Preface

The expansion of scientific knowledge and the development of technology are strongly connected with quantitative analysis of mathematical models. Accuracy and reliability are the main properties we wish to know about when considering a mathematical model. *Reliability of Mathematical Models* is a fundamental interdisciplinary problem, which has many aspects and includes subproblems related to different areas (natural sciences, computational methods, mathematical analysis, etc.). It is not surprising that many experts in the field of mathematical modelling consider the question

How accurate is a mathematical model?

as the most difficult to answer.

Natural sciences have developed a number of well-tested principles (e.g., conservation laws) that allow us to reject deliberately wrong models and to develop new ones, which are consistent with the physical axioms/laws. For example, a model does not deserve attention if it violates well-established physical laws or if it is in contradiction with laws and principles in other sciences. This "physical consistency" leaves only those models that are relevant from the physical point of view.

The second crucial step in the analysis of a mathematical model is verification of its mathematical correctness. It is commonly accepted that a mathematical model is well posed if it is free from mathematical contradictions (which arise, e.g., in the case of overdetermined systems or problems with inconsistent data) and possesses a solution that depends continuously on the problem data. As usual, we also need that the solution is unique within a certain suitable functional class. These questions together with the regularity theory (which states additional properties of solutions) are at the core of the modern theory of partial differential equations and there is an extensive literature devoted to this subject.

However, while being necessary, the above mentioned stages of verification are in general not sufficient for an unambiguous judgement on the suitability or unsuitability of the chosen mathematical model. Only quantitative verification enables us to make the final decision about the validity and accuracy of a model. Indeed, a model may be perfectly consistent from the viewpoint of physics and mathematics, but practically invalid because it produces wrong results. This situation may arise for many different reasons, for example due to instability of the model or because the model does not properly account for some essential physical effects (e.g., turbulence). In many cases, a particular phenomenon or process can be modelled by several different computer simulation codes based on competing mathematical models (which yield different results). It is often difficult to say whether the major differences came from the models or it is generated by computational methods, approximations, and algorithms. A similar question arises when experimental data are compared with results of computer simulations. If they are different, then we must understand the reason: is it the model itself or are the errors mainly associated with computations? In fact, we cannot answer this question unless the "modelling error" and the "approximation error" are clearly separated. Notice that the separation is always necessary, even in those cases where numerical results are in good agreement with experimental data. This fact does not fully confirm the validity of a model because modelling errors might be compensated by numerical ones (if they have opposite signs). Effects of this type are indeed known for some approximation methods.

This book presents a mathematical theory developed for explicit evaluation of modelling errors. It summarises our experience gained by studying this problem for about 20 years. Clearly, the theme in the title of the book is extremely wide and we are forced to confine ourselves to only one class of deterministic models. The main goal of our analysis is to create a unified approach to quantitative analysis of the accuracy of mathematical models associated with variational and saddle point problems in mathematical physics. Though the book is focused on the modelling errors, we also discuss approximation errors that arise if a mathematical model is approximated in order to obtain a numerical solution. For example, in the dimension reduction, homogenization, and simplification models, the overall error contains two major components: a modelling one and an approximation one. This fact leads to estimates of the difference between a numerical solution of a simplified mathematical model and the exact solution of the original (complicated) problem and makes the whole analysis fully practical. The reader will find several numerical examples of this kind. However, in the book we do not focus on estimates of approximation errors, which are well known and presented in numerous publications (including several monographs). Instead, we focus our attention on the errors that arise due to differences in mathematical models ("complicated" and "simplified"). The corresponding estimates of modelling errors contain only known data and solutions of "simplified" models. For example, the solution of a dimensionally reduced 2D model (or a suitable approximation of it) is used in order to approximate the solution a full-scale 3D problem and have a computable and guaranteed bound of the error arising in this process.

Basically, the book deals with stationary models, but the proposed concepts and methods of analysis can be naturally generalized to many evolutionary models. The reader will find several comments and references that could help in studying accuracy of time-dependent models. Moreover, in Chapter 6 we deduce estimates of errors generated by semi-discrete (incremental) approximations of parabolic-type problems.

As implied by the title, the main subject of the book is *modelling error*. Depending on the context, this term has two close but nontheless different meanings. First, the modelling error is a quantity (or a collection of quantities) that measures how a mathematical model differs from a physical phenomenon or process under consideration. This error is always present because mathematical models describe physical phenomena with a limited accuracy. Modelling error of this kind can be evaluated only by a systematic comparison of the data obtained in the respective physical and mathematical experiments. Here, the main mathematical problem to be solved is the *fully guaranteed estimation of computational errors*. We briefly discuss it at the end of Chapter 2 and refer the reader to the relevant literature. However, the book is mainly devoted to modelling errors of another kind, namely, those that arise if we compare solutions of different mathematical models related to one and the same object. For example, in *dimension reduction models*, we compare solutions of three-dimensional (3D) models of an elastic body with solutions of simplified two-dimensional (2D) models (which contain errors caused by a dimension reduction method). Analogously, models arising in *homogenization theory* contain errors arising when the original periodic structure is replaced by the corresponding homogenized model.

The book consists of six chapters. Chapter 1 contains all preliminary information subsequently used in different parts of the book. Also, it includes a special section related to functional inequalities and respective constants.

Chapter 2 gives a fairly complete exposition of the mathematical theory that allows us to estimate the distance to exact solutions of elliptic boundary value problems. The main attention is paid to the *error identities* (such as (2.21), (2.26), or (2.29)) that are further used in error analysis. They are derived for a wide class of problems related to the variational functional $J(v) = G(\Lambda v) + F(v)$, where G and F are convex functionals and Λ is a differential operator. This class encompasses the majority of linear and nonlinear elliptic problems, including variational inequalities. We show that error identities define error measures, which are natural for the problem in question and serve as a source of computable two-sided error bounds for these measures.

We should emphasize that the derivation of error bounds is based on purely functional arguments and do not use special properties of approximations or properties of the method by which they were constructed. Besides, the error bounds do not contain analytic quantities, which could be uncontrollably large (or even unbounded) as, e.g., H^2 regularity constants of problems with smooth but oscillatory coefficients. This fact is rather essential for the analysis of modelling errors because we are able to keep maximal generality of the results and are not confined to considerations of some specially selected methods and models.

We can apply the estimates to approximations of quite different types obtained by, e.g., reconstruction of dimensionally reduced models, regularisation, penalisation, linearisation, etc. General results are illustrated by several examples related to particular classes of problems. Special attention is paid to linear elliptic problems of divergence type. At the end of the chapter, we discuss possible applications of the estimates to validation of a mathematical model based on analysis of physical data and direct comparison of them with results of computational experiments. The estimates could guarantee the accuracy of computational data and confirm that they possess the same level of accuracy as in physical experiments. In this case, we are indeed able to draw reliable conclusions on the validity (accuracy) of a mathematical model within the selected range of physical data (parameters, geometry, other conditions).

Chapter 3 is concerned with dimension reduction models. First, we consider diffusion-type equations in "thin" domains. Formally this means that one characteristic size of the domain is much smaller than the other. No other essential restrictions on the shape and other properties of the domain and coefficients are imposed and we can analyse different models of lower dimensions based on various representations of the solution in the "degenerate" direction. Explicitly computable bounds of the errors are obtained for plate-type domains with plane faces as well as for domains with curvilinear faces. Finally, we investigate problems arising in linear elasticity.

Simplification of models is widely used in applied analysis. It has various forms related to geometry, coefficients, boundary conditions, etc. Modelling errors of this type appear in *defeaturing* (simplification) of mathematical relations when complicated coefficients (boundary conditions, geometrical details) are approximated by simpler ones. In Chapter 4 we study the main question that always arises:

What we loose in the process of simplification?

If one is able to answer it, then we get a certain accuracy level within which a simplified model can be successfully used instead of the original one. We consider two main cases: simplification of the coefficients of a partial differential equation and simplification of the underlying geometry.

Boundary value problems with *periodic structures* arise in various applications. Chapter 5 is devoted to mathematical models of homogenization theory, which is the major tool used to quantitatively analyse media with periodic structures (e.g., see [46, 92, 146] and other publications cited in the chapter). Typically, a *homogenized* boundary value problem is a problem with specially constructed smooth coefficients. It has been proved that the functions constructed by this procedure converge (with respect to some topology) to the exact solution as the cell size ε tends to zero. Moreover, known *a priori* error estimates qualify the convergence rate in terms of ε. However, *a priori* convergence estimates give only qualitative information on the behaviour of the error. In general, they are unable to provide a sharp and reliable quantitative information on the difference between the exact solutions of the original problem and the respective homogenized counterpart.

In contrast, the goal in Chapter 5 is to develop *error majorants* which allow to evaluate the *quality* of the model and its discretization in a split and a posteriori way (but not to develop new advanced homogenization *models*, which is also an important topic of intensive research in applied analysis).

To highlight the principal ideas in a most transparent way and to keep this exposition self-contained, we have chosen a relatively simple, first-order homogenization model and we obtain fully guaranteed and computable bounds of the difference between the exact solution of a particular elliptic boundary value problem with periodic coefficients and an abridged problem generated by homogenization. The difference is measured in terms of the energy norm of the basic problem and also in the combined primal-dual norm. Using the technique discussed in Chapter 2, we obtain two-sided bounds of the modelling error, which depend only on the solution of the homogenized problem, auxiliary problems defined on the periodicity cell, and known data. The estimates include only global constants associated with embedding-type inequalities in the domain and in the periodicity cell. Also, they contain constants in some new regularity type estimates for functions defined in convex domains. Formally, the estimates are valid for any number of cells and could be used for thin periodic structures as well as for coarse ones (though in the latter case errors generated by a homogenized model may be quite large). If the overall number of cells increases, then the respective modelling error decreases. We prove that the error majorant behaves accordingly, i.e., if the parameters of the majorant are selected in an appropriate manner, then it decreases with the same rate as the true error.

Finally, in Chapter 6 we consider various situations where one model is converted into another one. Usually this is done in order to obtain a more convenient problem (from the computational point of view) that can be solved by well developed numerical methods and/or standard computational software. A typical example of this kind is provided by a wide collection of methods sharing the name *penalization*. In these methods, various additional conditions imposed on the exact solutions are accounted in a weaker sense (as penalties). Penalization is widely used in the analysis of applied problems (if the "exact" incorporation of some constraints is difficult) and the question

How different are the solutions of the original and penalized problems?

is the first to be answered. Certainly asymptotic type estimates expressed in terms of the penalization parameter(s) are known for a rather wide collection of problems. We present estimates of a different type: they show the distance to the exact solution in terms of a fully computable functional, which contains only known constants and quantities that come from the solution of the penalized problem (or its numerical approximation). The well-known *fictitious domains method* (see, e.g., [126]) uses related ideas in order to reduce problems with complicated geometry to problems defined in simple domains (e.g., rectangles) where numerical approximations use simple meshes. We present the respective estimates and examples that demonstrate the efficiency of the approach.

Similar ideas of model transformation are used in the *regularization method*. We discuss it on the example of the Bingham problem, where the nondifferentiable term in the energy functional is replaced by a smoothed one. *Linearization* of nonlinear models is one of the most common approaches used in both theoretical and computational analysis of mathematical models. We consider applications of our error estimation method to this case and deduce error estimates in several examples. The estimates provide quantitative qualification of the linearized model, which enables the scientist to judge whether it can be successfully used as a replacement of the original one.

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