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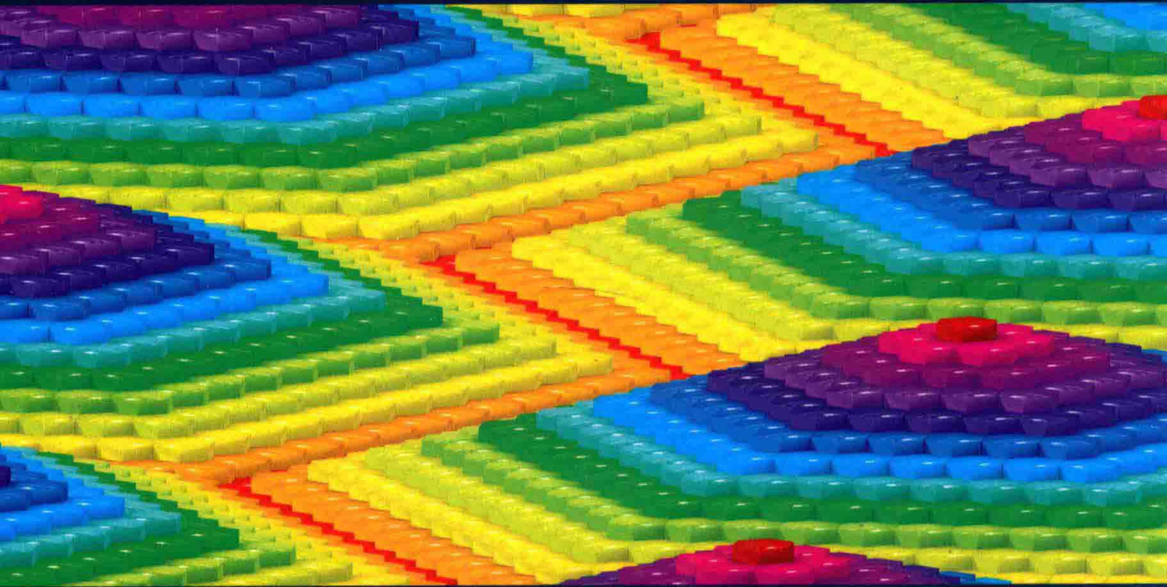

Volume 2

Discrete-continuum Coupling Method to Simulate Highly Dynamic Multi-scale Problems

Simulation of Laser-induced Damage in Silica Glass

Mohamed Jebahi, Frédéric Dau
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coordinated by
Ivan Iordanoff

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Discrete-continuum Coupling Method to Simulate Highly Dynamic Multi-scale Problems

Preface

Smart materials, added value manufacturing and factories for the future are key technological subjects for the future product developments and innovation. One of the key challenges is to play with the microstructure of the material to not only improve its properties but also to find new properties. Another key challenge is to define micro- or nanocomposites in order to mix physical properties. This allows enlarging the field of possible innovative material design. The other key challenge is to define new manufacturing processes to realize these materials and new factory organization to produce the commercial product. From the material to the product, the numerical design tools must follow all these evolutions from the nanoscopic scale to the macroscopic scale (simulation and optimization of the factory). If we analyze the great amount of numerical tool development in the world, we find a great amount of development at the nanoscopic to the microscopic scales, typically linked to *ab initio* calculations and molecular dynamics. We also find a great amount of numerical approaches used at the millimeter to the meter scales. The most famous one in the field of engineering is the finite element method. However, there is a numerical death valley to pass through, from micrometers to several centimeters. This scale corresponds to the need for taking into account discontinuity or microstructures in the material behavior at the sample scale or component scale (several centimeters). Since the 2000s, some attempts have been carried out to apply the discrete element method (DEM) for simulation of continuous materials. This method has been developed historically for true granular materials, such as sand, civil engineering grains and pharmaceutical powders. Some recent developments give new and simple tools to simulate quantitatively continuous materials and to pass from microscopic interactions at the material scale to the classical macroscopic properties at the component scale (stress and strain, thermal conductivity, cracks, damages, electrical resistivity, etc.).

In this set of books on discrete element model and simulation of continuous materials, we propose to present and explain the main advances in this field since 2010. The first book explained in a clear and simple manner the numerical way to build a DEM simulation that gives the right (same) macroscopic material properties, e.g. Young's modulus, Poisson's ratio, thermal conductivity, etc. Then, it showed how this numerical tool offers a new and powerful method for analysis and modeling of cracks, damages and finally failure of a component. In this second book, we present the coupling (bridging) between the DEM method and continuum numerical methods, such as the constrained natural element method. This allows us to focus DEM in the parts where the microscopic properties and discontinuities lead the behavior and leave continuum calculation where the material can be considered as continuous and homogeneous. Coupling scales for highly dynamic problem has been a challenge for a long time. This book shows how to choose the coupling parameters properly to avoid spurious wave reflection and to allow the passage of all the dynamic information both from fine to coarse model and from coarse to fine model. The second part demonstrates the ability of the coupling method to simulate a highly nonlinear dynamical problem: the laser shock processing of silica glass.

A further book in this set presents the numerical code developed under the free License GPL 'GranOO': www.granoo.org. All the presented developments are implemented in a simple way on this platform. This allows scientists and engineers to test and contribute to improving the presented methods in a simple and open way.

Now, dear readers let us open this book and welcome in the DEM community for the material of future development ...

Ivan IORDANOFF
Bordeaux, France
August, 2015

Introduction

I.1. Bridging the scales in science and engineering

Over the past few decades, numerical simulation has firmly established itself as a partner to experiment with unraveling the fundamental principles behind continuous material behaviors. Starting from the 1960s, this approach received strong scientific interest which led to the development of a great number of numerical methods. These methods can be divided into continuum methods (CMs) and discrete methods (DMs). Undoubtedly, the CMs are the most commonly used to solve problems at the engineering (macroscopic) scale, at which the mechanical behavior of materials can generally be described by continuum mechanics. However, their application to investigate microscopic effects, which can have a profound impact on what happens at larger space and time scales, faces several difficulties. Although solutions that are more or less reliable have been proposed in the literature to get over these difficulties, an accurate description of numerous engineering problems remains very challenging for CMs. Some difficulties, associated with reliance of these methods on a predefined mesh and/or unsuitability in dealing with discontinuities, are still not adequately ironed out. In contrast, the DMs naturally provide solutions for most of these outstanding difficulties. These are based on discrete mechanics and do not rely on any kind of mesh. Using DMs, the studied domain is modeled by a set of discrete bodies allowing discontinuities to be naturally taken into account. Although these methods were originally developed to study naturally discrete problems, their features have been proven to be very attractive for several continuous problems involving complex microscopic effects, e.g. damage, fracture and fragmentation. Application of such methods to overcome the CM limitations is then well worth exploring. Nevertheless, the lack of theoretical framework allowing these methods to properly model continua has restricted their application on this kind of problem until very recently.

Modeling continuous problems with DMs mainly faces two significant challenges. The first challenge concerns the choice of the cohesive links between the neighboring discrete bodies and the identification of their microscopic parameters so as to ensure the expected macroscopic mechanical behavior. The second challenge concerns the construction of the discrete domain which must take into account the structural properties of the original problem domain, e.g. homogeneity and isotropy, and must ensure independence of the macroscopic mechanical behavior on the discrete bodies number. The first book of this set, *Discrete Element Method to Model 3D Continuous Materials* [JEB 15], tried to tackle these challenges and to provide a comprehensive methodology allowing for correct discrete element modeling of continuous materials. This methodology was developed for a particular discrete element method (DEM) in which a given material is modeled by a set of rigid spheres in interaction with each other by three-dimensional (3D) cohesive beam bonds. As shown in [JEB 15], several conditions must be satisfied to properly model continua using the proposed DEM variation. The development of this DEM variation, in addition to the ever-increasing power and affordability of fast computers, has brought discrete element modeling of continuous material within reach. Nowadays, such a method presents a prominent tool for elucidating complex mechanical behaviors of continuous materials [AND 12b, JEB 15]. It was successfully applied to investigate several challenging problems that cannot be easily treated by CMs [AND 13, AND 12a, TER 13, JEB 13a, JEB 13b]. The major drawback of this method is that it is very time-consuming compared to CMs and the computation time can quickly become crippling, especially in the case of a large studied domain. However, in modern material science and engineering, real materials usually exhibit phenomena requiring multi-scale analysis. These phenomena require on one scale a very accurate and computationally expensive description to capture the complex effects at this scale and on another scale a coarser description is sufficient and, in fact, necessary to avoid prohibitively large computation. Therefore, in a view of expanding the scope of proposed DEM and alleviating its limitations, it would be beneficial to couple this approach with a CM, such that the computation effort can be distributed as needed.

In many mechanical problems, the notion of multi-scale modeling arises quite naturally. Indeed, most of the material behaviors at the macroscopic scale, which is the scale of interest for engineering applications, are determined by microscopic interactions between atoms. This is why such a notion has become a special area of interest for many scientists. Consequently, several multi-scale coupling methods have been developed over the last three decades. In a pioneer work, Ben Dhia [BEN 01, BEN 05, BEN 98] developed the Arlequin approach as a general framework which allows the intermixing of various mechanical models for structural analysis and computation. Abraham *et al.* [ABR 98, BRO 99] developed a methodology that couples the tight-bending quantum mechanics with molecular dynamics (MD) such that the two Hamiltonians are averaged in a bridging region. A damping was used in this region to reduce spurious reflections at the interface between the two models. Nevertheless, the choice of the damping coefficient remains difficult. Smirnova *et al.* [SMI 99] proposed a combined MD and finite element method (FEM) model with a transition zone in which the FEM nodes coincide with the positions of the particles in the MD region. The particles in the transition zone interact with the MD region via the interaction potential. At the same time, they experience the nodal forces due to the FEM grid. Belytschko and Xiao [BEL 03, XIA 04] developed a coupling method between the molecular dynamics and continuum mechanics models based on the bridging domain technique. In this method, the two models are overlaid at the interface and constrained with a Lagrange multiplier model in the bridging region. Fish *et al.* [FIS 07] formulated an atomistic-continuum coupling method based on a blend of the continuum stress and the atomistic force. In terms of equations, this method is very similar to the Arlequin approach [BEN 01, BEN 05, BEN 98]. In an interesting work, Chamoin *et al.* [CHA 10] analyzed the main spurious effects in the atomic-to-continuum coupling approaches and they proposed a corrective method based on the computation and injection of dead forces in the Arlequin formulation to offset these effects. Aubertin *et al.* [AUB 10] applied the Arlequin approach to couple the extended finite element method (X-FEM) with MD to study dynamic crack propagation. Bauman *et al.* [BAU 09] developed a 3D multi-scale method, based on the Arlequin approach, between highly heterogeneous particle models and nonlinear elastic continuum models. For more details, several papers reviewing these methods can be found in the literature [LU 05, XU 09, JEB 14, CUR 03]. Based on these papers, three approaches can mainly be used to couple DEM with CMs: the hierarchical, concurrent and hybrid hierarchical-concurrent coupling approach.

The hierarchical coupling approach, also called sequential, serial, implicit or message passing, is the most widely used and computationally the most efficient. This approach aims to piece together a hierarchy of numerical methods in which the coarse-scale model uses information obtained by the more detailed fine-scale model. The homogenization methods for multi-phase media are typical examples of the hierarchical coupling approach. The response of a representative volume element at a fine scale is first computed, and from this, a stress-strain law is extracted to describe the mechanical behavior of the homogenized material at coarser scale. The hierarchical approach is generally well suited for problems in which the different analysis scales are decoupled or weakly coupled. In other words, it can be used when the large-scale variations appear homogeneous and quasi-static from the fine scale point of view.

The concurrent coupling approach, also called parallel or explicit, consists of linking numerical models of different scales together in a single combined model, such that the fine-scale model communicates directly and instantly with the coarse-scale model through some coupling procedure. Both compatibility and momentum balance are enforced across the interface between the coupled models. This type of coupling approach is well suited to study multi-scale problems in which the behavior at each scale depends strongly on what happens at the other scale. A variation of the concurrent approach, generally referred to as semi-concurrent, is that in which the coupled models run together and communicate instantly with each other but are not intimately coupled. Compatibility and momentum balance are only satisfied approximately. The advantages of this approach lie in the fact that the coupled models can be computed by separate software. The FE^2 multi-scale approach of Feyel and Chaboche [FEY 00] is an example of this variation.

In some multi-scale problems, the involved scales can be weakly coupled at the beginning of the computation up to a certain response limit, and subsequently become highly dependent. Therefore, it would be computationally beneficial to combine the above two coupling approaches to study such problems. This has led to the development of the hybrid hierarchical-concurrent (or hierarchical-semi-concurrent) coupling approach. The hierarchical approach is used as long as the requested fine-scale information is available. When this information is no longer accessible, due to strain localization, for example, the concurrent (or semi-concurrent) approach is invoked. If the fine-scale response is history dependent, it is necessary to reconstruct at least an approximate history. An example of this approach is the adaptive multi-scale approach developed by Akbari *et al.* [AKB 12] to study the quasi-brittle crack propagation in metals. In this approach, the FE^2 technique is used in the safe regions of the studied domain. When strain localization appears, the concurrent coupling approach is used to solve the problem exactly at the material heterogeneities scale. Compared to the first two coupling approaches, the hybrid hierarchical-concurrent (hierarchical-semi-concurrent) coupling approach is relatively recent, and is, at present, the subject of several studies [AKB 12, NUG 07].

The choice of one of the above multi-scale approaches to couple DEM and CMs depends on the type and nature of the mechanical problems to be studied. This point will be discussed in the next section.

I.2. Scope and objective

The ever-accelerating progress in applied science and engineering has given rise to numerous interesting problems that require multi-scale modeling to accurately handle the relevant phenomena, while reducing the computation time. Of particular interest are the fast dynamic problems which generally involve strongly dependent multi-scale effects. Due to their complexity, these problems so far present a central issue for traditional numerical methods. In contrast, the DEM variation proposed [JEB 15], which is well adapted for highly dynamic analysis, can give answers to several outstanding questions related to such problems. In order to benefit from the DEM strengths in solving such problems, this book focuses on this type of problem. A common feature of most of these problems is that the regions requiring fine-scale analysis by DEM are generally small with respect to the full studied domain. Modeling such problems with DEM-CM coupling approach can thereby considerably reduce the computation costs without affecting the solution accuracy. Therefore, the first objective of this book aims to develop a robust multi-scale discrete-continuum coupling approach between DEM and a CM, adapted for highly dynamic problems. Among the cited coupling approaches, the concurrent approach offers several potential benefits with regard to this objective. Indeed, this approach is the most suitable to model strongly dependent multi-scale phenomena which are frequently encountered in complex highly dynamic problems. This approach is then retained to couple DEM with a CM to be chosen. As already known, numerous CMs used to model material behaviors can be found in the literature [LIU 03, LUC 77, ZIE 05c, ZIE 05a, ZIE 05b, CHI 11]. Each method has its features and specificities. The choice of the most appropriate CM to be coupled with DEM is thus not straightforward. To simplify this task, the most commonly used CMs will be classified according to their advantages and drawbacks with respect to the aim of the present work. Based on this classification, the method that best meets the expectation of this work will be retained for coupling with DEM. Then, a concurrent coupling approach adapted for highly dynamic multi-scale problems will be developed between these two methods.

With the development of the discrete-continuum coupling approach, several interesting complex applications in fast dynamics become affordable. One particular application is the laser shock processing (LSP) of materials. Since its first industrial application in the 1970s, LSP has become widely used in various engineering areas to improve the near-surface mechanical properties of metals, to remove matter by cutting or drilling, to harden or texture surfaces, etc. The ever-increasing use of this process has created a need for more in-depth studies to deal with some outstanding challenges. Despite the current experimental advances in this direction, some of these challenges still remain to be solved. Therefore, numerical simulation has become essential to support the experimental studies. To numerically study an LSP test from a mechanical point of view, it is necessary to know the mechanical loading generated by the laser–matter interaction. Several models aiming to approximate this loading exist in the literature [MAI 08, KHA 05, COL 06, FRO 93]. However, the various simplifying assumptions underlying these models have made them inaccurate in the general case. Application of the developed discrete element method-constrained natural element method (DEM-CNEM) coupling approach as an inverse technique to enrich the results of these models, based on the final experimental results of an LSP test, would be an avenue worth exploring. Nevertheless, implementation of this idea requires preliminary simulations to ensure that this coupling approach can correctly predict the important mechanical phenomena frequently encountered in LSP. This is the second goal of this work which aims to study qualitatively the complex LSP mechanical phenomena. The mechanical loading applied in this study is inspired by those obtained using a specialized laser–matter interaction software. Several interesting materials are routinely used in different laser applications and require additional investigation in their response to laser radiation. Of particular interest is silica glass which is the dominant constitutional material of the optical equipment in laser devices. This material is known to exhibit anomalous behavior in its thermal and mechanical properties [BRÜ 70, BRÜ 71]. Furthermore, certain properties of this glass such as Young's modulus, shear modulus and density show anomalous dependence on the fictive temperature. Because of its complex mechanical behavior, numerical study of this material remains a central issue for several researchers. These reasons have made silica glass an attractive material to be studied numerically. Therefore, it was selected as a part of the LSP application to be studied by the DEM-CM coupling approach. More precisely, the proposed coupling approach will be applied to simulate, from a mechanical point of view, the LSP of silica glass.

I.3. Organization

Following this introduction, the current book is divided into two parts. Part 1 deals with the first objective of this book which is the development of a discrete-continuum coupling approach adapted for highly dynamic multi-scale problems. This part consists of three chapters:

– Chapter 1 reviews some important aspects related to discrete-continuum coupling in dynamics. First, the main coupling challenges to be addressed are detailed. Then, the different concurrent coupling techniques reported in the literature are reviewed. Based on this review, the most appropriate technique is retained to concurrently couple DEM and a CM to be chosen.

– Chapter 2 aims to select the appropriate CM that will be used as a part of the discrete-continuum coupling. First, the most commonly used CMs in computational mechanics are reviewed and classified. Based on this classification, the method that best meets the expectations of the current work is chosen. Finally, the main specificities of the retained method are briefly recalled.

– Chapter 3 focuses on the development of the discrete-continuum coupling method between DEM and the chosen CM. After detailing how the coupling approach is performed, a parametric study of the different coupling parameters is performed. This study aims to draw recommendations simplifying the choice of these parameters in practice, and then to simplify the application of the coupling method on complex problems. Finally, the developed coupling approach is validated using several dynamic reference tests.

Part 2 is dedicated to the application of the developed discrete-continuum coupling approach to qualitatively study the LSP of silica glass, which is the second goal of this book. This part is also divided into three chapters:

– Chapter 4 gives some background knowledge of the different disciplines that interact to accomplish the second objective of this book. First, the laser–matter interaction theory is briefly recalled to identify the important phenomena that must be taken into account to correctly simulate the LSP of silica glass. Then, some important experimental works on the mechanical response of silica glass under different loadings are reviewed. This review serves to provide the main specificities of the silica glass mechanical behavior that is modeled using the proposed coupling approach.

– Chapter 5 focuses on the modeling of silica glass mechanical behavior. A new model intended to faithfully reproduce the different specificities of the silica glass response under highly dynamic loadings is proposed. This model is based on the normal stress in the cohesive beam bonds between discrete elements. Validation of this model is first performed in quasi-statics to simplify the analysis of the potential difficulties, and subsequently in fast dynamics by simulation of high-velocity impact tests of silica glass plates. To describe the silica glass brittle fracture, the virial-stress-based model developed in the first book of this series [JEB 15] is used. The main specificities of this model are briefly recalled at the end of this chapter.

– Chapter 6 investigates the ability of the developed discrete-continuum coupling approach to correctly predict the important mechanical effects characterizing an LSP experiment. To this end, a test of LSP of silica glass is reproduced numerically using this approach as well as the silica glass models detailed in the previous chapter.

Finally, this book ends with several conclusions and outlooks.

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