Numerical Methods and Modelling Methodologies in Computational Biomechanics

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PREFACE

Writing a book on numerical methods in computational biomechanics is not an easy task for several reasons. First of all, the audience. This is a book aimed at both undergraduate and graduate students, members of the academy, and also professionals in engineering and applied sciences. They all have different levels of knowledge and understanding of the topics. But despite this, and knowing the risk we are taking, we will still dare to do it.

Computational mechanics is one of the most fascinating fields of engineering and applied sciences. Perhaps one of the main aspects is that numerical simulation and computational modelling in biomechanics allow the analyst to better understand both biological and mechanical environments often immeasurable and inaccessible such as strains, stresses, and fluid flows (blood, air, etc.) in living organisms. The mechanical environment of in vivo systems can provide information about the state of health, predict the onset of disease, or assess the outcome of treatments. Therefore, models (and modelling) help researchers to organize and understand our observations and to predict the responses of living things under specific environments.

During the first half of the 20th century, researchers and modellers explored (and continue to explore) different biological scenarios using conservation laws, constitutive relationships, and appropriate numerical methods to create an in silico biological laboratory. Biological models address the complex challenges we face when trying to understand the behaviour of biological systems and human diseases, often from a multidisciplinary point of view.

In recent history, the complexity of models in the field of hardware-based science and engineering has experienced rapid growth, driven in part by theoretical understanding and the development of numerical formulations capable of being applied to simulations involving a large number of physical phenomena that interact with each other in a particular setting. The increasing demand in resources and computational effort caused by the complexity of the models has been largely mitigated by the increasing advancement of modern computing platforms. However, advanced methodologies capable of formulating and solving computational problems with precision and stability are of vital importance in seeking to address the complexity of multiphysics in biological problems, which is one of the main goals of this book.

A single example will suffice to illustrate what we are saying: the problem of the isotropic infinite medium subjected to a concentrated load was solved in 1848 by Lord Kelvin who provided the fundamental solution to the elastic problem, namely the Green's function of the Navier equations. With these equations and using the Principle of Superposition it is possible to determine, at least theoretically, the solution for the infinite medium and any external action constituted by loads. But given the immense volume of mathematical difficulties that the elasticist has to face in order to solve problems, the great majority of them do not yet have an analytical solution, nor will they in the near future. During the first half of the 20th century, the photoelastic method was the best resource available to solve a large number of problems, especially stress concentration in mechanical parts.

Numerical procedures and methods have been used to obtain approximate solutions, such as the Finite Difference method which, given its limitations, has been of little use when dealing with complex biomechanical simulation. In the middle of the 20th century, simultaneously with the birth of the computer, the Finite Element method emerged transforming the solution of the anisotropic elastic medium into the resolution of large linear systems of algebraic equations. Later, the Boundary Element method appeared which also transformed the elastic problem into the solution of a linear system of algebraic equations. Both methods, Finite Element and Boundary Element, are powerful. They are able to adaptively limit errors and are applicable not only to the elastic problem but to many other problems in physics. The development of numerical methods has then been possible thanks to the computer, an indispensable tool given the large number of equations to be solved.

Thus, this book collects a broad overview of numerical methods for simulation and modelling in biomechanics, covering methods such as Finite Volume, Finite Element and Boundary Element. Its application to computational biomechanics is discussed, showing studious readers various ways to simulate applied biomechanics problems.

The methodology proposed by the authors of this book contributes to the rapidly changing field of numerical simulation and its applications to complex biophysical problems. The topics are presented and discussed in careful detail and with full attention to the balance between theory and practice. The book can serve as a guide to code development in the field of computational simulation.

The diversity of the disciplines covered in the book gives it a singular character which we hope readers will find not only enjoyable but also of great use in seeking to understand the complex scenarios that engineers and analysts face when trying to simulate, and learn from, biomechanical problems in tissues, organs and human beings.

The Authors
Barcelona & Bogotá
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I

Introduction and theoretical background

CHAPTER 1

INTRODUCTION

1.1 An overview of numerical methods in computational biomechanics

This book proposes a practical and engineering view of computational biomechanics, covering a wide range of biomechanical topics using solid and fluid continuum mechanics. Several numerical simulation methods are presented so that the reader can compare their advantages and limitations in various applications. Domain methods have indisputable advantages over boundary methods in well-known and bounded domain applications. However, in problems where the domain is uncertain, not fully defined or very far away, boundary methods outperform domain methods in most cases.

The text is the result of the research undertaken by the authors over the last several years into the development of a comprehensive system of computational tools capable of addressing many aspects of the biophysical phenomena involved in bone tissue simulation including tissue differentiation, properties characterization, biomechanics, flow in porous media, as well as the complex interactions among them. To this end, the authors present the problem by using a rigorous formulation of existing biological and biomechanical processes, followed by a thorough comparison between them and the development of various state-of-the-art numerical techniques in bone tissue analysis.

Therefore, in this work the necessary fusion between mathematics, classical mechanics, and physics with medicine and biology is proposed, generating useful results for all and in particular for the patient who is the greatest beneficiary. The notable scenario that preceded this pairing is found with Giovanni Alfonso Borelli (Naples 1608, Rome 1679), an eminent mathematician and physicist who, upon contacting doctor Marcelo Malpighi (Bolonia 1628, Rome 1694), encouraged him to enter medicine.

Malpighi said: "The laws of the Universe are always on the side of the most sensitive observer." He was the attending physician of Pope Innocent XII (1691-1694) and he is considered the founder of Histology. His contributions delved into the physiology of the animal and plant kingdoms. He investigated brain anatomy, describing the distribution of the cortex, spinal cord tracts, and their connections to the cerebrum and cerebellum.

From these studies, and enthused by the glandular structure that he had investigated, he concluded: "The brain was of a glandular nature and secreter of vital spirits." This was in 1656, when he coincided at the University of Pisa with Giovanni Alfonso Borelli, professor of mathematics, whose house was a veritable laboratory that was enriched by the patronage of Grand Duke Ferdinand II. Borelli had the idea that men could fly like birds. In his research and experimentation, he discovered that birds have pectoral muscles that represent one sixth of their weight and can produce a force equal to 10,000 times their mass, unimaginable for humans. Borelli's greatest contribution to science was the application of physical and mathematical laws to biological processes, all within the Iatromechanics school, in which he was perhaps the most remarkable and well-known member.

Focusing on the numerical methods of analysis of the continuum, the first attempts to solve what is now called the elastic problem date back to the time of Galileo in the 17th century, when the elastic medium, and hence its properties and constitutive laws, were not yet known. It was not until the beginning of the 19th century, more than a century after the formulation of Hooke's Law, that the French mathematicians, physicists and engineers of the time (Cauchy, Poisson, Navier, Lamé, etc.) were able to establish the equations and general principles of the Theory of Elasticity. Since then, much progress has been made in solving the elastic problem and in determining analytical solutions to particular problems.

The discretization of continuous problems has been treated differently by mathematicians and engineers. Mathematicians have developed, on the one hand, general techniques directly applicable to the solution of the differential equations that govern the problem and, on the other hand, approximate techniques to determine the stationarity of the “functionals”. Engineers have tried to approach the problem in a more intuitive way by creating a direct analogy between real discrete elements and finite portions of a continuous domain to approximate the solution. Figure 1.1 schematically shows the evolution of mathematical techniques and methodologies that have shaped the most widely used numerical methods in engineering today.

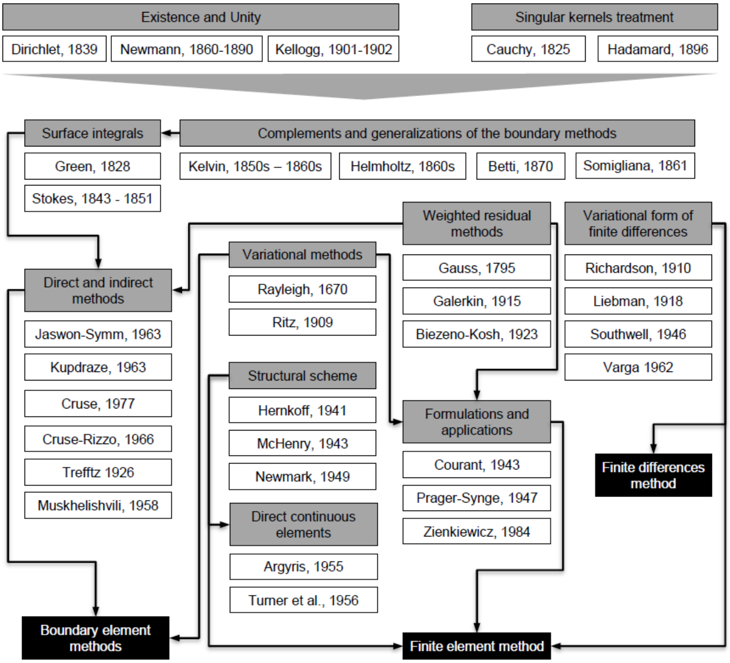

Figure 1.1: Summary of the evolution of numerical methods commonly used in engineering and applied sciences (adapted from Gonzalez *et al.* (2009)).

Regarding the modelling process, perhaps one of the most important obstacles that the analyst faces is: How to model the physical problem? The question is not easy and admits varied answers. Basically, two large categories can be established in the simulation process: the physical model, which interprets the real structure, and the mathematical model, which represents the physical model. For modelling purposes, the first thing to be determined is what type of representation should be used: plane stresses, plane strains, axisymmetry, 3D general solids, etc. (in the case of stress analysis of the continuous medium).

The best model to use is undoubtedly a general three-dimensional model (3D general solid) that considers the non-linear effects of both material and geometry. However, this is often difficult given its high cost and demand for human and computational effort. That is why sometimes simpler and cheaper two-dimensional models are used. Usually, but not always, and depending on the complexity of the real problem, the use of three-dimensional models involves higher costs by an order of magnitude than two-dimensional models. Likewise, it must be taken into account that determining the "exact" answer to the problem is impossible, since no matter how complex is the model used, it will never be possible to represent all the complexity and the number of variables that characterize the model.

Parallel to the development of theoretical models, there have been great advances in the computational field. The study of bone mechanics is linked to major obstacles such as complicated geometries, anisotropy, non-homogeneity in the properties of materials, particular boundary conditions, etc. Therefore, numerical simulation has prevailed to provide an approximate solution to these complex problems.

Let us turn to theories of bone adaptation which are one of the most relevant applications in bone biomechanics. There are a large number of computational approaches for the simulation of the bone adaptation process, some of them based on beam theory (Cowin *et al.*, 1985) while others are based on the boundary element method (Sadegh *et al.*, 1993). However, the numerical method that has been commonly used is the finite element method (Beaupré *et al.*, 1990; Doblare & Garcia, 2002; Hart *et al.*, 1992).

The modern treatment of the subject begins with Pauwels (1960) who proposed that the tissue growth and remodelling are achieved by the transformation of mechanical energy into the energy required for the chemical reactions involved in these processes to take place. Hydrostatic compression applied to mesenchymal tissue favoured cartilage formation, while deformation favoured connective tissue formation, and a combination of both led to fibrocartilage formation. According to this hypothesis, bone can only form after soft tissues offer sufficient stability. Subsequently, Carter *et al.* (1988) proposed a callus model using the finite element method to test the Pauwels hypothesis. They were the first to define a model focused on the study of the mechanical factors that affect tissue differentiation and, therefore, the evolution of healing, proposing one of the most important semi-quantitative hypotheses in the field of bone repair (Lacroix & Prendergast, 2002).

Focusing now on modelling in either elastic or elastoplastic domains, critical zones generally appear; these are zones where the stresses are concentrated, presenting high gradients. Stress concentrations on some areas of the model may be a result of poorly refined discretizations in the areas of concentration, or due to sudden changes in geometry or boundary conditions (loads or links). That is, there are stress concentrations caused by the definition of the mathematical model and the characteristics of the real situation. For example, point loads generate high stresses in the model response. The solution to this could be to apply the concentrated load as an equivalent stress over a very small area or edge. When it comes to high stresses caused by sudden changes in geometry such as sharp corners, one solution is to round off these corners to make them more representative of the real situation. This leads to a greater effort in defining the mesh as the area must be refined but, instead, a more real model is obtained, without “artificial” concentration of stresses. For instance, a practical case of undeniable importance is the insertion of implants in traumatology, where we should emphasize that improvement in osseointegration of the implant into the bone is a key factor for the effective and long-term implantation of any kind of implants.

Another classic issue of great importance is to decide which numerical method should be used in which application. In the vast majority of practical cases, the simple discretization of the boundary necessarily leads to a much smaller system of equations, compared to any method that requires the discretization of the entire domain (e.g. finite element method). On the other hand, in a homogeneous problem, the system of matrices generated by the boundary methods is non-symmetric and completely filled, while the system generated for the (much larger) finite element solutions is relatively sparsely populated and usually symmetric.

We should keep in mind that the Finite Element Method (FEM) is an approximate analysis tool and not a “magic” method. Analysis by the FEM will not give more or better results than those that the data can represent. That is, if the data entered is reliable and correct, the results will be reliable and correct. In certain applications of biological systems, it may be more appropriate to use approaches such as the Finite Volume Method (FVM). This is particularly true when considering phenomena involving biofluid flows, or transport phenomena in biological systems in general. As in the case of FEM, it should be kept in mind that the results obtained with FVM are approximations that, although precise or accurate, should be carefully examined and always validated against experimental or observational data.

Given the nature of the fundamental solutions, the results obtained by the Boundary Element Method (BEM) automatically satisfy admissible boundary conditions at infinity, so problems with boundaries at infinity do not require subdivisions at those boundaries, while in the case of finite elements or finite volumes, infinite boundaries must be approximated by a considerable number of distant elements. Also, for those systems characterized by semi-infinite regions with part of their surface free of charge and with the choice of the appropriate singular solution, the BEM does not require the complete discretization of such surfaces.

This is an appropriate moment to comment on the trend of analysis methods, within the complete conceptualization-analysis-design-manufacturing process: it is foreseeable that the analysis tools (FEM, FVM, and BEM) will improve further and allow the analyst to devote more attention to the definition of the model than to its analysis. In particular, less complex problems (typically based on linear behaviour models and subjected to static actions) can be analysed with tools that calculate the “error” committed and proceed to refine those critical areas of the mesh where the error is greater, to repeat the cycle again until the global error falls below a prescribed tolerance. All this iterative cycle of analysis will be automatic and will require practically no intervention from the analyst.

Several illustrative examples have been included in the text, so that the reader can check the usefulness and power of the numerical methods described in solving problems in biomechanics and biological processes.

Finally, the authors extend their deep and sincere thanks to all those people who contributed to this book and who made it possible for this work to see the light of day.

1.2 Why was this book written?

Today there is a growing need for engineering and practical approaches to make it easier for broad sectors of the engineering and biomedical community to understand computational mechanics. Therefore, this book focuses on numerical methods for biomechanical analysis.

The book covers an extensive number of topics of interest to biomechanicists, from basic aspects of solid mechanics to cases of utility in professional activity. The authors believe that this book can serve as a manual in biomechanics to guide the use of numerical methods, which is undoubtedly useful for all those involved in the field. It is a book that could serve both as a class textbook as well as in undergraduate courses in orthopedics and biomechanics.

In biomechanics, there are many interrelated concepts. In many cases, having analytical techniques and numerical methods together will help in better understanding the relationship between the concepts. Moreover, being able to study the worked examples illustrating the concepts of biomechanics will help consolidate the learning.

1.3 Who is this book useful for?

This book will be very useful for undergraduate and graduate engineering students, lecturers in both undergraduate and postgraduate schools, engineers, practitioners and biomechanical specialists, as well as orthopedic surgeons and clinicians.

The book is well presented, with clear organization and precise writing. It covers a wide range of aspects of biomechanics, from theoretical subjects to practical applications. This book will also be a comprehensive and unified text for those involved in biomechanical research and teaching, showing several numerical methods available for analysing real biomechanical and biological models. We maintain an introductory tone throughout the book, accompanied by numerous illustrations, which will undoubtedly facilitate its understanding and encourage follow-up by the studious reader.

This book is also oriented to professionals in engineering and applied sciences, both academics and those in professional practice. But it will also appeal to anyone wishing to deepen their knowledge of modern analysis methods, and whose curiosity takes them beyond the simple execution of a computer program.

In summary, it is a text for undergraduate and graduate students, academics and professionals, which can be used in undergraduate and introductory courses in graduate biology, medicine, and engineering. Each chapter is self-contained, that is, it can be followed without a strict need to refer to other chapters, although it is recommended that you read and follow the text sequentially.

1.4 Organization of the book

This book has nine chapters and one appendix, organized into **four main parts**, as described below:

PART I: INTRODUCTION AND THEORETICAL BACKGROUND. This opening part contains chapters devoted to the formulation and generalities of numerical methods and simulation. **Chapter 1** examines some history and how to conceptualize continuous problems. **Chapter 2** covers the basic foundations of tensor analysis when applied to continuum mechanics. **Chapter 3** briefly describes the necessary concepts of solid mechanics, emphasizing the Principle of Virtual Works and the constitutive laws of the material, while **Chapter 4** shows the formulation in fluid mechanics, discussing Newtonian and non-Newtonian fluids as well as laminar and turbulent flows.

PART II: NUMERICAL METHODS AND ALGORITHMS IN BIOMECHANICS. This section includes chapters concerned with numerical methods in biomechanical analysis. **Chapter 5** deals with the classical mathematical tools used in numerical methods. **Chapter 6** shows the formulation of various numerical methods such as the Finite Element method, the Finite Volume method and the Boundary Element method.

PART III: MODELLING IN BIOMECHANICS: AN ENGINEERING APPROACH. This part is made up of chapters devoted to the formulation of specific problems in biomechanics. **Chapter 7** shows how to model and analyse hard tissues of the human body, discussing the classic problems of bone fractures and their healing as well as the effect of piezoelectricity on bone remodelling. **Chapter 8** deals with biological problems governed by fluid mechanics. The computational simulation of bio-fluids is revisited from a general point of view, with special emphasis on air flow in the respiratory system. Finally, **Chapter 9** is dedicated to the simulation of biological processes, such as the diffusion of nutrients in vertebral discs, simulation in mechanobiology and bone ossification, among other areas.

Appendix A contains concepts of variational calculus, necessary for a correct formulation of numerical methods.

CHAPTER 2

TENSOR ANALYSIS IN CONTINUUM MECHANICS

Physical entities can be mathematically represented by means of tensors of different rank according to their characteristics. In particular, a scalar quantity is a zero-order tensor which is completely defined by its magnitude. Density, temperature, and energy are examples of this entity type. In contrast, a first-order tensor is known as a vector and is defined by its magnitude and direction. Some vectors in continuum mechanics are velocity, displacement, and force.

Second-order tensors represent physical entities whose description requires two vectors. For example, the stress state of a material point is defined by a vector of the internal force per unit surface and the unit vector normal to the plane where it acts. Likewise, the n-order tensors represent entities than have been defined by n vectors.

2.1 Convention of tensors, matrices and their components

In this book, the convention used to indicate the scalar, vector and tensor quantities is as follows:

- An italicized letter of the Latin or Greek alphabet indicates a scalar quantity, such as density ρ, temperature $\hat{t}$ or work W.

- A boldface lowercase letter of the Latin alphabet represents a vector, such as displacement $\mathbf{u}$, velocity $\mathbf{v}$ or force $\mathbf{f}$.

- A boldface uppercase letter of the Latin alphabet or a boldface letter of the Greek alphabet indicates a second- or higher-order tensor. For example, the constitutive tensor $\mathbf{D}$ of rank 4 or the second-order tensor of stress $\boldsymbol{\sigma}$ or strain $\boldsymbol{\varepsilon}$.

The matrices are presented using boldface italic letters of the Latin or Greek alphabet between square brackets. For example, the column matrix of displacement components $[\boldsymbol{u}]$, the square matrix of stress components $[\boldsymbol{\sigma}]$ or the transformation matrix $[\boldsymbol{T}]$.

The matrices in Voigt notation are denoted by a boldface letter of Sans Serif or Greek font between curly brackets. The elastic constitutive matrix $\{\mathsf{D}\}$, the column vector of the displacement $\{\mathsf{u}\}$ or the column matrix of the stress $\{\boldsymbol{\sigma}\}$ are examples of this notation type.

Each component of a vector, tensor or matrix is denoted by the same letter of the mathematical entity with a subscript for vectors, two subscripts for second-order tensors or matrices, and n subscripts for n-order tensors. For example, v_i is a component of the vector $\mathbf{v}$, C_{ij} is a component of the second-order tensor $\mathbf{C}$ or the matrix $[\boldsymbol{C}]$, and D_{ijkl} is a component of the fourth-order tensor $\mathbf{D}$. The subscripts i, j, k and l are integer values from 1 to 3 for three-dimensional spaces, and from 1 to 2 for two-dimensional spaces.

2.2 Index notation and the summation convention

The index notation and the summation convention allow us to write the tensor and vector operations, omitting the symbol of summation. In this notation, the product between components of two vectors or tensors with a *shared index* establishes a summation with respect to this index; while the other indices named *free indices*, determine the components of the obtained entity.

For example, the operation in index notation $\alpha = a_i b_i$ corresponds to $\alpha = \sum_{i=1}^{3} a_i b_i$, where the index i is shared between the components and the result is a scalar quantity because there are no free indices.

In another example, the operation in index notation $a_i = C_{ij} b_j$ indicates that $a_i = \sum_{j=1}^{3} C_{ij} b_j$, where the index j is shared between the components and the result is a vector quantity because there is a free index i.

Likewise, if two or more indices are shared by two tensors in a product then two or more summation are carried out with respect to each repeated index. For example, the operation $C_{ij} = D_{ijkl} A_{kl}$ corresponds to $C_{ij} = \sum_{k=1}^{3} \sum_{l=1}^{3} D_{ijkl} A_{kl}$. In this operation, the indices k and l are shared by the components and the indices i and j are free.

In particular, the operation $\sum_{i=1}^{3} C_{ii}$ of the components of a second-order tensor is represented as C_{ii} in index notation.

Additionally, the summation symbol can be omitted when the derivatives of the components of a vector or tensor field with respect to the components of the position vector are summed. For example, $\alpha = \sum_{i=1}^{3} \partial a_i/\partial x_i$ is presented in index notation as $\alpha = \partial a_i/\partial x_i$, or $b_i = \sum_{j=1}^{3} \partial A_{ij}/\partial x_j$ corresponds to $b_i = \partial A_{ij}/\partial x_j$.

2.3 Matrices

A matrix is a rectangular arrangement of coefficients ordered in rows and columns that can simultaneously describe an equation's scalar set. The coefficients of a matrix are represented by the same character in italic font with two subscripts that indicate the row and column of its position. A matrix $[\boldsymbol{A}]$ with m rows and n columns is defined as:

$$[\boldsymbol{A}] = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{bmatrix} \tag{2.1}$$

where A_{ij} is the coefficient located in i-row and j-column of the matrix.

2.4 The Kronecker delta function and the permutation function

Kronecker delta δ_{ij} is a function that depends on the integer variables i and j as follows:

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases} \tag{2.2}$$

This function can represent the component δ_{ij} of the identity matrix or the second-order unit tensor.

The permutation function $\hat{p}_{ijk}$ is defined in terms of the integer variables i, j and k, thus:

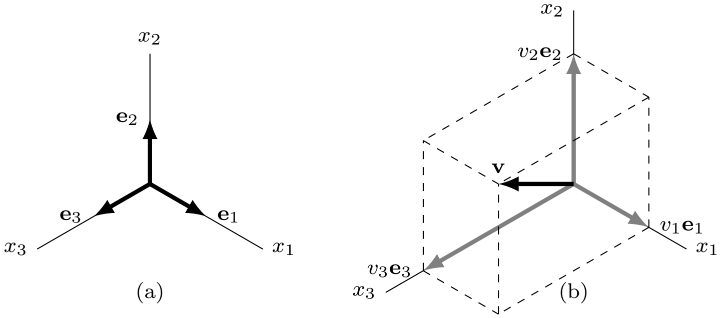

Figure 2.1: Vector defined in the original coordinate system: (a) unit base vector and (b) arbitrary vector **v** and its components.

$$\begin{aligned}\hat{p}_{ijk} &= \frac{1}{2}(i-j)(j-k)(k-i) \\ &= \begin{cases} 1 & \text{if } i,j,k = 1,2,3 \text{ or } 2,3,1 \text{ or } 3,1,2 \\ -1 & \text{if } i,j,k = 1,3,2 \text{ or } 3,2,1 \text{ or } 2,1,3 \\ 0 & \text{if } i=j \text{ or } i=k \text{ or } j=k \end{cases}\end{aligned} \tag{2.3}$$

This function allows us to obtain the cross product between vectors and the determinant of a square matrix and of a second-order tensor.

2.5 Vectors

A Cartesian coordinate system is defined by the axes x_1, x_2 and x_3, complying with the right-hand rule. The vector is a mathematical entity with magnitude and orientation, represented on the Cartesian coordinate system. In particular, the unit base vector of the axis x_1 named $\mathbf{e}_1$ is a vector with unit magnitude and direction parallel to the axis x_1. Likewise, $\mathbf{e}_2$ and $\mathbf{e}_3$ are the unit base vectors of the x_2- and x_3-axis, as shown in Figure 2.1(a). Consequently, $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ are mutuality orthogonal vectors that conform a orthonormal base in $\mathcal{R}^3$.

An arbitrary vector $\mathbf{v}$ is expressed as the linear combination of vectors parallel to the coordinate axes, thus:

$$\mathbf{v} = v_1\mathbf{e}_1 + v_2\mathbf{e}_2 + v_3\mathbf{e}_3 \equiv v_i\mathbf{e}_i \tag{2.4}$$