

# Preface

## Background

Numerical simulation using computers has increasingly become a very important approach for solving problems in engineering and science. It plays a valuable role in providing tests and examinations for theories, offering insights to complex physics, and assisting in the interpretation and even the discovery of new phenomena. Grid or mesh based numerical methods such as the finite difference methods (FDM) and the finite element methods (FEM) have been widely applied to various areas of computational fluid dynamics (CFD) and computational solid mechanics (CSM), and are currently the dominant methods in numerical simulations for solving problems in engineering and science.

Despite the great success, grid-based numerical methods suffer from difficulties in some aspects, which limit their applications in many complex problems. The major difficulties are inherited from the use of grid or mesh. Because the entire formulation is based on the grid/mesh, a time-consuming and costly process of generating/regenerating a quality grid/mesh is necessary. The use of grid/mesh can lead to difficulties in dealing with problems with free surface, deformable boundary, moving interface (for FDM), and extremely large deformation (for FEM).

A recent strong interest is focused on the next generation computational methods — meshfree methods, which are expected to be superior to conventional grid-based FDM and FEM in many applications. A large number of meshfree methods have been proposed for different applications, as detailed in the recent monograph on meshfree methods by G. R. Liu (2002). These

meshfree methods share some common features, but are different in the function approximation, the approaches for creating discretized system equations and the detailed implementation process.

This book will be focusing on a class of meshfree particle methods (MPMs), in particular, the smoothed particle hydrodynamics (SPH) method and its variations. The reasons for devoting this volume to the SPH method are listed as follows.

1. The SPH method is capable of dealing with problems with free surface, deformable boundary, moving interface as well as extremely large deformation.
2. The SPH method, as one of the oldest MPMs, is quickly approaching its mature stage.
3. With the continuing improvements and modifications, the accuracy, stability and adaptivity of the SPH method have reached an acceptable level for practical engineering applications.
4. Applications of the SPH method are very wide, ranging from micro-scale to macro-scale and even to astronomical scale, and from discrete systems to continuum systems.
5. Some commercial codes have incorporated the SPH processor into their software packages with many successful practical applications.

The authors and their research teams started to work on SPH since 1997, when they were searching for an alternative numerical approach for simulating explosion of high explosives, underwater explosion, etc. They were using the FEM, FVM, and ALE for explosion related projects (Lam and Liu et al. 1996; Liu and Lam et al. 1998; Zhao et al., 1998; Chong et al. 1998a; b; 1999; etc.). It was very often to encounter unexpected terminations during the computation due to mesh distortion related problems. It had been a constantly painful daily struggle to adjust all kinds of parameters in the codes that they used, and then re-run the simulation, hoping to get a successful run at the end. The research works using these methods were indeed not very productive, but there were no other choices. An alternative method without using a mesh is definitely necessary for these problems. The quest of the authors' teams for such an alternative method has led to their active venturing into the meshfree methods.

The SPH method was then chosen as one of the alternatives due to the above-mentioned reasons. The successful applications of the SPH method to many explosion related problems have encouraged the authors and their team members to further extend the SPH method for high velocity impact and penetration problems. These applications will be presented in detail in this book after a systematic presentation on the basic idea, theory, and the formation of the SPH method of various versions.

## **This book**

For the very first time, the SPH method is presented in detail in a book form. The book aims to provide an introduction to the SPH method for readers who are interested in learning, using or further developing the method. It covers the theoretical background, numerical techniques, code implementation issues and many different applications.

The book is written for senior university students, graduate students, researchers and professionals both in engineering and science. The presented techniques, intriguing applications and sample code will be useful to mechanical, civil, and aeronautical and astronautically students, engineers, researchers and professionals in both CFD and CSM areas.

Substantial efforts have been made in presenting the materials in an easy-to-understand manner, so that the 3<sup>rd</sup> year undergraduates in engineering or science schools can understand most of the materials discussed in this book. Background knowledge on the grid-based numerical methods such as FEM (see, e.g., Liu and Quek, 2003) and FDM is not required but would be helpful in understanding the procedure and the method, and in reading the book. Basic knowledge on CFD will also help in reading the book, and a section is therefore provided to prepare the students for the knowledge on fundamental equations that governs the fluid flows.

In theories, the kernel approximation in continuous form and particle approximation in discretized form are described, as these two approximations form the foundation for the SPH methods. The reproducibility of the SPH approximation is investigated, which is accompanied with systematically derived consistency conditions in both continuous and discretized forms. The continuous consistency conditions result in a generalized approach to construct analytical smoothing functions that play a key role in the SPH formulation. The discretized consistency conditions provide means to restore the particle inconsistency in the conventional SPH, and lead to the development of the corrective smoothed particle method (or CSPM). A discontinuous SPH (or DSPH) formulation is presented to simulate discontinuous phenomena such as shock waves. The DSPH formulation improves the boundary deficiency and restores consistency in the discontinuous region. An adaptive SPH (or ASPH) that provides better directional smoothing features is also introduced.

In numerical techniques, some detailed treatments such as artificial viscosity, artificial heat, physical viscosity, variable smoothing length, zero-energy mode problem, artificial compressibility, solid boundary treatment, choice of time step are addressed for enhancing the stability in the computational process and the accuracy of the results.

In applications, many interesting and practical examples are presented. The applications are dispersed in different chapters when addressing the corresponding topics. Except for some routine cases for benchmarking the SPH

method, most of the presented applications are quite difficult for the grid-based numerical methods. These includes incompressible flows, free surface flows, high compressible flows, high explosive (HE) detonation and explosion, underwater explosion and water mitigation of explosive shocks, high velocity impact and penetration, and multiple scale simulations coupled with the molecular dynamics method. The presented numerical examples demonstrate the powerful capabilities of the SPH method and offer ample opportunities to further improve and extend the SPH method for more complex and practical applications in engineering and science.

In implementation, this book also discusses some important issues in the computer coding of the SPH method, including basics of parallel coding. A source code in FORTRAN 77 is provided with detailed descriptions.

Numerical simulations using the SPH method are a relatively new area of research, and are still under continuing development. There are problems awaiting further improvements in the SPH method. These problems in turn offer ample opportunities for researchers to develop more advanced particle methods as the next generation of numerical methods. The authors hope that the formulation and the source code provided in this book can serve the purpose to have a smoother start to efficiently learn, test, practise and further develop the SPH methods.

## Outline of the book

This book provides a comprehensive introduction to the SPH method and its variations such as the CSPM, DSPH, and ASPH. It is organized in a total of ten chapters that are briefed as follows.

**Chapter 1** introduces some background knowledge of numerical simulation. The features and limitations of the grid-based numerical methods are discussed. The basic ideas of meshfree and particle methods are briefed. Some general features of the meshfree particle methods, especially smoothed particle hydrodynamics, are described. The invention, development, applications and extensions of the SPH method are briefly addressed.

**Chapter 2** provides the fundamentals of the SPH method such as the basic concepts and the essence of SPH formulations. The essential formulations will be useful in the later Chapters.

**Chapter 3** presents a general approach to construct analytical smoothing functions for the meshfree methods including SPH. The approach not only systematically derives the constructing conditions for the smoothing function, but also addresses the related particle consistency problem in the SPH method. The efficiency of the approach has been demonstrated by developing various existing smoothing functions including a newly constructed smoothing function.

**Chapter 4** describes the implementation of the SPH method on the Navier-Stokes equation, and presents some applications to some general fluid dynamic problems. Some numerical aspects such as artificial viscosity, artificial heat, physical viscosity, variable smoothing length, zero-energy mode problem, artificial compressibility, solid boundary treatment, choice of time step are discussed. Nearest neighbor particle searching (NNPS) algorithms and pair interaction technique for particle interaction are described. The implemented three-dimensional SPH code is applied to solve different flow problems.

**Chapter 5** proposes a smoothed particle hydrodynamics formulation, which is superior to the traditional SPH and the corrective smoothed particle method (CSPM) in simulating discontinuous phenomena. With this formulation, the solution accuracy near the boundaries and the discontinuities are both considerably improved.

**Chapter 6** presents the application of SPH to high explosive (HE) detonations process, and the later expansion process. An adaptive procedure to evolve the smoothing length is employed to meet the needs of simulating large deformation and explosion events. Besides some basic numerical examples, explosions of shaped charge are also simulated using the SPH method with some revealing results.

**Chapter 7** introduces the application of SPH to the simulation of the early time phenomena such as shock waves in underwater explosions. A particle-to-particle interface treat technique is employed, which allows the kernel and particle approximations among particles from different materials, and applies a special penalty force to penetrating particles. A comparison investigation is also carried out on the real and the artificial detonation models of HE as well as their influences to the entire underwater explosion shock simulations. This chapter also presents an investigation on the water mitigation problems using the SPH method. Contact and non-contact water mitigation simulations have been carried out and are compared with the case without water to study the water mitigation effects.

**Chapter 8** investigates the hydrodynamics with material strength using both the SPH method and the adaptive smoothed particle hydrodynamics (ASPH) that is a modified version of SPH. A comparison study of SPH and ASPH and their applications in hydrodynamics with material strength is presented. The constitutive model and equation of state for the material are incorporated into the SPH and ASPH equations. Two numerical tests of impact and penetration are presented.

**Chapter 9** presents an approach for coupling length scale (CLS) via combining SPH with molecular dynamics (MD). The molecular dynamics is applied to the atomic-sized regions for accuracy, whereas SPH is applied to other peripheral regions for efficiency. Handshaking MD/SPH is implemented by allowing interaction between SPH particles and MD atoms. The validity of this

novel particle-particle CLS approach is preliminarily demonstrated by the simulation of the Poiseuille flow and Couette flow of simple fluids.

**Chapter 10** addresses issues related to the computer implementation of the SPH method. The general procedure for Lagrangian particle simulation is described. Computer implementations of the SPH method on serial and parallel computers are also addressed. A sample SPH code is presented. The main features of the sample code, more detailed descriptions and the source code of the related subroutines are given. The programs demonstrate most of the concepts and techniques related to the MPMs related to SPH.

Chapters 1 to 4 are essential for the SPH method, and may be read orderly before reading other chapters. Chapters 5 to 9 are mainly applications and special topics of the SPH method. They may be read independently in any order depending on the interests of the readers. Proper cross-references are provided when substantial materials and issues are shared between these chapters. Chapter 10 provides a SPH code and the detailed descriptions. It may be read after Chapter 4 for the beginners and any time for the experienced users who are interested only in using the source code.

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