Journal of Computational Physics 336 (2017) 492–512

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

3D level set methods for evolving fronts on tetrahedral meshes with adaptive mesh refinement

Nathaniel R. Morgan *, Jacob I. Waltz

X-Computational Physics Division, Los Alamos National Laboratory, P.O. Box 1663, Los Alamos, NM, USA

A R T I C L E   I N F O

Article history:
Received 9 November 2015
Received in revised form 8 February 2017
Accepted 9 February 2017
Available online 2 March 2017

Keywords:
Level set
Hamilton–Jacobi
Eulerian
Adaptive mesh refinement (AMR)
Advection
Point-centered
Finite difference
Tetrahedral meshes
3D

A B S T R A C T

The level set method is commonly used to model dynamically evolving fronts and interfaces. In this work, we present new methods for evolving fronts with a specified velocity field or in the surface normal direction on 3D unstructured tetrahedral meshes with adaptive mesh refinement (AMR). The level set field is located at the nodes of the tetrahedral cells and is evolved using new upwind discretizations of Hamilton–Jacobi equations combined with a Runge–Kutta method for temporal integration. The level set field is periodically reinitialized to a signed distance function using an iterative approach with a new upwind gradient. The details of these level set and reinitialization methods are discussed. Results from a range of numerical test problems are presented.

1. Introduction

The level set approach was first proposed by Osher and Sethian [32] to model evolving fronts with curvature. In the level set approach, the front is modeled using a higher dimensional function ϕ, where $\phi = 0$ represents the front. The regions where the level set function is greater than zero correspond to the first material, and the regions where the level set function is less than zero correspond to the second material. The level set field is either (1) advected through the mesh using a velocity field that is specified or calculated by solving ancillary equations, or (2) is evolved in the surface normal direction. The level set approach has been applied to a range of applications [34,31], examples include multi-material flows [40,14,30,18], flows with phase transition [37,35,36,27] and high-explosive (HE) detonation fronts [3,5].

Simulating the propagation of detonation fronts has a range of challenges. Aslam et al. [3] and Bdzil et al. [5] proposed using the level set approach [32] to capture the details of a high-explosive detonation front on the continuum scale under a set of physical assumptions. The zero contour of the level set field is used to represent the detonation front. The regions where the level set function is greater than zero correspond to the unburned high-explosive, and the regions where the level set function is less than zero correspond to the reactants. The approach in [3] assumes a uniform, Cartesian structured mesh and addresses 2D geometries. This type of computational mesh requires special treatments to handle complex geometries, which can be challenging if extended to 3D. In [3], internal boundary conditions are applied to the uniform Cartesian mesh using additional, separate level set functions to address curved, irregularly shaped boundaries. This internal boundary

* Corresponding author.
E-mail address: nmorgan@lanl.gov (N.R. Morgan).

http://dx.doi.org/10.1016/j.jcp.2017.02.030

condition enforcement has similarities to the ghost fluid approach [14,15,13,27], because constraints on the level set field for the high-explosive detonation front are applied to nodes near the boundary. An alternate approach to handle arbitrary, irregular geometries is to use tetrahedral cells that can conformally mesh complex geometries. Other notable advantages of tetrahedral cells include reduced complexity in mesh reconnection and preserving tetrahedral cells with AMR. Likewise, arbitrary polygonal cells [6] can be decomposed into tetrahedral cells. Due to these advantages, this paper addresses the extension of the level set method to evolving fronts on 3D tetrahedral cells, which requires finding robust solutions to nonlinear Hamilton–Jacobi equations of the general form $\frac{\partial \phi}{\partial t} + H(\nabla\phi, \mathbf{x}) = R(\phi, \mathbf{x})$, where $H(\nabla\phi, \mathbf{x})$ is a Hamiltonian.

Level set methods research has heavily focused on developing methods for fixed, structured Cartesian meshes [34,31], and for spatially adaptive methods, the focus has been on developing methods for adaptive mesh refinement (AMR) of a Cartesian mesh [38,21,26]. Sussman *et al.* [38] proposed a level set method for 2D Cartesian meshes with AMR and used the method to simulate incompressible two-phase flows with surface tension. Losasso *et al.* [21] used a particle level set method [12] with AMR on a 3D Cartesian mesh to simulate the dynamics of a water-air interface. Min and Bibou [26] followed the work in [21] and developed a level set method for 3D adaptive Cartesian meshes.

Level set methods research with unstructured meshes has principally focused on developing methods for 2D triangular meshes. Abgrall [1] developed a finite difference method for solving the Hamilton–Jacobi equations on 2D triangular meshes. Barth and Sethian [4] developed both finite difference and Petrov–Galerkin methods for 2D triangular meshes. Li and Yan [19] followed the work by Barth and Sethian and proposed a finite element method for 2D triangular meshes. Work by Abgrall [2] addresses boundary conditions for Hamilton–Jacobi equations on triangular meshes. High-order methods for solving the Hamilton–Jacobi equations on 2D triangular meshes were created by Zang and Shu [48] followed by Zhu and Qiu [49]. Zang and Shu [48] developed weighted essentially nonoscillatory (WENO) methods and Zhu and Qiu [49] developed Hermite WENO methods for 2D triangular meshes.

Previous research with tetrahedral meshes has focused on advecting the level set field using a specified or externally calculated velocity field. A coupled level set volume of fluid method (CLSVOF) was developed by Lv et al. [23] and was used with a finite volume method to simulate free-surface flows on tetrahedral meshes. The velocity field in [23] was either prescribed or was obtained by solving the incompressible Navier–Stokes equations that govern fluid motion. Follow-on work by Kees et al. [17] used a finite element method coupled with a conservative level method to simulate the dynamics of free-surface flows. These papers only consider the case of advecting the level set field through a tetrahedral mesh using a velocity field derived externally (*e.g.,* user prescribed, derived from solving the Navier–Stokes equation, etc.); in contrast, we seek to develop methods that are suitable for both advecting the level set field and for evolving a front in the surface normal direction. Methods for this second case are required, for instance, to simulate the propagation of detonation fronts on an unstructured mesh.

The goals of this research effort are to develop methods to solve Hamilton–Jacobi equations for several distinct Hamiltonians on 3D unstructured tetrahedral meshes with AMR and iteratively reinitialize the level set field to a signed distance function; as a result, this work deviates from the research discussed above. In this paper, (1) we present new 3D level set methods that robustly evolve fronts in the surface normal direction or with a specified velocity on unstructured tetrahedral meshes coupled with AMR, (2) we present a new method to calculate a stable upwind gradient on unstructured tetrahedral meshes, and (3) we use this new method to calculate a stable upwind gradient to iteratively reinitialize the level set field to a signed distance function on unstructured tetrahedral grids. The focus of the paper is on the numerics of the new methods and not necessarily on the physics of a particular application. The new methods presented in the paper have potential utility in a wide range of applications.

The layout of the paper is briefly described. The nomenclature used in the paper is presented in Section 1.1. The governing equations are presented in Section 2. The details on the numerical approach for evolving the level set field are discussed in Section 3. The iterative reinitialization approach is discussed in Section 4. The approach for temporal integration is described in Section 5. Adaptive mesh refinement is discussed in Section 6. Analysis is presented in Section 7 to show that the new methods are numerical consistent. Lastly, the test problems are presented in Section 8.

1.1. Nomenclature

The nomenclature used in this paper is illustrated in Fig. 1. Vectors and tensors are both denoted with bold font. Subscripts denote spatial locations and superscript letters denote temporal values such as n, $n+\frac{1}{2}$, or $n+1$ respectively. The level set field, ϕ, is stored at the nodes, α, of the mesh. The level set unit normal direction is $\mathbf{n}$. A neighboring node to α is denoted with β, and an edge e connects nodes α and β. A quantity at the center of a tetrahedral cell is denoted with a subscript z.

Central difference gradients can be calculated at the node α and at the cell center z. Each central difference gradient is found by integrating along the boundaries of the corresponding control volumes (CV). The nodal CV, which is also called the dual grid, encompasses the node α. The CV for the cell is the tetrahedron.

The nodal CV surface is decomposed into smaller facets, which are denoted with a subscript i. The vertices of the facet are the face, edge, and zone (f, e, z). The outward surface area normal of a facet on the nodal CV is $\mathbf{S}_i$, and the corresponding unit normal is $\mathbf{s}_i$. All nodal control volume facets around a node is expressed as $i \in \alpha$.

A tetrahedral cell is decomposed into 4 sub-cells that are hexahedra and these sub-cells are termed corners. The quantities in a corner are denoted with a subscript c. The outward corner area normal of a tetrahedron is $\mathbf{A}_c$. All corners in a