Numerical Methods for Partial Differential Equations - Notes - v0.2.0-dev

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Preface

Every theory section in these notes has been taken from the sources:

- Course slides. [1]

About:

GitHub repository

These notes are an unofficial resource and shouldn't replace the course material or any other book on numerical methods for partial differential equations. It is not made for commercial purposes. I've made the following notes to help me improve my knowledge and maybe it can be helpful for everyone.

As I have highlighted, a student should choose the teacher's material or a book on the topic. These notes can only be a helpful material.

Contents

1 Basic Concepts

In this course, we introduce numerical methods for the solution of **Partial Differential Equations** (PDEs), with focus on the **Finite Element** (FE) **method**[1] and the use of the computer for the construction of the PDEs numerical solution.

We will consider the numerical approximation of elliptic and parabolic PDEs by considering their variational formulation, Galërkin and FE approximations in 1D/2D/3D, the theoretical properties and practical use of the methods, algorithmic aspects, and interpretation of the numerical results.

Advanced topics include the approximation of saddle-point PDEs (Stokes equations), vectorial, nonlinear, and multiphysics differential problems, domain decomposition methods exploiting the properties of the PDEs, and the introduction to parallel computing for the FE method, i.e., in the *High Performance Computing* (HPC) framework.

Finally, the course will feature the use of the `deal.II` software library, a C++ open source FE library, and ParaView for the visualization of numerical solution and scientific computing data.

[1]The **Finite Element Method (FEM)** is a popular method for numerically solving differential equations arising in engineering and mathematical modeling. Typical problem areas of interest include the traditional fields of structural analysis, heat transfer, fluid flow, mass transport, and electromagnetic potential. Computers are usually used to perform the calculations required. With high-speed supercomputers, better solutions can be achieved, and are often required to solve the largest and most complex problems. (source)

1.1 Mathematical Models and Scientific Computing

Definition 1: Mathematical Model

A **Mathematical Model** is a **set of** (algebraic or differential) **equations that is able to represent the features of a complex system or process**.

Why do they exist?

Models are **developed** to:

- Describe
- Forecast
- Control

The **behavior or evolution of such systems**.

We are interested in the physics models. **Physics-based models** are those **mathematical models that are derived from physical principles** (like conservation laws of mass, momentum, energy, etc.) **and that encode natural laws of leading to (differential) equations whose solutions are often represented in the form of functions**. However, the analytical solution of such models is rarely available in closed form, for which numerical approximation methods are instead employed.

Definition 2: Numerical Modelling

Numerical Modelling indicates **sets of numerical methods that determine an approximate solution of the original** (often infinite-dimensional) **mathematical model**, by turing it into a *discrete problem* (algebraic, finite-dimensional), whose dimension (size) is typically very large.

Definition 3: Scientific Computing

Scientific Computing is **a branch** of Mathematics **that numerically solves** (differential) **mathematical models by building approximate solutions though the use of a calculator**.

For numerical models of large size, parallel architectures for calculators and the HPC framework are typically used.

❓ Why did we introduce mathematical models and physical models?

Because they are connected and used together. Mathematical models are conventionally used altogether with theoretical (mathematical) models and experimental tests. Unfortunately, in several cases theoretical models are not available (like in Computational Medicine) or experimental tests are not meaningful or cannot be performed (for example, for nuclear testing). Physics-based models have witnessed an increasing role in the modern society in virtue of the massive developments of Scientific Computing and computational tools.

Since a large amount of data is becoming available from multiple sources nowadays, data-driven models are fundamentals. **Data-driven models** are those mathematical models built from meaningful data that do not rely on physical principles, because the latter are not available or are not reliable, and whose construction calls for statical learning methods.

Physics-based mathematical models (**mathematical problems**) are a fundamental pillar in the understanding and prediction of several physical phenomena and processes (**physical problems**). However, these mathematical models lead to problems that can rarely be solved analytically, or in an exact way (**exact solution**), especially for PDEs: with only a few exceptions, it is not possible to write their solution explicitly.

Numerical methods and numerical approximation techniques (**numerical problems**) serve the purpose to determine an **approximate solution** of a mathematical model. When the calculator is used to determine such approximate solution, the latter is called **numerical solution** (see the Figure 1).

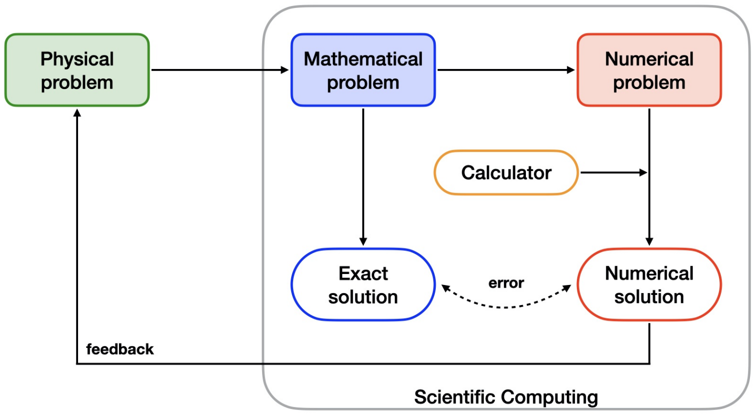

Figure 1: Scientific Computing.

1.2 Differential Models and PDEs

Definition 4: Partial Differential Equation (PDE)

A **differential equation** (model) is an equation that involves **one or more derivatives of an unknown function**. In an **Ordinary Differential Equation** (ODE), **every derivative of the unknown solution is with respect to a single independent variable**. If instead, derivatives are partial, then we have a **Partial Differential Equation (PDE)**.

In other words, it is a differential equation where its derivatives are partial.

There are different types of PDEs, and their nature depends on the conditions and their type. Mathematically, we can represent a **differential model** (equation) as follows:

$$\mathcal{P}(u; g) = 0 \qquad \text{differential equation (mathematical problem)} \tag{1}$$

Where:

- $\mathcal{P}$ indicates the ***model***;
- u is the ***exact solution***, a function of one or more independent variables (space and/or time variables);
- g indicates the ***data***.

1.2.1 ODEs

Ordinary Differential Equation (ODE) is also known as **initial value problem**.

I°ODE - Cauchy problem

A **first order** ODE, a **Cauchy problem**, is a differential problem, whose:

- ***Solution*** $u = u(t)$ is a function of a single independent variable t, often interpreted as time.
- A ***single condition*** is assigned on the solution, at a point (usually, the left end of the integration interval).

Its form is the following find $u : I \subset \mathbb{R} \to \mathbb{R}$ such that:

$$\begin{cases} \dfrac{\mathrm{d}u}{\mathrm{d}t}(t) = f(t, u(t)) \quad t \in I \\ u(t_0) = u_0 \end{cases} \tag{2}$$

Where:

- $I = (t_0, t_f] \subset \mathbb{R}$ is a ***time interval***;
- u_0 is the ***initial value*** assigned at $t = t_0$;
- $f : I \times \mathbb{R} \to \mathbb{R}$

Meaning. The equation describes the **evolution of a scalar quantity** u **over time** t, **without distribution in space**.

Vectorial problems. In vectorial problems, the **unknown is a vector-valued function** $\mathbf{u} = \mathbf{u}(t)$, where $\mathbf{u} = (u_1, \ldots, u_m) \in \mathbb{R}^m$, with $m \geq 1$. The first order Cauchy problem reads: find $\mathbf{u} : I \subset \mathbb{R} \to \mathbb{R}^m$ such that:

$$\begin{cases} \dfrac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}(t) = \mathbf{f}(t, \mathbf{u}(t)) \quad t \in I \\ \mathbf{u}(t_0) = \mathbf{u}_0 \end{cases}$$

Where $\mathbf{u}_0 \in \mathbb{R}^m$ is the initial datum and $\mathbf{f} : I \times \mathbb{R}^m \to \mathbb{R}^m$.

II°ODE - Cauchy problem

A **second order Cauchy problem** sees second order time derivatives and two initial conditions. It reads as: find $u : I \subset \mathbb{R} \to \mathbb{R}$ such that:

$$\begin{cases} \dfrac{\mathrm{d}^2u}{\mathrm{d}t^2}(t) = f\left(t, u(t), \dfrac{\mathrm{d}u}{\mathrm{d}t}(t)\right) \quad t \in I \\ \dfrac{\mathrm{d}u}{\mathrm{d}t}(t_0) = v_0 \\ u(t_0) = u_0 \end{cases} \tag{3}$$

Where the initial data are u_0 and v_0, while $f : I \times \mathbb{R} \times \mathbb{R} \to \mathbb{R}$.

1.2.2 PDE, boundary value problem in 1D

The **Boundary value problem in 1D** is characterized by a **single independent variable** x, which represents the **space coordinate in an interval** $\Omega = (a, b) \in \mathbb{R}$ (1D).

The problem involves **second order derivatives of the unknown solution** $u = u(x)$ with respect to x. The value of u, or the **value of its first derivate**, is a **set at the two boundaries of the domain** (interval) Ω, that is at $x = a$ and $x = b$ (the domain boundary is $\partial\Omega = \{a, b\}$).

Let us consider the following **Poisson problem** with (homogeneous) Dirichlet boundary conditions: find $u : \Omega \subset \mathbb{R} \to \mathbb{R}$ such that:

$$\begin{cases} -\dfrac{\mathrm{d}^2 u}{\mathrm{d}x^2}(x) = f(x) \quad x \in \Omega = (a, b) \\ u(a) = u(b) = 0 \end{cases} \tag{4}$$

This equation models a **stationary phenomenon** (the time variable doesn't appear in fact) and represent a **diffusion model**.

Example 1

For example, the diffusion model models the diffusion of a pollutant along a 1D channel $\Omega = (a, b)$ or the vertical displacement of an *elastic thread* fixed at its ends. In the first case, $f = f(x)$ indicates the source of the pollutant along the flow, while in the second case, f is the traverse force acting on the elastic thread, in the hypothesis of negligible mass and small displacements of the thread.

⚖ Boundary value problem in 1D vs ODE

We remark that the **boundary value problem in 1D is a particular case of PDEs**, even if it involves only derivatives with respect to a single independent variable x. Indeed, even if apparently similar to a second order ODE, the boundary value problem is in reality substantially **different** from an ODE:

- In ODE, two conditions are set at $t = t_0$;
- In the boundary value problem in 1D, one condition is set at $x = a$ and the other one at $x = b$.

The conditions in the boundary value problem determine to the so-called global nature of the model.

1.2.3 PDE, initial and boundary value problem in 1D

Initial and boundary value problem in 1D is a type of problems that concern equations that **depend on space and time**:

- The **unknown solution** $u = u(x, t)$ both depends on the space coordinate $x \in \Omega \subset \mathbb{R}$ in 1D;
- The **time variable** $t \in I \subset I$.

In this case, the initial conditions at $t = 0$ must be prescribed, as well as the boundary conditions at the ends of the interval in 1D.

The **Heat equation**, also known as **Diffusion equation**, with Dirichlet boundary conditions assumes the following form: find $u : \Omega \times I \to \mathbb{R}$ such that:

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,t) - \mu \dfrac{\partial^2 u}{\partial x^2}(x,t) = f(x,t) & x \in \Omega = (a,b), t \in I \\ u(a,t) = u(b,t) = 0 & t \in I \\ u(x,t_0) = u_0(x) & x \in \Omega = (a,b) \end{cases} \tag{5}$$

Example 2

For example, the unknown function $u(x, t)$ describes the temperature in a point $x \in \Omega = (a, b)$ and time $t \in I$ of a metallic bar covering the space interval Ω. The diffusion coefficient μ represents the thermal response of the material and it is related to its thermal conductivity. The Dirichlet boundary conditions express the fact that the ends of the bar are kept at a reference temperature (zero degrees in this case), while at time $t = t_0$ the temperature is assigned in each point $x \in \Omega$ through the initial function $u_0(x)$. Finally, the bar is subject to a heat source of linear density $f(x, t)$.

1.2.4 PDE, boundary value problem in multidimensional domains

The Poisson problem (equation 4, page 9) can be **extended in multidimensional domains** $\Omega \subset \mathbb{R}^d$, with $d = 2, 3$; the solution is $u = u(\mathbf{x})$, where $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$. This leads to the following Poisson problem with (homogeneous) Dirichlet boundary conditions: find $u : \Omega \subset \mathbb{R}^d \to \mathbb{R}$ such that:

$$\begin{cases} -\Delta u = f & \text{in } \Omega \text{ (i.e. } \mathbf{x} \in \Omega) \\ u = 0 & \text{on } \partial\Omega \text{ (i.e. } \mathbf{x} \in \partial\Omega) \end{cases} \tag{6}$$

Where:

- The **Laplace operator**:

$$\Delta u(\mathbf{x}) := \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}(\mathbf{x})$$

- The **domain** $\Omega \subset \mathbb{R}^d$ is endowed with boundary $\partial\Omega$;
- $f = f(x)$ is the ***external forcing term***.

This equation is used **for example** to **model the vertical displacement of an elastic membrane fixed at the boundaries**.

1.2.5 PDE, initial and boundary value problem in multidimensional domains

The **multidimensional** counterpart of the **heat equation** (5, page 10) reads: find $u : \Omega \times I \to \mathbb{R}$ such that:

$$\begin{cases} \dfrac{\partial u}{\partial t} - \mu \Delta u = f & \mathbf{x} \in \Omega, t \in I \\ u(\mathbf{x}, t) = 0 & \mathbf{x} \in \partial\Omega, t \in I \\ u(\mathbf{x}, t_0) = u_0(\mathbf{x}) & \mathbf{x} \in \Omega \end{cases} \tag{7}$$

Where u_0 is the **initial datum**. The **solution** is $u = u(\mathbf{x}, t)$.

1.2.6 Classification of PDEs

A PDE is a relationship among:

- The partial derivatives of a function $u = u(\mathbf{u}, t)$, that is the PDE **solution**;
- **Spatial coordinates** $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$ on which the solution depends (if the problem is defined in a spatial domain $\Omega \subset \mathbb{R}^d$).
- **Time variable** t.

Therefore, a PDE can be written as:

$$\mathcal{P}\left(u, \frac{\partial u}{\partial t}, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_d}, \dots, \frac{\partial^{p_1+\dots+p_d+p_t} u}{\partial x_1^{p_1} \dots \partial x_d^{p_d}\, \partial t^{p_t}}, \mathbf{x}, t; g\right) = 0 \tag{8}$$

Where $p_1, \dots, p_d, p_t \in \mathbb{N}$ and g are the data.

Definition 5: PDE order

The **PDE order** is the **maximum order of derivation** that appears in $\mathcal{P}$, that is:

$$q = p_1 + \dots + p_d + p_t \tag{9}$$

Definition 6: PDE is linear

The **PDE is linear** if $\mathcal{P}$ **linearly depends** on u and its **derivatives**.

Classification

Let us focus on linear PDEs of order $q = 2$ with constant coefficients, so that the general PDE formulation is:

$$\mathcal{L}u = g$$

Where $\mathcal{L}$ is a second order, **linear differential operator**. When only two independent variables (our case) x_1 and x_2 are considered, the operator $\mathcal{L}$ applied to the function u reads:

$$\mathcal{L}u = A \cdot \frac{\partial^2 u}{\partial x_1^2} + B \cdot \frac{\partial^2 u}{\partial x_1\, \partial x_2} + C \cdot \frac{\partial^2 u}{\partial x_2^2} + D \cdot \frac{\partial u}{\partial x_1} + E \cdot \frac{\partial u}{\partial x_2} + F \cdot u$$

For some constant coefficients $A, B, C, D, E, F, G \in \mathbb{R}$. If $d = 2$ (our case), the **independent variables** can represent the *space coordinates*:

- $x_1 = x$
- $x_2 = y$

After introducing the **PDE discriminant** (a quantity that helps determine the type of PDE):

$$\Delta := B^2 - 4AC \tag{10}$$

The PDE can be classified as:

- **Elliptic PDE** if $\Delta < 0$
- **Parabolic PDE** if $\Delta = 0$
- **Hyperbolic PDE** if $\Delta > 0$

What are the implications of PDE classification?

The different nature of the PDE impacts on:

- **Type** and **amount of data to prescribe as boundary**;
- **Initial conditions** to ensure the well-posedness of the problem (existence and uniqueness of the solution);
- The **phenomena that can be described** by the PDE;
- The **information that encapsulates**.

In general:

- **Elliptic PDE** typically describes **stationary phenomena**, without time evolution of quantities.
- **Parabolic PDE** describes **wave propagation phenomena** with infinite velocity of propagation.
- **Hyperbolic PDE** describes **wave propagation phenomena** but with finite velocity of propagation.

1.3 Numerical Methods

Since in most cases of practical interest we **cannot solve a PDE analytically**, we need to use **numerical methods** that allow us to construct an *approximation* u_h of the *exact solution* u, for which the corresponding *error* $(u - u_h)$ can be quantified and/or estimated.

$$\begin{array}{cc} \mathcal{P}(u; g) = 0 & \text{PDE (mathematical problem)} \\ \downarrow & \textit{numerical method} \\ \mathcal{P}_h(u_h; g_h) = 0 & \text{approximate PDE (numerical problem)} \end{array}$$

Where:

- g_h is an approximation of the data g;
- $\mathcal{P}_h$ is a characterization of the approximate problem.

The subscript h indicates a **discretization parameter** that characterizes the numerical approximation. Conventionally, the smaller is h, the better is the approximation of u made by u_h. Furthermore, the error $(u - u_h)$ tends to zero as h gets smaller and smaller. In this course, we will specifically introduce the FE method (page 4) to build the numerical approximation of PDEs.

Summary Notation

Notation	Description
$\mathcal{P}(u; g) = 0$	PDE (mathematical problem)
u	***exact solution*** of a PDE
u_h	***approximate solution*** of a PDE
$(u - u_h)$	***error*** (quantified and/or estimated; tends to zero if h is smaller)
h	***discretization parameter*** ($\downarrow$ smaller h, better approximation; $\uparrow$ higher h, poor approximation)
$\mathcal{P}_h(u_h; g_h) = 0$	approximate PDE (numerical problem)
g_h	***approximation*** of the ***data*** g
$\mathcal{P}_h$	***characterization*** of the approximate problem.

Table 1: Notation used to approximate the PDE with numerical methods.

References

[1] Quarteroni Alfio Maria. Numerical methods for partial differential equations. Slides from the HPC-E master's degree course on Politecnico di Milano, 2024.

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