Cahn-Hilliard model for multiphase flows

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Multiphase flows are of enormous interest in a broad range of applications, from turbulent flows in industrial reactors to labs-on-a-chip in microfluidic devices.

Two different approaches are used in the simulation of multiphase problems. The sharp-interface models describe the interface between fluids as a discontinuity, relaying on independent sets of the Navier-Stokes equation for each fluid domain. On the contrary, in the diffusive interface family the interface is represented as a thin continuous layer where the fluid composition changes smoothly, and uses a unified system of equations for the complete simulation domain.

The Cahn-Hilliard method, belonging to the diffusive interface family, is a promising method to simulate multiphase flows, which is drawing increasing attention. Its main strength lays on its capability to deal with complex topological changes, such as splitting or merging interfaces. Other attracting characteristics are its thermodynamically consistent nature and the simplicity of its implementation [1].

The Cahn-Hilliard method introduces a scalar phase variable, ϕ, which represents the local composition of the fluid, and a scalar transport equation to govern the dynamics of ϕ:

$$\frac{\partial \phi}{\partial t} + u \cdot \nabla \phi = \kappa \nabla^2(\psi) \tag{1}$$

where κ is the so called mobility parameter and ψ is the chemical potential of the system, defined as:

$$\psi = \alpha h'(x) - \beta \nabla^2 \phi \tag{2}$$

Its first component describes the change in free energy due to bulk mixing and is usually modelled throught $h = \frac{(\phi+1)^2(\phi-1)^2}{4}$, a double well potential. The second term depicts the increase in free energy due to the interface formation and α and β are constants used to control the relative weight of the two terms. The latter two can be linked to the surface tension ($\sigma = \sqrt{\frac{\alpha\beta}{18}}$) and the interface thickness ($\epsilon = \sqrt{\frac{\alpha}{\beta}}$). Additionally, a surface tension force term is added to the momentum equations and a generalized pressure gradient term is needed to impose the incompressibility condition[2].

$$\rho(\phi)\left[\frac{\partial u}{\partial t} + u \cdot \nabla u\right] = -\nabla \tilde{p} + \nabla \cdot (\mu(\phi)(\nabla u + \nabla u^T)) + \psi \nabla \phi \tag{3}$$

The dimensionless numbers associated to this model are:

- Cahn number, $Cn = \frac{\sqrt{\alpha/\beta}}{L}$. Represents the ratio between the characteristic length scales of the interface and the flow
- Peclet number $Pe = \frac{UL}{\kappa\beta}$. Describes the ratio between convective and diffusive transport of the phase variable
- Capillary number $Ca = \frac{\mu U}{\sigma}$. Describes the ratio between viscous forces (or inertial forces) surface tension force and viscous (or inertial) forces

In order to approach the "sharp-interface limit" and correctly model the underlying physics, the values of the value of the Cahn and Peclet numbers have to be chosen carefully. [3]

We have developed an accurate solver of the CH-NS system for pipe flow using a high-order finite-difference method in the radial direction and the Fourier pseudospectral method in the azimuthal and axial directions. It has been successfully applied to simulate several interesting cases, such as core annular flow and a rising droplet.

Furthermore, a different approach is being developed, based on the finite volumes method and the FASTEST3D framework, developed at the Friedrich-Alexander Universität in Erlangen. This approach has the potential to be used in problems with more complex geometries

References

[1] John W. Cahn, John E. Hilliard *Free Energy of a Nonuniform System. I. Interfacial Free Energy.* Journal of Chemical Physics 1958

[2] David Jacqmin *Calculation of Two-Phase Navier-Stokes Flows Using Phase-Field Modeling.* Journal of Computational Physics 1999

[3] F. Magaletti, F. Picano, M. Chinappi, L. Marino, C.M: Casciola *The sharp-interface limit of the Cahn-Hilliard/Navier-Stokes model for binary fluids.* Journal of Fluid Mechanics 2013