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A gradient augmented level set method for unstructured grids

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ABSTRACT

We present and test a gradient augmented level set method for unstructured grids, which has been designed to allow for easy integration in parallel flow solvers. The means to this end is a Hermite formulation, where the gradient is stored and advected as an independent variable, along with the level set function. The method uses narrow-band storage in conjunction with a Fast Marching Method, which is also designed to take advantage of the gradient augmentation. We demonstrate through standard passive advection test cases that the proposed method is able to compute interface motion with performance comparable to popular high-performing methods on structured grids.

1. Introduction

Modern fluid simulation of practical problems usually involve complex geometries, variable spatial resolution and parallel computing. The introduction of phase interfaces adds to the complexity. Whereas there exists an abundance of methods and algorithms to track fluid interfaces, much fewer possess the generality that allow them to be implemented with an unstructured, parallel solver.

Volume Of Fluid (VOF) methods and Level Set methods are two of the most popular interface capturing approaches used on stationary grids. In the original VOF method [1], the volume fraction of fluid in the computational cell is used to identify and track the surface, ideally conserving mass. However, VOF encounters a common problem: a characteristic of a fluid surface or interface is that it represents a discontinuity, which does not readily lend itself to polynomial interpolation schemes. While several variants of shock capturing schemes exist, these introduce significant numerical diffusion when applied to discontinuities. Thus, in [1], the surface is reconstructed in a geometric fashion, where chunks of fluid are transfered from one cell to the other. To maintain a sharp interface, additional ad-hoc procedures are introduced after advection. This is a relatively crude process, and it is particularly challenging on unstructured grids. Thus, while conserving mass, VOF has in many cases difficulties with accurately representing the motion of an interface; see [2] for a modern example.

Level set methods, on the other hand, convert the scalar function, in which the interface is embedded, to a form more suitable for polynomial interpolation schemes. This is done through the solution of a reinitialization equation – most often an eikonal equation – which converts the level set function into a signed distance function. Since the distance to the interface is not a conserved quantity, level set methods using this approach do not conserve mass exactly. While the signed distance function represents the interface in a relatively smooth manner, numerical diffusion is still present, and this often causes unacceptably high local mass loss or gain, especially in regions of high curvature.

Several strategies exist to counteract this. The conceptually simplest is to increase the resolution of the grid near the interface, either through adaptive mesh refinement [3], or a finer, separate background grid [4]. Another approach is to

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increase the numerical accuracy. The WENO-type high-order, shock-capturing schemes [5] are popular for structured grids. Implementation on unstructured grids is however more complicated [6], and a general drawback of WENO schemes is that the numerical stencils are rather large, thus complicating data transfer in parallel settings.

A simpler approach is the use of Lagrangian particles to track the interface. The Particle Level Set method [7] is one such method, where particles of finite radius are placed tangent to the interface to correct numerical error in the Eulerian solution. By using Lagrangian interface tracking in conjunction with the level set method, topology changes may be simplified as compared to a purely Lagrangian method. While the original Particle Level Set method used a WENO scheme for the grid-based advection, it was discovered in [8] that since the accuracy mainly depends on the particle correction, a first order semi-Lagrangian scheme for the grid-based quantities is sufficient. Lagrangian augmentation of the interface advection has many attractive features. But like all of the discussed methods, it introduces an additional layer of complexity. Moreover, as the interface is stretched or compressed, so are the particles. This necessitates particle seeding or deletion. When seeding new particles, some kind of interpolant must be used to approximate the interface position from the grid data, and the accuracy of the interface reconstruction is limited by this interpolant. Due to the relatively limited information contained in each particle (position, radius and sign), and the fact that the corrections are made on a per-particle basis, a relatively dense particle distribution is required. In [7], a default of 64 particles per cell per phase was used in 3D. Particles were seeded in a band that spanned around three cells from the interface, yielding a large number of particles. In [9], gradient and curvature information were also embedded in Lagrangian particles and used in conjunction with a level set method. The information transfer from particle to grid was however done by a first order Taylor expansion only, and it remains unresolved how reseeding and topology change should be treated in a robust manner.

If local mass conservation is a pressing issue, the signed distance function may be replaced by a smeared-out approximation of the volume fraction [10,11], however, this may decrease the accuracy of the numerical schemes. Global mass conservation can always be assured by iterating a scheme that moves the interface in the normal direction [12]. This may be an acceptable approach if the local mass loss/gain is low, but over longer periods of time leads to unphysical results.

As mentioned above, high-order schemes can reduce the mass loss, but these often require large stencils. Cubic Hermite interpolation is one of the exceptions – all data required to construct the interpolant is contained within a single cell. The gradients may be obtained by a transport equation, which is derived by taking the gradient of the scalar advection equation, or its discrete analogue. While maintaining compact stencils, this also introduces additional effective resolution, at the expense of increased data storage. Transporting the gradient as an independent quantity has been used in Cubic Interpolated Pseudo-particle/Constrained Interpolation Profile (CIP) [13,14] methods for some time, however, only recently has this approach spread to level set [15] and VOF methods [16]. In [15], a semi-Lagrangian scheme based on tensor product cubic Hermite splines was used. This required a structured grid, and the issue of reinitialization was not treated. Specifically designed for use with the advection scheme proposed in [15], a reinitialization procedure using a Fast Marching Method (FMM) was introduced in [17]. Combined, these two should constitute a good choice for structured grids.

In [18], flow simulations using semi-Lagrangian gradient transport and the tetrahedral cubic Hermite interpolant described in [19] were presented, though interface advection was not treated. Other interesting approaches to high-order semi-Lagrangian advection schemes are found in [20,21]. In [20], a method for structured grids which uses a narrow-band formulation with arbitrary order Gauss–Lobatto stencils is presented. In [21], a conservative, 2D unstructured scheme is formulated using a combination of point values updated by a semi-Lagrangian scheme, and area average updated by a Finite Volume scheme. These are only a few examples of the versatility of semi-Lagrangian schemes. An additional advantage is that they are not limited by the Courant–Friedrichs–Lewy (CFL) condition, as the characteristics may be traced back across several cells during one time step [22].

In the present work, we extend the work of [15] to general 3D unstructured grids, and include reinitialization of the signed distance property, which is integrated into the gradient-augmented setting. This is done by a Fast Marching Method which computes both the level set function and its gradient. For the FMM, we apply Huygens' principle to obtain a local approximation of the distance function. This approach requires local solutions of a small optimization problem, and differs from the Finite Difference (FD) approach used in [17]. Huygens' principle leads to the same type of update rule as presented in e.g. [23,24], which are based on a control-theoretic approach. We use a narrow-band method with storage based on a tetrahedral subgrid, meaning that general, unstructured primal grids are decomposed into tetrahedra.

To avoid overshoots and generation of artifacts in high-curvature areas, we develop a gradient limiting algorithm which is demonstrated to be important for the overall accuracy. The proposed method can readily be incorporated into a parallel setting, as we adhere strictly to compact stencils. While this has been done, the detailed parallel implementation and performance are not the focus of the present work. It should be noted that in the Finite Element framework, another approach with many of the same attractive features we seek already exists. The Discontinuous Galerkin Method has been applied with the level set approach on unstructured grids [25,26] with excellent results.

The rest of the article is organized as follows. A brief description of the level set method, narrow-band and grid structure is given in Section 2. Cubic Hermite interpolants for 1-, 2- and 3-simplices are described in Section 3, followed by an explanation of the semi-Lagrangian advection scheme for function value and gradient in Section 4 and the reinitialization procedure for the level set function in Section 5. We test the method on standard passive advection cases in Section 6, and discuss the overall method and results in Section 7. To promote readability, much of the discretization details, examples and theoretical support are left to Appendices.