DIFFUSE INTERFACE MODELS AND THEIR APPLICATION IN FLOAT FORMING

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Abstract. Diffuse interface models have been successfully used as a tool for mathematical description of the motion of several immiscible fluids and their mutual interaction. Multicomponent flows of this type are of interest in many engineering applications. A practical example of such a multicomponent system is glass/tin/nitrogen system that must be studied in modelling of the float glass process (Pilkington process).

The diffuse interface models allow for consistent incorporation of the surface tension effects. The interface between the components is in this case treated as a thin layer across which the components are allowed to mix. The main challenge in the numerical simulations is the very fine spatial resolution required for capturing the dynamics of the interface. We have recently developed a variant of the model that is applicable in a general non-isothermal setting. We will discuss the numerical issues and challenges that must be addressed in simulations of the problems that might be of relevance in modelling of the float glass process.

1. Introduction

In this contribution we are interested in mathematical description of simultaneous flow of several immiscible fluids in a fixed domain. Flows of this type formally belong to a wider class of so-called *multiphase flows* in which the flow and interaction of different materials, commonly referred to as *phases*, is of interest. These can be materials with different state (gas, liquid, solid) and/or materials with generally different chemical properties (like immiscible fluids).

Physical processes involving multiphase flows are frequently met in many industrial applications. Very often, it is of importance to provide reliable computer simulations of such processes enabling their optimization from various aspects. The need to model and simulate the processes on the computer results from the fact that it is often not feasible to carry out experiments at operational conditions.

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From this point of view, modelling of multicomponent flows has been a very challenging topic for decades and the problem has been tackled by variety of different numerical and modelling approaches. The two main model concepts can be distinguished based on the different treatment of the interfaces between the phases. Each phase in the system can be described by the so-called *order parameter* (or phase-field variable), which is typically the volume fraction of the phase, and the interface between each two phases can be characterized by the "abrupt change" of the respective order parameter.

In the first modelling approach the interfaces are considered as being *sharp*. In this case the respective order parameter is discontinuous across the interface and one needs to supply the transition conditions at the interfaces in the form of jump conditions. In numerical simulations one also needs to employ some kind of interface tracking technique which often brings implementation difficulties.

In the second modelling approach the interfaces are considered as being *diffuse*, meaning that they are treated as narrow transition zones of finite thickness across which the phases are allowed to mix. The respective order parameter thus changes smoothly across the interfacial layer in this case. The interface itself then can be captured as an appropriate set of contours of the respective order parameter. This methodology also allows for consistent incorporation of surface tension effects inside the interfacial layer. Nice overview of various diffuse interface models is presented in Kim (2012), including numerous references to the previously mentioned interface tracking techniques. In Section 2 of this document we briefly discuss the derivation of a certain class of diffuse interface models based on the theory of interacting continua.

Natural requirement to keep the interfacial layer as narrow as possible contrasts with the fact that we need to cover it with a sufficient number of computational points in order to capture the dynamics of the interfaces properly. One possible way of how to deal with this problem is to exploit the parallelization approach to the scientific computing. In Section 3 we briefly discuss one of the state-of-the-art approaches designed to tackle large systems of equations describing the flow dynamics, which have been successfully tested at large scale HPC infrastructure.

Our research is motivated by the applicability of diffuse interface models in the *float glass process*, see Pilkington (1969), an ingenious technology based on the idea of floating the ribbon of molten glass on top of a bath of molten tin in a chemically controlled atmosphere. In the context of preceding paragraphs, this process, or more precisely its initial stage, involves three imiscible fluid phases that do not chemically interact. These are the molten glass (1), the molten tin (2) and the protective atmosphere (3). Some practical issues concerning the implementation of diffuse interface models in the context of this complicated problem were recently discussed in Řehoř et al. (2017).

2. Diffuse interface models

Our derivation of diffuse interface models is based on the description of multicomponent systems that is commonly adopted in the theory of mixtures[1]. The separation of phases (components), reflecting their immiscibility, is ensured by the special choice of the Helmholtz free energy which subsequently yields a class of so-called Cahn-Hilliard-Navier-Stokes (CHNS) type models.

[1]Note that *multicomponent flows* are usually characterized by mixing of components at the molecular level within the whole domain (not only in some narrow interfacial layer). Moreover, chemical interaction between the components is generally allowed. From these points of view, multicomponent flows represent a more general concept compared to multiphase flows discussed above.

More specifically, our thermodynamically consistent derivation of these type of models follows the idea presented in Heida et al. (2012) with some subtle deviations. For example, instead of mass fractions or partial densities, we consider volume fractions as an appropriate choice of the order parameters that are supposed to add up to unity at each point of the fixed domain (at least in cases with incompressible phases). A hierarchy of different CHNS type models can be obtained with respect to different choices of the averaged velocity field as well as some other factors, see for example Lowengrub and Truskinovsky (1998), Aland and Voigt (2012), Abels et al. (2012).

To give a specific example of such a model let us examine the general N-component incompressible CHNS type model that is given by the system of partial differential equations for the unknown field quantities $\phi_1, \dots, \phi_{N-1}$ (volume fractions), $\boldsymbol{v}$ (velocity) and p (pressure), namely

$$\frac{\partial \phi_i}{\partial t} + \operatorname{div}(\phi_i \boldsymbol{v}) = \operatorname{div}\left(M_0 \sum_{j=1}^{N-1} \ell_{ij} \nabla \mu_j \right), \quad i = 1, \dots, N-1, \tag{2.1a}$$

$$\mu_i = \frac{b}{\varepsilon} \frac{\partial F}{\partial \phi_i} - \frac{a\varepsilon}{2} \sum_{j=1}^{N-1} \lambda_{ij} \Delta \phi_j, \quad i = 1, \dots, N-1, \tag{2.1b}$$

$$\operatorname{div} \boldsymbol{v} = 0, \tag{2.1c}$$

$$\varrho(\boldsymbol{\phi}) \frac{\partial \boldsymbol{v}}{\partial t} + (\nabla \boldsymbol{v})\,(\varrho(\boldsymbol{\phi}) \boldsymbol{v} + \boldsymbol{J}) = -\nabla p + \operatorname{div}(2\nu(\boldsymbol{\phi}) \mathbb{D}) - \frac{a\varepsilon}{2} \sum_{i,j=1}^{N-1} \lambda_{ij} \operatorname{div}(\nabla \phi_j \otimes \nabla \phi_i) + \varrho(\boldsymbol{\phi}) \boldsymbol{b}, \tag{2.1d}$$

where the first two equations describe the time evolution of $(N-1)$ order parameters[2] $\boldsymbol{\phi} = (\phi_1, \dots, \phi_{N-1})$, the third one is the incompressibility condition for the averaged velocity field, and finally the last equation represents the balance of linear momentum for the physical system as a whole. Here a and b are constants related to the choice of the nonlinear potential F that comes from the bulk part of the Helmholtz free energy, M_0 is the so-called mobility, ε is the characteristic scale of the interfacial thickness, λ_{ij} and ℓ_{ij} are constants given by a combination of surface tensions between the phases, and finally $\boldsymbol{J}$ represents the total diffusive mass flux across the interfaces within the system. The quantities $\varrho(\boldsymbol{\phi})$ and $\nu(\boldsymbol{\phi})$ represent homogenized density and dynamic viscosity respectively. In other words, these quantities are obtained as linear combinations of the respective constant material parameters associated with the phases. In practical simulations one often faces the problem to overcome the issues like spurious numerical oscillations that usually appear as a result of big differences in the values of material parameters, see Řehoř et al. (2017).

This particular model in the context of two-phase flows was originally derived by Abels et al. (2012). The three-phase variant, with neglected $\boldsymbol{J}$ on the left hand side of (2.1d), was proposed by Boyer and Lapuerta (2006), see also Boyer and Minjeaud (2014). We have recently extended the above model by adding the equation for the temperature in a consistent way.

3. Efficient numerical solution of multiphase flows

The system of equations (2.1) is extremely difficult to solve numerically since it is highly nonlinear and all equations are strongly coupled. Moreover, as we have mentioned, we need a fine resolution of the mesh close to the interfaces. As a consequence, after the discretization and linearization, we are facing the problem of solving a large scale system of linear algebraic equations, which is not feasible with conventional sparce direct solvers.

[2] The remaining phase is described by $\phi_N = 1 - \sum_{j=1}^{N} \phi_j$.

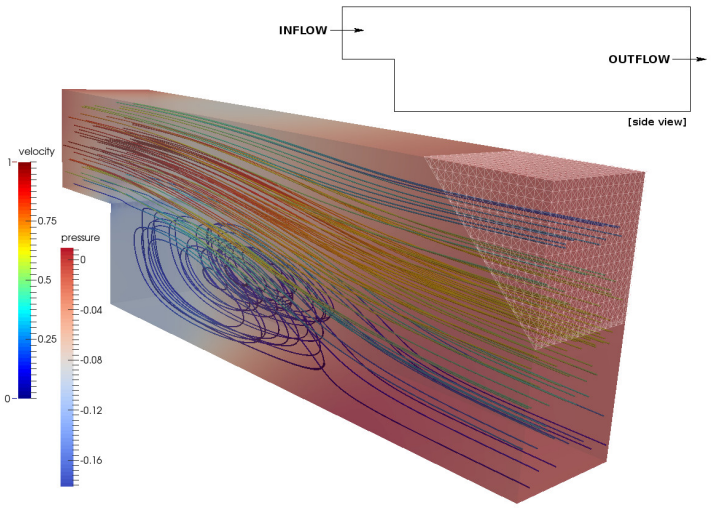

Figure 1: Flow of a single-component fluid, described by the incompressible Navier-Stokes equations, over a backward-facing step in 3D. The figure shows pressure distribution in the domain together with a set of streamlines illustrating that particles introduced at the inflow pass over the step and exit at the outflow, while some other particles remain in the recirculating region behind the step. This is one of the academic problems appropriate for the testing of robustness of numerical solvers in question with respect to changing parameters of the model (e.g. viscosity, mesh refinement).

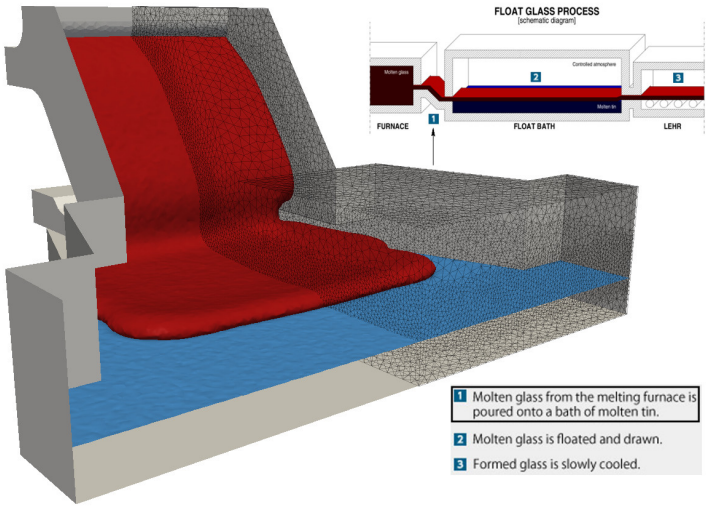

Figure 2: The tested numerical solvers have been applied in large scale numerical simulations of the first stage of the industrial float glass process (Pilkington process). The figure shows the impact of the molten glass onto the bath of molten tin. It is an example of a complicated multicomponent flow in which the flow dynamics is described by the incompressible Navier-Stokes equations with variable density and viscosity.

Recently we have tested an implementation of the model (2.1) that enables to use *algebraic multigrid* and *Krylov subspace methods* to resolve the underlying system of algebraic equations corresponding to Navier-Stokes part of the model (equations (2.1c)–(2.1d)). The key aspect of the implementation lies in the construction of pressure-convection-diffusion (PCD) preconditioners, see Elman et al. (2014). We

have implemented and tested two different variants of PCD in academic setting, see Figure 1. Both of them seem to share the potential to be useful also in the context of multiphase flows, see Figure 2.

A different promising strategy for the efficient resolution of systems of the type (2.1), which is based on *projection methods*, has been presented in the recent works Dong (2014), Dong (2015), Dong (2017).

References

Abels, H., H. Garcke, and G. Grün (2012). Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities. *Math. Models Methods Appl. Sci. 22*(3), 1150013, 40.

Aland, S. and A. Voigt (2012). Benchmark computations of diffuse interface models for two-dimensional bubble dynamics. *International Journal for Numerical Methods in Fluids 69*(3), 747–761.

Boyer, F. and C. Lapuerta (2006, 7). Study of a three component Cahn-Hilliard flow model. *ESAIM: Mathematical Modelling and Numerical Analysis 40*, 653–687.

Boyer, F. and S. Minjeaud (2014). Hierarchy of consistent n-component cahn–hilliard systems. *Mathematical Models and Methods in Applied Sciences 24*(14), 2885–2928.

Dong, S. (2014). An efficient algorithm for incompressible N-phase flows. *Journal of Computational Physics 276*, 691–728.

Dong, S. (2015). Physical formulation and numerical algorithm for simulating N immiscible incompressible fluids involving general order parameters. *Journal of Computational Physics 283*, 98–128.

Dong, S. (2017). Wall-bounded multiphase flows of n immiscible incompressible fluids: Consistency and contact-angle boundary condition. *Journal of Computational Physics 338*, 21 – 67.

Elman, H. C., D. J. Silvester, and A. J. Wathen (2014). *Finite elements and fast iterative solvers: with applications in incompressible fluid dynamics* (2nd ed.). Numerical Mathematics and Scientific Computation. Oxford University Press.

Heida, M., J. Málek, and K. R. Rajagopal (2012). On the development and generalizations of Cahn-Hilliard equations within a thermodynamic framework. *Z. Angew. Math. Phys. 63*(1), 145–169.

Kim, J. (2012). Phase-field models for multi-component fluid flows. *Commun. Comput. Phys. 12*(3), 613–661.

Lowengrub, J. and L. Truskinovsky (1998). Quasi-incompressible Cahn-Hilliard fluids and topological transitions. *R. Soc. Lond. Proc. Ser. A Math. Phys. Eng. Sci. 454*(1978), 2617–2654.

Pilkington, L. A. B. (1969). Review lecture. The float glass process. *Proc. R. Soc. A-Math. Phys. Eng. Sci. 314*(1516), 1–25.

Řehoř, M., J. Blechta, and O. Souček (2017). On some practical issues concerning the implementation of Cahn–Hilliard–Navier–Stokes type models. *International Journal of Advances in Engineering Sciences and Applied Mathematics 9*(1), 30–39.