Model Predictive Control of Variable Density Multiphase Flows Governed by Diffuse Interface Models

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Abstract: We present a nonlinear model predictive framework for closed-loop control of two-phase flows governed by Cahn-Hilliard Navier-Stokes system with variable density. The control goal consists in achieving a prescribed concentration distribution in the Cahn-Hilliard part through distributed and/or boundary control of the flow part. Special emphasis is taken on quick control responses which are achieved through the inexact solution of the optimal control problems appearing in the model predictive control strategy. The resulting control concept is known as instantaneous control and is applied to feedback control of the Navier-Stokes system in e.g. Choi et al. (1999); Hinze (2005a); Hinze and Volkwein (2002). We provide numerical investigations which indicate that instantaneous wall parallel boundary control of the flow part is well suited to achieve a prescribed concentration distribution in the variable density Cahn-Hilliard Navier-Stokes system.

Keywords: Model predictive control, Flow control, Variable-densities Cahn-Hilliard Navier-Stokes equations, Instantaneous control

1. INTRODUCTION

We present a nonlinear model predictive framework for closed-loop control of two-phase flows governed by Cahn-Hilliard Navier-Stokes system with variable density. The control goal consists in achieving a prescribed concentration distribution in the Cahn-Hilliard part through distributed and/or boundary control of the flow part. Special emphasis is taken on quick control responses which are achieved through the inexact solution of the optimal control problems appearing in the model predictive control strategy. The resulting control concept is known as instantaneous control. Instantaneous control in the context of flow control is proposed in e.g. Choi (1995); Choi et al. (1999); Hinze and Kunisch (2000), and for distributed control of the Navier-Stokes system is analyzed in Hinze (2005a), where among other things it is shown that the method is able to steer the system exponentially fast to a prescribed flow profile supposing certain smallness assumptions on the initial conditions. For an overview in the field of nonlinear model predictive control we refer to Nevistic and Primbs (1997); Qin and Badgwell (2003) and also to the monograph Grün and Pannek (2011), where also further references can be found.

The outline of this paper is as follows. In section 2 we describe the concept of model predictive control. In section 3 we give a brief introduction to the variable density Cahn-Hilliard Navier-Stokes system, including its numerical treatment. In section 4 we describe the instantaneous control strategy for this system and demonstrate its performance in section 5 by two numerical examples. Some conclusions are given in section 6.

2. MODEL PREDICTIVE CONTROL

The aim of model predictive control (MPC) consists in steering or keeping the state of a dynamical system to or at a given desired trajectory, see e.g. Grün and Pannek (2011). To fix the concept, let us first consider an abstract dynamical system with initial condition \( x^0 \), state \( x(t) \), observation \( y(t) \) and control \( u(t) \):

\[
\dot{x}(t) + Ax(t) = b(x,t) + Bu(t), \quad \text{state},
\]

\[
y(t) = Cx(t), \quad \text{observation},
\]

\[
x(0) = x^0, \quad \text{initial condition}.
\]

Our aim consists in constructing a nonlinear feedback control law \( K \) with \( Bu(t) = K(y(t)) \) which steers the observable part of the dynamical system to the desired trajectory \( \bar{y}(t) \) in the observation space, i.e.

\[
y(t) \to \bar{y}(t), \quad (t \to \infty).
\]

For ease of notation let us for the moment set \( B = id \) and \( C = id \), i.e. we assume full observability and allow fully distributed controls. In section 4 we apply the concept to control the phase field in a Cahn-Hilliard Navier-Stokes system with different densities (Abels et al. (2012)) by wall tangential boundary control of the flow part. The according control and observation operators \( B \) and \( C \) are also specified there.

To prepare for model predictive control, system (1) is discretized in time using the semi-implicit Euler method...
on a time grid \( 0 = t_0 \leq t_1 \leq \ldots \) with \( t_{k+1} - t_k = \tau_k \) for \( k = 0, 1, 2, \ldots \). Here \( x^k \) denotes the state at time \( t_k \) and \( b^k \) denotes the nonlinearity \( b(x^k, t_k) \). For given initial state \( x^0 \) we obtain the time discrete model
\[
(1 + \tau_k A)x^{k+1} = x^k + \tau_k b^k + u^{k+1}, \quad k = 0, 1, \ldots \quad (2)
\]
and consider for given time horizon \( L > 0 \) and \( \alpha > 0 \) the optimal control problem
\[
\min J(x^{j+1}, \ldots, x^{j+L}, u^{j+1}, \ldots, u^{j+L}) \quad \text{s.t.} \quad (2) \quad (P_k)
\]
where
\[
J(x^{j+1}, \ldots, x^{j+L}, u^{j+1}, \ldots, u^{j+L}) := \sum_{i=1}^{L} \left( \frac{1}{2} \| u^{k+i} - x^{k+i} \|^2 + \frac{\alpha}{2} \| u^{k+i} \|^2 \right).
\]
Let us note that problem \((P_k)\) for \( L = 1 \) admits a unique solution. However, for \( L > 1 \) solutions in general need not be unique since \((2)\) then represents a nonlinear constraint. In that case we assume that \((P_k)\) admits a solution.

The idea of model predictive control now is to solve minimization problem \((P_k)\) to obtain a sequence of optimal controls \( u = (u^{k+1}, \ldots, u^{k+L}) \) and to use \( u^{k+1} \) to steer the system to the next time-instance.

**Instantaneous Control**

The solution of the full optimization problem \((P_k)\) forms the bottleneck of the MPC approach if fast control responses are required, in particular if the prediction horizon (i.e. \( L \)) is large. In this case the use of an approximate solution to \((P_k)\) in the MPC algorithm forms an option. Various techniques are available for an approximate solution of \((P_k)\); reduced order modeling techniques replace the large-scale time discrete system in \((P_k)\) by a low-dimensional surrogate model and solve the modified optimization problem for an approximate optimal control instead, see e.g. Hinze and Volkwein (2005). Here we follow a different approach called instantaneous control, which uses an inexact solution of problem \((P_k)\). In its simplest form the algorithm uses the control obtained by performing only one steepest descent step for \((P_k)\). In this particular situation instantaneous control performs the following steps for a given initialization \( u_0^{k+1}, \ldots, u_0^{k+L} \):

1. Solve \((2)\) for \( x^{k+1}, \ldots, x^{k+L} \) with \( u^{k+1} := u^0_0 + (i = 1, \ldots, L) \),
2. solve the adjoint system of \((2)\) with right hand side \((x^{k+1} - x^{k+1}, \ldots, x^{k+L} - x^{k+1})^T\) for \( \lambda^{k+1}, \ldots, \lambda^{k+1} \),
3. set \( d = \alpha(u_0^{k+1}, \ldots, u_0^{k+L})^T + (\lambda^{k+1}, \ldots, \lambda^{k+1})^T \),
4. determine a suitable stepsize \( \theta > 0 \),
5. set \( u^{k+1} := u_0^{k+1} - \theta d, \quad k = k + 1 \).

Here we use the adjoint calculus to express the derivatives of the cost functional \( J \), see e.g. Hinze et al. (2009).

Let us recall that in the case \( L = 1 \) problem \((P_k)\) is a linear quadratic optimal control problem, so that the optimal stepsize \( \theta \) for minimizing \( J \) in direction \( d \) is given by
\[
\theta_{opt} = \frac{(x^0_0 - x^{k+1}, x(d)) + \alpha \| u(d) \|^2}{\| x(d) \|^2 + \alpha \| d \|^2}.
\]
Here, for given \( \kappa \) the vector \( x(\kappa) \) denotes the solution to \((2)\) with \( u^{k+1} := \kappa \).

### 3. The Governing Equations

We consider an immiscible fluid consisting of two components \( A \) and \( B \) with different densities. To model the underlying dynamics we here use a diffuse interface approach based on the model derived in (Abels et al., 2012, 3.), for which among other things sharp interface analysis and energy-inequalities are available.

For the time discretization of the related Cahn-Hilliard Navier-Stokes system with double-obstacle free energy we use a semi-implicit Euler scheme (see e.g. Kay et al. (2008)) and relax the variational inequality associated with the double-obstacle potential, see Blowey and Elliott (1991), using a Moreau-Yosida regularization proposed in Hintermüller et al. (2011). For details of this discretization-relaxation approach we refer to Hintermüller et al. (2012). At a given time instance \( t \) we in the present situation obtain the problem:

\[
\text{find } (y, p, c, w) \in H^3_0(\Omega) \times L^2_0(\Omega) \times H^1(\Omega) \times H^1(\Omega) \text{ such that}
\]

\[
\begin{align}
\xi(p - y_{old}) & - \text{div}(2\eta D y) + \nabla p \\
+ ((p y + f) \cdot \nabla) y + \sigma \text{div} (\nabla c \otimes \nabla c) - p G & = 0 \\
\text{div } y & = 0, \quad (3) \\
\xi(c - c_{old}) - m \Delta w + y_{old} \nabla c & = 0 \\
-\sigma \epsilon \Delta c - w + \lambda(c) - \sigma c_{old}^{-1} c_{old} & = 0, \quad (5)
\end{align}
\]

which is supplemented with the boundary values

\[
\nabla c \cdot \nu = \nabla w \cdot \nu = 0.
\]

Here, \( \Omega \subset \mathbb{R}^n, (n = 2, 3) \) denotes the flow domain with outer unit normal \( \nu \). The concentration order parameter associated with the mass concentrations \( c_A \) and \( c_B \) in the fluid phases \( A \) and \( B \) defined on \( \Omega \), respectively, in the unrelaxed case is \( c = (c_A - c_B)/(c_A + c_B) \in [-1, 1] \) with \( c \equiv 1 \) in the pure \( A \)-phase and \( c \equiv -1 \) in the pure \( B \)-phase region. The term \( \lambda(c) = s \max(0, c - 1) + s \min(0, c + 1) \) realizes the Moreau-Yosida relaxation of the constraint \( |c| \leq 1 \) with \( s > 0 \) denoting the relaxation parameter. Initially, i.e. for \( t = 0 \), we have \( c(0, \cdot) = 0 \) in \( \Omega \). With \( y \) we denote the volume averaged velocity, see (Abels et al., 2012, 2.) and \( p \) denotes the pressure of the fluid. \( \rho = \frac{\epsilon a_A + \epsilon a_B + \epsilon a_{AB}}{2} \) denotes the mean density, and \( \eta = \frac{\epsilon a_A + \epsilon a_B + \epsilon a_{AB}}{2} \) the mean viscosity of the fluid. The quantity \( w \) represents the chemical potential. \( G \) denotes the gravitational force, \( D y := \frac{1}{2}(\nabla y + (\nabla y)^T) \) the stress tensor, and \( j = -m \nu y \nabla w \) the flux arising from the chemical potential, where \( m \) is the mobility of the fluid. The subscript \( \text{old} \) denotes to the respective quantities at the previous time step. Furthermore, the parameter \( \tau \) denotes the time stepsize, \( \xi := \frac{1}{\tau} \), the constant \( \epsilon \) is related to the thickness of the diffuse interface, and the constant \( \sigma \) is related to the surface energy density, see (Abels et al., 2012, 4., 4.3.4). Finally, \( H^1(\Omega) \) denotes the Sobolev space of square integrable functions possessing square integrable weak derivatives, \( H^1_0(\Omega) \) its subspace with zero traces at the boundary of \( \Omega \), and \( L^2(t) = \{ v \in L^2(\Omega) | \int_0^t v dx = 0 \} \).

For the analysis of (3)–(6) and the numerical treatment with semi-smooth Newton methods we refer to Hintermüller et al. (2011, 2012).
The construction of the controller now is based on per-
through distributed and/or tangential Dirichlet boundary
with $c$. For the spatial treatment of the Cahn-Hilliard part (5)–(6) we use the adaptive approach presented in Hintermüller et al. (2012, 2011). We emphasize that we use different spatial meshes for the Cahn-Hilliard and the Navier-Stokes part. In the present paper the discretization used for solving the Navier-Stokes part is build upon a refined Cahn-Hilliard mesh.

4. AN INSTANTANEOUS CONTROLLER FOR TWO-PHASE-FLOWS

We now describe how the instantaneous control strategy with one steepest descent step for $L = 1$ can be applied to obtain a controller for multi-phase flows governed by the Cahn-Hilliard Navier-Stokes system. The controlling objective is given by

$$ J(u) = \frac{1}{2} \| c(u) - c_d \|^2_{L^2(\Omega)} + \frac{\alpha}{2} \| u \|^2_U $$

with $c(u)$ denoting the phase-field, which is controlled through distributed and/or tangential Dirichlet boundary flow control $u$. Here, $c_d(t)$ denotes the desired concentration trajectory at time instance $t$. This might be an ideal trajectory precomputed by an open loop optimization run, or a concentration state which represents certain desired concentration features. The control operator is then given by $\mathcal{C}(y, p, c, w) := c \in L^2(\Omega)$.

Let us first consider distributed control in the domain $\Omega$, so that with $U := L^2(\Omega)^n$ the control operator is defined by $B(u) := (u, 0, 0, 0)$, i.e. it maps controls to the feasible right hand sides of (3)-(6). To begin with we assume that the flow can be controlled by volume forces at every single point of the domain. Though this scenario is not realizable in practice, it shows what one best can achieve in practice through controlling the system in the flow part.

At a given time instance we consider the optimization problem

$$ \min_{u \in U} J(u) = \frac{1}{2} \| c(u) - c_d \|^2_{L^2(\Omega)} + \frac{\alpha}{2} \| u \|^2_U $$

s.t.

$$ \xi \rho_{old} y - \text{div}(\eta_{old} \nabla y) + \nabla p = f(c_{old}, y_{old}) + u $$

$$ \text{div} y = 0 $$

$$ c - \tau m \Delta w = c_{old} - \tau y \nabla c_{old} $$

$$ -\sigma \Delta c - w = \sigma c^{-1} c_{old} - \lambda $$

$$ y = \nu \cdot \nabla c = \nu \cdot \nabla w = 0 $$

The construction of the controller now is based on performing one steepest descent step to $u$ at a given control $u$ to decrease the value of $J(u)$. Here, $J$ is a tracking-type functional with $\alpha > 0$ penalizing the control cost, and the concentration is a function of the control, i.e. $c = c(u)$, realized through the system (7)–(11). The right hand side in (7) is given by

$$ f(c_{old}, y_{old}, u) = \xi \rho_{old} y_{old} - \rho_{old} y_{old} \cdot \nabla y_{old} $$

$$ -\sigma \text{div}(\nabla c_{old} \otimes \nabla c_{old}) + \rho_{old} G $$

and the control $u$ thus enters the Navier-Stokes system as a volume force on the right hand side. Let us note that (7)–(11) represents a linear system, which for a given control $u$ in general can be solved faster than (5)–(6) supplied with an additional distributed forcing term $u$ in (7). This is our motivation to consider the linear system (7)–(11) instead of (5)–(6). However, we stress that the time discretization related to (7)–(11) is not suitable for simulation purposes, since e.g. mass is not conserved.

4.1 Adjoint representation of the gradient $\nabla J(u)$

Using adjoint calculus Hinze et al. (2009) one easily verifies that

$$ \nabla J(u) = \alpha u + p $$

where $p$ is related to $u$ through the adjoint system

$$ p_2 - \tau m \Delta p_1 = 0 $$

$$ -\sigma \Delta p_2 - p_1 = c(u) - c_d $$

$$ \xi \rho_{old} p_4 - \text{div}(\eta_{old} \nabla p_4) + \nabla p_4 = -\tau p_1 \nabla c_{old} $$

$$ \text{div} p_3 = 0 $$

with $(p_1, p_2, p_3, p_4) \in H^{-1}(\Omega) \times H^1(\Omega) \times H_0^1(\Omega)^n \times L^2(\Omega)$ denoting the adjoint variable, and $c(u)$ denoting the solution to (7)–(11) for given $u$.

4.2 Obtaining the steepest descent stepsizes

To achieve sufficient decrease in the value of $J(u)$ through

$$ u := u - \nabla J(u) $$

the choice of the stepsize $\theta$ is crucial. In the present situation the functional $J$ is quadratic, since (7)–(11) forms a linear system with a well defined, linear and continuous solution operator. Now, for given $u \in U$, let $g := \nabla J(u)$ and denote by $c(g)$ the concentration defined through the system

$$ \xi \rho_{old} y - \text{div}(\eta_{old} \nabla y) + \nabla p = g $$

$$ \text{div} y = 0 $$

$$ c - \tau m \Delta w = -\tau y \nabla c_{old} $$

$$ -\sigma \Delta c - w = 0 $$

If $g \neq 0$, the optimal stepsize $\theta$ is well defined and satisfies

$$ \theta = \arg\min_{\theta \in R} J(u - \theta g) $$

A short calculation shows

$$ \theta = \frac{\| c(u) - c_d, c(g) \|^2_{L^2(\Omega)} + \alpha \| u, g \|^2_{L^2(\Omega)}}{\| c(g) \|^2_{L^2(\Omega)} + \alpha \| g \|^2_{L^2(\Omega)}} $$

so that in the present situation the computation of the optimal steepest descent stepsize requires one additional linear system solve.

The controller step for a given initial control guess $u_0 \in U$ now performs the steps;

- Compute $c(u_0)$,
- compute $p_3(u_0)$,
- set $g = \nabla J(u_0)$,
- compute $c(g)$,
- compute $\theta$ with $u = u_0$, $c(g)$ and $g$,
- update $u = u_0 - \theta g$,
• compute $c(u)$.

In total the numerical amount of work consists of four linear system solves.

Subsequently we use $u^0 = 0$ as initial control in the controller step. On the discrete level the functions $y, p, c, g, p_1, \ldots, p_4$ have to be replaced by their finite element counterparts. However, recalling the representation of $g$, the control $u = -\theta g$ is implicitly discretized through the discrete counterpart of $p_3$ (see Hinze (2005b)).

### 4.3 Tangential dirichlet boundary control

Tangential dirichlet boundary control is a practicable control procedure which is mass-conserving. The related optimization problem reads

$$
\min J(u) = \frac{1}{2} ||c(u) - c_d||_{L^2(\Omega)}^2 + \frac{\alpha}{2} ||u||^2_U \quad (P_D)
$$

subject to

$$\xi \rho_{old} y - \text{div} (\eta_{old} \nabla y) + \nabla p = f(c_{old}, y_{old}),$$

$$\text{div} y = 0,$$

$$c - \tau_m \Delta w = c_{old} - \tau y \nabla c_{old},$$

$$-\sigma \epsilon \nabla c = -\epsilon \nabla c_{old} - \lambda(c_{old}),$$

$$\nu \cdot \nabla c = \nu \cdot \nabla w = 0 \text{ on } \partial \Omega,$$

$$\nu \cdot y = 0 \text{ on } \partial \Omega,$$

$$\nu \cdot y = u \text{ on } \partial \Omega.$$  

Here $\nu^\perp$ denotes the unit tangential field to the boundary $\partial \Omega$, where we assume that we have an orthonormal basis of the tangential space available at every point of $\partial \Omega$ and (22) is satisfied for this basis. The right hand side in (16) is the same as in (12). The control space $U$ is either $L^2(\Omega)^{(n-1)}$, or $H^{1/2}(\Omega)^{(n-1)}$, where we note that in the $L^2$ case the system (16),(17),(21),(22) has to be understood in the very weak sense. The control operator is defined by $B(u) := \left( -\int_{\partial \Omega} u \nu \cdot \partial_\nu \cdot \right. \delta, 0, 0, 0, 0).$

The corresponding adjoint system again is (15), while the gradient in the $L^2$ case now takes the form

$$\nabla J_p(u) = c u - \nu \theta(c_{old}) \nabla p_3 \nu.$$  

In the $H^{1/2}$ case the function $\nu^\perp y(c_{old}) \nabla p_3 \nu$ has to be replaced by its Riesz representer associated to the $(H^{1/2}, H^{-1/2})$ pairing. The system to be solved for obtaining the optimal stepsize $\theta$ changes accordingly.

### 5. NUMERICAL TESTS

#### Distributed Control

Here we report on the effectiveness of the instantaneous control strategy described in the previous section. We use fully distributed flow control with control gain of morphing a circle (which represents a stable state) into a square (which represents an unstable state). We set $\Omega := (0,1)^2$, $c_0(x,y) := -\tan \left( \frac{\sqrt{(x-0.5)^2 + (y-0.5)^2} - 0.25}{\epsilon \sqrt{2}} \right)$ which describes a circle with radius $r = 0.25$ and midpoint located at $M = (0.5,0.5)$. The parameter $\epsilon$ corresponds to the interfacial thickness. Inside the circle we have $c_0 \approx 1$ while $c_0 \approx -1$ outside the circle, see Fig. 1 (left), where black indicates $c \approx 1$ and white indicates $c \approx -1$. Control is applied to the flow field with control gain of steering $c$ to the desired state $c_d$ with values 1 in the square with edge length ensuring $(c_0,1) = (c_d,1)$ and center at $(0.35,0.35)$, see Fig. 1 (right). This requirement is meaningful, since our time discretization scheme (3)–(6) is mass-conserving.

We further use $\rho_1 = \rho_2 = 1$, $\eta_1 = \eta_2 = 0.02$, and set $G := 0$. The mobility is $m = 0.0001$, and $\sigma := \epsilon = 1/(40\pi)$. The time stepping is adapted to fulfill the CFL-condition, which in the present example gives time steps of size about 0.0035.

Fig. 2 shows the stabilized state $c$ at time $t = 2$ together with the stabilized flowfield (left) and the temporal behaviour of $\|c - c_d\|$ in the case of distributed control.

### Tangential Dirichlet Boundary Control

We next show an example using tangential Dirichlet boundary control in the rising bubble benchmark Hysing et al. (2009), see Fig. 3 (left). Due to gravitational force the bubble intends to rise. Using Dirichlet boundary control we are able to prevent the bubble from rising and to stabilise it at the bottom of the flow column.

As domain we choose $\Omega := (0,1) \times (0,1.5)$, $c_0(x,y) := -\tan \left( \frac{\sqrt{(x-0.75)^2 + (y-0.75)^2} - 0.25}{\epsilon \sqrt{2}} \right)$ which represents a circle with radius $r = 0.25$ located at $M_{c_0} = (0.75,0.75)$. Again, the parameter $\epsilon$ corresponds...
to the interfacial thickness. Inside the circle we have \( c_0 \approx 1 \), while \( c_0 \approx -1 \) outside the circle, see Fig. 3 (left). The desired state \( c_d \) is a circle with same radius and midpoint located at \( M_{cd} = (0.5,0.5) \), see Fig. 3 (right). Furthermore, \( \rho_1 = 500, \rho_2 = 100, \eta_1 = 50, \) and \( \eta_2 = 1 \), and \( G = (0,-0.98) \). The mobility is \( \mu = 10^{-5}, \sigma = 25, \) and \( \epsilon = 0.01 \). Values are similar to the ones used for benchmarking in Hysing et al. (2009).

In Fig. 4 we show an intermediate state and the final stabilised state. At the left boundary one sees the tangential boundary control, while on the right part of the plots we show some streamlines of the velocity field. We note that the state is symmetric.

Fig. 5 shows that the instantaneous feedback controller with tangential Dirichlet boundary control indeed steers the system into the desired state very fast and stabilizes it there.

6. CONCLUSIONS

We present a nonlinear model predictive framework for closed-loop control of two-phase flows governed by Cahn-Hilliard Navier-Stokes system with variable density. Special emphasis is taken on quick control responses which are achieved through the inexact solution of the optimal control problems appearing in the model predictive control strategy. The resulting control concept is known as instantaneous control, which in the present paper is successfully applied with distributed and tangential Dirichlet boundary control of the flow part to achieve a prescribed concentration distribution in the variable density Cahn-Hilliard Navier-Stokes system. In particular, the controller is able to prevent the bubble in the rising bubble benchmark from Hysing et al. (2009) from rising using tangential Dirichlet boundary control.

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