Optimal control for mass conservative level set methods

von

C. Basting & D. Kuzmin

No. 370 2013
Optimal Control for Mass Conservative Level Set Methods

Christopher Basting\textsuperscript{a}, Dmitri Kuzmin\textsuperscript{a}

\textsuperscript{a}Applied Mathematics III, University Erlangen-Nuremberg, Cauerstr. 11, 91058 Erlangen

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.

Keywords: transport equations, evolving interfaces, level set methods, finite elements, mass conservation, optimal control, PDE-constrained optimization

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. 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 \cite{14, 11, 12}. 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 \( \Phi \) by the signed distance to the interface. This approach offers further advantages such as the smoothness of \( \Phi \) 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 \cite{1, 13} or various PDE-based reinitialization techniques \cite{12, 17}. A promising new approach is the use of minimization-based redistancing \cite{2} 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 [13] 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 [7]. 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.

In the original optimization-based mass correction method [7], 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 $\Gamma$ inside a bounded domain $\Omega$ is based on an implicit representation of $\Gamma$ in terms of a scalar indicator function $\Phi(x, t)$ such that

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

The evolution of $\Phi$ is governed by the transport equation

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

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

The usual initial condition for $\Phi$ is given by the signed distance function (SDF)

$$\Phi(x, 0) = \pm \text{dist}(x, \Gamma_0).$$  \hfill (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 $\Gamma$ separate two incompressible fluids with densities $\rho_1$ and $\rho_2$. The corresponding subdomains are denoted by $\Omega_1(t) := \{ x \in \Omega \mid \Phi(x, t) > 0 \}$ and $\Omega_2(t) = \Omega \setminus (\Omega_1(t) \cup \Gamma(t))$. To tell the fluids apart, we will use the Heaviside function $H : \Phi : \Omega \times [0, \infty) \to \mathbb{R}$ s.t.

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

(4)

The total mass contained in $\Omega_1$ is given by the volume integral

$$m_1(t) = \int_{\Omega_1(t)} \rho_1 \, dx = \int_{\Omega} \rho(x, t) H(\Phi(x, t)) \, dx,$$

(5)

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

$$\rho(\Phi(x, t)) := (\rho_1 - \rho_2)H(\Phi(x, t)) + \rho_2.$$  

(6)

Using this formalism, the continuity equation

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

(7)

can be written in the equivalent form

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

(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 [6, 8, 9, 10, 15, 16, 18]. Our approach [7] 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 [7]. Let $H(\Phi)$ denote the Heaviside function defined by (4). Consider the modified conservation law

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

(9)

The gradient of the control $u$ will correct the convective flux so as to enforce conservation of mass while minimizing deviations from a non-conservative numerical solution $\tilde{\Phi}$ to the level set equation (2). One can easily show that the integral conservation law holds for any scalar $u$ satisfying the homogeneous Neumann boundary condition

$$n \cdot \nabla u = 0 \quad \text{on } \partial \Omega,$$

(10)
where \( \mathbf{n} \) denotes the outward-pointing normal to the outer boundary \( \partial \Omega \) of the domain.

Integrating by parts in the variational form of (9) and invoking (10), we obtain

\[
\int_\Omega \left[ \frac{\partial H(\Phi)}{\partial t} w + (\nabla u - H(\tilde{\Phi}) \mathbf{v}) \cdot \nabla w \right] \, d\mathbf{x} = 0, \quad \forall w,
\]

(11)

where \( w \) is an admissible test function. The surface integral containing \( H(\tilde{\Phi}) \) vanishes because we have \( \tilde{\Phi} < 0 \) on the outer boundary \( \partial \Omega \). The choice \( w \equiv 1 \) yields

\[
\frac{d}{dt} \int_\Omega H(\Phi) \, d\mathbf{x} = \frac{dm_1(t)}{dt} = 0.
\]

(12)

The optimal control problem for correcting a non-conservative approximation \( \tilde{\Phi} \) is as follows [7]: Find a pair \((\Phi, u)\) that solves (11) while minimizing the cost functional

\[
J(\Phi, u, \tilde{\Phi}) = \frac{1}{2} \| \Phi - \tilde{\Phi} \|^2_{L^2(\Omega)} + \beta \frac{1}{2} \| u \|^2_{H^1(\Omega)},
\]

(13)

where \( \beta > 0 \) is the Tikhonov regularization parameter. Since the control variable \( u \) is scalar-valued, we refer to this optimization problem as the scalar control approach.

4. Vector control approach

Let us now consider an alternative formulation in which the conservation law

\[
\frac{\partial H(\Phi)}{\partial t} + \nabla \cdot (H(\tilde{\Phi}) \mathbf{v} - \mathbf{u}) = 0
\]

(14)

incorporates a vector-valued control \( \mathbf{u} = (u_1, u_2) \) instead of \( \nabla u \). To guarantee global mass conservation, we impose the natural boundary condition

\[
\mathbf{n} \cdot \mathbf{u} = 0 \quad \text{on} \ \partial \Omega.
\]

(15)

The variational formulation of the so-defined boundary-value problem reads

\[
\int_\Omega \left[ \frac{\partial H(\Phi)}{\partial t} w + (\mathbf{u} - H(\tilde{\Phi}) \mathbf{v}) \cdot \nabla w \right] \, d\mathbf{x} = 0, \quad \forall w.
\]

(16)

Plugging \( w \equiv 1 \), we obtain the integral form (12) of the mass conservation law.

An appropriate cost functional for the proposed vector control approach is given by

\[
J(\Phi, \mathbf{u}, \tilde{\Phi}) = \frac{1}{2} \| \Phi - \tilde{\Phi} \|^2_{L^2(\Omega)} + \frac{\beta_1}{2} \| u_1 \|^2_{L^2(\Omega)} + \frac{\beta_2}{2} \| u_2 \|^2_{L^2(\Omega)},
\]

(17)

where \( \beta_1 > 0 \) and \( \beta_2 > 0 \) serve as regularization parameters. Since the vector control \( \mathbf{u} \) does not need to be differentiated in (16), less regularity is required and the Tikhonov regularization terms are defined using the \( L^2(\Omega) \) norm rather than the \( H^1(\Omega) \) norm.
5. Finite element discretization

In what follows, we adopt the discretize-then-optimize approach to PDE-constrained optimization. Let us discretize the level set equation (2) and the state equations (11), (16) in time using the standard two-level θ-scheme and a constant time step ∆t. The sequence of discrete time levels is defined by the formula \( t^n = n \Delta t \), where \( n = 0, 1, \ldots, M \).

The discretization in space is performed using linear finite elements on a triangular mesh. Let \( \varphi_i \) denote the global basis function associated with the mesh node \( x_i \). The numerical approximations to the state variable \( \Phi \) and control variable \( u \) are given by

\[
\Phi_h(x, t) = \sum_j \Phi_j(t) \varphi_j(x), \quad u_h(x, t) = \sum_k u_k(t) \varphi_k(x).
\]

The finite element discretization of the level set equation (2) can be written as

\[
M \ddot{\Phi}^{n+1} + \theta \Delta t C(v) \dot{\Phi}^{n+1} = M \Phi^n - (1 - \theta) \Delta t C(v) \Phi^n.
\] (18)

The mass matrix \( M \) and the discrete transport operator \( C(v) \) are defined by

\[
m_{ij} = \int_{\Omega} \varphi_i \varphi_j \, dx, \quad c_{ik}(v) = \int_{\Omega} \varphi_i v \cdot \nabla \varphi_k \, dx.
\]

The discrete form of the state equation (11) with \( \Delta t \) absorbed into \( u \) reads [7]

\[
g(\Phi^{n+1}) + S u^{n+1} = g(\Phi^n) + \theta \Delta t f(\dot{\Phi}^{n+1}) + (1 - \theta) \Delta t f(\Phi^n),
\] (19)

where \( S \) is the discrete Laplacian operator with entries

\[
s_{ij} = \int_{\Omega} \nabla \varphi_i \cdot \nabla \varphi_j \, dx.
\]

The components of \( f \) and \( g \) depend on \( H(\Phi_h) \) as follows:

\[
f_i(\Phi) = \int_{\Omega} H(\Phi_h) v \cdot \nabla \varphi_i \, dx = \int_{\Omega} v \cdot \nabla \varphi_i \, dx,
\]

\[
g_i(\Phi) = \int_{\Omega} H(\Phi_h) \varphi_i \, dx = \int_{\Omega} \varphi_i \, dx.
\]

In the vector control version, the discretization of (16) leads to

\[
g(\Phi^{n+1}) + C_1 u_1^{n+1} + C_2 u_2^{n+1} = g(\Phi^n) + \theta \Delta t f(\dot{\Phi}^{n+1}) + (1 - \theta) \Delta t f(\Phi^n),
\] (20)

where the skew-symmetric matrices \( C_1 \) and \( C_2 \) with entries

\[
c_{1,ij} = \int_{\Omega} \frac{\partial \varphi_i}{\partial x} \varphi_j \, dx, \quad c_{2,ij} = \int_{\Omega} \frac{\partial \varphi_i}{\partial y} \varphi_j \, dx
\]

represent the two components of the discrete divergence operator applied to \( u \).
At each time step, the vector control for the level set evolution equation is implemented using the following predictor-corrector algorithm (cf. [7]):

1. Calculate the non-conservative approximation \( \Phi^{n+1}_h \) by solving (18).
2. Find \( (\Phi^{n+1}_h, u^{n+1}_h, \tilde{\Phi}^{n+1}_h) \) minimizing \( J(\Phi^{n+1}_h, u^{n+1}_h, \tilde{\Phi}^{n+1}_h) \) subject to (20).

Following the proof of the discrete conservation property for the scalar control approach [7], it is easy to verify that the discrete counterpart of (12) holds:

\[
\int_{\Omega} [H(\Phi^{n+1}) - H(\Phi^n)] d\mathbf{x} = \sum_i [g_i(\Phi^{n+1}) - g_i(\Phi^n)] = \theta \Delta t \sum_i f_i(\tilde{\Phi}^{n+1}) + (1 - \theta) \Delta t \sum_i (c_{1,i}u_{1,k} + c_{2,i}u_{2,k}) = 0, \tag{21}
\]

where the partition of unity property \( \sum_i \varphi_i = 1 \) of the basis functions \( \varphi_i \) was exploited.

6. Optimality conditions for the scalar control approach

Now that the problem is discretized, we can derive the first-order optimality conditions. Let the residual of the discrete state equation (19) be denoted by

\[
q(\Phi, u, \tilde{\Phi}) = g(\Phi) - g(\Phi^n) + Su - [\theta \Delta t f(\tilde{\Phi}) + (1 - \theta) \Delta t f(\Phi^n)].
\]

For the discrete scalar control problem, the Lagrangian is given by

\[
\mathcal{L}(\Phi, u, p) = \frac{1}{2} \Phi^T M \Phi - \Phi^T M \tilde{\Phi} + \frac{1}{2} \tilde{\Phi}^T M \Phi + \frac{\beta}{2} u^T (M + S) u + p^T q(\Phi, u, \tilde{\Phi}),
\]

where \( p \) is the vector of Lagrange multipliers. To obtain the KKT conditions for the discrete optimization problem, \( \mathcal{L}(\Phi, u, p) \) is differentiated w.r.t. \( \Phi, u, \) and \( p \). This gives

\[
M \Phi^{n+1} + K(\Phi^{n+1}) p^{n+1} = M \tilde{\Phi}^{n+1}, \tag{22}
\]

\[
\beta (M + S) u^{n+1} + S p^{n+1} = 0, \tag{23}
\]

\[
q(\Phi^{n+1}, u^{n+1}, \tilde{\Phi}^{n+1}) = 0, \tag{24}
\]

where \( K(\Phi) \) is a weighted mass matrix defined by

\[
k_{ij}(\Phi) = \int_{\Omega} \varphi_i \varphi_j H'(\Phi_h) d\mathbf{x}.
\]

Note that \( H'(\Phi_h) = \delta(\Phi_h) \) is the Dirac delta function that picks out the interface \( \Gamma \) converting a volume integral into a surface integral. As shown in [5, 11], we have

\[
\int_{\Omega} \varphi_i \varphi_j \delta(\Phi_h) |\nabla \Phi_h| d\mathbf{x} = \int_{\Gamma(\Phi_h)} \varphi_i \varphi_j d\mathbf{x}.
\]

For a distance function \( \Phi_h \) satisfying the Eikonal equation

\[
|\nabla \Phi_h| = 1, \tag{25}
\]
the formula for \( k_{ij}(\Phi) \) simplifies to

\[
k_{ij}(\Phi) = \int_{\Gamma(\Phi_h)} \varphi_i \varphi_j \, dx.
\] (26)

In our numerical studies, we calculate the entries of \( K \) using this simplification even if \( \Phi_h \) is initialized by a signed distance function but never reinitialized.

We remark that the above approach to assembly of \( K \) is different from the one presented in [7]. Instead of using special numerical quadrature formulas to integrate a regularized Heaviside function, we calculate the entries of \( K \) by integrating products of basis functions over the zero level set of \( \Phi_h \). Using linear elements on triangles, this task can be easily accomplished by finding the triangles where the level set function changes its sign and splitting them into subcells in which \( \Phi_h \) is non-positive or non-negative.

To write \( r(\Phi, u, \tilde{\Phi}) \) as a matrix-vector product, we linearize \( g(\Phi) \) as follows:

\[
g(\Phi) \approx K(\Phi) \Phi.
\]

The nonlinear system (22)–(24) is solved using a fixed-point iteration method:

1. Set \((\Phi^{(0)}, u^{(0)}, p^{(0)}) := (\tilde{\Phi}, 0, 0) \) and \( m := 1 \).
2. Assemble the residual vector

\[
\begin{bmatrix}
    r_{\Phi}^{(m-1)} \\
    r_{u}^{(m-1)} \\
    r_{p}^{(m-1)}
\end{bmatrix} =
\begin{bmatrix}
    M(\tilde{\Phi}^{(n+1)} - \Phi^{(m-1)}) - K(\Phi^{(m-1)})p^{(m-1)} \\
    -\beta(M + S)u^{(m-1)} - Sp^{(m-1)} \\
    -q(\Phi^{(m-1)}, u^{(m-1)}, \tilde{\Phi}^{(n+1)})
\end{bmatrix}.
\]

3. If the norm of the residual is smaller than a prescribed tolerance, stop.
4. Update the approximate solution:

\[
\begin{bmatrix}
    \Phi^{(m)} \\
    u^{(m)} \\
    p^{(m)}
\end{bmatrix} =
\begin{bmatrix}
    \Phi^{(m-1)} \\
    u^{(m-1)} \\
    p^{(m-1)}
\end{bmatrix} + A^{-1}
\begin{bmatrix}
    r_{\Phi}^{(m-1)} \\
    r_{u}^{(m-1)} \\
    r_{p}^{(m-1)}
\end{bmatrix}
\]

using the preconditioner

\[
A :=
\begin{bmatrix}
    M & 0 & K(\Phi^{(m-1)}) \\
    0 & \beta(M + S) & S \\
    K(\Phi^{(m-1)}) & S & 0
\end{bmatrix}.
\]

5. Increase \( m \) by 1 and go to step 2.

Clearly, the ‘inversion’ of \( A \) in step 4 is performed by solving the linear system

\[
A \begin{bmatrix}
    \delta \Phi^{(m)} \\
    \delta u^{(m)} \\
    \delta p^{(m)}
\end{bmatrix} =
\begin{bmatrix}
    r_{\Phi}^{(m-1)} \\
    r_{u}^{(m-1)} \\
    r_{p}^{(m-1)}
\end{bmatrix}.
\]

As long as some entries of \( K = K(\Phi^{(m-1)}) \) are nonzero, we can show that this problem has a unique solution. On the one hand, the block-diagonal matrix \( A \) defined by

\[
A :=
\begin{bmatrix}
    M & 0 & 0 \\
    0 & \beta(M + S)
\end{bmatrix}
\]
is positive-definite by definition and, therefore, \( \ker(A) = \{0\} \). On the other hand, the stiffness matrix \( S \) is symmetric positive semi-definite and \( \ker(S) = \text{span}(1, 1, \ldots, 1)^\top \).

In order to prove that \( A \) is non-singular, it remains to show that the matrix block
\[
B := [K S]^\top
\]
is full rank (see, for example, Theorem 3.2 in [3]). The entries of \( K \) are all non-negative and, by assumption, some of them are strictly positive. It follows that
\[
\ker(B) = \ker(K) \cap \ker(S) = \{0\}.
\]
Let \( n \) denote the number of rows and columns of the square matrices \( M, S \) and \( K \). Since the dimensions of the kernel and image of \( B \) are related by the formula
\[
\dim \ker(B) + \dim \im(B) = n,
\]
we conclude that \( B \) is full rank and, therefore, the system matrix \( A \) is non-singular.

Note that the all-at-once preconditioner \( A \) is slightly different from the one employed in [7], where the matrix block \( K \) in the bottom left corner of \( A \) was replaced by a multiple of the mass matrix \( M \) to perform pseudo-time relaxation for the state equation.

7. Optimality conditions for the vector control approach

In the vector control version, the residual of the discrete state equation (20) is given by
\[
q(\Phi, u_1, u_2, \tilde{\Phi}) = g(\Phi) - g(\Phi^n) + C_1 u_1 + C_2 u_2 - [\theta \Delta t f(\tilde{\Phi}) + (1 - \theta) \Delta t f(\Phi^n)]
\]
and the Lagrangian associated with the discrete optimization problem becomes
\[
\mathcal{L}(\Phi, u_1, u_2, p) = \frac{1}{2} \Phi^\top M \Phi - \Phi^\top M \tilde{\Phi} + \frac{1}{2} \tilde{\Phi}^\top M \tilde{\Phi} + \frac{\beta}{2} (u_1^\top M u_1 + u_2^\top M u_2) + p^\top q(\Phi, u_1, u_2, \tilde{\Phi}).
\]
Differentiation w.r.t. \( \Phi, u_1, u_2, \) and \( p \) yields the first-order optimality conditions. The resultant nonlinear discrete problem is solved using the fixed-point iteration method.

The linearized \( 4 \times 4 \) block KKT system to be solved at the \( m \)-th iteration reads
\[
\begin{bmatrix}
M & 0 & 0 & K(\Phi^{(m-1)}) \\
0 & \beta M & 0 & C_1^\top \\
0 & 0 & \beta M & C_2^\top \\
K(\Phi^{(m-1)}) & C_1 & C_2 & 0
\end{bmatrix}
\begin{bmatrix}
\delta \Phi^{(m)} \\
\delta u_1^{(m)} \\
\delta u_2^{(m)} \\
\delta p^{(m)}
\end{bmatrix}
= \begin{bmatrix}
r_\Phi^{(m-1)} \\
r_{u_1}^{(m-1)} \\
r_{u_2}^{(m-1)} \\
r_p^{(m-1)}
\end{bmatrix},
\]
where
\[
\begin{bmatrix}
r_\Phi^{(m-1)} \\
r_{u_1}^{(m-1)} \\
r_{u_2}^{(m-1)} \\
r_p^{(m-1)}
\end{bmatrix}
= \begin{bmatrix}
M(\tilde{\Phi}^{(n+1)} - \Phi^{(m-1)}) - K(\Phi^{(m-1)}) p^{(m-1)} \\
-\beta M u_1^{(m-1)} - C_1^\top p^{(m-1)} \\
-\beta M u_2^{(m-1)} - C_2^\top p^{(m-1)} \\
-q(\Phi^{(m-1)}, u^{(m-1)}, \tilde{\Phi}^{(n+1)})
\end{bmatrix}.
\]
The existence of a unique solution can be shown as in the scalar control case. Even though the system size is increased significantly compared to the scalar control approach, the discrete saddle point problem with the system matrix

\[
A = \begin{bmatrix}
M & 0 & 0 & K(\Phi^{(m-1)}) \\
0 & \beta M & 0 & C_1^T \\
0 & 0 & \beta M & C_2^T \\
K(\Phi^{(m-1)}) & C_1 & C_2 & 0
\end{bmatrix}
\]

is better suited for the design of efficient solution techniques. In contrast to the scalar control approach which leads to a biharmonic problem for \( p \), the Schur complement operator of the vector control approach is of Laplacian type. Moreover, the use of the \( L^2 \) norm in Tikhonov regularization terms improves the conditioning of the diagonal blocks.

8. Numerical examples

In this section, we perform a numerical evaluation and comparison of the scalar and vector control approaches to enforcing mass conservation in level set algorithms. In all numerical experiments, the domain of interest is the unit square \( \Omega = (0, 1) \times (0, 1) \) and the incompressible velocity field is given by the formula

\[
v(x, y) = (0.5 - y, x - 0.5)^T, \quad (x, y) \in \Omega,
\]

which describes a counterclockwise rotation about the point \((0.5, 0.5)\). For this particular choice of \( v \), the exact solution to the level set transport equation (2) coincides with the initial distance function \( \Phi_0 \) after each full revolution (i.e., at time instants \( t = 2\pi k, \ k \in \mathbb{N} \)). Thus, we can assess the quality of numerical approximations by comparing them to the initial data. Of particular interest is the ability of the proposed numerical algorithms to preserve the total mass and the initial shape of the evolving interface.

At the inlet \( \Gamma_{in} := \{x \in \partial \Omega \mid n(x) \cdot v(x) < 0 \} \), Dirichlet boundary conditions are prescribed using the exact solution. In the numerical study to be presented, the second-order accurate Crank-Nicolson scheme (\( \theta = \frac{1}{2} \)) is used for temporal discretization. All computations are performed using linear finite elements on structured triangular meshes.

8.1. Rotating circle

In the first numerical example, we rotate a circle of radius 0.1 initially centered at \((0.5, 0.75)\) as depicted in Figure 1. The methods under investigation are the non-conservative level set algorithm and the optimization-based procedures with scalar and vector-valued controls. Figure 2 displays the numerical results (mesh size \( h = \frac{1}{32} \)) after one full revolution. All three methods preserve the zero level set fairly well. However, the evolution of mass depicted in Figure 3 reveals that the standard level set method leads to mass conservation errors. Both optimization-based methods conserve the mass perfectly but require numerical solution of several sparse linear systems at each time step (one per fixed-point iteration). Figure 4 shows the number of iterations required to reach a certain level of accuracy (residual of the state equation < \( 10^{-10} \)). The vector control version requires slightly more iterations than the scalar approach. Additionally, the numerical cost of the vector control solution is higher due to the larger system size. However, the costs can be significantly reduced by exploiting the nicer structure of the underlying saddle point system and designing a suitable Schur complement preconditioner.
8.2. Zalesak’s disc

In the second and more challenging experiment, the zero level set of the initial data is given by Zalesak’s slotted disc [20] depicted in Figure 5. The numerical results in Figures 6 and 7 show the loss in mass for the standard level set method after one full revolution. To speed up convergence, we equipped the fixed-point iteration method with Anderson acceleration [19]. For non-linear problems, a remarkable relation to the quasi-Newton method with Broyden update was shown in [4]. In each iteration, a least squares problem is solved to determine the weights for an optimal linear combination of the last iterates. The additional computational effort essentially boils down to the solution of a small QR problem. However, the convergence behavior is influenced by the choice of parameters, as illustrated in Figure 8. For well-chosen parameter settings, fewer iterations are needed to reach the desired tolerance in the scalar control case. Using the same set of parameters in the vector control case, about one additional iteration per time step is required.

9. Conclusions

In this paper, we presented conservative level set algorithms based on PDE-constrained optimization with scalar and vector controls. We have shown that both approaches yield perfectly conservative solutions and mainly differ in the computational effort involved. Even though the vector control approach significantly increases the size of the linear systems to be solved, the additional computational cost may be compensated by exploiting the nicer structure of the underlying saddle point problem. The design of efficient iterative solvers for such systems appears to be a promising direction for future work.

We envisage that the signed distance property can be maintained by incorporating the residual of the Eikonal equation into the cost functional. Preliminary numerical studies indicate that the optimal control approach makes it possible to correct mass conservation errors and the gradients of the level set function in a single postprocessing step.
Figure 2: Rotation of a circle: Heaviside function after one revolution ($t = 2\pi$) for the non-conservative level set method (left) and the conservative method with scalar control (right).

Acknowledgements

The authors would like to thank Dr. John Shadid and Dr. Eric Cyr (Sandia National Laboratories, Albuquerque) for inspiring discussions which have led to the development of the vector control approach presented in this paper. This research was supported by the National Science Foundation under grant DMS-1015002.

References

Figure 3: Rotation of a circle: evolution of the total mass.


Figure 4: Rotation of a circle: number of fixed-point iterations per time step.

Figure 5: Zalesak’s disc: Heaviside function and level set function of the initial data / exact solution.
Figure 6: Zalesak’s disc: Heaviside function after one revolution ($t = 2\pi$) for the non-conservative level set method (red) and the conservative method with vector control (green).

Figure 7: Zalesak’s disc: evolution of the total mass.
Figure 8: Zalesak's disc: number of fixed-point iterations per time step.
G. Eichfelder, J. Povh: On the set-semidefinite representation of nonconvex quadratic programs over arbitrary feasible sets (30.06.2011)


N. Ray, T. van Noorden, F. Frank, P. Knabner: Colloid and Fluid Dynamics in Porous Media including an Evolving Microstructure (05.03.2012)


J. Hoffmann, S. Kräutle, P. Knabner: A general reduction scheme for reactive transport in porous media (20.04.2012)

S. Kräutle: Existence of solutions of reactive transport problems with mass action kinetics and species-dependent diffusion on large time intervals (20.04.2012)


Ch. Basting, D. Kuzmin: A minimization-based finite element formulation for interface-preserving level set reinitialization (04.10.2012)

D. Kuzmin: An optimization-based approach to enforcing mass conservation in level set methods (11.10.2012)


R. Prignitz, E. Bänsch: Particulate flows with the subspace projection method (30.10.2012)


A.M. Khludnev, G.R. Leugering: Delaminated thin elastic inclusions inside elastic bodies (25.01.2013)

F. Brunner, F. Radu, P. Knabner: Analysis of an upwind-mixed hybrid finite element method for transport problems (01.02.2013)

A.M. Khludnev, G.R. Leugering: On Timoshenko thin elastic inclusions inside elastic bodies (06.03.2013)

J. Jahn: Vectorization in set optimization (06.03.2013)


R. Becker, M. Bittl, D. Kuzmin: Analysis of a combined CG1-DG2 method for the transport equation (12.09.2013)


C. Basting, D. Kuzmin: Optimal control for mass conservative level set methods (01.10.2013)