Computational explosion mechanics and related progress

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Explosion mechanics is the theoretical basis for the design of highly efficient arms and ammunition and industrial explosion safety. Because it involves the complex physical and mechanical behaviors of multi-materials under extreme conditions, such as high speed, high temperature and high pressure, it is almost impossible to give exact solutions for explosion problems. As explosion occurs in a very short time and has a strong destructive effect, there will be limited amounts of experimental data obtained during the explosion process. With the continuous development of numerical methods and computer performance, computational explosion mechanics has become a new interdisciplinary branch of explosion mechanics, material dynamics, computational mathematics and computer technology, and greatly promoted the development of explosion mechanics and weapons equipment. Since the late 1960s, US-led western developed countries have developed more than one hundred calculation codes of explosion mechanics.

Based on the simulation software for explosion mechanics, calculations about three-dimensional physical processes on a system scale during the course of weapon system development have been performed, which resulted in the development of a number of high efficiency arms and ammunition. Such research institutions as the Beijing Institute of Technology, the Chinese Academy of Engineering Physics, the Institute of Applied Physics and Computational Mathematics, the Institute of Mechanics of the Chinese Academy of Sciences, Peking University, the University of Science and Technology of China and other research institutions have developed different numerical methods for explosion mechanics, dynamic constitutive models and software development.

Finite Difference Method and Finite Element Method are the most common methods of the discrete methods adopted in computational explosion mechanics. The former is a representative method by which time and space are covered with cells to gain approximate numerical solutions after partial differential equations (governing equations) are established. The latter is a representative method by which continuous space is decomposed into finite elements. Classed by coordinates, Eulerian method and Lagrangian Method are two common methods utilized in computational explosion mechanics. On the base of these two methods, two hybrid methods, ALE (Arbitrary Lagrange Euler) and CLE (Coupled Lagrange Euler), are developed. Eulerian method has an advantage in treating the large deformation of materials, which always occurs in explosion mechanics. However, it is difficult to handle mixed cells using this method if the studied system includes multi-materials because a transition region forms along the interface which becomes fuzzy between materials. How to determine the position of interfaces and how to calculate the physical quantities in the mixed cells have been difficult problems in Eulerian codes. PIC (Particle in Cell) method and VOF (Volume of Fluid) method are the traditional methods to solve the interface problems in Eulerian codes. Youngs method can determine the interface clearly by transporting fluid of cells around the interface, becoming the mainstream of VOF methods. The original Youngs method just determines the interface in a mixed cell, and cannot determine the transport order and quantity of material. That is a problem of Eulerian methods. A modified Youngs method is adopted in [1], in which the material’s fractions are adopted to determine the transport order of material. Ref. [2] proposes an interface treatment method, in which the interface curve of material is traced by a series of straight-line segments which connect head and tails, and the material interface is determined by marker line located on the grid lines. Ref. [3] proposed a hybrid VOF and PIC multi-material interface treatment method, in which PIC method is utilized in the important regions, and continuous method is used in the other, resulting in high precision and high efficiency of algorithm by which the deformation of material is tracked successfully during penetration. Another method, Level Set, has been proposed and widely used in recent years. In [4], Level Set method combined with Ghost Fluid method is employed to track the
interface. Numerical results, such as shock-wave action, implosion and velocity filed shock effect on bubbles, show that the algorithm improves the capability of disposing interface of the original Level Set method. Local hybrid Level Set method is used in [5], in which non-mass Lagrangian particles are introduced into the Level Set method and the governing equations are discrete by an improved CE/SE method. Combining Local hybrid Level Set method with three chemical reaction models, the simulations of shock-wave reflecting over wedges, explosive welding and two-phase detonating in gas-droplet system show that the algorithm can compute multi-materials and achieve high accuracy, wide application range and good compatibility. The study of high accuracy scheme used in explosive simulation is currently one of the hot. For example, WENO scheme and two-step chemical reaction model is presented in [6], and the influence of obstacle in a two-end-enclosed duct on the propagation of flame of coal gas explosion and on over-pressure explosion is studied by combining numerical simulation with experiments. In [7,8], a fifth-order WENO in space and a third-order Rung-Kutta time stepping method is used to examine the feature of the detonation for gas. Simulation of turbulence also is a difficulty in computational explosion mechanics. The Smagorinsky turbulence model and lager eddy simulation method are used in [9] to simulate the LANL’s shock tube experiment of shocked SF6 gas cylinder with the initiate state of SF6 gas cylinder described by dissipative ITL (interface transition layer), and the results show that the width and height of the column agree with the experimental results.

However, the actual explosion mechanics problems are three-dimensional models, and only a few problems can be simplified to two-dimensional models. For example, the two-dimensional penetration model can only dispose vertical problems, but most cases are oblique penetrations, which belong to three-dimensional models. Furthermore, the numerical results of two-dimensional models do not agree well with the reality. It is imperative to study on three-dimensional Computational Explosion Mechanics, but this work is more difficult compared with the two-dimensional problems. Firstly, the geometric topology of three-dimensional problems is more complicated. Although the traditional two-dimensional interface treatment methods can be extended to dispose three-dimensional multi-materials in theory, it is not easy in fact. In [10] based on fuzzy mathematics theory, fuzzy interface treatment changes the perspective of traditional interface treatment methods. The key idea of this method is that the interface is not determined exactly, but the transport order and quantity of material are determined by fuzzy weight. This method results in simple logic and small computation. Secondly, three-dimensional problems are large scale. Owing to the limited processing speed and relatively small size of local memory and storage in single computer, the parallel computation is an indispensable technique for running large-scale simulations. A dynamic parallel strategy base on the domain decomposition method is presented in [11]. Using this algorithm, the computational domain can be expanded and loaded adaptively in balance, and the calculation scale is enlarged, and the calculation speed is accelerated.

Because material constitutive models are key issues in the computational explosion mechanics, we have to study the dynamic mechanical properties of materials and develop relevant constitutive models. Ren et al. [12] investigated the dynamic behavior of alumina by plate impact experiments and obtained Hugoniot elastic limit, the free surface velocity profile and stress histories. Based on the experimental data a Hugoniot curve was fitted, from which a high pressure state equation was derived. All these experimental data were applied in the numerical simulation of the fracture process of alumina by the way of finite element code. The numerical results showed that predictions of stress histories agreed with the experimental results. They also found that the nucleation and the growth of the cracks played an important role in the macroscopic fracture of the alumina target. Ning et al. [13] developed a micromechanical damage model, which considered the nucleation and growth process of microcracks. By the verification of the model, they found that the nucleation parameters and the initiate size of cracks had strong influence on the dynamic fracture strength.

In order to describe the complicate mechanic responses for concretes under shock loadings, Ning et al. [14] developed a damage coupled with plasticity constitutive model based on the continuum damage mechanics theory and the Perzyna viscoplastic constitutive equation. This model assumes that the concrete contains a large number of microcracks and microvoids. When subjected to shock loadings, the concrete may be damaged for nucleation, growth and coalescence of micro-cracks. Meanwhile, the collapse of microvoids produces a compaction of the concrete. However, this model does not consider the interaction between microcracks and microvoids. Liu et al. [15] took concrete as a four-phase composite made of the intact matrix and three mutually perpendicular groups of penny-shaped micro-cracks. Based on Mori-Tanaka’s average stress concept and Eshelby’s equivalent inclusion theory, they developed a dynamic constitutive model for concrete subjected to impact loading and gave a micro-crack damage evolution equation. The advantage of using the micromechanics to study the dynamic properties of concrete is that the evolution process of inner microscopic structure in concrete can be described. Liu et al. [16] investigated the dynamic responses of the reinforced concrete under impact loadings by using one stage light gas guns. They obtained stress-strain curves of the reinforced concrete at different impact velocities, which produced the high strain rate up to 1x10^6 and high pressure up to 1.5 GPa. Through theoretical analysis, they pointed out that the concrete had a significant nonlinearity and rate sensitivity. Song et al. [17] developed a four-stage analytical model for the dynamic perforation of
stiffened plates by rigid projectiles. By adopting an energy method, the model could be used to predict accurately the residual velocity of the projectiles. Analyzing by the model, they found that the residual velocity depends on the size of reinforcement ribs.

With the developments of the modern geotechnical engineering, such as underground constructions of nuclear waste disposal, energy-efficient buildings and the underground storage of carbon dioxide, more and more researchers had started to study the influence of the temperature on the basic mechanical properties of unsaturated soils. On the basis of the theory of multiphase porous-media, Cai et al. [18,19] investigated the effective stress theory, the characteristic of deformations and the constitutive relation of unsaturated soils. They proposed a constitutive model of soil considering the effect of gas phase and the temperature, which had been verified by experimental results. Above studies of material dynamic constitutive relation play an important role in computational explosion mechanics. For more and more new materials arise, such as composite energetic materials [20] and metallic foams [21], it is necessary to develop the corresponding dynamic constitutive model for them.

In recent years, great progresses have been made in some research fields associated with explosion shock problems, such as explosion testing technology, material synthesis and fluid-solid interactions, which can provide a reliable reference for computational explosion mechanics.

According to the aero-optics, a collimated light beam will be refracted if it propagates through the real explosion flow field with index-of-refraction variations, and its wavefront will be distorted. If we measure the deflection angle of the light beam, the gradient of the wavefront can be obtained using the Malus law, and the wavefront aberration can be computed with a reconstruction algorithm. Based on the BOS of Schlieren mode, Tian et al. [22] proposed a new wavefront measurement technique, which was called the BOS-based wavefront technique. It could measure transient wavefront quantitatively with high temporal resolution, high temporal correlation resolution and relatively high spatial resolution. The existing methods for measuring aero-optical aberration suffered from several problems, such as low spatiotemporal resolution, sensitivity to environment, and integral effects, Yi et al. [23,24] developed a visualization technique, which could measure fine structures of supersonic flows, and proposed a new method for measuring aero-optical aberration of supersonic flow. Based on this method, the wavefront aberration induced by a cross-section of supersonic flow field could be measured by ray-tracing. This method has high spatial and temporal resolutions, and could avoid the integral effects and could be used to study the flow field of interest locally. It also could avoid the influence from the test section wall boundary layers and environmental disturbances.

The turbulence problems of hypersonic vehicles are still not well understood. The flow structure in an internal combustion chamber and around a vehicle contains complicated physical phenomena, such as shock wave/boundary layer interactions between shocks. For compressible high-speed turbulent flows, Han et al. [25] presented a new compressibility modification k-ε model, including the shock unsteadiness effect and the previous compressibility modification of the pressure dilatation and dilatational dissipation rate. The model could improve the predictions through inhibiting excessive growth of turbulent kinetic energy, which was very effective for both the supersonic mixing layer and supersonic flows with transverse injection. The more obvious effects of the modified models would be obtained if the flow separated stronger.

Fluid-solid interaction dynamics is attracting more and more concerns in engineering applications for both fluid and solid mechanics. Fluid-solid interactions are complex and universal. Wang et al. [26] proposed a numerical method to simulate the coupled phenomena in a fluid-flexible-structure system. In this study, a two-dimensional panel method was used to calculate the hydrodynamic forces and a modal superposition method was used to solve the governing equation of an Eulerian beam. This method is not only effective for the simulations of the stable boundary and the flow-induced vibration of a single beam, but also effective for the simulations of coupled-flapping of two parallel flexible beams.

Because diamonds are multifunctional super-hard materials with a set of excellent performances, many researchers have done great work on diamond synthesis. In Xiao et al.’s works [27], high-quality type-Ib tower-shape diamond single crystals were synthesized in cubic anvil high pressure apparatus. Using two kinds of carbon diffusing fields (type-B and type-G), many diamond single crystals were synthesized. The effects of carbon diffusing fields on the crystal quality were studied. The results showed that considerable inclusions appear in tower-shape diamond crystals when using type-B diffusing field.

Computational explosion mechanics is a new interdisciplinary science, which is in the development process and is still at a beginning stage of understanding. It is an urgent need to promote the development of computational explosion mechanics for national defense constructions and the designs of weapons and ammunitions. Developing large-scale digital softwares with our own intellectual property is a great challenge for the researchers of computational explosion mechanics.

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