Journal of Computational and Applied Mathematics 270 (2014) 343–352

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

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

Optimal control for mass conservative level set methods

Christopher Basting *, Dmitri Kuzmin

Department of Mathematics, LS III, Dortmund University of Technology, Vogelpothsweg 87, D-44227 Dortmund, Germany

ARTICLE INFO

Article history:
Received 27 September 2013
Received in revised form 17 December 2013

Keywords:
Evolving interfaces
Level set methods
Finite elements
Mass conservation
Optimal control
PDE-constrained optimization

ABSTRACT

This paper presents two different versions of an optimal control method for enforcing mass conservation in level set algorithms. The proposed PDE-constrained optimization procedure corrects a numerical solution to the level set transport equation so as to satisfy a conservation law for the corresponding Heaviside function. In the original version of this method, conservation errors are corrected by adding the gradient of a scalar control variable to the convective flux in the state equation. In the present paper, we investigate the use of vector controls. The alternative formulation offers additional flexibility and requires less regularity than the original method. The nonlinear system of first-order optimality conditions is solved using a standard fixed-point iteration. The new methodology is evaluated numerically and compared to the scalar control approach.

1. Introduction

Evolving interfaces commonly occur in two-phase fluid dynamics, image processing, and many other fields of science and technology. In a typical mathematical model, a moving boundary separates two materials with different physical properties or defines the geometry of a deformable object. The numerical solution of such problems requires an accurate localization of the interface, and a variety of algorithms have been developed for this purpose. A particularly popular interface-capturing technique is the *level set method* in which the interface is implicitly defined by the zero level set of an auxiliary function [1–3]. The evolution of the level set function is governed by a transport equation. The attractive features of the level set approach include the simplicity of interface reconstruction, as well as the straightforward definition of normals and curvatures.

It is common practice to initialize the level set function Φ by the signed distance to the interface. This approach offers further advantages such as the smoothness of Φ and its capability to serve as proximity indicator in the context of adaptive mesh refinement. In the process of convection, the signed distance function property is generally lost. This deficiency is usually rectified by using geometric redistancing procedures [4,5] or various PDE-based reinitialization techniques [3,6]. A promising new approach is the use of minimization-based redistancing [7] which leads to a nonlinear elliptic problem.

The level set method is known to be non-conservative and may fail to preserve the total mass or volume confined by the interface. Many approaches to maintaining mass conservation have been proposed in recent years. For example, Smolianski [5] shifts the convected level set function by a constant to compensate a loss or gain of mass. This manipulation may result in global non-physical displacements of the interface. The mass lost in one place might reappear in another place, and only global conservation is guaranteed for fluids consisting of multiple disconnected components.

The second author has recently proposed an optimization-based approach to enforcing mass conservation in level set methods [8]. The key idea is to constrain the level set function in such a way that a local conservation law holds for the corresponding Heaviside function. The control variable adjusts itself so that conservation of mass is enforced and deviations from the target state are minimized. The target is defined as the solution to the standard level set transport equation. This approach offers great flexibility since additional design criteria can be easily incorporated into the cost functional.

* Corresponding author. Tel.: +49 91318567227.
E-mail addresses: christopher.basting@math.fau.de (C. Basting), kuzmin@math.uni-dortmund.de (D. Kuzmin).

0377-0427/$ – see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.cam.2013.12.040

In the original optimization-based mass correction method [8], the gradient of the control is added to the convective flux. This formulation imposes stringent regularity requirements on the control. Moreover, the Schur complement operator associated with the KKT system of optimality conditions is of biharmonic type. This has led us to explore the possibility of replacing the gradient of a scalar control by a vector-valued control. Even though this increases the size of the system, the discrete saddle point problem has nicer properties. In particular, the Schur complement operator is of Laplacian type. Furthermore, milder smoothness assumptions need to be made on the control and, due to the increased dimension of the control, more flexibility can be expected.

In this paper, we review and generalize the optimal control approach to the design of conservative level set methods. Following the discretize-then-optimize approach, we present the finite element discretization before deriving the optimality conditions of first order. The nonlinear saddle point problem is solved using a linearization which is slightly different from the one employed in the original paper. In the numerical study below, we compare the PDE-constrained optimization methods based on scalar and vector-valued control, in particular regarding the number of fixed-point iterations per time step.

2. Level set method

The level set approach to simulating the evolution of a moving interface Γ inside a bounded domain Ω is based on an implicit representation of Γ in terms of a scalar indicator function $\Phi(\mathbf{x}, t)$ such that

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

The evolution of Φ is governed by the transport equation

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

where $\mathbf{v}$ is a given velocity field. In applications to two-phase fluid dynamics, $\mathbf{v}$ is usually determined by solving the incompressible Navier–Stokes equations.

The usual initial condition for Φ is given 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 again after a certain number of time steps.

For simplicity, we restrict ourselves to two-phase flow applications. Let the interface Γ separate two incompressible fluids with densities ρ_1 and ρ_2. The corresponding subdomains are denoted by $\Omega_1(t) := \{\mathbf{x} \in \Omega \mid \Phi(\mathbf{x}, t) > 0\}$ and $\Omega_2(t) = \Omega \setminus (\Omega_1(t) \cup \Gamma(t))$. To tell the fluids apart, we will use the Heaviside function $H \circ \Phi : \Omega \times [0, \infty) \to \mathbb{R}$ s.t.

$$H(\Phi(\mathbf{x}, t)) = \begin{cases} 1 & \text{if } \Phi(\mathbf{x}, t) > 0, \\ 0 & \text{if } \Phi(\mathbf{x}, t) < 0. \end{cases} \tag{4}$$

The total mass contained in Ω_1 is given by the volume integral

$$m_1(t) = \int_{\Omega_1(t)} \rho_1 \mathrm{d}\mathbf{x} = \int_{\Omega} \rho(\mathbf{x}, t) H(\Phi(\mathbf{x}, t)) \mathrm{d}\mathbf{x}, \tag{5}$$

where we have used the definition of the piecewise-constant density

$$\rho(\Phi(\mathbf{x}, t)) := (\rho_1 - \rho_2) H(\Phi(\mathbf{x}, t)) + \rho_2. \tag{6}$$

Using this formalism, the continuity equation

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

can be written in the equivalent form

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

At the continuous level, the solution to the level set equation (2) satisfies conservation laws (7) and (8). However, numerical solutions to (2) are generally non-conservative, whence the volume of the incompressible fluids may change in an unpredictable manner. Many postprocessing techniques and hybrid algorithms have been developed for improving the mass conservation properties of level set algorithms [9–15]. Our approach [8] to this problem is based on the use of PDE-constrained optimization.

3. Scalar control approach

In this section, we review the mass correction algorithm proposed in [8]. Let $H(\Phi)$ denote the Heaviside function defined by (4). Consider the modified conservation law

$$\frac{\partial H(\Phi)}{\partial t} + \nabla \cdot (H(\tilde{\Phi})\mathbf{v} - \nabla u) = 0 \quad \text{in } \Omega. \tag{9}$$