Journal of Computational Physics 349 (2017) 176–190

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

An improved 2D MoF method by using high order derivatives

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ARTICLE INFO

Article history:
Received 29 March 2017
Received in revised form 31 July 2017
Accepted 15 August 2017
Available online xxxx

Keywords:
Interface reconstruction
Moment of Fluid
Multi-material flow

ABSTRACT

The MoF (Moment of Fluid) method is one of the most accurate approaches among various interface reconstruction algorithms. Alike other second order methods, the MoF method needs to solve an implicit optimization problem to obtain the optimal approximate interface, so an iteration process is inevitable under most circumstances. In order to solve the optimization efficiently, the properties of the objective function are worthy of studying. In 2D problems, the first order derivative has been deduced and applied in the previous researches. In this paper, the high order derivatives of the objective function are deduced on the convex polygon. We show that the nth ($n \geq 2$) order derivatives are discontinuous, and the number of the discontinuous points is two times the number of the polygon edge. A rotation algorithm is proposed to successively calculate these discontinuous points, thus the target interval where the optimal solution is located can be determined. Since the high order derivatives of the objective function are continuous in the target interval, the iteration schemes based on high order derivatives can be used to improve the convergence rate. Moreover, when iterating in the target interval, the value of objective function and its derivatives can be directly updated without explicitly solving the volume conservation equation. The direct update makes a further improvement of the efficiency especially when the number of edges of the polygon is increasing. The Halley's method, which is based on the first three order derivatives, is applied as the iteration scheme in this paper and the numerical results indicate that the CPU time is about half of the previous method on the quadrilateral cell and is about one sixth on the decagon cell.

1. Introduction

Simulation of fluid with multiple-materials is a great challenge in computational mechanics. Depending on the different description of grid motion, the computational grid can be classified into the Lagrange frame and Eulerian frame. In the Lagrangian frame, the computational grid is fixed with the material so the material interface will always be coincident with the cell boundaries which can be tracked innately. However, in the Lagrangian frame, the computation will fall into stagnation with the increasing grid distortion because the fluid material always experiences a large deformation with respect to time. On the contrary, in the Eulerian frame, the grid is fixed in space to overcome the distortion. Since the material will advect across the cell's boundaries during the simulation, the interface information is lost when using the Eulerian frame. Therefore, in order to track the material interface, extra effort is required.

The level-set method and the VoF-PLIC (Volume of Fluid with Piecewise Linear Interface Reconstruction) method are the two major approaches for interface reconstruction. The level-set method [1–3] reconstructs the material interface by

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http://dx.doi.org/10.1016/j.jcp.2017.08.031
0021-9991/

an implicit distance function whose zero contour represents the location of the material interface. This method avoids the complex geometric analysis but the level-set function must be solved in high order accurate to avoid serious dissipation which leads to a high level of volume loss especially in the unstructured grid [2]. The VoF-PLIC method [4–9] explicitly reconstructs such an approximate linear interface in the mix cells that the total volume conservation of each material is preserved. Since the VoF-PLIC method is independent of grid type, it can be performed on both structured and unstructured grid.

In the VoF-PLIC method, an approximate interface $\boldsymbol{n} \cdot \boldsymbol{x} + d = 0$ in the mixed cell is constructed in two steps. The first step determines the normal $\boldsymbol{n}$ of the linear interface, while the second step calculates the constant d which satisfies the local volume enforcement requirement, namely the volume fraction of the polygon below the approximate material interface must be exactly equal to the given volume fraction in the mixed cell. The second step in different kinds of VoF-PLIC method is almost the same because the constant d can be uniquely calculated as long as $\boldsymbol{n}$ and volume fraction are given [10,11].

Therefore, the most important part of the VoF-PLIC method is the first step because the estimation of $\boldsymbol{n}$ influences the accuracy of interface reconstruction significantly. Youngs' method [4,9,12] calculates the normal $\boldsymbol{n}$ by the volume fraction gradient which is constructed from the adjacent cells. Although the normal can be calculated directly without iteration in the Youngs' method, it is only first order accurate and can not reconstruct the linear interface precisely. For the sake of the second order accurate, additional requirement is proposed besides the matching of volume fraction. LVIRA (Least square Volume Interface Reconstruction Algorithm) [7] estimates the normal by finding a linear interface, which will be extended outside the mix cell, gives a best approximation to the given volume fraction in adjacent cells. ELVIRA (Efficient least squares VoF interface reconstruction algorithm) [7] presents an alternative minimization approach by determining the normal from six candidates which is also second order accurate and does not require iterative process. Swartz method [13,14] calculates the normal by finding a common linear interface for a pair of neighbor mixed cells which rigorously satisfies the given volume fraction. These methods are second order accurate but an implicit optimization is usually required except for the ELVIRA method which can only be performed on structured grid. All of these methods need the volume fraction from the adjacent cells and extra treatments have to be implemented on the boundary, thus increasing difficulty in programming and parallelization.

The MoF (Moment of Fluid) method [15–17] is a new approach to calculate the interface normal which not only uses the volume fraction but also takes use of the material centroid in the mixed cell. It calculates the normal $\boldsymbol{n}$ by finding a linear interface which fulfills the local volume enforcement requirement and minimizes the discrepancy between the given reference material centroid and the approximate material centroid. The MoF method is also second order accurate and previous researches find that it is more accurate than the VoF-PLIC methods in fluid simulation [18]. Despite its higher accuracy, another attractive superiority of the MoF method is that its implementation could work as a cell-by-cell black-box routine without the requirement from neighbor cells. Alike other second order method, an implicit nonlinear optimization problem is also needed to be solved and an iteration process is inevitable under most circumstances. In order to improve the convergence rate, the derivative-based iteration scheme is preferred. Although the objective function is nonlinear and implicit, the analytical first order derivative has been deduced in the previous researches [11,19] so that the value of the objective function and its first order derivative can be calculated simultaneously. Therefore, iteration schemes based on first order derivative, such as the cubic interpolation method [11,20], are commonly used in the MoF method.

The efficiency of the MoF method is important. The majority of the CPU time is consumed in this process especially in the Eulerian codes [21] or the MMALE codes with sub-scale closure model [22] since the interface must be reconstructed in every time step under these situations. Therefore, in order to further improve the efficiency, the properties of the objective function are worthy of studying. In this paper, the high order derivatives of the objective function are deduced on the convex polygon. We find that the nth ($n \geq 2$) order derivatives are discontinuous, and the number of the discontinuous points is two times the number of the polygon edge. A rotation algorithm is proposed to successively calculate these discontinuous points, thus the interval where the optimal solution is located can be determined. In the target interval, the high order derivatives of the objective function are always continuous so the iteration schemes based on high order derivatives can be used to improve the convergence rate. Moreover, when iterating in the target interval, the value of objective function and its derivatives can be directly updated without explicitly solving the volume conservation equation. The direct update makes a further improvement of the efficiency especially when the number of edges of the polygon is increasing. The Halley's method, which is based on the first three order derivatives, is applied as the iteration scheme in this paper and the numerical results indicate that the CPU time is about half of the previous method on the quadrilateral cell and is about one sixth on the decagon cell.

The rest of this paper is organized as follows. In Section 2, we will briefly review the concept of local volume enforcement requirement. In Section 3, the basic idea of the MoF method is introduced. Afterwards, the high order derivatives of the objective function are deduced in Section 4 and the discontinuity of the high order derivatives is analyzed in Section 5. Then in Section 6, we will develop a direct update of the value and the derivatives of the objective function without explicitly solving the volume conservation equation. Before the numerical tests, full steps of our algorithm are summarized in Section 7. Finally, a series of numerical tests will be conducted in Section 8 and the conclusion is drawn in Section 9.