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Analysis and applications of the Voronoi Implicit Interface Method

R.I. Saye, J.A. Sethian *

Department of Mathematics and Lawrence Berkeley National Laboratory, University of California, Berkeley, Berkeley, CA 94720, United States

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ABSTRACT

We analyze a new mathematical and numerical framework, the "Voronoi Implicit Interface Method" ("VIIM"), first introduced in Saye and Sethian (2011) [R.I. Saye, J.A. Sethian, The Voronoi Implicit Interface Method for computing multiphase physics, PNAS 108 (49) (2011) 19498–19503] for tracking multiple interacting and evolving regions ("phases") whose motion is determined by complex physics (fluids, mechanics, elasticity, etc.). From a mathematical point of view, the method provides a theoretical framework for moving interface problems that involve multiple junctions, defining the motion as the formal limit of a sequence of related problems. Discretizing this theoretical framework provides a numerical methodolology which automatically handles multiple junctions, triple points and quadruple points in two dimensions, as well as triple lines, etc. in higher dimensions. Topological changes in the system occur naturally, with no surgery required. In this paper, we present the method in detail, and demonstrate several new extensions of the method to different physical phenomena, including curvature flow with surface energy densities defined on a per-phase basis, as well as multiphase fluid flow in which density, viscosity and surface tension can be defined on a per-phase basis.

We test this method in a variety of ways. We perform rigorous analysis and demonstrate convergence in both two and three dimensions for a variety of evolving interface problems, including verification of von Neumann–Mullins' law in two dimensions (and its analog in three dimensions), as well as normal driven flow and curvature flow with and without constraints, demonstrating topological change and the effects of different boundary conditions. We couple the method to a second order projection method solver for incompressible fluid flow, and study the effects of membrane permeability and impermeability, large shearing torsional forces, and the effects of varying density, viscosity and surface tension on a per-phase basis. Finally, we demonstrate convergence in both space and time of a topological change in a multiphase foam.

1. Introduction

Many scientific and engineering problems are characterized by a large number of different regions that touch in many different configurations, and whose interaction depends on local geometries, complex physics, intricate jump conditions, and other associated boundary conditions and constraints. Examples include the motion of foams, crystal grain growth, and multicellular structures in man-made and biological materials, as well as mathematical problems, such as geometric motion, domain decomposition and surface area minimization problems.

There are a host of mathematical and computational challenges associated with computing the solutions to these problems. Often, the physics, chemistry, and mechanics that drive the interface motion are complex, requiring the solution of

* Corresponding author.
E-mail address: sethian@math.berkeley.edu (J.A. Sethian).

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fluid mechanical equations with specified jumps, elasticity solvers with different properties in each membrane, as well as diffusion and transport effects of species both within and across the region boundaries, etc. It is challenging to construct good and well-posed mathematical models that adequately describe the fundamental forces. At the same time, formulating a consistent mathematical model and numerical methodology for the interface motion itself can be daunting, especially in the presence of multi-junction points (triple points, quadruple points, etc.) in two dimensions and analogous structures in three dimensions, including triple lines where multiple surfaces meet, etc.

1.1. Mathematical formulations

From a mathematical perspective, formulating a consistent model is a significant part of the challenge. In general, the motion of triple points in two dimensions and triple lines in three dimensions (as well as objects with higher degrees of connectedness) must be specified, either explicitly or implicitly through requirements on the curves (in 2D) and surfaces (in 3D) that connect them. As examples of how such motion may be specified for a purely geometric motion given by curvature flow in two dimensions:

- One option might be to employ curvature flow on each interface, with the additional requirement that triple points remain fixed in time: in this case, the equilibrium solution is a network of straight lines.
- Another option might allow triple points to move in order to minimize the total length of the network of two dimensional curves connecting the triple points: this motion would satisfy Young's law for triple point angles. (In the simplest scenario, Young's law states that triple points make 120° angles.) This case is of physical relevance, since various physical situations demonstrate triple point angle conditions, including crystal grain growth and soap bubble foams. In this situation, generally speaking, quadruple points are unstable: they will quickly destabilize into two nearby triple points.
- A third option might be to disallow triple points and only allow quadruple points: this could lead to an equilibrium solution that resembles a quadrilateral mesh.

In this work, we concentrate mainly on the case relevant to many physical problems in which triple points are allowed to move, often satisfying certain triple point angle conditions that naturally arise from the type of physics being considered. This will carry over to three-dimensional analogs with no change to the fundamental formulation.

1.2. Numerical formulations

From a numerical perspective, we want a stable method that correctly includes the prescribed motion at triple points, correctly represents moving-interface boundary conditions and associated physics, performs efficiently and accurately, and handles rapid changes in topology and structure.

A variety of numerical methods have been proposed to track the evolution of these multiphase problems. Somewhat broadly, major approaches include:

- *Front tracking methods*: Here, the interface is explicitly represented with a Lagrangian geometric representation, typically taken as connected line segments in two dimensions and triangles in three dimensions (see, for example, [7,6,13]). Junctions (e.g. triple points) have shared nodes, and the positions of the elements making up the front are updated in time. In these methods, an explicit surgery mechanism for topological change is required, which may be challenging in three dimensions due to a range of possible types of topology change. For multiphase systems, Young's law, which determines the angles in a triple point, is explicitly assumed and enforced as a boundary condition.
- *Volume of fluid methods*: Here, each phase/region is described by a characteristic function, which has a value of one inside the phase and zero outside [18]. In discrete form, these become volume fractions on a mesh, in which multiple phases can occupy the same cell, with respective volume fractions adding up to one. The values of these fractions inside the cells are updated according to local reconstruction algorithms based on neighboring cell values. Junctions correspond to mixed regions with more than two phases in a cell [4,8].
- *Level set methods*: Level set methods, introduced by Osher and Sethian [19], embed the interface as the zero level set of an implicitly defined signed distance function, and rely in part on the theory of curve and surface evolution given in [24] and on the link between front propagation and hyperbolic conservation laws discussed in [25]. Level set methods recast interface motion as a time-dependent Eulerian initial value partial differential equation, and use viscosity solutions of the appropriate differential equations to update the position of the front, using an interface velocity that is derived from the relevant physics both on and off the interface. Topological change is handled as a straightforward part of the implicit embedding, and geometric quantities such as normal directions and curvature are naturally calculated. The appropriate viscosity solutions are obtained by exploiting schemes from the numerical solution of hyperbolic conservation laws to build appropriate finite difference and finite element approximations, and the underlying level set methods are made computationally efficient through the use of adaptive narrow banding, see [1]. For a general review, see [27].

  The extension of these methods to multiphase systems typically involves using multiple level set functions, one for each phase/region (or some other encoding scheme): the first such method was introduced in [17]. These different