^{n} \frac{\partial \sigma_{1j}}{\partial x_j} \\ \vdots \\ \displaystyle\sum_{j=1}^{n} \frac{\partial \sigma_{nj}}{\partial x_j} \end{pmatrix}.$$

1.3 Cross product and curl

Cross product in $\mathbb{R}^3$

Let us introduce the cross product of two vectors $u, v \in \mathbb{R}^3$:

$$u \times v = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} \times \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} u_2 v_3 - u_3 v_2 \\ u_3 v_1 - u_1 v_3 \\ u_1 v_2 - u_2 v_1 \end{pmatrix}.$$

Curl operator

With the help of the cross product, we can define the rotation or curl of a vector field $\mathbf{v} : \mathbb{R}^3 \to \mathbb{R}^3$:

$$\operatorname{rot} \mathbf{v} = \nabla \times \mathbf{v} = \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} \times \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{pmatrix} \partial_y v_3 - \partial_z v_2 \\ \partial_z v_1 - \partial_x v_3 \\ \partial_x v_2 - \partial_y v_1 \end{pmatrix}.$$

In index notation, using the Levi-Civita symbol ε_{ijk}:

$$(\nabla \times \mathbf{v})_i = \sum_{j,k=1}^{3} \varepsilon_{ijk} \partial_j v_k.$$

1.4 Divergence theorem and integration by parts

Proposition 1.4.1 (Gauss' divergence theorem / Gauss-Green theorem)*.* Let $\Omega \subset \mathbb{R}^d$ be bounded and open, and let $\partial\Omega$ be of class C^1. Let $f \in C^1(\overline{\Omega})$. Then,

$$\int_\Omega \operatorname{div} f \, dx = \int_{\partial\Omega} f \cdot n \, ds.$$

The outer normal of $\partial\Omega$ is given by n.

Proposition 1.4.2 (Partial integration)*.* Let $f, g \in C^1(\overline{\Omega})$. Then,

$$\int_\Omega \partial_i f \, g \, dx = -\int_\Omega f \, \partial_i g \, dx + \int_{\partial\Omega} f g \, n_i \, ds \quad \text{for } i = 1, \ldots, d.$$

Here we consider $D \subset \mathbb{R}^d$ ($d = 1, 2, 3$) the computational geometry and ∂D its boundary. Generally, we have three classes fo PDEs.

- **Elliptic equation:** describing phenomena that do not change from moment to moment, as when a flow of heat or fluid takes place within a medium with no accumulations. The Laplace equation, $\Delta f = 0$ is the simplest such equation describing this condition in multi dimensions. In addition to satisfying a differential equation within the region, the elliptic equation is also determined by its values (boundary values) along the boundary of the region, which represent the effect from outside the region. These conditions can be either those of a fixed temperature distribution at points of the boundary (Dirichlet problem) or those in which heat is being supplied or removed across the boundary in such a way as to maintain a constant temperature distribution throughout (Neumann problem).

We shall study partial differential equations of the form

$$LU = f, \qquad \text{in} D \tag{1.2a}$$

$$u = 0, \qquad \text{on} \partial D \tag{1.2b}$$

where L is the linear second order differential operator

$$Lu = \sum_{i,j=1}^{d} -\frac{\partial}{\partial x_i}\left(a_{ij}\frac{\partial u}{\partial x_j}\right) + cu \tag{1.3}$$

with a_{ij}, $i, j = 1 \cdots , d$, and c are given coefficients depending only on the space coordinates x_i. We shall assume that there is a value a_0 such that $a_{ij} > a_0$ for all $i, j = 1, \cdots , d$, and that these coefficients are symmetric in the sense that $a_{ij} = a_{ji}$ as well as $c \geq 0$. Therefore, we have

$$Lu = -\nabla \cdot (a\nabla u) + cu \tag{1.4}$$

the famous elliptic equations are

1. The Laplace equation
2. The Poisson equation
3. The nonlinear Poisson-Boltzmann equation
4. The diffusion-reaction equation

- **Parabolic equation:** Unlike elliptic equations, which describes a steady state, parabolic (and hyperbolic) evolution equations describe processes that are evolving in time. For such an equation the initial state of the system is part of the auxiliary data for a well-posed problem. The theory of second order parabolic equations of the form

$$Lu = \sum_{i,j=1}^{d} a_i(x,t)\frac{\partial^2 u}{\partial x_j^2} + \sum_{i,j=1}^{d} b_i(x,t)\frac{\partial u}{\partial x_j} + c(x,t)u - \frac{\partial u}{\partial t} = f \tag{1.5}$$

The archetypal parabolic evolution equation is the "heat conduction" or "diffusion" equation. In this course also we consider

1. The Boltzmann-transport equation
2. The Cahn-Hilliard-Cook equation
3. The stochastic Swift-Hohenberg equation

- **Hyperbolic equation:** The most popular is wave equation. The acoustic Wave equation describes sound waves in a continuum (i.e., liquid or gas), and in this context sound is interpreted as a pressure disturbance. The equation in 1-D case can be written as

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{1.6}$$

The equation has the property that, if u and its first time derivative are arbitrarily specified initial data on the line $t = 0$ (with sufficient smoothness properties), then there exists a solution for all time t.

Sobolev spaces: Fix $1 < p < \infty$ and let k be a nonnegative integer. We define now certain function spaces, whose members have weak derivatives of various orders lying in various L^p spaces.

An L^p space may be defined as a space of functions for which the p-th power of the absolute value is Lebesgue integrable, or equivalently,

$$\|f\|_p = \left(\int_S |f|^p \mathrm{d}\mu \right)^{1/p} < \infty \tag{1.7}$$

The Sobolev space

$$W^{k,p}(U) \tag{1.8}$$

consists of all locally summable functions $u : U \to \mathbb{R}$ such that for each multi index a with $|\alpha| \leq k$, $D^\alpha u$ exists in the weak sense and belongs to $L^p(U)$.

If $p = 2$, we usually write

$$H^k(U) = W^{k,2}(U) \qquad (k = 0, 1, \cdots). \tag{1.9}$$

The letter H is used, since $H^k(U)$ is a **Hilbert space**. Note that $H^0(U) = L^2(U)$.

$$\|u\|_{W^{k,p}(U)} := \begin{cases} \left(\sum_{|\alpha| \leq k} \int_U |D^\alpha u|^p dx \right)^{1/p} & (1 \leq p < \infty), \\ \sum_{|\alpha| \leq k} \text{ess sup}_U |D^\alpha u|^p & (p = \infty) \end{cases} \tag{1.10}$$

Boundary conditions

Let us assume $D \subset \mathbb{R}^d,\ d = 1, 2, 3$ is the computational geometry and ∂D is its boundary. We have the following types of boundary conditions:

- **Dirichlet boundary condition**: it is imposed on an ordinary or a partial differential equation, it specifies the values that a solution needs to take on along the boundary of the domain. For the ODE

$$u'' + u = 0, \tag{1.11}$$

the Dirichlet boundary conditions on the interval $[a, b]$ take the form

$$u(a) = \alpha \qquad u(b) = \beta \tag{1.12}$$

where α and β are given numbers. For a PDE, such as

$$\nabla^2 u + u = 0, \tag{1.13}$$

the Dirichlet boundary conditions on a domain $D \subset \mathbb{R}^n$ take the form

$$u(x) = f(x) \qquad \forall x \in \partial D, \tag{1.14}$$

where f is a known function defined on the boundary ∂D.

- **Neumann boundary condition**: it is imposed on an ordinary or a partial differential equation, the condition specifies the values in which the derivative of a solution is applied within the boundary of the domain. For the ODE

$$u'' + u = 0, \tag{1.15}$$

the Neumann boundary conditions on the interval $[a, b]$ take the form

$$u'(a) = \alpha \qquad u'(b) = \beta \tag{1.16}$$

where α and β are given numbers. For a PDE, such as

$$\nabla^2 u + u = 0, \tag{1.17}$$

the Dirichlet boundary conditions on a domain $D \subset \mathbb{R}^n$ take the form

$$\frac{\partial u}{\partial \mathbf{n}}(x) = f(x) \qquad \forall x \in \partial D, \tag{1.18}$$

The normal derivative, which shows up on the left side, is defined as

$$\frac{\partial u}{\partial \mathbf{n}}(x) = \nabla u(x) \cdot \hat{\mathbf{n}}(x) \qquad \forall x \in \partial D, \tag{1.19}$$

$\hat{\mathbf{n}}$ is the unit normal, and the 'dot' represents the inner product operator.

- **Robin boundary conditions** are a weighted combination of Dirichlet boundary conditions and Neumann boundary conditions. This contrasts to mixed boundary conditions, which are boundary conditions of different types specified on different subsets of the boundary. It has the form

$$au + b\frac{\partial u}{\partial n} = g \qquad \partial D \tag{1.20}$$

for some non-zero constants a and b and a given function g defined on ∂D.

- **Mixed boundary conditions**: a solution u to a partial differential equation on a domain D with boundary ∂D, it is said to satisfy a mixed boundary condition if, consisting ∂D of

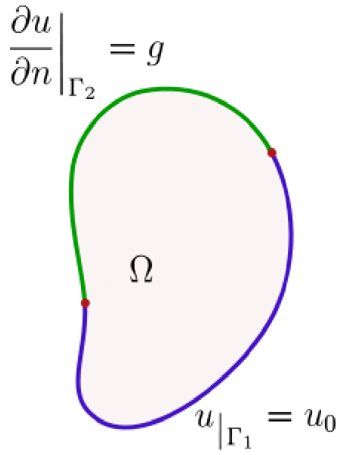

FIGURE 1.1: Green: Neumann boundary condition; purple: Dirichlet boundary condition.

two disjoint parts, Γ_1 and Γ_2, such that $\partial D = \Gamma_1 \cup \Gamma_2$; u verifies the following equations:

$$u|_{\Gamma_1} = u_0 \qquad \text{and} \qquad \frac{\partial u}{\partial n}|_{\Gamma_2} = g \tag{1.21}$$

where u_0 and g are given functions defined on those portions of the boundary (see Figure 1.1 for a better illustration).

1.5 Transport equation

The transport equation describes how a scalar quantity is transported in a space. Usually, it is applied to the transport of a scalar field (e.g. chemical concentration, material properties or temperature) inside an incompressible flow. From the mathematical point of view, the transport equation is also called the convection-diffusion equation, which is a first order PDE (partial differential equation). The convection-diffusion equation is the basis for the most common transportation models.

One of the simplest partial differential equations is the transport equation with constant coefficients. This is the PDE

$$u_t + b \cdot Du = 0 \qquad \text{in} \mathbb{R}^n \times (0, \infty) \tag{1.22}$$

If $u \in W^{k,p}(U)$, we define its norm to be

where b is a fixed vector in $\mathbb{R}^n$, $b = (b_1, \dots, b_n)$ and $u : \mathbb{R}^n \times [0, \infty] \to \mathbb{R}$ is the unknown. Here $x|(x_1 \dots, x_n)$ denotes a typical point in space, and $t > 0$ denotes a typical time. We write $Du = D_x u = (u_{x_1}, ..., u_{x_n})$ for the gradient of u with respect to the spatial variables x.

We have the following transport initial value problem

$$\begin{cases} u_t + b \cdot DU = 0 & \text{in } \mathbb{R}^n \times (0, \infty), \\ u = g & \text{on } \mathbb{R}^n \times t_0 \end{cases} \tag{1.23}$$

Here $b \in \mathbb{R}^n$ and $g : \mathbb{R}^n \to R$ are known, and the problem is to compute u by given (x, t). Also, we have the nonhomogeneous problem

$$\begin{cases} u_t + b \cdot DU = f & \text{in } \mathbb{R}^n \times (0, \infty), \\ u = g & \text{on } \mathbb{R}^n \times t_0 \end{cases} \tag{1.24}$$

The Boltzmann equation or **Boltzmann transport equation (BTE)** describes the statistical behaviour of a thermodynamic system not in a state of equilibrium, devised by Ludwig Boltzmann in 1872. The classic example of such a system is a fluid with temperature gradients in space causing heat to flow from hotter regions to colder ones, by the random but biased transport of the particles making up that fluid. In the modern literature the term Boltzmann equation is often used in a more general sense, referring to any kinetic equation that describes the change of a macroscopic quantity in a thermodynamic system, such as energy, charge or particle number.

The starting point is the Boltzmann transport equation in the form

$$\partial_t f + \{\mathcal{E}, f\}_{XP} + \mathcal{Q}[f] = 0, \tag{1.25}$$

where the Poisson bracket is defined as

$$\{g, f\}_{XP} := \nabla_P g \cdot \nabla_X f - \nabla_X g \cdot \nabla_P f. \tag{1.26}$$

Here $f(X, P, t)$ is the kinetic particle density, $X \in \mathbb{R}^3$ is position, $P \in \mathbb{R}^3$ is momentum, t is time, $E(X, P)$ is the energy, and $\mathcal{Q}$ is the scattering operator.

1.6 Poisson equation

Among the most important of all partial differential equations are undoubtedly Laplace's equation

$$\Delta u = 0 \tag{1.27}$$

and Poisson equation

$$-\Delta u = f \tag{1.28}$$

or more complicated

$$-\nabla \cdot (c \nabla u) = f \tag{1.29}$$

Physical interpretation: Gauss's law may be expressed as

$$\Phi_E = \frac{Q}{A} \tag{1.30}$$

where Φ_E is the electric flux through a closed surface S enclosing any volume V, Q is the total charge enclosed within V, and A is the electric constant. The electric flux Φ_E is defined as a surface integral of the electric field:

$$\Phi_E = \oiint_S E \cdot dK \tag{1.31}$$

where E is the electric field, dK is a vector representing an infinitesimal element of area of the surface and $\cdot$ represents the dot product of two vectors (inner product). Equivalently, we have

$$\nabla \cdot D = \rho_f, \tag{1.32}$$

where D is the displacement filed (accounts for the effects of free and bound charge within materials), and ρ_f is free charge density. In physics, a constitutive equation or constitutive relation is a relation between two physical quantities that is specific to a material or substance, and approximates the response of that material to external stimuli, usually as applied fields or forces. We have the constitutive equation

$$D = AE \tag{1.33}$$

where A is dielectric constant (permittivity) of the medium and E is the electric field. Substituting this into Gauss's law and assuming A is spatially constant in the region of interest yields

$$\nabla \cdot E = \frac{\rho}{A} \tag{1.34}$$

In the absence of a changing magnetic field, B, Faraday's law of induction gives

$$\nabla \times E = -\frac{\partial B}{\partial t} = 0 \tag{1.35}$$

Since the curl of the electric field is zero, it is defined by a scalar electric potential field V

$$E = -\nabla V \tag{1.36}$$

The derivation of Poisson's equation under these circumstances is straightforward. Substituting the potential gradient for the electric field,

$$\nabla \cdot E = \nabla \cdot (-\nabla V) = -\nabla^2 V = \frac{\rho}{A} \tag{1.37}$$

directly produces Poisson's equation for electrostatics, which is

$$\nabla^2 V = -\frac{\rho}{A}. \tag{1.38}$$

The **Poisson-Boltzmann equation** arising in the Debye-Hückel theory as a second order nonlinear partial differential equation describes the electrostatic potential. It is used for a wide range of applications, including the computation of the electrostatic potential at the solvent-accessible molecular surface, the computation of encounter rates between molecules in the solution, the computation of the free energy of association and its salt dependence, and the combination of classical molecular mechanics and dynamics.

The equation defined for 1-1 electrolytes as

$$-\nabla \cdot (A\nabla V) + 2\varphi \sinh(\beta(V - \Phi_F)) = 0$$

holds and models screening by free charges. Here φ is the ionic concentration, the constant β equals $\beta := q/(k_B T)$ in terms of the Boltzmann constant k_B and the temperature T, and Φ_F is the Fermi level.

1.7 Heat equation

Next we study the heat equation

$$u_t - \Delta u = 0 \tag{1.39}$$

and the nonhomogeneous heat equation

$$u_t - \Delta u = f \tag{1.40}$$

We assume $U \subset \mathbb{R}^n$, the function $f : U \times [0, \infty) \to R$ is given. The heat equation, also known as the diffusion equation, describes in typical applications the evolution in time of the density u of some quantity such as heat, chemical concentration, etc. If $V \subset U$ is any smooth subregion, the rate of change of the total quantity within V equals the negative of the net flux through ∂V:

$$\frac{d}{dt}\int_V u dx = -\int_{\partial V} F \cdot \nu dS, \tag{1.41}$$

F being the flux density. Thus

$$u_t = -\text{div} F, \tag{1.42}$$

as V was arbitrary. In many situations F is proportional to the gradient of u but points in the opposite direction (since the flow is from regions of higher to lower concentration):

$$F = -aDu \qquad (a > 0). \tag{1.43}$$

Substituting into (1.42) will lead to

$$u_t = a\text{div}(Du) = a\Delta u, \tag{1.44}$$

which for $a = 1$ is the heat equation. The heat equation appears as well in the study of Brownian motion.

1.8 Wave equation

The wave equation is an important second-order linear partial differential equation for the description of waves as they occur in classical physics such as mechanical waves (e.g. water waves, sound waves and seismic waves) or light waves. It arises in fields like acoustics, electromagnetics, and fluid dynamics.

The wave equation alone does not specify a physical solution; a unique solution is usually obtained by setting a problem with further conditions, such as initial conditions, which prescribe the amplitude and phase of the wave. Another important class of problems occurs in enclosed spaces specified by boundary conditions, for which the solutions represent standing waves, or harmonics, analogous to the harmonics of musical instruments.

The wave equation, and modifications of it, are also found in elasticity, quantum mechanics, plasma physics and general relativity.

Here we investigate the wave equation

$$u_{tt} - \Delta u = 0 \tag{1.45}$$

and the nonhomogeneous wave equation

$$u_{tt} - \Delta u = f, \tag{1.46}$$

subject to appropriate initial and boundary conditions. Here $t > 0$ and $x \in U$, where $U \subset \mathbb{R}^n$ is open and the function $f : U \times [0, \infty) \to R$ is given.