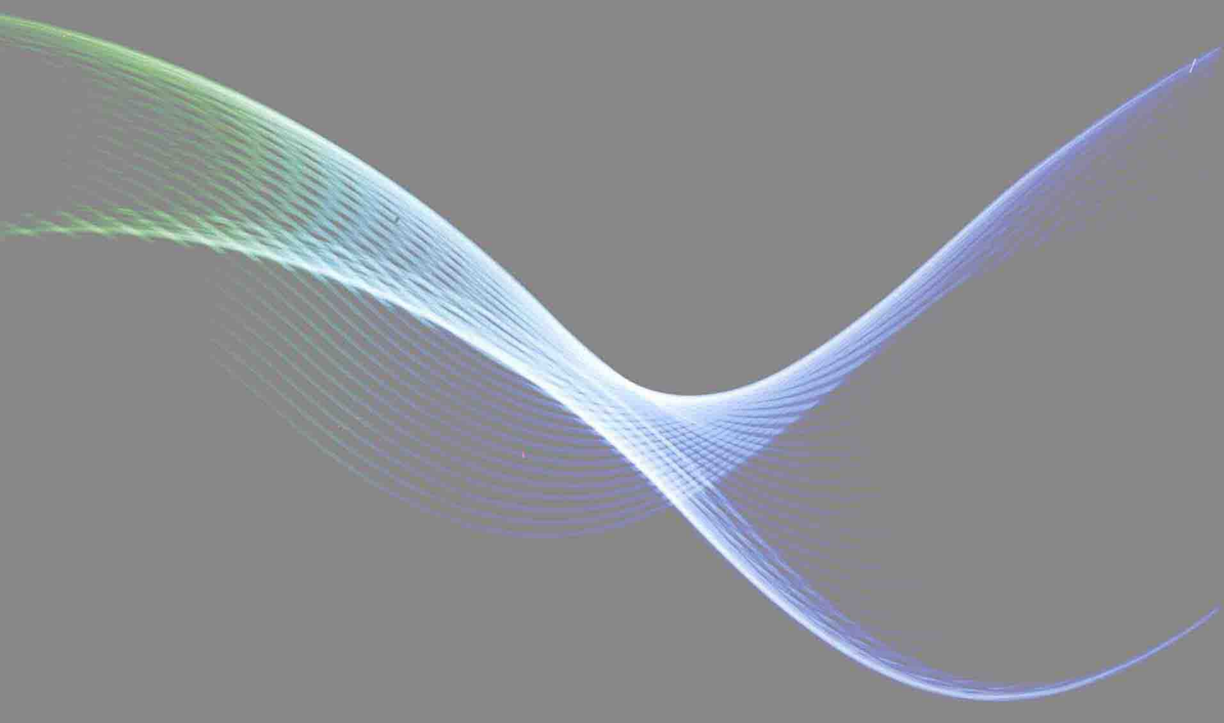
# NUMERICAL METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

## An Introduction

Vitoriano Ruas



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# NUMERICAL METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

## AN INTRODUCTION FINITE DIFFERENCES, FINITE ELEMENTS AND FINITE VOLUMES

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# NUMERICAL METHODS FOR PARTIAL DIFFERENTIAL EQUATIONS

*A Alex, Léo & Romy*

*En hommage à mes maîtres de l'école parisienne d'analyse numérique*

# Preface by Eugenio Oñate

Numerical methods have become nowadays indispensable tools for the quantitative solution of the differential equations that express the behaviour of any system in the universe. Examples are found in the study of engineering systems such as mechanical devices, structures and vehicles, and of biological and medical systems such as human organs, prosthesis and cells, to name a few. Numerical methods are applicable to the solution of differential equations that represent mathematical models of an underlying real system. These models are conceptual representation of reality using mathematics. It is interesting that in mechanics (which governs the behaviour of all engineering systems and many problems in physics) these models are obtained by simple balance (or equilibrium) laws applied to infinitesimal parts of the continuous system and its boundary. The beauty of the modelling process is that many times the resulting differential equations, even if they have the same mathematical form, are applicable to many different real life problems. A typical example is the Poisson equation that is used to represent the behaviour of such different problems as the heat conduction in a body, the seepage flow in a porous media, the flow of an incompressible fluid and the torsion of a bar, among others. Clearly a mathematical model represents a simplification of reality using geometrical data and physical properties of the constituent materials that are close enough to those of the real system under study and at the same time help to express its behaviour in mathematical form. On the other hand, the numerical solution of the resulting governing differential equations of the mathematical model introduces a series of simplifications. Numerical methods work on discretized forms of the model geometry which is split into simple geometrical entities, such as triangles and tetrahedra in two (2D) or three (3D) dimensions, respectively, as is typical in finite element or finite volume procedures or Cartesian grids, as is done in finite difference methods. The balance equations for each discretization unit (an element, a volume or a cell) are obtained in terms of a finite set of parameters and then used to obtain (assemble) the behaviour of the whole system by expressing the satisfaction of the balance laws at all the discrete points of the discrete system. The so-called discretization process leads to a system of algebraic equations that typically involve several millions of unknown parameters for real life problems. These equations are solved in modern computers using state of the art of computer science technology. This explains why numerical methods are many times referred to as computational methods. The two terms are in fact equivalent. The simplifications made along the modelling and numerical solution path lead to a final quantitative solution that is only approximate. The quantification of the modelling and numerical solution errors are topics of much current research. The timely book of Professor Ruas fits precisely in the context described above as it provides a comprehensive insight on the derivation and best use of numerical methods for solving a number of differential equations that govern a wide class of practical problems. The emphasis is in providing the reader with the knowledge and tools to assess the performance and reliability of a particular numerical method via the study of its stability, consistency, convergence and approximation order. The book uses simple one-dimensional (1D) problems for introducing the three basic numerical methods addressed in the book: finite differences, finite elements and finite volumes. A quantitative reliability analysis of the three families of methods is presented as well as the extension of the methods to transient situations and 2D problems. A convergence analysis for a well know multidimensional scalar problem (the Poisson equation) is also included. The book devotes a chapter to presenting higher order Lagrange finite elements and the extension of the finite element method to 3D problems. A final chapter describes a number of interesting topics such as the numerical solution of bi-harmonic equations in rectangles, the solution of the advection- diffusion equation, an outline of a posteriori error estimation and adaptive numerical solution procedures and a brief introduction to the numerical solution of nonlinear partial differential equations. Other numerical techniques are briefly presented in the Appendix.

I consider the book of Professor Ruas a valuable contribution to the extensive literature on numerical methods for partial differential equations. The book addresses modern and practical issues that are of paramount importance for the use of numerical methods with enough confidence. It is written in a clear form with many examples that help to understand the different concepts. I believe that it will be very useful to students in mathematics, physics, engineering and general sciences, as well as to the practitioners of numerical methods.

Barcelona, October 12, 2015
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# Preface by Larisa Beilina

This book presents the basics of the mathematical theory for three main numerical methods applied to the solution of Partial Differential Equations: the Finite Element Method (FEM), the Finite Difference Method (FDM) and the Finite Volume Method (FVM).

Author's proposal contains a lot of new material, such us several optimal results, which have not been considered before. An outstanding advantage of Professor Ruas' book is the fact that the basic FEM, FDM and FVM, are studied in a simple and popular fashion, although their reliability is addressed with all rigor by exploiting the concepts of method's stability, consistency and convergence. Main attention is given to low order methods as the most employed ones in real-life applications.

The first two chapters in the book describe the three discretization methods and present in a simplified framework the mathematical analysis applied to the one-dimensional boundary value problem in space. The next chapter considers discretization methods for time-dependent boundary value problems, as well as corresponding stability, consistency and convergence results. Then further chapters of the book gradually take the reader to the discretization and analysis of spatial and time-dependent PDEs in higher dimensions. More precisely, in a very easy form the FEM with piecewise-linear functions as well as the Vertex and Cell-centred FVM are explained, and convergence and reliability analysis of these methods are presented. Several important extensions of the FEM with Lagrange elements of degree greater than or equal to one applied to the solution of elliptic PDE in two and three dimensions are consistently shown. Finally, some basic numerical methods for the solution of non-linear PDEs are also described.

Several numerical examples appended to every chapter, run with codes written in MATLAB or in FORTRAN 95, illustrate approximation properties of numerical methods. At the end of every chapter a number of useful exercises are proposed in order to help the reader to consolidate understanding of the material presented therein, for a number of applied problems.

This book is undoubtedly of great interest for undergraduate and graduate students in computational and applied mathematics, as well as for researchers and engineers working in the field of numerical methods for PDEs.

Gothenburg, October 30, 2015
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The author is most grateful to his colleague and friend Marco Antonio S. Ramos for a scrupulous and diligent help with coding and numerical examples.

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# About the Companion Website

This book is accompanied by a companion website:

www.wiley.com/go/ruas/numericalmethodsforpartial

The website includes:

- Host codes
- Solutions for the exercises

# Introduction

In the realm of spirit, seek
clarity; in the material world,
seek utility.
Gottfried Wilhelm Leibniz

Since Leonhard Euler, **numerical methods** gradually became the currently widespread techniques to solve real-life problems governed by **differential equations**. It was, however, the invention of modern computers in the middle of the 20th century that significantly pushed this branch of applied science to play such a prominent role in contemporary technological development. Supercomputers among other high-performance machines became available since the 1980s, and this has favoured an even more spectacular evolution of numerical methods for differential equations, as tools capable of producing exploitable responses out of mathematical models of the kind.

In case a system of differential equations is expressed in terms of more than one independent variable, a system member is referred to as a **partial differential equation** (i.e. a **PDE**) and otherwise as an **ordinary differential equation**, (i.e. an **ODE**). About 100 years ago, numerical methods became practitioners' preferred alternative to solve PDEs, whose analytical solution is out of reach. This book is intended for presentation, to specialists acting in various technological and scientific fields, of basic elements on numerical methods to solve PDEs. Although the equations can be posed in any kind of spatial domain, here we confine ourselves to the case of **boundary value problems**, supplemented with **initial conditions** in case they are also time-dependent. This implies assuming that an equation's definition domain is bounded. Moreover, except for a few cases, the presentation is restricted to equations in terms of real independent variables, whose solution range is a subset of the real line.

It is well-known that PDEs model the behaviour of relevant unknown quantities in a large amount of situations of practical interest. These cover domains as diverse as engineering, physics, geo- and biomedical sciences, chemistry and economics, among many others. For example, in aircraft design the knowledge of the way air flows about fuselages is of paramount importance, as much as mastering the propagation of acoustic waves in vehicle interiors is a must in modern automobile design. Also in recent decades, more and more such models are being employed in the search for better understanding of human body systems. This is surely helping to prevent highly lethal diseases such as cardiovascular ones.

Of course, whenever possible, analytical methods should be employed to solve certain types of PDEs. Among these, the method of separation of variables is an outstanding example. However, for different reasons, including model complexity, irregular geometries or inaccurate field data, it is no point trying to determine exact analytical solutions to PDEs in most cases. Instead, numerical methods, naturally designed for use in a computational environment, provide a valid alternative to mathematical expressions representing solutions to the theoretical model. These can be as diverse as fluid velocity, blood pressure, electromagnetic fields, structural stresses, species fractions in biological evolution or chemical reactions, among many others having their behavior modelled by a PDE. That is why running a computer code, in which a numerical solution procedure is implemented, is called a **numerical simulation**. Indeed, the thus generated numerical values replace, in a way, a physical response to input data characterising a specific application.

## Aim

The purpose of this book is to study numerical methods for solving PDEs, designed to possibly generate accurate substitutes of unknown fields, in terms of which the equations are expressed. Generally speaking, instead of values provided by a solution's analytical expression at every point of the physical domain in which a given phenomenon or process is being modelled by a PDE, in the numerical approach only solution's approximate values or related quantities at a finite number of points are determined. Owing to this feature, the underlying numerical method is also known as a **discretisation method**. Otherwise stated, the term **discrete** qualifies numerical solution techniques, as much as the terms **analytical** and **continuous** do for procedures aimed at finding exact mathematical expressions for a solution, when they exist.

To a large extent PDEs, being used in mathematical modelling, are of the second order, which means that the highest partial derivative order of the unknown fields appearing in the equations is two. For this reason, a particular emphasis is given to this class of PDEs throughout the text. However, for the sake of conciseness and clarity, we will confine the whole presentation of the numerical methods to the case of **linear differential equations**. Nevertheless, the types of linear PDEs to be studied are the most frequently encountered in practical applications, namely, **elliptic, parabolic and hyperbolic equations**. We assume throughout the text that the reader is familiar with basic concepts of linear PDEs of these representative types. Nevertheless, it would not be superfluous to recall the criteria that characterise them, by restricting the definitions to the case where the solution $w$ of a linear second-order PDE is a function of two independent variables $r$ and $s$, and moreover to the case of constant coefficients, that is, an equation of the form

$$A\frac{\partial w^2}{\partial r^2} + 2B\frac{\partial w^2}{\partial r \partial s} + C\frac{\partial w^2}{\partial s^2} + D\frac{\partial w}{\partial r} + E\frac{\partial w}{\partial s} + Fw = G,$$

where $G$ is a given function and $A^2 + B^2 + C^2 > 0$. Letting $\Delta = B^2 - AC$, we have:

- If $\Delta > 0$, the equation is hyperbolic;
- If $\Delta = 0$, the equation is parabolic;
- If $\Delta < 0$, the equation is elliptic.

One of the main differences between the three types of equations relies on the boundary and/or initial conditions that must be prescribed, in order to ensure existence and uniqueness of a solution. This issue will be clarified in Chapter 3, as far as the first two types of PDEs are concerned, and in Chapter 4, whose purpose is the study of the Poisson equation, the most typical elliptic PDE.

As many authors believe, in starting from linear PDEs, it is easier to take on otherwise challenging and complicated problems in more advanced studies. Furthermore, this linear approach has an undeniable virtue: if a numerical method is unreliable to find solutions to a simplified linear (i.e. a linearised form), of a true nonlinear model, let alone its application to the latter.

## Scope

First of all, we should emphasise that in contemporary numerical simulations of complex physical events, powerful computational tools such as graphics processing units (GPUs) are at practitioners' disposal. Moreover, high-performance techniques to optimise simulation codes, in order to save RAM and storage in general and make them run faster, have been in current use for the past few decades. Here one might think of **vectorisation**, a technique aimed at speeding up matrix and vector arithmetics, featuring more recent scientific computing-oriented programming languages such as FORTRAN 95 and MATLAB. **Parallel computing** based on distributed systems consisting of a computer network or several processors running concurrently in parallel, in order to accomplish different tasks of large-scale numerical processing, has been a facility in use in research centers and industries around the world for a few decades now. Although we are convinced that the reader should be aware of these possibilities, we do not address them at all because our book is an introductory one. In other words, its scope is limited to the study of numerical methods in the framework of rather simple model problems, whose solutions do not require sophisticated tools employed in intensive computer simulations.

The subject this book deals with is continuously evolving. New proposals for the numerical solution of PDEs of particular types are being published in specialised journals practically every week. However, a glance at the present state of the art suffices to show out that a milestone was reached about 50 years ago. At that time, the concepts lying behind three big families of discretisation methods to solve PDEs became well accepted in the worldwide scientific and industrial communities. More precisely, we mean the **finite difference method** (FDM), the **finite element method** (FEM) and the **finite volume method** (FVM), which we chose to study in detail in this book, as techniques playing central roles among several ingredients, in a recipe for the computational determination of **numerical solutions** to PDEs.

The FDM is the oldest and the simplest numerical method to solve differential equations. It has been known since Euler's work in the 18th century, and countless specialists in numerical mathematics contributed to its development up to now. Its routine use among specialists in the numerical solution of PDEs dates back to the beginning of the 20th century. Pioneering work of **Courant**, **Friedrichs** and **Levy** in Europe and in the United States (cf. [55]) set the bases to justify the method's effectiveness and reliability. Almost in parallel, **Gerschgorin** [85] derived decisive results in the framework of numerical analysis as applied to PDEs. Much later, other prominent members of the Russian school such as **Godunov** [91] and **Marchuk** [133] gave relevant contributions in this direction. The latter also collaborated hand in hand with **Lions** (cf. [127]), the respected founder of the prolific Paris school of analysis and numerical mathematics for PDEs in the late 1960s. However as Lions himself and his disciples realised very soon, the development of the FDM was considerably slowing down in the last third of the 20th century, because of its limitation to handle efficiently complex geometries and/or boundary conditions. Nevertheless, the author should stress that, owing to its simplicity and easy implementation, as a rule the FDM should be preferred to other methods, as long as severe applicability restrictions do not come into play. This certainly explains why the method is still very popular today.

In contrast, from the mid-1950s on, the FEM gradually emerged as a flexible tool capable of giving appropriate responses to most geometric and mathematical challenges encountered in practical applications of PDEs, more particularly in engineering. At that time, work on this new numerical simulation technique was carried out simultaneously in several places, in connection with big-aircraft industry among other major building or manufacturing enterprises. The method was tailored to its present form by people like **Clough**, **Turner** [196] and co-workers in the United States; **Argyris** [8] in Germany and in England; **Zienkiewicz** [210] in Wales; **Fraeijs de Veubeke** in Belgium [75] and **Arantes e Oliveira** in Portugal [7], among many other names.

A little later the FVM appeared as a new tool, aimed at overcoming the aforementioned limitation of the FDM. Scientists like **Samarskii** and **Tikhonov** [193] from the the Russian school can be credited as outstanding developers of the FVM, as much as **Spalding** and **Patankar** in the United Kingdom (cf. [151] and [152]). A remarkable growth of the method's user community followed, and to date several commercial simulation codes widely in use in industry are FVM-based, more particularly in fluid dynamics. Such a great success seems to be due to the fact that the principles the method is based upon are close to those of physics. Indeed, by using this method, local mass or heat fluxes, discharges among many other fundamental physical quantities, can be easily controlled in a direct and transparent manner. This is certainly very appealing to industry designers who ordinarily are not available to undertake too many technical interventions in order to run a simulation code, or to post-process numerical results.

On the other hand, the FEM is by far the richest among these three numerical methods, in terms of both versions and applicability. The number of efficient FEM packages available, as applied to a wide spectrum of technological domains, is very large, and this is particularly true of structural analysis. Actually, the range of the FEM and its multiple variants to solve countless classes of problems governed by PDEs is steadily growing, and is practically unlimited. This has certainly something to do with the method's great versatility. However, it is true that in some domains such as fluid dynamics, good use and understanding of the FEM require some more mathematical insight, which is perhaps the reason why the FVM is often preferred in such applications.

These preliminary considerations on the strengths and weaknesses of the three methods will be enriched by additional comments to be made as they are presented and studied along the chapters.

## Approach

It is important to recall that values provided by the numerical solution procedure are only **approximations** of those of the theoretical solution, at least in an overwhelming majority of cases. But then a fundamental question arises: How reliable are such approximations as compared to the corresponding values the model would provide if it could be solved analytically? An attempt is made to give precise answers to this question without resorting to functional analysis, in contrast to what many authors do.

Actually, in a book aimed at being used in the framework of an introductory and intensive course it would be advisable to avoid as much as possible going into details on mathematical aspects of the numerical methods being presented. Addressing rather their functional features, such as limits and merits in practical terms, or implementation, might be considered more appropriate. However, many authors are persuaded that, for a better comprehension of numerical methods, mastering underlying basic mathematical concepts is of paramount importance. As a former assistant of the late Professor **Daniel Euvrard** at the Division of Mechanics of the University of Paris 6, the author believes to have learned well with him the right approach to motivate into the subject students in fields other than mathematics, and to convince them why a numerical method is reliable or not. Nevertheless, in his book, he declined to go into ultimate considerations on such aspects of numerical methods. This is perhaps because he felt this would require mathematical concepts supposedly not mastered by his students. Within a certain time after Daniel Euvrard passed away, the author endeavoured to find means to render complete and rigorous reliability studies of numerical methods for PDEs accessible to final-term undergraduate or graduate students in any scientific domain. In a sense, this book is the outcome of what the author believes to be the ideal pedagogic approach, after a rather long maturation period.

More precisely, we shall introduce and thoroughly exploit the concepts of **stability**, **consistency**, **convergence** and **order** of a numerical method to solve PDEs, as fundamental tools to understand why they work or not, or how well they work. This is because both the stability and the consistency of a numerical method imply that it is reliable. More precisely, convergence to an equation's exact solution is guaranteed at a certain rate related to the method's order. However, it must be emphasised again that this book utilises neither high-level nor abstract mathematics to qualify numerical methods. Indeed, only the mathematical knowledge a student in scientific or technical fields is supposed to master, when she or he reaches the stage of studying numerical methods for PDEs is taken for granted. Nevertheless in some cases, optimality in the mathematical sense is sacrificed, so as to make possible such an approach.

In short, in many respects, this book can be viewed as original. The following issues should definitively be underlined:

- The pre-requisites for full understanding of this book's material are differential & integral calculus in multiple variables, besides elementary analysis, tensor calculus, numerical analysis and linear algebra. Of course, basics of differential equations including linear PDEs are supposed to be known.
- The reliability analyses for the three methods are carried out in a unified framework, by exploiting in a structured and visible manner the equivalence between convergence and the pair of properties stability and consistency, that is to say, the **Lax–Richtmyer equivalence theorem** [123].
- In addition to this unified treatment, here and there new techniques are employed to derive known results, thereby simplifying their proof.
- Emphasis is given to low-order methods, as practitioners' overwhelming default options for everyday use.
- In the chapters, any time a particular PDE's feature is important for better comprehension of a numerical solution method, the corresponding property is duly presented, recalled or cited from the literature.

- The book is placed halfway between texts addressed to students in mathematics and those for students in other sciences. This means that a balanced emphasis is given to both practical considerations and a rigorous mathematical treatment.
- To the best of the author's knowledge several optimal results rigorously established in the text cannot be found elsewhere, not even in more advanced books. In this sense, although this one is basically education oriented, marginally it can also be a valid reference for research work on numerical methods for PDEs.

More commonplace features are lists of exercises proposed at the end of each chapter. Most of them are just complements to theoretical studies, in order to help the student to consolidate her or his understanding of a particular issue. In some cases, exercises are simply a way to abridge the text itself. In addition to this, several numerical examples are supplied using codes programmed either in **FORTRAN 95** language or in a **MATLAB** environment. Almost all the given examples are academic in the sense that their exact solution is known beforehand. This is because they are essentially aimed at either illustrating or assessing methods' approximation capabilities. By adding this kind of stuff to all chapters, our approach turns out to be similar to the one adopted in some text books on the subject such as **Hughes'** [100]. However, in contrast to this one, the latter are either devoted to a single type of method or addressed to a specific scientific community. In short, coding was just aimed at supporting the material addressed in the book and in no case a goal itself. This is the reason why we did not care about using techniques such as vectorisation, parallelism or computational tools more powerful than an ordinary laptop for running our examples. The reader will certainly realise it by examining some of the programs incorporated into the text.

The general subject organisation throughout the book is as follows. For the sake of clarity and objectiveness, the basic concepts inherent to numerical methods are first presented in the framework of differential equations whose spatial definition domain is one-dimensional, more specifically a bounded interval of the real line. Nevertheless, this presentation is enriched by the treatment of the **time-dependent case**. This means equations having the time as an independent variable, besides the space variable, which model the so-called **transient problems**. Once these concepts are introduced in such a simplified framework, their application to problems defined in domains of higher dimensions can be assimilated more smoothly as we believe. However, we only apply to two-dimensional problems (surely closer to real-life ones!) the conclusions in terms of reliability that the previous studies allow for. A point of view shared by many authors is that this is good pedagogy, since properties that hold for a multidimensional problem can often be regarded as mere extrapolations of valid ones for lower dimensional counterparts.

From the beginning, we should point out that in a significant majority of cases, a numerical method to solve boundary value problems leads to the solution of **systems of linear algebraic equations**. Since such systems play a central role in the framework of numerical methods for PDEs, throughout the text the acronym **SLAE** will be used instead of the expression in full. The SLAE unknowns are usually approximations of the solution function at a set of points of a discretisation lattice. As pointed out above, for this reason numerical methods are often referred to as discretisation methods. Notice, however, that SLAE unknowns can also be other expressions, depending on the solution function, such as derivatives, integrals or combinations of all these.

Owing to the topic's relevance, we supply right after this Introduction some reminders of linear algebra as related to SLAEs, which will be particularly useful throughout the text.

Whenever necessary, these will be complemented with further details on a method to solve SLAEs particularly pertinent to a subject addressed in a given chapter.

## Book's outline

Following the introductory section on linear algebra, we describe in Chapter 1 the three discretisation methods named above, as applied to a one-dimensional model problem. Chapter 2 is devoted to mathematical analyses of these methods in such a simplified framework; more precisely, the basic concepts that characterise the reliability of a numerical method for solving a PDE are introduced. In Chapter 3, we apply the same concepts in order to examine schemes for time-dependent counterparts of the model problem. In Chapter 4, we describe the use of the three approaches to solve problems posed in two spatial dimensions without time dependence. The aim of Chapter 5 is the rigorous mathematical study of numerical methods in two space variables. Besides the problems addressed in Chapter 4, their time-dependent counterparts are also considered. This chapter is by far the heaviest part of the book in terms of calculations, which could be left aside in a short or intensive course. In this case, the student could just concentrate on the final results. Chapter 6 brings about several important extensions of the material studied in all the previous chapters, in terms of practical applications, including three-dimensional modelling. Chapter 7 is a complementary one; specific numerical methods are considered for a few scattered but relevant classes of linear PDEs that are not studied in the previous chapters. In the final section of Chapter 7, some basics of the numerical solution of nonlinear PDEs close the book. This outline is completed by those supplied at the beginning of each chapter, specifying its organisation and providing a brief summary of its different sections.

To conclude, we must underline that in contemporary numerical simulations, users can count on numerous methodological options. At an introductory level, however, it would be out of purpose to attempt to address them all. That is what motivated our choice of three methods out of several other techniques for solving PDEs. Nevertheless, for the reader's information and better guidance, we added an Appendix, where main lines are highlighted of several numerical methods of current use not covered by the book. More specifically, brief descriptions are given of the boundary element method, discontinuous Galerkin methods, meshless methods, spectral methods, hybrid finite elements, iso-geometric analysis, the virtual element method, domain decomposition techniques and multigrid methods.

## WARNING

Throughout the text, the range of any subscript or superscript is assumed to be sufficiently large, for the surrounding statements or formulae involving it to make sense.

Incidentally it should be stressed that, to a great extent, numerical analysis is the art of handling concepts closely related to integer symbols standing for array subscripts, grid point positions, time stages or iteration numbers in recursive procedures, among many other abstract things of unspecified dimensions or sizes. For this reason, the reader should be aware that following such notations requires much attention. Moreover, symbol-correct typing forces authors on the subject to make an iterative improvement of their texts, a process that usually converges very slowly, and eventually never converges ...