Journal of Computational and Applied Mathematics 258 (2014) 78–86

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

An optimization-based approach to enforcing mass conservation in level set methods

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A R T I C L E I N F O

Article history:
Received 10 October 2012
Received in revised form 8 July 2013

Keywords:
Transport equations
Evolving interfaces
Level set methods
Finite elements
Mass conservation
PDE-constrained optimization

A B S T R A C T

This paper presents a new conservative level set method for numerical simulation of evolving interfaces. A PDE-constrained optimization problem is formulated and solved in an iterative fashion. The proposed optimal control procedure constrains the level set function to satisfy a conservation law for the corresponding Heaviside function. The target value of the state variable is defined as the solution to the standard level set transport equation. The gradient of the control variable corrects the convective flux in the nonlinear state equation so as to enforce mass conservation while minimizing deviations from the target state. A relaxation term is added when it comes to the design of an iterative solver for the nonlinear system. The potential of the optimization-based approach is illustrated by two numerical examples.

1. Introduction

Many problems in science in engineering are characterized by the presence of evolving interfaces that divide the domain of interest into two or more time-dependent subdomains. One of the most popular approaches to numerical solution of such free boundary problems is the *level set method* which traces its origins to the work of Dervieux and Thomasset [1,2] and Osher and Sethian [3]. The crux of the level set formulation is an implicit representation of the interface as the zero level set of an auxiliary function whose evolution is governed by a scalar transport equation [4–6]. The reasons for the popularity of this interface capturing technique include simplicity of interface reconstruction and straightforward definition of normals and curvatures. However, the level set method is generally nonconservative and may fail to preserve the total mass/volume in applications to immiscible incompressible fluids [7–9].

The ongoing quest for a conservative level set algorithm has produced a large number of publications in which various improvements to the original formulation are proposed. As shown by Smolianski [9], global mass conservation can readily be enforced by adding a constant to the convected level set function. Obviously, there is a danger that the mass lost in one place might reappear in another place. If one fluid consists of multiple disconnected components, global mass correction does not guarantee that the mass/volume of each component is conserved. In the method developed by Lesage et al. [8], the correction to the level set function is proportional to the residual of a *dual level set* equation. If the local conservation principle holds in the neighborhood of a mesh vertex, then the corresponding nodal value of the level set function remains unchanged. However, some nonphysical mass exchange between the remaining nodes may still occur since the weights are defined using a global constant.

Another popular approach to improving mass conservation properties of level set methods involves solving a continuity equation for the volume fraction of one phase. Hybrid algorithms based on this idea include the coupled level set and volume-of-fluid (CLSVOF) method of Sussman and Puckett [10,11], the mass-conserving level set (MCLS) formulation of

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0377-0427/$ – see front matter © 2013 Published by Elsevier B.V.
http://dx.doi.org/10.1016/j.cam.2013.09.009

van der Pijl et al. [12], and the variational mass correction technique of Kees et al. [7]. The conservative level set method of Olsson and Kreiss [13,14] operates directly with a regularized characteristic function and can be classified as a *diffuse interface* method.

In this paper, we use PDE-constrained optimization tools (cf. [15–19]) to enforce mass conservation. The regularized Heaviside function is treated as a derived quantity which must satisfy a conservation law written in terms of the level set function (*state variable*) and an adjustable flux potential (*control variable*). The objective function is defined so as to minimize the difference between the conservative and nonconservative approximations. The reasons that speak in favor of the optimization-based approach are twofold. In contrast to global mass correction methods, the lost mass reappears in the region of its origin, and a local conservation principle is guaranteed to hold at the discrete level. Moreover, the corresponding PDE constraint is formulated without resorting to VOF-based reconstructions of Heaviside functions which could distort the interface and/or produce mass conservation errors. This is the main difference compared to the method developed by Kees et al. [7].

After presenting the basic (nonconservative) level set algorithm and formulating the PDE-constrained optimization problem, we describe the iterative solution strategy and relevant implementation details. The paper concludes with a preliminary numerical study of mass conservation properties for solid body rotation of a circle and a slotted disc. This research was motivated by applications to two-phase fluid dynamics but the proposed mass correction technique is readily applicable to any kind of evolving interfaces since it is independent of the way in which the velocity field is defined and calculated.

2. The level set algorithm

Consider a free interface Γ evolving inside a bounded domain Ω. The outer boundary of Ω is denoted by $\partial\Omega$. In level set methods [4–6], the shape of Γ is implicitly defined by a scalar indicator function $\phi(\mathbf{x}, t)$ such that

$$\Gamma(\phi) = \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) = 0\}. \tag{1}$$

In applications to two-phase fluid dynamics, the convective transport of ϕ by a given velocity field $\mathbf{v}$ is described by the hyperbolic equation

$$\frac{\partial \phi}{\partial t} + \mathbf{v} \cdot \nabla\phi = 0 \quad \text{in } \Omega. \tag{2}$$

It is common practice to initialize ϕ by the signed distance function (SDF)

$$\phi(\mathbf{x}, 0) = \pm\,\mathrm{dist}(\mathbf{x}, \Gamma_0). \tag{3}$$

Since the SDF property is generally lost as time evolves, the solution to (2) is commonly reinitialized to become a SDF after a certain number of time steps. This task can be accomplished using geometric redistancing [20,9] or PDE-based reinitialization techniques [21–23]. Regardless of what approach is adopted, it is essential to guarantee that the employed post-processing technique does not displace the interface. In our recent publication [21], we present a new minimization-based interface-preserving reinitialization procedure. This methodology builds on ideas introduced by Li et al. [24] in the context of distance regularized level set evolution (DRLSE) for image segmentation.

3. Conservation laws

If the interface separates two incompressible fluids, the piecewise-constant density ρ is defined in terms of the level set function ϕ as follows:

$$\rho(\mathbf{x}, t) = (\rho_1 - \rho_2)H(\mathbf{x}, t) + \rho_2, \tag{4}$$

where $H : \Omega \times [0, \infty) \mapsto \mathbb{R}$ is the Heaviside function

$$H(\mathbf{x}, t) = \begin{cases} 1 & \text{if } \phi(\mathbf{x}, t) > 0, \\ 0 & \text{if } \phi(\mathbf{x}, t) < 0. \end{cases} \tag{5}$$

The total mass contained in $\Omega_1(t) := \{\mathbf{x} \in \Omega \mid \phi(\mathbf{x}, t) > 0\}$ is given by [7]

$$m_1(t) = \int_{\Omega_1(t)} \rho_1 \,\mathrm{d}\mathbf{x} = \int_\Omega \rho H \,\mathrm{d}\mathbf{x}. \tag{6}$$

The differential form of the integral conservation law $\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho \,\mathrm{d}\mathbf{x} = 0$ reads

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho\mathbf{v}) = 0 \quad \text{in } \Omega \tag{7}$$

or, equivalently,

$$\frac{\partial H}{\partial t} + \nabla \cdot (H\mathbf{v}) = 0 \quad \text{in } \Omega, \tag{8}$$

where the partial derivatives are defined in the sense of distributions.