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Robust Finite Volume Modeling of 3-D Free Surface Flows on Unstructured Meshes *

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Abstract

The numerical simulation of incompressible fluids possessing multiple distinct, immiscible fluids are of great interest to the engineering community. These flows contain interfaces which can merge and tear as a result of interface physics such as phase change and surface tension. The arbitrarily complex interface topologies inevitably requires an underlying Eulerian formulation. Volume tracking methods are in wide use today, having proven themselves to be topologically robust and relatively easy to implement. The basis in volume fractions also allows the straightforward incorporation of interfacial physics. The formulation of kernel-based continuum surface tension models for these methods has demonstrated acceptable results for orthogonal grids. Attaining accurate, high order results however, on unstructured meshes is necessary if surface tension-driven flows are to be reliably modeled within the confined, complex geometries of most industrial processes. In the following, we investigate the accuracy and convergence of our interface topology estimates and surface tension model on 3-D tetrahedral meshes. We use various ellipsoids to scrutinize our algorithm, which is based on a convolution (hybrid) method to determine the interface unit normal and mean curvature.

Introduction

The use of convolutions with smooth kernels to model surface tension forces in volume tracking methods has been investigated over the past few years ([AP95] – [WKP99]). Here we use the sixth degree kernel introduced in [WKP99], denoted $\boldsymbol{K}(r,\epsilon)$, where r is the distance from the center of the convolution and ϵ is a representative size of the support of the kernel. The gradient of a scalar function (typically volume fractions) is approximated by the convolution of the scalar function with the derivative of the kernel. For instance, given a scalar function f, a smooth approximation to the derivative along the x axis at the point $\boldsymbol{x}$ is given by

$$\frac{\partial f(\mathbf{x})}{\partial x} \approx \int_\Omega \frac{\partial \boldsymbol{K}}{\partial x}(\boldsymbol{x}' - \boldsymbol{x}) f(\boldsymbol{x}') d\boldsymbol{x}'. \quad (1)$$

where Ω represents the entire computational domain.

For a point along the interface, these approximate gradients can be use to construct an approximation to the unit normal to the interface, $\mathbf{n}$.

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The mean curvature of the interface (κ) is found as the divergence of the unit normal, i.e.

$$\kappa = -\nabla \cdot \mathbf{n}. \qquad (2)$$

It has been shown that a simple discretization of the unit normals leads to a much more accurate approximation to κ on orthogonal meshes([WKP99]). This approach avoids convolving the second derivatives of the kernel $\boldsymbol{K}$ with the scalar function f. This idea should logically extend to unstructured meshes, although the discrete divergence operator is now more complicated.

The accuracy of the unit normal and curvature to an interface is tested by approximating the topology of several ellipsoids on unstructured meshes. The meshes consists of a varying number of tetrahedral cells within a unit cube, the meshes have been arbitrarily generated with no knowledge of the interface location. Ellipsoids of increasing slenderness are used to pose problems of greater difficulty for the algorithm. In future work, the topological terms will be used to determine surface tension forces normal to the interface.

Unstructured Tetrahedron Meshes

The meshes used for these calculations consist of arbitrary tetrahedral cells partitioning a unit cube. No orientation towards the interface location was used to generate the meshes. The fluid flow algorithm treats the tetrahedron as "degenerative hexahedron" where one face has collapsed to a point and another face has been collapsed to a line. This allows the fluid flow algorithm to also treat the tetrahedral mesh as a generic set of hexahedra. Because of the nature of how the mesh is treated, the unstructured tetrahedral mesh offers the most demanding test for fluid flow or heat transfer simulations. Figure 1 shows a plane cut through the middle of the unit cube for several meshes, the planes are shown on the $x = 0.5$ surface. The figures demonstrate that these meshes certainly do pose a viable test domain for even the simplest of flow problems.

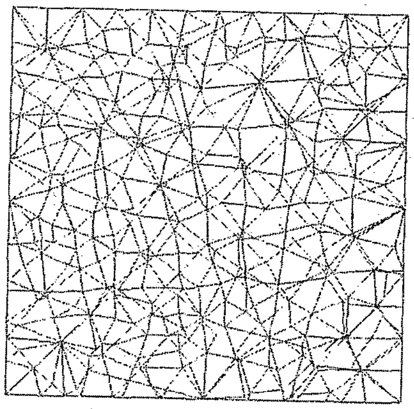
Interface Topology

The methodology to determine the unit normal to the interface, $\mathbf{n}$, and the mean curvature of the interface κ has been discussed in the introduction. A more detailed analysis of this method is presented in [WKP99]. In each cell containing the interface, the approximated normals are used to construct a piecewise planar approximation to the interface which satisfies the discrete volume fraction of the cell.

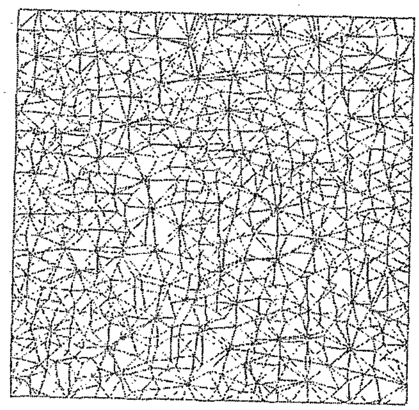
Figures 2 and 3 show the computed unit normals and reconstructed interface for different ellipsoids on the unstructured meshes of Figure 1. Figures 4 and 5 show the reconstructed interface along with the cell edges of all the cells that contain the interface.

Test Problems

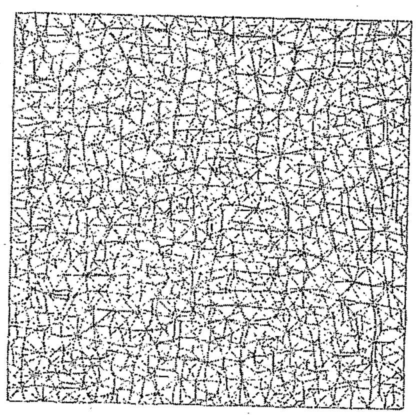
The hybrid convolution method for determining interface topologies is tested on several ellipsoids. Ellipsoids make nice test forms since they can vary in slenderness (eccentricity) to simulate tearing or merging of fluid. The first ellipse is more circular (lower eccentricity) and has axis of length 0.20, 0.20, 0.35 along the x, y and z axis, respectively. The kernel used for the calculations on this ellipsoid has a radius of support of 0.125. This ellipsoid is shown in Figures



(a) 7454 cells



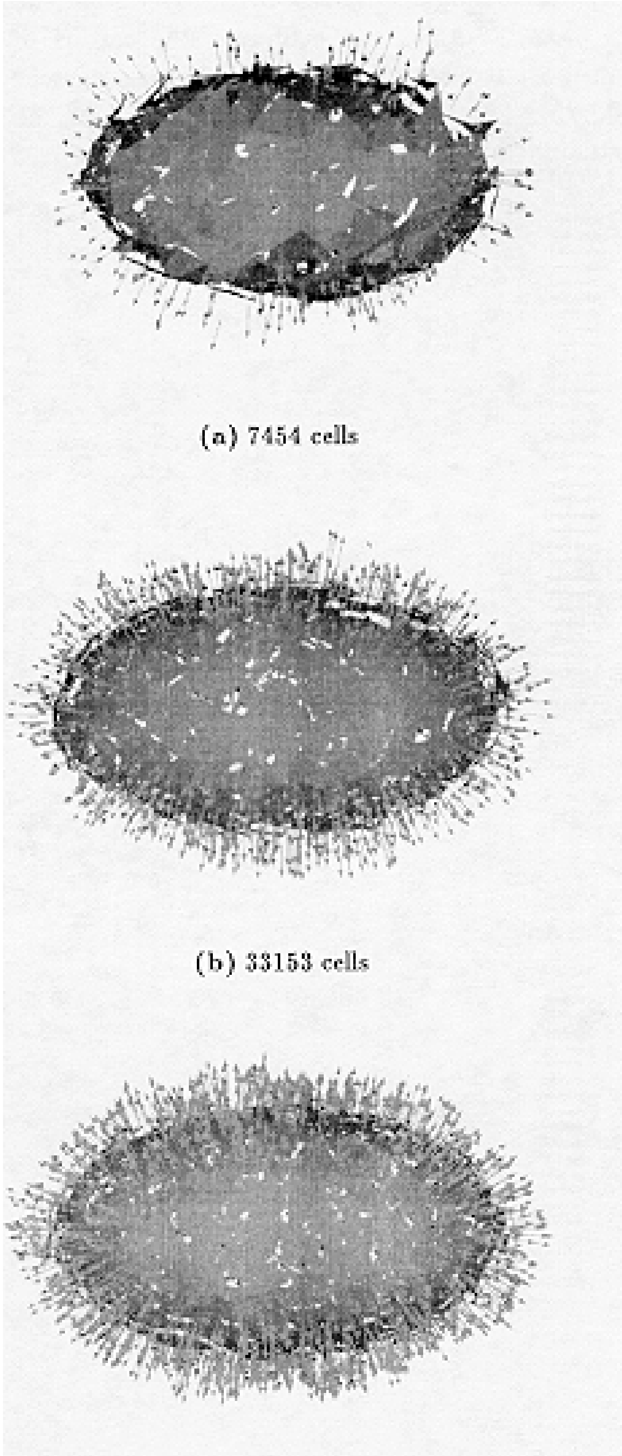
(b) 33153 cells



(c) 65590 cells

Figure 1: Cutplane at $x = 0.5$ for three different unstructured tetrahedral meshes of increasing resolution.

2 and 4. The second ellipse is more slender, with axis lengths of 0.15, 0.15, 0.40 along the x y and z axis respectively. The radius of support for kernel in these calculations was 0.075. This ellipsoid and the results of the calculations are seen in Figures 3 and 5.

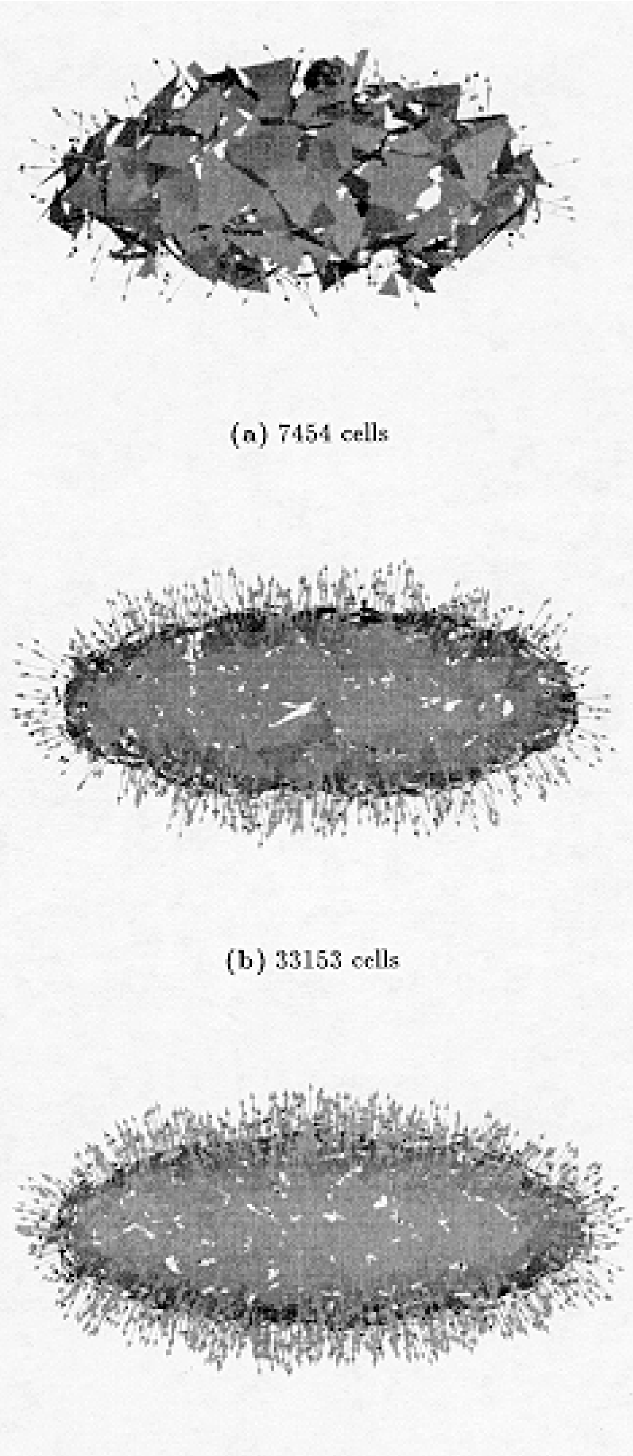


(a) 7454 cells

(b) 33153 cells

(c) 65590 cells

Figure 2: Piecewise planar reconstructed interface for an ellipsiod on unstructured tetrahedron meshes. Ellipsoid axis are of lengths 0.20, 0.20, 0.35.

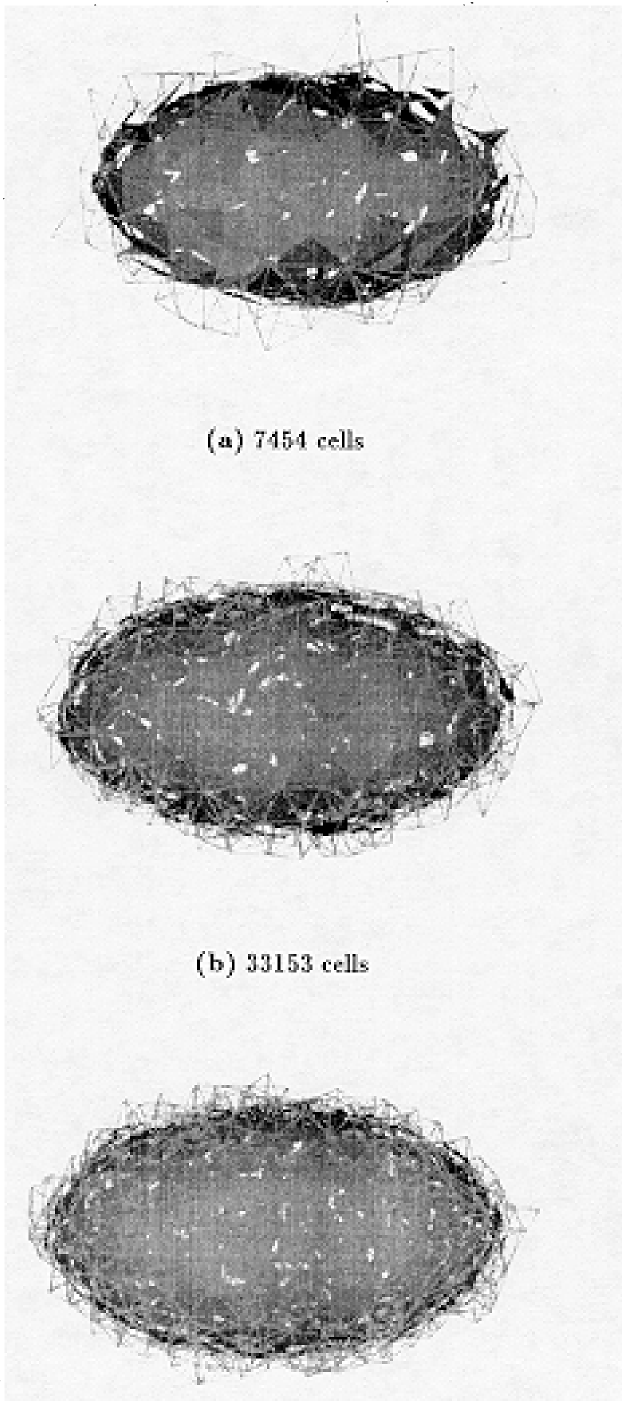


(a) 7454 cells

(b) 33153 cells

(c) 65590 cells

Figure 3: Piecewise planar reconstructed interface for an ellipsiod on unstructured tetrahedron meshes. Ellipsoid axis are of lengths 0.15, 0.15, 0.40.

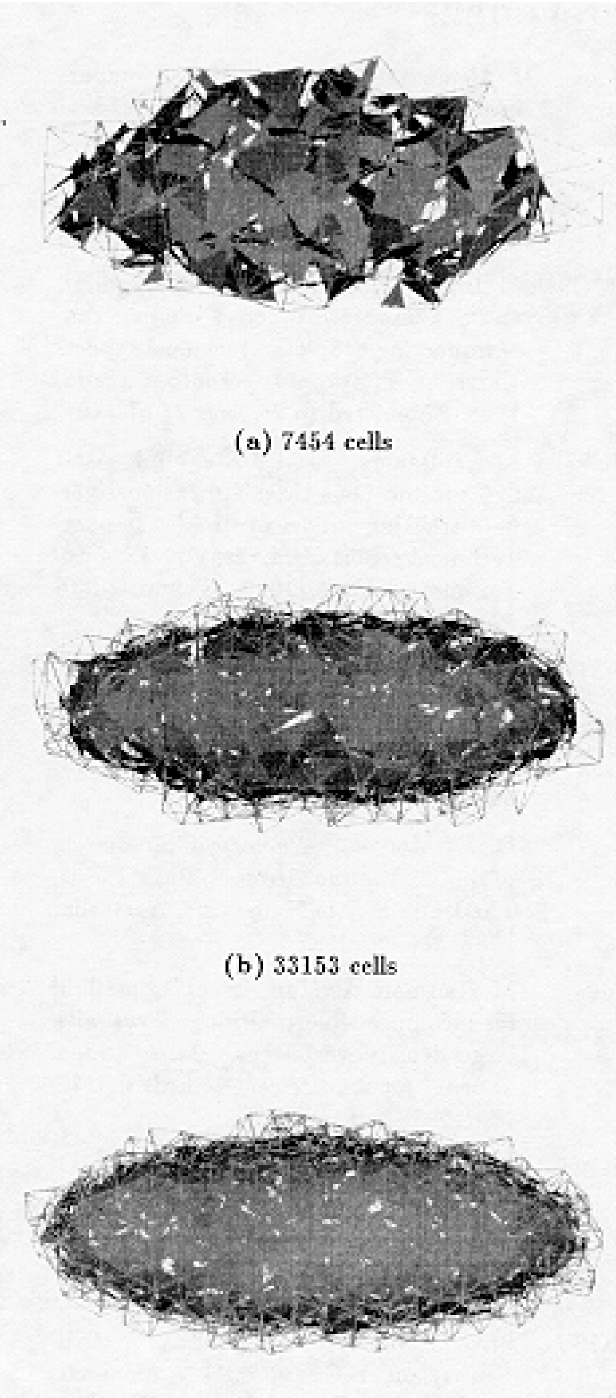


(a) 7454 cells

(b) 33153 cells

(c) 65590 cells

Figure 4: Piecewise planar reconstructed interface for an ellipsiod on unstructured tetrahedron meshes. Ellipsoid axis are of lengths 0.20, 0.20, 0.35.



(a) 7454 cells

(b) 33153 cells

(c) 65590 cells

Figure 5: Piecewise planar reconstructed interface for an ellipsiod on unstructured tetrahedron meshes. Ellipsoid axis are of lengths 0.15, 0.15, 0.40.

References

[AP95] I. Aleinov and E. G. Puckett. Computing surface tension with high-order kernels. In H. A. Dwyer, editor, *Proceedings of the Sixth International Symposium on Computational Fluid Dynamics*, pages 13–18, Lake Tahoe, NV, 1995.

[BAMC98] M. Bussman, S. D. Aziz, J. Mostaghimi, and S. Chandra. Modeling the fingering of impacting droplets. Technical report, University of Toronto, Toronto, Canada, 1998. Submitted to *Physics of Fluids*.

[BMC97] M. Bussman, J. Mostaghimi, and S. Chandra. On a three-dimensional volume tracking model of droplet impact. Technical report, University of Toronto, Toronto, Canada, 1997. Submitted to *Physics of Fluids*.

[Mor97a] J. P. Morris. Simulating surface tension with smoothed particle hydrodynamics. *International Journal for Numerical Methods in Fluids*, 1997. Submitted.

[Mor97b] D. E. Morton. *Numerical Simulation of an Impacting Drop*. PhD thesis, The University of Melbourne, Australia, 1997.

[Rud98] M. Rudman. A volume-tracking method for incompressible multifluid flows with large density variations. *International Journal for Numerical Methods in Fluids*, 1998. In Press.

[WKP99] M. Williams, D.B. Kothe, and E.G. Puckett. Convergence and accuracy of continuum surface tension models. In Wei Shyy, editor, *Fluid Dynamics at Interfaces*. Cambridge Univ. Press, 1999.

[WKP2] M. Williams, D.B. Kothe, and E.G. Puckett. Appoximating Interface Topologies with Applications for Interface Tracking Algorithms. 37th AIAA Aerospace Sciences Meeting and Exhibit, Reno NV, 1990