Preface

In spite of the impressive progress made during the last decades in mathematical modelling and techniques of scientific computing, many problems in science and engineering remain intractable. Among them, we can cite those related to high-dimensional models (i.e., in dynamics of complex fluids, quantum chemistry), for which classical mesh-based approaches fail due to the exponential increase of the number of degrees of freedom. Other challenging scenarios are those requiring many direct solutions of a given problem (i.e., in optimization, inverse identification, uncertainty quantification) or those needing very fast solutions (i.e., for real-time simulation, simulation-based control).

Over the last 10 years, the authors of the present book and their collaborators have been developing a novel technique, called Proper Generalized Decomposition (PGD), that has proven capable of tackling these challenging issues. The PGD builds, by means of a successive enrichment strategy, a numerical approximation of the unknown fields in a separated form involving a *priori* unknown functions of individual or clustered coordinates of the problem. Although first introduced and successfully demonstrated in the context of high-dimensional problems, the PGD allows for a completely new approach for addressing more standard problems in science and engineering. Indeed, many challenging problems can be efficiently cast into a multidimensional framework, thus opening entirely new solution strategies in the PGD framework. For instance, the material parameters and boundary conditions appearing in a particular mathematical model can be regarded as extra-coordinates of the problem in addition to the usual coordinates such as space and time. In the PGD framework, this enriched model is solved only once to yield a general or parametric solution that includes all particular solutions for specific values of the parameters. Thus, optimization of complex problems, uncertainty quantification, simulation-based control, and real-time simulation become feasible, even in highly complex scenarios. Once the PGD-separated representation of the parametric solution has been computed offline, its online use only requires one to particularize the solution for a desired set of parameter values. Obviously, this task can be performed very fast and repeatedly in real time, by using light computing platforms such as smartphones or tablets.

The PGD is a numerical technique based on separated representations. The use of separated representations is not new. Indeed, the reader probably remembers the *method of separation of variables* discussed in his/her introductory course on

partial differential equations. The basic idea behind this analytical procedure is to assume that the exact solution $u(x, y)$, say of Laplace's equation in a square domain, can be written as an infinite sum of terms, each one consisting of a function of x multiplied by a function of y. When feasible, the method of separation of variables often yields accurate solutions with only a small number of terms. It is unfortunately unable to address nonlinearities or complex geometries, so that the student is quickly introduced to the powerful and flexible alternative of *mesh-based numerical techniques*. Here, an approximation of the solution is computed at a finite number of mesh points distributed in the computational domain, by means of an appropriate technique (e.g. finite elements or finite differences). Suitable interpolation is then used to evaluate the solution anywhere in the computational domain. Powerful numerical methods have been developed to a significant extent over the last decades in virtually all fields of science and engineering. The concurrent explosive increase in computing resources has made possible the numerical simulation of problems of great complexity.

Mesh-based numerical techniques are not feasible, however, for solving mathematical problems defined in spaces of high dimension. The reason is that their number of degrees of freedom grows exponentially with the dimensionality of the problem. High-dimensional models abound in many fields, such as quantum mechanics or kinetic theory of complex materials. In vast contrast, the complexity of the PGD grows linearly with the problem's dimension.

Numerical schemes based on separated representations have been used for decades in the scientific community, under different forms. In quantum chemistry, Hartree-Fock and post-Hartree-Fock approaches exploit this formalism. In the 1980s, P. Ladevèze proposed a space-time separated representation to develop a nonincremental solver for transient problems in computational solid mechanics. It is in the particular context of high-dimensional kinetic models of polymeric fluids that A. Ammar, F. Chinesta, and R. Keunings devised the first version of the PGD strategy in the early 2000s. During the last decade, these authors and other colleagues further developed the PGD and applied it successfully to a wide variety of problems.

The PGD has now attracted the attention of a large number of research groups worldwide. The number of research papers on this topic is growing strongly, and so is the need for an introductory book. The present text is thus the first available book describing the PGD. Our aim has been to provide a very readable and practical introduction, i.e., a "primer", that will allow the reader to quickly grasp the main features of the method. Prerequisites are limited to a basic course in mathematical modeling and numerical methods. Throughout the book, we show how to apply the PGD to problems of increasing complexity, and we illustrate the methodology by means of carefully selected numerical examples. In addition, the reader will have free access to the Matlab software used to generate these examples at http://extras.springer.com. Finally, we provide references to a large number of recent research publications on the PGD that will allow the reader to go beyond the present introduction.

It is a pleasure to acknowledge all our coauthors of PGD-related research publications. In particular, we wish to thank Amine Ammar, Elias Cueto, Antonio Huerta, and Pierre Ladevèze, who from the very beginning contributed significantly to the development of the PGD.

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A Primer

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