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Computational Engineering – Introduction to Numerical Methods

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With 204 Figures

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Preface

Due to the enormous progress in computer technology and numerical methods that have been achieved in recent years, the use of numerical simulation methods in industry gains more and more importance. In particular, this applies to all engineering disciplines. Numerical computations in many cases offer a cost effective and, therefore, very attractive possibility for the investigation and optimization of products and processes.

Besides the need for developers of corresponding software, there is a strong – and still rapidly growing – demand for qualified specialists who are able to efficiently apply numerical simulation tools to complex industrial problems. The successful and efficient application of such tools requires certain basic knowledge about the underlying numerical methodologies and their possibilities with respect to specific applications. The major concern of this book is the impartation of this knowledge in a comprehensive way.

The text gives a practice oriented introduction in modern numerical methods as they typically are applied in engineering disciplines like mechanical, chemical, or civil engineering. In corresponding applications the by far most frequent tasks are related to problems from heat transfer, structural mechanics, and fluid mechanics, which, therefore, constitute a thematical focus of the text.

The topic must be seen as a strongly interdisciplinary field in which aspects of numerical mathematics, natural sciences, computer science, and the corresponding engineering area are simultaneously important. As a consequence, usually the necessary information is distributed in different textbooks from the individual disciplines. In the present text the subject matter is presented in a comprehensive multidisciplinary way, where aspects from the different fields are treated insofar as it is necessary for general understanding.

Following this concept, the text covers the basics of modeling, discretization, and solution algorithms, whereas an attempt is always made to establish the relationships to the engineering relevant application areas mentioned above. Overarching aspects of the different numerical techniques are emphasized and questions related to accuracy, efficiency, and cost effectiveness, which are most relevant for the practical application, are discussed. The following subjects are addressed in detail:

- *Modelling:* simple field problems, heat transfer, structural mechanics, fluid mechanics.
- *Discretization:* connection to CAD, numerical grids, finite-volume methods, finite-element methods, time discretization, properties of discrete systems.
- *Solution algorithms:* linear systems, non-linear systems, coupling of variables, adaptivity, multi-grid methods, parallelization.
- *Special applications*: finite-element methods for elasto-mechanical problems, finite-volume methods for incompressible flows, simulation of turbulent flows.

The topics are presented in an introductory manner, such that besides basic mathematical standard knowledge in analysis and linear algebra no further prerequisites are necessary. For possible continuative studies hints for corresponding literature with reference to the respective chapter are given.

Important aspects are illustrated by means of application examples. Many exemplary computations done "by hand" help to follow and understand the numerical methods. The exercises for each chapter give the possibility of reviewing the essentials of the methods. Solutions are provided on the web page *www.fnb.tu-darmstadt.de/ceinm/*. The book is suitable either for self-study or as an accompanying textbook for corresponding lectures. It can be useful for students of engineering disciplines, but also for computational engineers in industrial practice. Many of the methods presented are integrated in the flow simulation code FASTEST, which is available from the author.

The text evolved on the basis of several lecture notes for different courses at the *Department of Numerical Methods in Mechanical Engineering* at *Darmstadt University of Technology*. It closely follows the German book *Numerik im Maschinenbau* (Springer, 1999) by the author, but includes several modifications and extensions.

The author would like to thank all members of the department who have supported the preparation of the manuscript. Special thanks are addressed to Patrick Bontoux and the MSNM-GP group of CNRS at Marseille for the warm hospitality at the institute during several visits which helped a lot in completing the text in time. Sincere thanks are given to Rekik Alehegn Mekonnen for proofreading the English text. Last but not least the author would like to thank the Springer-Verlag for the very pleasant cooperation.

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1

Introduction

In this introductory chapter we elucidate the value of using numerical methods in engineering applications. Also, a brief overview of the historical development of computers is given, which, of course, are a major prerequisite for the successful and efficient use of numerical simulation techniques for solving complex practical problems.

1.1 Usefulness of Numerical Investigations

The functionality or efficiency of technical systems is always determined by certain properties. An ample knowledge of these properties is frequently the key to understanding the systems or a starting point for their optimization. Numerous examples from various engineering branches could be given for this. A few examples, which are listed in Table 1.1, may be sufficient for the motivation.

Table 1.1. Examples for the correlation of properties with functionality and efficiency of technical systems

Property	Functionality/Efficiency
Aerodynamics of vehicles	Fuel consumption
Statics of bridges	Carrying capacity
Crash behavior of vehicles	Chances of passenger survival
Pressure drop in vacuum cleaners	Sucking performance
Pressure distribution in brake pipes	Braking effect
Pollutants in exhaust gases	Environmental burden
Deformation of antennas	Pointing accuracy
Temperature distributions in ovens	Quality of baked products

In engineering disciplines in this context, in particular, solid body and flow properties like

- deformations or stresses,
- flow velocities, pressure or temperature distributions,
- drag or lift forces,
- pressure or energy losses,
- heat or mass transfer rates, ...

play an important role. For engineering tasks the investigation of such properties usually matters in the course of the redevelopment or enhancement of products and processes, where the insights gained can be useful for different purposes. To this respect, exemplarily can be mentioned:

- improvement of efficiency (e.g., performance of solar cells),
- reduction of energy consumption (e.g., current drain of refrigerators),
- increase of yield (e.g., production of video tapes),
- enhancement of safety (e.g., crack propagation in gas pipes, crash behavior of cars),
- improvement of durability (e.g., material fatigue in bridges, corrosion of exhaust systems),
- enhancement of purity (e.g., miniaturization of semi-conductor devices),
- pollutants reduction (e.g., fuel combustion in engines),
- noise reduction (e.g., shaping of vehicle components, material for pavings),
- saving of raw material (e.g., production of packing material),
- understanding of processes, ...

Of course, in the industrial environment in many instances the question of cost reduction, which may arise in one way or another with the above improvements, takes center stage. But it is also often a matter of obtaining a general understanding of processes, which function as a result of long-standing experience and trial and error, but whose actual operating mode is not exactly known. This aspect crops up and becomes a problem particularly if improvements (e.g. as indicated above) should be achieved and the process – under more or less changed basic conditions – does not function anymore or only works in a constricted way (e.g., production of silicon crystals, noise generation of high speed trains, ...).

There are fields of application for the addressed investigations in nearly all branches of engineering and natural sciences. Some important areas are, for instance:

- automotive, aircraft, and ship engineering,
- engine, turbine, and pump engineering,
- reactor and plant construction,
- ventilation, heating, and air conditioning technology,
- coating and deposition techniques,
- combustion and explosion processes,

- production processes in semi-conductor industry,
- energy production and environmental technology,
- medicine, biology, and micro-system technique,
- weather prediction and climate models, ...

Let us turn to the question of what possibilities are available for obtaining knowledge on the properties of systems, since here, compared to alternative investigation methods, the great potential of numerical methods can be seen. In general, the following approaches can be distinguished:

- theoretical methods,
- experimental investigations,
- numerical simulations.

Theoretical methods, i.e., analytical considerations of the equations describing the problems, are only very conditionally applicable for practically relevant problems. The equations, which have to be considered for a realistic description of the processes, are usually so complex (mostly systems of partial differential equations, see Chap. 2) that they are not solvable analytically. Simplifications, which would be necessary in order to allow an analytical solution, often are not valid and lead to inaccurate results (and therefore probably to wrong conclusions). More universally valid approximative formulas, as they are willingly used by engineers, usually cannot be derived from purely analytical considerations for complex systems.

While carrying out experimental investigations one aims to obtain the required system information by means of tests (with models or with real objects) using specialized apparatuses and measuring instruments. In many cases this can cause problems for the following reasons:

- Measurements at real objects often are difficult or even impossible since, for instance, the dimensions are too small or too large (e.g., nano system technique or earth's atmosphere), the processes elapse too slowly or too fast (e.g., corrosion processes or explosions), the objects are not accessible directly (e.g., human body), or the process to be investigated is disturbed during the measurement (e.g., quantuum mechanics).
- Conclusions from model experiments to the real object, e.g., due to different boundary conditions, often are not directly executable (e.g., airplane in wind tunnel and in real flight).
- Experiments are prohibited due to safety or environmental reasons (e.g., impact of a tanker ship accident or an accident in a nuclear reactor).
- Experiments are often very expensive and time consuming (e.g., crash tests, wind tunnel costs, model fabrication, parameter variations, not all interesting quantities can be measured at the same time).

Besides (or rather between) theoretical and experimental approaches, in recent years numerical simulation techniques have become established as a widely self-contained scientific discipline. Here, investigations are performed by means of numerical methods on computers. The advantages of numerical simulations compared to purely experimental investigations are quite obvious:

- Numerical results often can be obtained faster and at lower costs.
- Parameter variations on the computer usually are easily realizable (e.g., aerodynamics of different car bodies).
- A numerical simulation often gives more comprehensive information due to the global and simultaneous computation of different problem-relevant quantities (e.g., temperature, pressure, humidity, and wind for weather forecast).

An important prerequisite for exploiting these advantages is, of course, the reliability of the computations. The possibilities for this have significantly improved in recent years due developments which have contributed a great deal to the "booming" of numerical simulation techniques (this will be briefly sketched in the next section). However, this does *not* mean that experimental investigations are (or will become) superfluous. Numerical computations surely will never completely replace experiments and measurements. Complex physical and chemical processes, like turbulence, combustion, etc., or non-linear material properties have to be modelled realistically, for which as near to exact and detailed measuring data are indispensable. Thus, both areas, numerics *and* experiments, must be further developed and ideally used in a complementary way to achieve optimal solutions for the different requirements.

1.2 Development of Numerical Methods

The possibility of obtaining approximative solutions via the application of finite-difference methods to the partial differential equations, as they typically arise in the engineering problems of interest here, was already known in the 19th century (the mathematicians Gauß and Euler should be mentioned as pioneers). However, these methods could not be exploited reasonably due to the too high number of required arithmetic operations and the lack of computers. It was with the development of electronic computers that these numerical approaches gained importance. This development was (and is) very fast-paced, as can be well recognized from the maximally possible number of floating point operations per second (Flops) achieved by the computers which is indicated in Table 1.2. Comparable rates of improvement can be observed for the available memory capacity (also see Table 1.2).

However, not only the advances in computer technology have had a crucial influence on the possibilities of numerical simulation methods, but also the continuous further development of the numerical algorithms has contributed significantly to this. This becomes apparent when one contrasts the developments in both areas in recent years as indicated in Fig. 1.1. The improved

Table 1.2. Development of computing power and memory capacity of electronic computers

Year	Computer	Floating point operations per second (Flops)	Memory space in Bytes
1949	EDSAC 1	$1 \cdot 10^2$	$2 \cdot 10^3$
1964	CDC 6600	$3 \cdot 10^6$	$9 \cdot 10^5$
1976	CRAY 1	$8 \cdot 10^7$	$3 \cdot 10^7$
1985	CRAY 2	$1 \cdot 10^9$	$4 \cdot 10^9$
1997	Intel ASCI	$1 \cdot 10^{12}$	$3 \cdot 10^{11}$
2002	NEC Earth Simulator	$4 \cdot 10^{13}$	$1 \cdot 10^{13}$
2005	IBM Blue Gene/L	$3 \cdot 10^{14}$	$5 \cdot 10^{13}$
2009	IBM Blue Gene/Q	$3 \cdot 10^{15}$	$5 \cdot 10^{14}$

capabilities with respect to a realistic modeling of the processes to be investigated also have to be mentioned in this context. An end to these developments is not yet in sight and the following trends are on the horizon for the future:

- Computers will become ever faster (higher integrated chips, higher clock rates, parallel computers) and the memory capacity will simultaneously increase.
- The numerical algorithms will become more and more efficient (e.g., by adaptivity concepts).
- The possibilities of a realistic modeling will be further improved by the allocation of more exact and detailed measurement data.

One can thus assume that the capabilities of numerical simulation techniques will greatly increase in the future.

Along with the achieved advances, the application of numerical simulation methods in industry increases rapidly. It can be expected that this trend will be even more pronounced in the future. However, with the increased possibilities the demand for simulations of more and more complex tasks also rises. This in turn means that the complexity of the numerical methods and the corresponding software further increases. Therefore, as is already the case in recent years, the field will be an area of active research and development in the foreseeable future. An important aspect in this context is that developments frequently undertaken at universities are rapidly made available for efficient use in industrial practice.

Based on the aforementioned developments, it can be assumed that in the future there will be a continuously increasing demand for qualified specialists, who are able to apply numerical methods in an efficient way for complex industrial problems. An important aspect here is that the possibilities *and also* the limitations of numerical methods and the corresponding computer software for the respective application area are properly assessed.

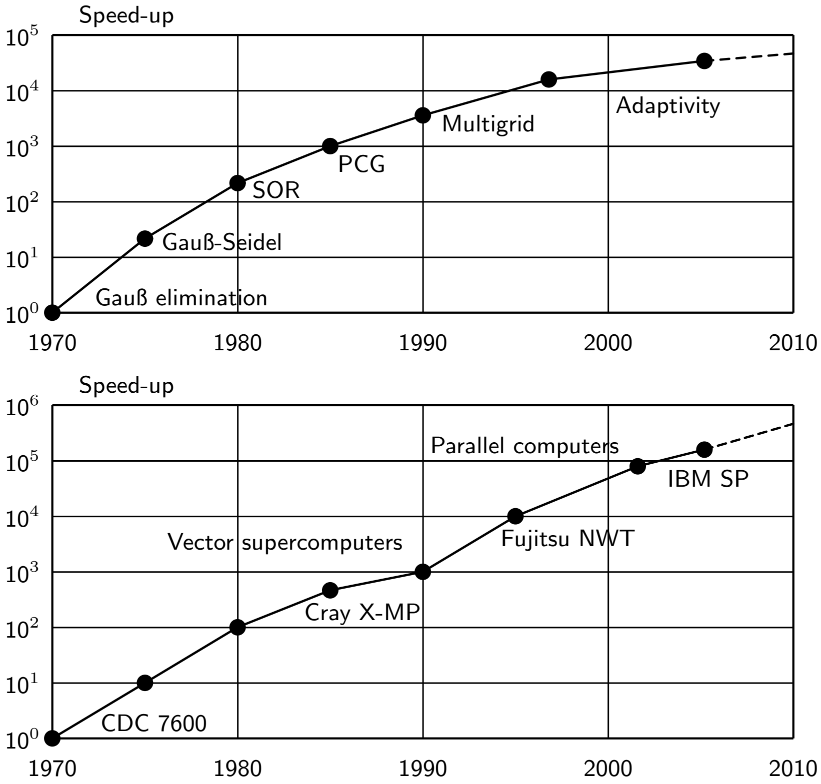

Fig. 1.1. Developments in computer technology (bottom) and numerical methods (top)

1.3 Characterization of Numerical Methods

To illustrate the different aspects that play a role when employing numerical simulation techniques for the solution of engineering problems, the general procedure is represented schematically in Fig. 1.2.

The first step consists in the appropriate mathematical modeling of the processes to be investigated or, in the case when an existing program package is used, in the choice of the model which is best adapted to the concrete problem. This aspect, which we will consider in more detail in Chap. 2, must be considered as crucial, since the simulation usually will not yield any valuable results if it is not based on an adequate model.

The continuous problem that result from the modeling – usually systems of differential or integral equations derived in the framework of continuum mechanics – must then be suitably approximated by a discrete problem, i.e., the unknown quantities to be computed have to be represented by a finite

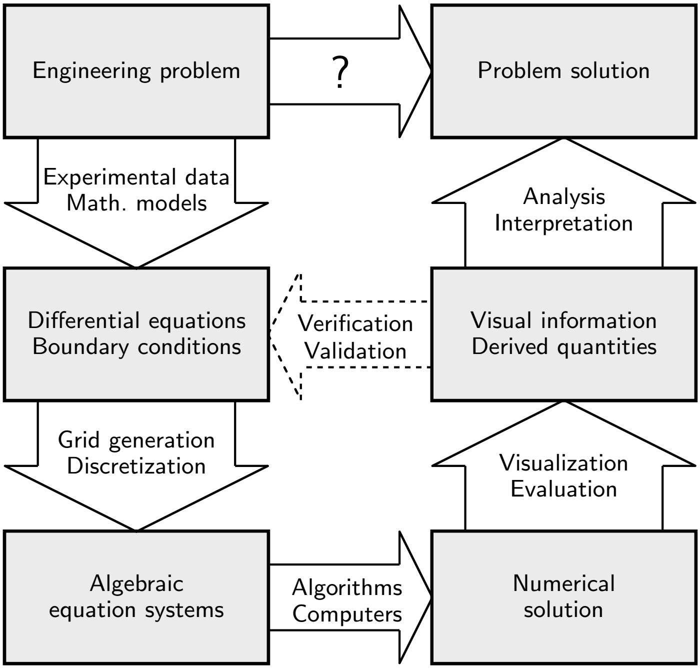

Fig. 1.2. Procedure for the application of numerical simulation techniques for the solution of engineering problems

number of values. This process, which is called *discretization*, mainly involves two tasks:

- the discretization of the problem domain,
- the discretization of the equations.

The discretization of the problem domain, which is addressed in Chap. 3, approximates the continuous domain (in space and time) by a finite number of subdomains (see Fig. 1.3), in which then numerical values for the unknown quantities are determined. The set of relations for the computation of these values are obtained by the discretization of the equations, which approximates the continuous systems by discrete ones. In contrast to an analytical solution, the numerical solution thus yields a set of values related to the discretized problem domain from which the approximation of the solution can be constructed.

There are primarily three different approaches available for the discretization procedure:

- the finite-difference method (FDM),
- the finite-volume method (FVM),
- the finite-element method (FEM).

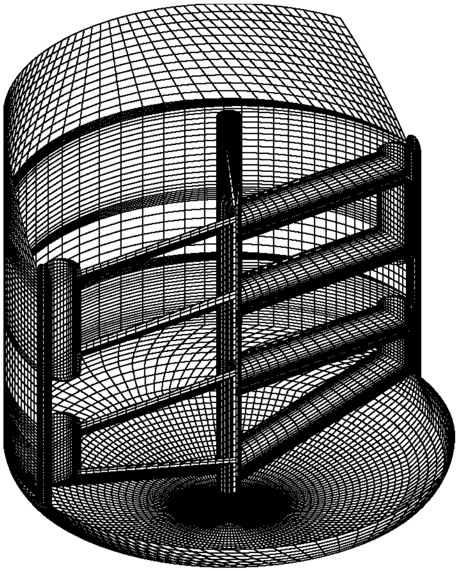

Fig. 1.3. Example for the discretization of a problem domain (surface grid of dispersion stirrer)

In practice nowadays mainly FEM and FVM are employed (the basics are addressed in detail in Chaps. 4 and 5). While FEM is predominantly used in the area of structural mechanics, FVM dominates in the flow mechanical area. Because of the importance of these two application areas in combination with the corresponding discretization technique, we will deal with them separately in Chaps. 9 and 10. For special puposes, e.g., for the time discretization, which is the topic of Chap. 6, or for special approximations in the course of FVM and FEM, FDM is often also applied (the corresponding basics are recalled where needed). It should be noted that there are other discretization methods, e.g., spectral methods or meshless methods, which are used for special purposes. However, since these currently are not in widespread use we do not consider them further here.

The next step in the course of the simulation consists in the solution of the algebraic equation systems (the actual computation), where one frequently is faced with equations with several millions of unknowns (the more unknowns, the more accurate the numerical result will be). Here, algorithmic questions and, of course, computers come into play. The most relevant aspects in this regard are treated in Chaps. 7 and 12.

The computation in the first instance results in a usually huge amount of numbers, which normally are not intuitively understood. Therefore, for the evaluation of the computed results a suitable visualization of the results is important. For this purpose special software packages are available, which meanwhile have reached a relatively high standard. We do not address this topic further here.

After the results are available in an interpretable form, it is essential to inspect them with respect to their quality. During all prior steps, errors are inevitably introduced, and it is necessary to get clarity about their quantity (e.g., reference experiments for model error, systematic computations for numerical errors). Here, two questions have to be distinguished:

- *Validation:* Are the proper equations solved?
- *Verification:* Are the equations solved properly?

Often, after the validation and verification it is necessary to either adapt the model or to repeat the computation with a better discretization accuracy. These crucial questions, which also are closely linked to the properties of the model equations and the discretization techniques, are discussed in detail in Chap. 8.

In summary, it can be stated that related to the application of numerical methods for engineering problems, the following areas are of particular importance:

- Mathematical modelling of continuum mechanical processes.
- Development and analysis of numerical algorithms.
- Implementation of numerical methods into computer codes.
- Adaption and application of numerical methods to concrete problems.
- Validation, verification, evaluation and interpretation of numerical results.

The corresponding requirements and their interdependencies are indicated schematically in Fig. 1.4.

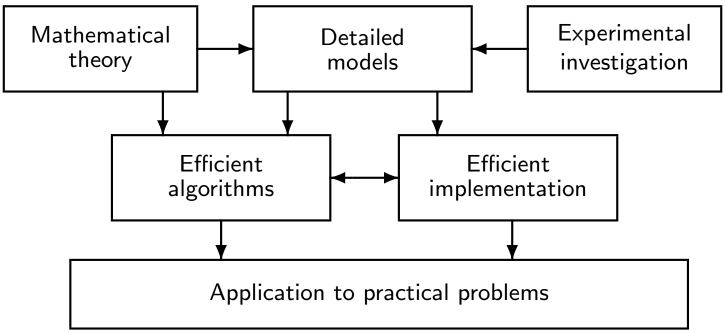

Fig. 1.4. Requirements and interdependencies for the numerical simulation of practical engineering problems

Regarding the above considerations, one can say that one is faced with a strongly interdisciplinary field, in which aspects from engineering science, natural sciences, numerical mathematics, and computer science (see Fig. 1.5) are involved. An important prerequisite for the successful and efficient use of

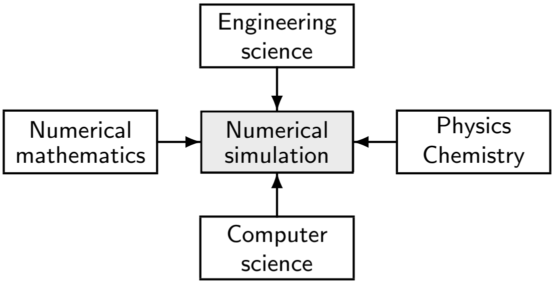

Fig. 1.5. Interdisciplinarity of numerical simulation of engineering problems

numerical simulation methods is, in particular, the efficient interaction of the different methodologies from the different areas.

2

Modeling of Continuum Mechanical Problems

A very important aspect when applying numerical simulation techniques is the "proper" mathematical modeling of the processes to be investigated. If there is no adequate underlying model, even a perfect numerical method will not yield reasonable results. Another essential issue related to modeling is that frequently it is possible to significantly reduce the computational effort by certain simplifications in the model. In general, the modeling should follow the principle already formulated by Albert Einstein: *as simple as possible, but not simpler*. Because of the high relevance of the topic in the context of the practical use of numerical simulation methods, we will discuss here the most essential basics for the modeling of continuum mechanical problems as they primarily occur in engineering applications. We will dwell on continuum mechanics only to the extent as it is necessary for a basic understanding of the models.

2.1 Kinematics

For further considerations some notation conventions are required, which we will introduce first. In the Euclidian space $\mathbb{R}^3$ we consider a Cartesian coordinate system with the basis unit vectors $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$ (see Fig. 2.1). The continuum mechanical quantities of interest are *scalars (zeroth-order tensors)*, *vectors (first-order tensors)*, and *dyads (second-order tensors)*, for which we will use the following notations:

- scalars with letters in normal font: a, b, $\ldots$, A, B, $\ldots$, α, β, $\ldots$,
- vectors with bold face lower case letters: $\mathbf{a}$, $\mathbf{b}$, $\ldots$,
- dyads with bold face upper case letters: $\mathbf{A}$, $\mathbf{B}$, $\ldots$

The different notations of the tensors are summarized in Table 2.1. We denote the coordinates of vectors and dyads with the corresponding letters in normal font (with the associated indexing). We mainly use the coordinate notation, which usually also constitutes the basis for the realization of a model within a