Journal of Computational Physics 270 (2014) 203–213

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

A conservative algorithm for parabolic problems in domains with moving boundaries

Igor L. Novak, Boris M. Slepchenko *

Richard D. Berlin Center for Cell Analysis and Modeling, Department of Cell Biology, University of Connecticut Health Center, 263 Farmington Avenue, Farmington, CT 06030, United States

ARTICLE INFO

Article history:
Received 18 July 2013
Received in revised form 28 January 2014
Accepted 13 March 2014
Available online 20 March 2014

Keywords:
Numerical algorithm
Moving boundaries
Parabolic equations
Exact mass conservation
Cell migration

ABSTRACT

We describe a novel conservative algorithm for parabolic problems in domains with moving boundaries developed for modeling in cell biology. The spatial discretization is accomplished by applying Voronoi decomposition to a fixed rectangular grid. In the vicinity of the boundary, the procedure generates irregular Voronoi cells that conform to the domain shape and merge seamlessly with regular control volumes in the domain interior. Consequently, our algorithm is free of the CFL stability issue due to moving interfaces and does not involve cell-merging or mass redistribution. Local mass conservation is ensured by finite-volume discretization and natural-neighbor interpolation. Numerical experiments with two-dimensional geometries demonstrate exact mass conservation and indicate an order of convergence in space between one and two. The use of standard meshing techniques makes extension of the method to three dimensions conceptually straightforward.

Published by Elsevier Inc.

1. Introduction

In this paper, we describe a fully conservative algorithm for solving parabolic problems in domains with moving boundaries. The work was motivated by the need to develop a capability of modeling cell migration within the Virtual Cell (VCell), a computational framework for simulating cellular phenomena in realistic geometries [1–5].

Mechanisms underlying dynamical changes of cell shape and cell migration have long been of interest to cell biologists and biophysicists [6,7]. Mathematical models of varying degree of complexity have been proposed [8–17], and a recently released computer program called 'Cytopede' was specifically designed for modeling mechanical and signaling behaviors of plated cells [18]. Implementation of numerical algorithms, required for the modeling of dynamic cell shape and cell migration, within a general-purpose computational framework will further facilitate research in this area.

Numerical methods for solving systems with time-dependent discontinuities constitute an area of active research in applied mathematics and computational physics. They involve particular techniques for tracking boundaries and are often classified as Lagrangian and Eulerian, depending on whether the spatial grids are moving or stationary [19]. The interface-tracking techniques used in Lagrangian methods treat dynamic discontinuities as explicit sharp interfaces. The moving grids, constructed so that they fit the boundary, are recomputed each time the surface is updated [20]. This type of approach is used in the Cytopede code [18] that simulates shape changes of fibroblasts cultured on flat surfaces. In Eulerian methods,

* Corresponding author. Tel.: +1 860 679 4025; fax: +1 860 679 1039.
E-mail address: boris@neuron.uchc.edu (B.M. Slepchenko).

http://dx.doi.org/10.1016/j.jcp.2014.03.014
0021-9991/Published by Elsevier Inc.

computations are performed on fixed grids, often based on structured meshes. These methods usually employ interface-capturing techniques in which the shape of the surface is defined implicitly. One class of interface-capturing techniques is level-set methods [21], in which the surface is determined by a zero level of an auxiliary volumetric scalar field.

There are also hybrid methods, in which an Eulerian approach to solving a governing equation is combined with a particular method of tracking or capturing the moving interface [22–26]. These methods are attractive as they avoid complexities of maintaining moving grids, which is particularly challenging in three dimensions, and have the advantages of using regular volumetric grids. Combining the Eulerian approach with interface-tracking techniques allows one to define explicit grids on the surface that are beneficial for cell-biological applications which often include membrane-bound molecules. However, exact mass conservation, another extremely valuable feature for applications in cell biology, becomes an issue in the hybrid methods, because the conservative discretization of equations subjected to boundary conditions at interfaces moving with respect to a fixed grid is nontrivial [23].

The conservative formulations of hyperbolic problems in domains with moving boundaries [23,25] interpret the intersection of the Cartesian cells with the regions on either side of a moving front as a collection of time-dependent control volumes, over which the conservation law is integrated in space–time to derive a finite-volume discretization. The presence of arbitrary small control volumes in this approach leads to a Courant–Friedrich–Lewy (CFL) stability issue, which is resolved differently by different methods.

In an algorithm proposed by Glimm and co-workers [23], the CFL singularities are resolved through merging the small control volumes with adjacent cells [27]. The method works in conjunction with robust front-tracking methods implemented in FronTier [28], a publicly available C++ library for accurate tracking of moving interfaces both in two (2D) and three dimensions (3D). A similar approach was used by Udaykumar and coworkers [29,30] in applications to solidification and fluid dynamics problems. Cell-merging, however, while well-defined in one and two dimensions, may not be straightforward to apply to 3D problems.

In the embedded boundary methods [24] based on the Volume-of-Fluid front-capturing techniques [31], cell-merging is avoided by performing two updates, a conservative update and a nonconservative, but CFL stable, update. The difference between the two updates is then redistributed to neighboring computational cells to maintain overall stability and local conservation. Recent improvements to the method have been shown to yield second-order accuracy in one dimension [25]. While the redistribution of mass is simpler to apply in multiple dimensions, maintaining the second-order accuracy of the method in 2D and 3D is a challenging problem.

In a recently published hybrid algorithm [26], specifically designed for applications to cell biology, the contour of a moving cell is captured by a level-set technique. Still, the algorithm constructs and maintains the grid on the contour by projecting nearby rectangular grid points onto the interface at each integration time step. The method employs finite-volume discretization with the grid becoming unstructured near the membrane. Because of non-conservative interpolation of displaced grid points, the method does not conserve mass locally, but global mass conservation is enforced on the assumption that the total mass inside the domain is known in advance.

This paper is focused on the description of a fully conservative discretization scheme for parabolic (diffusion–advection–reaction) equations with Rankine–Hugoniot boundary conditions imposed at moving interfaces. For simplicity, we defer the discussion of the front-tracking technique and assume that the position of a moving piecewise-linear interface is known at any time.

In our algorithm, spatial discretization is based on Voronoi decomposition [32] applied to a fixed set of regularly spaced gridpoints. Voronoi meshes were used previously in modeling cell migration by Bottino et al. [33] and in our algorithm for modeling diffusion on a surface coupled to diffusion in embedding volume [3]. Utilizing this meshing technique for purposes of the algorithm described in this article has a number of practical advantages. Voronoi polygons are well suited for conservative finite volume discretization. The procedure automatically generates control volumes of comparable sizes, and the CFL stability issue due to crossings of a moving front with the mesh does not arise. Thus, there is no need in our method to adjust positions of the grid points, nor it requires cell-merging or redistributing mass between control volumes. While the control volumes adjacent to a moving interface conform to the shape of the domain and are therefore irregular, they merge seamlessly with regular Voronoi cells in the interior of the domain. In fact, the procedure of Voronoi decomposition needs to be applied only to the gridpoints in the vicinity of the interface. Finally, the use of the standard meshing technique makes extension of the method to three dimensions conceptually straightforward.

Fully conservative formulation is achieved through finite-volume discretization and natural-neighbor interpolation [34] (interpolation is required to reinitialize unknowns at the nodes crossed by a propagating front and at their neighbors). The formulae of the natural-neighbor interpolation are derived from the requirement that mass be not relocated when boundaries between Voronoi cells are redrawn, thus preserving local mass conservation. Test cases with two-dimensional geometries demonstrate exact mass conservation and indicate an order of convergence of the error between 1 and 2.

2. Mathematical problem

Consider a system defined in a spatial domain $\Omega(t) \in R^n$ (n is the dimensionality of the space) whose boundary $\partial\Omega(t)$ changes with time. The system is governed by the continuity (mass conservation) equation,

$$\frac{\partial u}{\partial t} = -\operatorname{div}\mathbf{J} + R, \tag{1}$$