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Roman Trobec
Gregor Kosec

Parallel Scientific Computing

Theory, Algorithms, and Applications of Mesh Based and Meshless Methods

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Roman Trobec
Jožef Stefan Institute
Ljubljana
Slovenia

Gregor Kosec
Jožef Stefan Institute
Ljubljana
Slovenia

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To all who make our lives worthwhile.

Preface

The scientific computing and computer simulations on modern, powerful computers are tools that can reduce the costs of developing new machines, evaluate different environmental risks, simulate the evolution of different natural or technological phenomena, and conduct virtual experiments that are too dangerous or impossible to perform in laboratories, amongst many other possibilities.

This book is concentrated on the synergy between computer science and numerical analysis. It is written to provide a firm understanding of the described approaches to computer scientists, engineers or other experts who have to solve real problems. The meshless solution approach is described in more detail, with a description of the required algorithms and the methods that are needed for the design of an efficient computer program. Most of the details are demonstrated on solutions of practical problems, from basic to more complicated ones. We believe that this book will be a useful tool for any reader interested in solving complex problems in real computational domains.

We are grateful to all our colleagues who have contributed to this book through discussions or by reading the material, in particular to Marjan Šterk and Božidar Šarler who initiated and supported the research on meshless methods in our research community. Many thanks to Monika Kapus-Kolar and Matjaž Depolli, who carefully read our text and resolved many formal and linguistic inconsistencies. We are indebted to the Jožef Stefan Institute and the Slovenian Research Agency for their support of our work.

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Roman Trobec
Gregor Kosec

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Chapter 1
Introduction

Abstract The background and motivation for the development of solution methodologies for partial differential equations are given with an overview of the related work and the relevant publications.

Keywords Modeling · Partial differential equation · Numerical solution

1.1 Overview and Motivation

In the recent decades, scientific computing and numerical modeling have been drawing a lot of attention in research, due to their major contribution to a better understanding of Nature as well as in the development of advanced technologies. The modeling of more and more complex physical transport systems helps the community to address important issues like identifying environmental problems, improving technological processes, developing biomedical applications, etc. Many physical models are constituted through systems of coupled Partial Differential Equations (PDEs). Unfortunately, most of the PDEs that describe real-life problems do not possess a closed-form solution and, therefore, a suitable numerical approach is required. In the majority of numerical simulations, the Finite Volume Method (FVM), the Finite Difference Method (FDM), the Boundary Element Method (BEM), or the Finite Element Method (FEM) are used. However, there are also numerous scientific works related to the development and implementation of a relatively new class of simulation methods, referred to as meshless or meshfree methods.

Regardless of the numerical method, the solution algorithms are executed on computers, and so in most cases the accuracy of the computed solution is limited by the capacities of the available computer resources and by the efficiency of the computer programs implementation. Numerical modeling and computer science are, therefore, closely coupled scientific disciplines. The developments of computer technology are nowadays extremely vivid. Almost all modern computer platforms are parallel; most computers use several computing cores, sharing the same memory. For more complex computations, interconnected computers in computing clusters that work with a distributed memory are used. Moreover, the use of Graphical Processing Units

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(GPUs) and Field Programmable Gate Arrays (FPGAs) for accelerating numerical simulations are becoming more and more attractive.

To effectively analyze complex natural phenomena by means of numerical simulations, all the involved phases, i.e., the physical modeling, mathematical formulation of the numerical methods, and their computer implementation and execution, have to be adequately addressed. This book tackles, in limited detail, all three phases, where we focus our discussion on the phenomena that can be described with a coupled system of second-order PDEs and supporting constitutive equations. We are, in particular, interested in the computational aspects of local meshless numerical methods, which, unlike the usual mesh-based methods, like the FEM or the FDM, require no topological relations between the discretization nodes.

Two different classes of local meshless methods are analyzed, i.e., strong form and weak form meshless methods. Regardless of the form of the equations, the basic principle of the local meshless methods is to create a local approximation of the solution that can be further manipulated, in most cases, with partial differential operators. The Meshless Local Strong Form Method (MLSM) is a generalization of the methods in the literature known as the Diffuse Approximate Method (DAM) [1], Local Radial Basis Function Collocation Method (LRBFCM) [2], Generalized FDM [3], Collocated Discrete Least Squares (CDLS) meshless [4], and similar. Although each of the listed methods possesses some unique properties, there is not much difference in their basic conception. In this book, the MLSM is employed as a generic name incorporating the basic principles of the meshless local strong form methods. The MLSM can also be understood as a meshless generalization of the FDM.

Another well-known weak form meshless method considered in this book is the Meshless Local Petrov Galerkin method (MLPG) [5]. It has been derived from the Weighted Residual Method (WRM) and follows similar principles as the FEM. As such, the MLPG can also be understood as a meshless generalization of the FEM.

It is claimed that meshless methods also perform well in situations with complicated geometry and a nonuniform node arrangement and that in comparison with mesh-based methods, they result in a smoother solution. However, since these methods are still under development, they have in most numerical simulations [6–8] only been demonstrated on simple geometries with regular node arrangements. Direct comparisons of different meshless methods are also rarely found in the literature. In this book, we want to contribute to a better understanding of meshless approaches, with emphasis on aspects of computer execution and implementation. The analyses focus first on the solution to a simple case formulated with diffusion equation, to assess the convergence rate, stability, and other basic properties of the methods. After initial evaluation, more complex cases are solved, i.e., fluid flow, semiconductor simulations, and solid mechanics problems. For assessment by simulation, we use uniform and nonuniform node arrangements and simple as well as more complicated geometries. The obtained results are also analyzed in terms of computer execution performance on modern computer architectures.

The book offers a broad insight into meshless methods from various points of view. The solution procedure is formulated in such a way that even readers with