An Effective Three Dimensional MMALE Method for Compressible Fluid Dynamics

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Abstract

An effective second-order three-dimensional unstructured multimaterial arbitrary Lagrangian–Eulerian (MMALE) method was presented for compressible fluid dynamics, which uses Moment of Fluid (MOF) method to reconstruct material interface for immiscible fluids. It is of the explicit time-marching Lagrange plus remap type. Comparing with traditional ALE method, MMALE method permits multimaterials in a singel cell, thus has the extra advantage of accurately modeling problems involving severe mesh distortion as well as interface fragmentations and coalitions induced by strong shearing deformation. Because the stencil used in the staggered compatible discretization involves only the nearest neighbouring cells and the MOF algorithm does not need information from the neighboring cells, the MMALE method in this paper is suitable for parallel computation while keeps second-order accurate. Several numerical tests on three-dimensional structured and unstructured meshes have proved the accuracy and robustness of the present method.

Keywords: MMALE method, MOF method, compatible Lagrangian method, multimaterial fluid dynamics

Introduction

There are generally two kinds of numerical methods for the computation of fluid Dynamics according to the movement of the mesh during computation. The first one is Lagrangian method, in which the mesh is moving with material velocity. It has the advantage of capturing the material interface precisely and explicitly which is very important for moving boundary problems where material interfaces are of great concern, but with the limitation of severe grid distortion due to strong shear deformation which always stops the calculation. The second one is Eulerian method in which the mesh is fixed avoiding the problem of grid distortions but at the expense of precise material interface construction. In order to overcome the drawbacks of the two methods above, an arbitrary Lagrangian Eulerian (ALE) method was introduced to combine the advantages of both the Lagrangian and Eulerian approaches [Donea et al. (1982)]. In the ALE methodology, the mesh may be moved in some arbitrarily specified way to improve the resolution and enhance the robustness of the simulation. Most ALE algorithms consist of three phases, a Lagrangian phase in which the physical variables and mesh are updated, a rezoning phase for defining a new mesh with better quality, and a remapping phase wherein the physical variables are conservatively interpolated from the old Lagrangian mesh onto the new rezoned one. ALE algorithms have much more flexibilities to deal with multi-material problems such as strong fluid-structure interaction and inertial confinement fusion (ICF) problems.

For the traditional ALE method, only one material is allowed to be contained in each mesh cell, so the material interface must be described explicitly by cell edges. When the mesh and the interface deform severely, it is very difficult to generate a new mesh with good quality. In some cases such as interface fragmentations and coalitions emerge due to strong shearing deformation, it is even impossible to perform rezoning successfully and the traditional ALE method often fails. Thus, a new approach called multimaterial ALE method (MMALE) was developed for these problems [Peery et al. (2000)]. The MMALE method is based on a flexible strategy. It allows for multiple materials in a single cell and therefore affords additional flexibility over the traditional ALE method. In other words, MMALE methods permit the interface to cut through cell edges and pass across the cells, and no material-interface-fitted mesh is required, thus the difficulty of mesh adjustment in the rezoning phase is decreased. With these flexibilities, the MMALE method can accurately model problems involving severe mesh distortion as well as interface fragmentations and coalitions induced by strong shearing deformation.

In this paper an effective second-order three dimensional unstructured grid MMALE method was developed for simulating multi-material compressible fluid flows involving strong shearing deformation [Jia et al. (2013)]. It combined the staggered compatible Lagrangian method and momentum of fluid (MOF) algorithm for interface reconstruction, which has the advantages of second-order accuracy and compact stencils. Numerical results of several test problems including Rayleigh-Taylor instability have shown the accuracy and robustness of the method.

Numerical Method

The flowchart of our MMALE method is displayed in Fig. 1. In the initialization stage, the distribution of all the physical variables over the initial mesh is defined. The volume fractions and positions of material centroids are initialized using the method which is an extension of [Aulisa et al. (2007)].

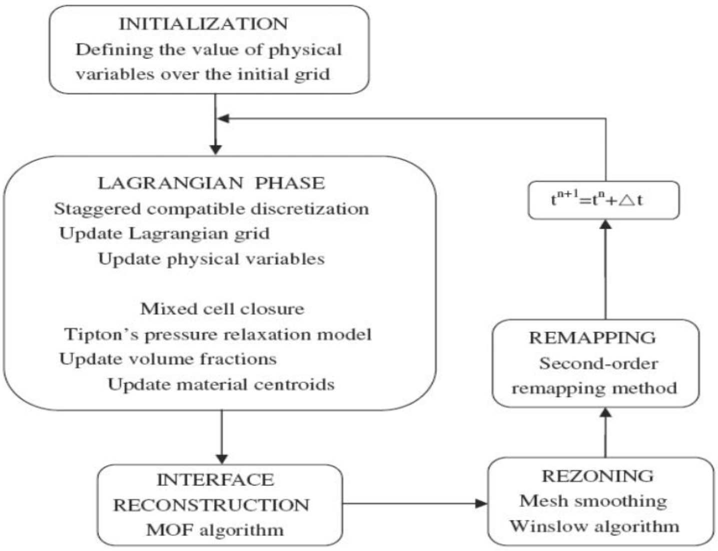

Figure 1. Flowchart of the multi-material ALE algorithm

During the Lagrangian phase, the gas dynamics equations of the Lagrangian form are solved using the staggered compatible discretization, the velocity, density, internal energy, pressure and the Lagrangian mesh are updated. For mixed cells, Tipton's pressure relaxation model is used to define a thermodynamic closure. The material centroids are updated using a method which can be seen as an extension from 2D to 3D of the method presented in [Kucharik et al. (2010)]. The interface reconstruction is performed using MOF algorithm [Ahn et al. (2007)]. In the rezoning phase, the quality of the Lagrangian mesh is improved by means of mesh smoothing using Winslow's algorithm [Winslow (1997)]. Finally, in the remapping phase, all the physical variables are conservatively interpolated from the Lagrangian mesh onto the new rezoned mesh using a cell intersection based second-order remapping method.

In the Lagrangian phase, it is assumed that the computational frame is following the material motion. For pure cells which contain just one material, staggered compatible discretization for Lagrangian gas dynamics is used to update the velocity and position of the node for the movement of the mesh [Caramana et al. (1998)]. For mixed cells containing more than one material, a thermodynamic closure model is needed to define how the volume fractions and the thermodynamic states of the individual materials evolve during the Lagrangian step.

There are several closure models in the literature. The first one is the mean strain rate model [Benson (1992); (1997)] in which each material in the mixed cell takes the mean strain rate of the cell. Actually, it simply assumes that the volume fraction of each material remains unchanged during the Lagrangian step, which may produce nonphysical results in some cases. The second one is the pressure equilibration model [Benson et al. (2004)]. It imposes instantaneous equilibration of the pressure at the cell level. The equilibration problem is nonlinear and sophisticated iteration schemes are necessary for a robust implementation. The third one is the pressure relaxation model [Tipton (1989); Kamm and Shashkov(2010)]. In this model, a relaxation mechanism like viscosity is introduced to make the pressure within a mixed cell move toward pressure equilibration. The forth one is the bulk modulus weighting model [Miller et al. (2007)]. In this model, when the mixed cell is in compression, the bulk modulus weighting algorithm is used; but the volume fraction keeps unchanged when the mixed cell is expanding. The fifth one is the contact mixture model, which was developed to permit slip and separation by solving the jump conditions for the stress and the strain rate across each interface [Benson (1997)]. The sixth one is a one-dimensional model called the sub-cell dynamics model [Barlow (2001)]. In this model, one first estimates the velocity normal to the interface between materials using the acoustic Riemann solver and then approximates the change of volume fraction for each material. In general, the first and the second closure models are very simple and only thermodynamic state dependent while the third and the fourth models are path or process dependent. The fifth and sixth models are more complex and more realistic which are wave structures dependent.

Among these models, the pressure relaxation model is used in this paper because it is more efficient and more effective for three-dimensional MMALE computation.

When the MOF interface reconstruction algorithm is coupled to a Lagrangian hydrodynamics scheme in MMALE methods, it is required that the positions of material centroids in mixed cells be updated during the Lagrangian phase. Following the idea of the constant parametric coordinate method presented in [Kucharik et al. (2010)], it is assumed that the parametric coordinates of the material centroids keep unchanged during the Lagrangian phase. It is proved in [Kucharik et al. (2010)] that this method gives a second-order approximation provided that the time step is small enough. Here we extend the method from 2D to 3D, and present a new approach to compute the parametric coordinates in a hexahedron [Jia et al. (2013)]. In this approach, a good approximation for the initial value of the parametric coordinates is given at first, and then Newton iteration is used to obtain accurate value of it. The convergence of this algorithm is quite fast.

Under the assumption that the materials of the fluid are immiscible, MOF algorithm is used to reconstruct the interface in mixed cells. MOF algorithm is second-order accurate. This method uses information not only about volume fraction but also about position of the centroid for each material. Also it provides automatic ordering of the materials in the process of interface reconstruction. In the case of three-dimensional unstructured meshes, the reconstructed interface is a plane which is chosen to match exactly the volume fraction and to provide the best possible approximation to the centroid positions of the materials.For more details about the numerical implementation refer to [Ahn and Shashkov (2007); Anbarlooei and Mazaheri(2009); Dyadechko and Shashkov (2008)].

In the remapping phase, the physical variables are interpolated from the Lagrangian mesh onto the rezoned mesh. In this paper, by simplifying and improving the method in [Goncharov and Yanilkin (2004)], we develop a second-order accurate remapping method on three-dimensional unstructured mesh [Jia et al. (2013)]. It is a cell-intersection-based method which calculates the volume and centroid of the intersection polyhedron between the old and new cells. It is suitable for remapping between two meshes with different topology.

Numerical Examples

Example 1 3D Periodic Vortex Problem

The three dimensional periodic vortex problem is constructed following the idea of manufactured analytical solution [Salari and Knupp (2000)]. It is the extension of the two-dimensional periodic vortex problem in [Shu (1998); Jia et al. (2013)]. The numerical results proved that MMALE method reaches second-order with mesh refinement.

Example 2 3D Noh Problem

The Noh problem [Noh (1987)] has been used extensively to validate Lagrangian and ALE schemes in the regime of strong shock waves. A perfect gas with $\gamma = 5/3$ is given an initial unit inward radial velocity. The initial thermodynamic state is given by ρ =1and p=0. A spherical shock wave is generated at the origin and moves with constant speed 1/3. At time t =0.6, the shock wave has radial coordinate 0.2. The density behind shock is ρ =64. The initial domain is [0, 1] ×[0, 1] ×[0, 1] decomposed with a 48×48×48 orthogonal mesh. At the initial time, in the vicinity of the spherical $x^2+ y^2+z^2= 1/4$, we place a layer of mixed cells. We note that in these mixed cells the two materials are indeed perfect gases with the same polytropic index γ, and that we treat them as mixed cells to compare the numerical solutions obtained by the MMALE method with the analytical solutions. To run this test we do not need MMALE strategy, traditional pure Lagrangian schemes usually performs well. However, we run this test with MMALE method just for the sake of validation.

The mesh and the interface at t = 0.6 obtained by Lagrangian computation (left) and by MMALE computation (right) are shown in Fig. 2. It can be seen that the final meshes obtained by Lagrangian computation and by MMALE computation both have good quality, the position of interface for both methods are almost the same. The density distributions at t =0.6 are shown in Fig. 3. The peak densities obtained by Lagrangian computation and by MMALE computation reach the value 52.6785 and 60.0365, respectively. It is obvious that MMALE result is better.

More numerical results can be found in reference [Jia et al. (2013)].

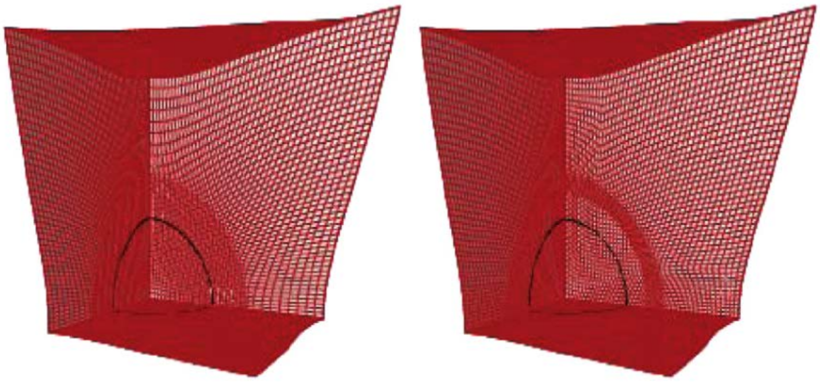

Figure 2. mesh and the interface of Noh problem (Left ,Lagrangian ; Right MMALE)

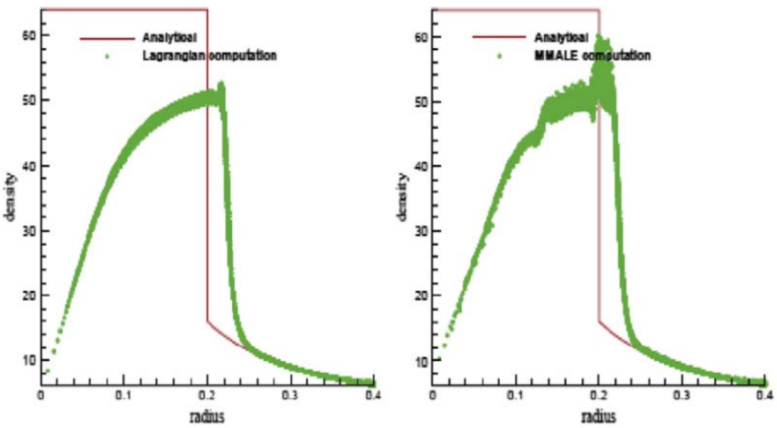

Figure 3. Density distribution at t=0.6 of Noh problem (Left ,Lagrangian ; Right MMALE)

Concluding Remark

A second order three dimensional unstructured MMALE method is presented in this paper, which uses MOF interface reconstruction for simulating multi-material compressible fluid flows involving strong shearing deformation. Numerical test proved the method is of second-order accuracy for continuous solutions. The application for 3D Noh Problem has shown the effectiveness and robust of the MMALE method.

Acknowledgements

This research was sponsored by the National Nature Science Foundation of China (11072040, 11472060), and Projects (2012A0202010, 2012A0201011, 2011B0201042, 2009A 0202014) supported by CAEP.

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