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Time integration for diffuse interface models for two-phase flow

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ABSTRACT

We propose a variant of the θ-scheme for diffuse interface models for two-phase flow, together with three new linearization techniques for the surface tension. These involve either additional stabilizing force terms, or a fully implicit coupling of the Navier–Stokes and Cahn–Hilliard equation.

In the common case that the equations for interface and flow are coupled explicitly, we find a time step restriction which is very different to other two-phase flow models and in particular is independent of the grid size. We also show that the proposed stabilization techniques can lift this time step restriction.

Even more pronounced is the performance of the proposed fully implicit scheme which is stable for arbitrarily large time steps. We demonstrate in a Taylor-flow application that this superior coupling between flow and interface equation can decrease the computation time by several orders of magnitude.

1. Introduction

The numerical simulation of two-phase flows has reached some importance in microfluidic applications. In the last decade, diffuse interface (or phase-field) models have become a valuable alternative to the more established sharp interface methods (e.g. Level-Set, Arbitrary Lagrangian–Eulerian, Volume-Of-Fluid). The advantages of diffuse interface methods include the possibility to easily handle moving contact lines and topological transitions as well as the fact that they do not require any reinitialization or convection stabilization. The corresponding equations involve a Navier–Stokes (NS) equation coupled to a convective Cahn–Hilliard (CH) equation. A lot of efficient spacial discretization techniques and solvers for these equations have been proposed (e.g. [20]). However, not much work has been done on time integration strategies and efficient coupling between the NS and the CH equation, which we will address in this paper.

But at first, let us introduce the diffuse interface method more carefully. The method was originally developed to model solid–liquid phase transitions, see e.g. [6,14,26]. The interface thereby is represented as a thin layer of finite thickness and an auxiliary function, the so-called phase field, is used to indicate the phases. The phase field function varies smoothly between distinct values in both phases and the interface can be associated with an intermediate level set of the phase field function. Diffuse interface approaches for mixtures of two immiscible, incompressible fluids lead to the NS–CH equations and have been considered by several authors, see e.g. [19,15,20,11]. The simplest model reads:

$$\rho(c)\left(\partial_t \mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u}\right) = -\nabla p + \nabla\cdot\left(\nu(c)\mathbf{D}(\mathbf{u})\right) + \mathbf{F} + \mu\nabla c, \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0, \tag{2}$$

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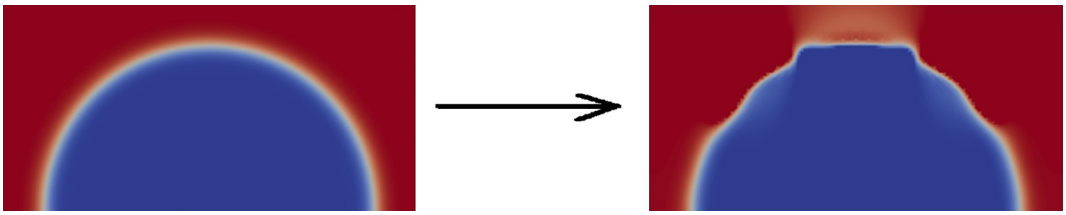

Fig. 1. Evolution of a semi-circular bubble under the diffuse interface model with too large time steps. Left: initial shape; Right: Evolved shape after ten time steps.

$$\partial_t c + \mathbf{u} \cdot \nabla c = \nabla \cdot \big(M(c) \nabla \mu\big), \tag{3}$$

$$\mu = \tilde{\sigma} \epsilon^{-1} W'(c) - \tilde{\sigma} \epsilon \Delta c, \tag{4}$$

in the domain Ω. Here $\mathbf{u}$, p, c and μ are the velocity, pressure, phase field variable and chemical potential, respectively. The function $W(c)$ is a double well potential, here we use $W = 1/4(c^2-1)^2$ which ensures that $c \approx \pm 1$ in two fluid phases, respectively.

The function $M(c)$ is a mobility, ϵ defines a length scale over which the interface is smeared out. In general for the diffuse interface fluid method, it is desirable to keep M small such that the phase field function is primarily moved by advection. At the same time the mobility needs to be big enough to ensure that the interface profile stays accurately modeled and the interface thickness is approximately constant. Furthermore, $\mathbf{D}(\mathbf{u}) = \nabla \mathbf{u} + \nabla \mathbf{u}^T$ is the strain tensor, $\rho(c)$, $\nu(c)$ and $\mathbf{F}$ are the (phase dependent) density, viscosity and body force. The parameter $\tilde{\sigma}$ is a scaled surface tension which is related to the physical surface tension by $\tilde{\sigma} = \sigma \frac{3}{2\sqrt{2}}$. There are efficient solvers available to discretize and solve Eqs. (1)–(4) in space (see e.g. [20]).

Surface tension is a major component of all multiphase fluid models and hence various spatial discretizations of the surface tension force for diffuse–interface models have been proposed (e.g. [22]). The surface tension force $\mu \nabla c$ introduces a strong coupling between the NS equation providing the flow field and the CH equation evolving the phase field. This is very similar to sharp interface models for two-phase flow where the same interface-to-flow coupling introduces a severe time step restriction of the form [7,9]:

$$\tau < C \rho^{\frac{1}{2}} h^{\frac{3}{2}} \sigma^{-\frac{1}{2}}. \tag{5}$$

Here, τ is the maximum time step size, ρ the average density of both fluids and h the grid size. The above CFL-like restriction is particularly strong for large effective surface tensions, e.g. when small physical length scales are considered. It is usually assumed that this restriction also holds for diffuse interface models (e.g. in [21]). In Section 6.1 we will show that this assumption is wrong.

However, also for diffuse interface models there is some time step restriction which can make computations extremely costly, even in cases when the interface is supposed to hardly move. Fig. 1 shows such a case of a perfectly circular interface, which is almost stationary. However, if too big time steps are chosen, even such an equilibrated surface will start to wobble and finally break up. In sharp interface models, there are techniques to overcome such time step restrictions [17]. To the best of the authors' knowledge there is no such technique available for diffuse interface models yet. We will develop techniques to improve the coupling between the NS and the CH equations, which will turn out to lift the time step restrictions significantly.

Apart from increasing the computational performance, there is a second reason to develop better time integration schemes for diffuse interface models. The simple time discretization schemes available often imply the need to stabilize the system by choosing a relatively high CH mobility. But this high artificial diffusion perturbs the simulation results since matched asymptotic analysis shows the convergence of diffuse–interface methods toward the sharp interface equations only for small CH mobility [1]. Therefore better time integration strategies would not only speed-up the simulations but also allow to take smaller (more physical) CH mobility and thus improve the accuracy of diffuse–interface methods.

The structure of the remaining paper is as follows. Sections 2 and 3 will introduce a simple variant of the θ scheme as well as a block Gauss–Seidel coupling strategy. The main attention is given to Section 4 where some new improved coupling techniques for diffuse interface models are presented. The solution of the resulting systems is discussed in Section 5. In Section 6 we perform numerical tests. In particular a CFL-condition for diffuse interface methods is numerically derived and it is shown that the new proposed coupling methods can, for some problems, result in an extreme gain of performance. Finally, conclusions are drawn in Section 7.

2. Time discretization: a variant of the θ-scheme

In this section we adopt the well-known θ-scheme for the time discretization of the NS–CH equations. Let the time interval $[0, T]$ be divided in N subintervals of size τ^n, $n = 1 \dots N$. We define the discrete time derivative of a (solution) variable v to be $d_t v^{n+1} := (v^{n+1} - v^n)/\tau^n$, where the upper index denotes the time step number. For a shorter notation we introduce