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Computation of multiphase systems with phase field models. (English) Zbl 1076.76517

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Summary: Phase field models offer a systematic physical approach for investigating complex multiphase systems behaviors such as near-critical interfacial phenomena, phase separation under shear, and microstructure evolution during solidification. However, because interfaces are replaced by thin transition regions (diffuse interfaces), phase field simulations require resolution of very thin layers to capture the physics of the problems studied. This demands robust numerical methods that can efficiently achieve high resolution and accuracy, especially in three dimensions. We present here an accurate and efficient numerical method to solve the coupled Cahn-Hilliard/Navier-Stokes system, known as Model H, that constitutes a phase field model for density-matched binary fluids with variable mobility and viscosity. The numerical method is a time-split scheme that combines a novel semi-implicit discretization for the convective Cahn-Hilliard equation with an innovative application of high-resolution schemes employed for direct numerical simulations of turbulence. This new semi-implicit discretization is simple but effective since it removes the stability constraint due to the nonlinearity of the Cahn-Hilliard equation at the same cost as that of an explicit scheme. It is derived from a discretization used for diffusive problems that we further enhance to efficiently solve flow problems with variable mobility and viscosity. Moreover, we solve the Navier-Stokes equations with a robust time-discretization of the projection method that guarantees better stability properties than those for Crank-Nicolson-based projection methods. For channel geometries, the method uses a spectral discretization in the streamwise and spanwise directions and a combination of spectral and high order compact finite difference discretizations in the wall normal direction. The capabilities of the method are demonstrated with several examples including phase separation with, and without, shear in two and three dimensions. The method effectively resolves interfacial layers of as few as three mesh points. The numerical examples show agreement with analytical solutions and scaling laws, where available, and the 3D simulations, in the presence of shear, reveal rich and complex structures, including strings.

MSC:

76D05	Navier-Stokes equations for incompressible viscous fluids
76M25	Other numerical methods (fluid mechanics) (MSC2010)
65M70	Spectral, collocation and related methods for initial value and initial-boundary value problems involving PDEs
35Q30	Navier-Stokes equations

Keywords:

Cahn-Hilliard equation; Navier-Stokes equations; Phase separation; Model H; Phase separation under shear flow; Interface capturing methods

Software:

FFTW

Full Text: DOI

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