Computational Mechanics Series

The Material Point Method

A Continuum-Based Particle Method for Extreme Loading Cases

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适于极端工况的粒子类方法（英文版）

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内 容 简 介

本书系统地论述了物质点法的理论、程序设计和应用，并提供了开源代码MPM3D-F90。英文版在中文版的基础上做了大幅修改和补充，增加和扩充了部分内容（如不可压物质点法、隐式物质点法、开源代码MPM3D-F90的描述与算例、多尺度物质点法等），并基于点面接触算法对耦合物质点有限元和自适应物质点有限元法进行了全面更新，力图反映物质点法的最新研究进展。

本书可供航天航空、力学、机械、汽车、土木、水利等专业的高年级本科生、研究生和教师使用，也可供相关领域的科技人员阅读参考。

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Dedication

To Yun and Ximing for their company and support!

Xiong Zhang

To Jessie and Ethan for their understanding and support!

Zhen Chen

To my parents!

Yan Liu

About the Authors

Xiong Zhang received his Ph.D. in Computational Mechanics from the Dalian University of Technology in 1992. He is now a professor in the School of Aerospace Engineering at Tsinghua University, and the Associate Editor of the *International Journal of Mechanics and Materials in Design*. His selected honors include the New Century Excellent Talents in University (Ministry of Education of China, 2004), the First prize (2008) and Second prize (2009) for Natural Science from the Ministry of Education of China, the ICACM Fellows Award (2011), the Beijing Municipal Famous Teacher Award for Higher Education (2015) and the Qian Lingxi Computational Mechanics Award (Achievement Award, 2016). His current research interests focus on numerical modeling of extreme events, such as hypervelocity impact, blast, bird impact, penetration, perforation and fluid–structure interaction. He has published 3 monographs and 3 textbooks in Chinese. He was included in the list of Elsevier's "Most Cited Chinese Researchers" in 2015.

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Preface

Simulation-based Engineering Science (SBES) has become the third pillar of modern science and technology, a peer alongside theory and physical experiment [1]. Computer modeling and simulation are now an indispensable tool for resolving a multitude of scientific and technological problems we are facing [2]. To model and simulate those extreme loading events such as hypervelocity impact, penetration, blast, machining, transient crack propagation and multiphase (solid–liquid–gas) interactions involving failure evolution, however, how to effectively describe localized large deformations, the transition from continuous to discontinuous failure modes, and fragmentation remains a challenging task.

Both Lagrangian and Eulerian approaches have been used in SBES to tackle different kinds of extreme events. Lagrangian methods have a computational grid embedded and deformed with the material [3,4]. As a result, material interfaces can be easily tracked, and history-dependent constitutive models can be readily implemented. However, Lagrangian methods suffer from the difficulties associated with grid distortion and element entanglement, which make Lagrangian methods unsuitable for solving problems involving localized large deformation, fragmentation, melting and vaporization. By contrast, in Eulerian methods, the computational grid is fixed in space, and mass flows through the grid. There is no difficulty associated with grid distortion and element entanglement in Eulerian methods so that they can easily solve the problems involving extreme deformation, fragmentation, melting and vaporization. However, special procedures are required to identify the material interfaces and history-dependency, which are very computationally intensive as compared with Lagrangian methods.

To take advantage of both Eulerian and Lagrangian methods while avoiding the shortcomings of each, the Material Point Method (MPM) has evolved over more than twenty years since its first journal paper was published in 1994 [5]. The MPM is an extension of the particle-in-cell (PIC) method in computational fluid dynamics to computational solid dynamics, formulated using the weak formulation and including the history-dependency of constitutive models.

It discretizes a continuum body into a set of material points (particles) moving through an Eulerian background grid. Hence, the MPM is a continuum-based particle method. The particles carry all material properties such as mass, velocity, stress, strain and state variables so that it is easy to track material interfaces and to implement history-dependent constitutive models. As the equations of motion are solved on the Eulerian background grid, there is no grid distortion or element entanglement, which makes the MPM robust in dealing with various types of extreme loading events.

After providing the necessary background information, this book describes the fundamental theory, implementation and application of the MPM as well as its recent extensions. It contains eight chapters. Chapter 1 briefly introduces the basic ideas and features of the Lagrangian methods, Eulerian methods, hybrid methods and meshfree methods, respectively. Chapter 2 reviews the Lagrangian and Eulerian descriptions of deformation and motion, as well as the strain and stress measures in large deformation theory. The governing equations of motion in an updated Lagrangian framework are given. Based on the updated Lagrangian description, Chapter 3 establishes the MPM formulation by discretizing a continuum body into a set of particles. Both explicit and implicit formulations are presented. The Generalized Interpolation Material Point (GIMP) method, contact algorithm, adaptive MPM, incompressible MPM and non-reflection boundary are discussed in detail. The computer implementation of the MPM and corresponding source codes are described in Chapter 4 based on our open source MPM code, MPM3D-F90. A user's guide and several numerical examples of the MPM3D-F90 code are also presented, for which the input data files can be downloaded from our web site: http://mpm3d.comdyn.cn. Chapter 5 first reviews the explicit finite element method, and then presents the material point finite element method, coupled material point finite element method, adaptive material point finite element method and hybrid material point finite element method as developed in the Computational Dynamics Lab of the School of Aerospace Engineering at Tsinghua University. Chapter 6 discusses the constitutive models which describe different types of material behaviors, with a focus on the extreme events. The computer implementation of these constitutive models is specified in detail, and corresponding source codes are provided. Chapter 7 introduces a multiscale MPM that could couple discrete forcing functions as used in molecular dynamics with constitutive models as used in the continuous approaches in a single computational domain. The mapping and remapping process in the MPM could effectively coarse-grain fine details. Chapter 8 describes the applications of the MPM and its extensions in those extreme events such as transient crack propagation, impact/penetration, blast, fluid–structure interaction, and biomechanical responses to extreme loading.

The most materials of this book were based on our MPM book in Chinese [6] with significant extensions and revisions. Zhen Chen added Sect. 3.2.3 and Chapter 7 while Yan Liu drafted Chapter 8. The remaining chapters were drafted by Xiong Zhang. Xiong Zhang and Zhen Chen have revised the whole book.

Finally, the first author wishes to acknowledge his students, S. Ma, P. Huang, Z.T. Ma, Y.P. Lian, H.K. Wang, W.W. Gong, S.Z. Zhou, P.F. Yang, X.X. Cui, P. Liu, Y.T. Zhang, X.J. Wang, Z.X. Hu, J.G. Li, Z.P. Chen and F. Zhang, for their contributions to the algorithm development and programming related to the book. Especially, Tamás Benedek who implemented a subroutine in MPM3D-F90 to output simulation results to ParaView [7] for postprocessing when he worked on his master thesis at Tsinghua University.

Contents

3. The Material Point Method

4. Computer Implementation of the MPM

Chapter 1

Introduction

Contents

Simulation-based Engineering Science (SBES) [2] is the third pillar of the modern science and engineering, a peer alongside theory and physical experiment [1]. Compared with physical experiment, SBES has the advantages of low cost, safety, and efficiency in solving various kinds of challenging problems. To better simulate those extreme events such as hypervelocity impact, penetration, blast, crack propagation, and multi-phase (solid–liquid–gas) interactions involving failure evolution, yet effectively discretize localized large deformation, the transition among different types of failure modes and fragmentation remains a very difficult task. Based on the way how deformation and motion are described, existing spatial discretization methods can be classified into Lagrangian, Eulerian, and hybrid ones, respectively.

1.1 LAGRANGIAN METHODS

In Lagrangian methods the computational grid is embedded and deformed with the material. Since there is no advection between the grid and material, no advection term appears in the governing equations, which significantly simplifies the solution process. The mass of each material element keeps constant during the solution process, but the element volume varies due to element deformation. Lagrangian methods have the following advantages:

1. They are conceptually more simple and efficient than Eulerian methods. Because there is no advection term that describes the mass flow across element boundaries, the conservation equations for mass, momentum, and energy are simple in form, and can be efficiently solved.

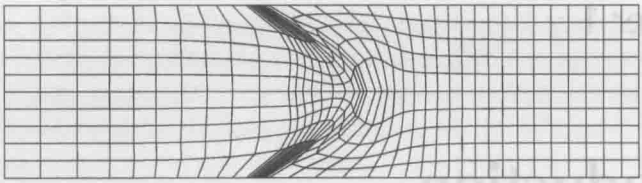

FIGURE 1.1 Lagrangian grid.

2. Element boundaries coincide with the material interfaces during the solution process so that it is easy to impose boundary conditions and to track material interfaces.
3. Since Lagrangian methods track the flow of individual masses, it is easy to implement history-dependent constitutive models.

Fig. 1.1 shows a typical Lagrangian grid which is embedded and deformed with the material. Severe element distortion results in significant errors in numerical solution, and even leads to a negative element volume or area which would cause abnormal termination of the computation. To obtain a stable solution with an explicit time integration scheme, the time step must be smaller than a critical time step which is controlled by the minimum characteristic length of all elements in the grid. Because severe element distortion would significantly decrease the characteristic element length, the time step in a Lagrangian calculation could become smaller and smaller, and finally approach zero, which makes the computation impossible to be completed. To complete a Lagrangian computation for an extreme loading case, a distorted grid must be remeshed and its result must be interpolated to the remeshed grid. The remesh or rezone technique has been successfully used in solving many 1D and 2D problems, but rezoning a complicated 3D material domain is still a challenging task. For a history-dependent material, the history variables are also required to be interpolated from the old grid to the new grid, which may further cause numerical error in stress calculation.

Another way to eliminate the element distortion is to use the erosion technique, which simply deletes the heavily distorted elements. An element is considered to be heavily distorted if its equivalent plastic strain exceeds a user-defined erosion strain value, or the critical time step size is less than a prescribed value. Introducing element erosion can resolve some of the issues related to the severe element distortion, but also introduce new issues. The global system will lose both mass and energy, which can severely affect the simulation outcome. Furthermore, the erosion technique cannot model the formation process of debris cloud and its interaction with other panels in hypervelocity impact simulation.

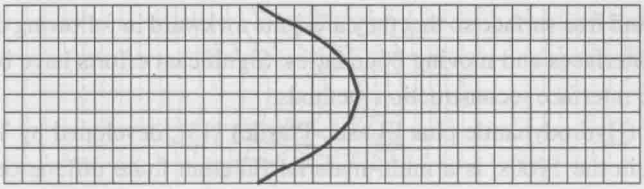

FIGURE 1.2 Eulerian grid.

Many Lagrangian codes have been developed, as shown in the open literature. The HEMP [8] was developed in the early 1960s by Wilkins at the Lawrence Livermore National Laboratory. The HEMP was an explicit Lagrangian finite-difference code that could handle large strains, elastic–plastic flow, wave propagation, and sliding interfaces. The EPIC code [9] was an explicit Lagrangian finite element code developed in the 1970s by Johnson. Both the rezoning and erosion techniques were employed in the EPIC to simulate high velocity impact and blast problems. The PRONTO3D code [10] was a 3D transient solid dynamics code developed at the Sandia National Laboratory for analyzing large deformations of highly nonlinear materials subjected to extremely high strain rates. This code was based on an explicit finite element formulation, and had been coupled with the smoothed particle hydrodynamics (SPH) method through a contact-like algorithm [11]. The DYNA2D and DYNA3D codes were developed in the 1970s at the Lawrence Livermore National Laboratory as explicit Lagrangian finite element codes and were successfully commercialized [12–14].

1.2 EULERIAN METHODS

For problems in which a material domain could become heavily distorted or different materials are mixed, an Eulerian method is more appropriate. In Eulerian methods, the computational grid is fixed in space and does not move with the material such that the material flows through the grid, as shown in Fig. 1.2.

There is no element distortion in Eulerian methods, but the physical variables, such as mass, momentum, and energy, advect between adjacent elements across their interface. The volume of each element keeps constant during the simulation, but its density varies due to the advection of mass. Eulerian methods are suited for modeling large deformations of materials so that most of computational fluid dynamics codes and early hydrocodes for impact and blast simulation employ Eulerian methods.

Eulerian methods only calculate the material quantities advected between elements without explicitly and accurately determining the position of material

interface and free surface so that they are quite awkward in following deforming material interfaces and moving boundaries. Significant efforts have been made to develop interface reconstruction methods.

HELP (Hydrodynamic plus ELastic Plastic) [15], developed by Walsh and Hageman in the 1960s, is a multi-material Eulerian finite difference program for compressible fluid and elastic–plastic flows. To treat the material interface or free surface, massless tracer particles are used, which define the surface position and move across the Eulerian grid. CTH [16] is an Eulerian finite volume code developed at Sandia National Laboratories to model multi-dimensional, multi-material, large deformation, and strong shock wave physics. The CTH code employs a two-step Eulerian solution scheme, a Lagrangian step in which the cells distort to follow the material motion, and a remesh step where the distorted cells are mapped back to the Eulerian mesh. Material interfaces are reconstructed using the Sandia Modified Young's Reconstruction Algorithm. The CTH has adaptive mesh refinement and uses second-order accurate numerical methods to reduce numerical dispersion and dissipation. It is still under development at Sandia National Laboratories [17].

The Zapotec developed at Sandia National Laboratories is a framework that tightly couples the CTH and PRONTO codes [18,19]. In a Zapotec analysis, both CTH and PRONTO are run concurrently. For a given time step, the Zapotec maps the current configuration of a Lagrangian body onto the fixed Eulerian mesh. Any overlapping Lagrangian material is inserted into the Eulerian mesh with the updated mesh data passed back to the CTH. After that the external loading on the Lagrangian material surfaces is determined from the stress state in the Eulerian mesh. These loads are passed back to PRONTO as a set of external nodal forces. After the coupled treatment is completed, both CTH and PRONTO are run independently over the next time step.

1.3 HYBRID METHODS

Both purely Lagrangian and purely Eulerian methods possess different shortcomings and advantages so that it is desirable to find new approaches to take advantage of both methods to better tackle challenging problems. The arbitrary Lagrangian–Eulerian (ALE) method [20] and the particle-in-cell (PIC) method [21,22] are two representatives.

1.3.1 Arbitrary Eulerian–Lagrangian Method and Its Variations

The ALE method was first proposed in the finite difference and finite volume context [23,24], and was subsequently adopted in the finite element context