COMPUTATION OF MULTIPHASE SYSTEMS WITH PHASE FIELD MODELS

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Phase fields models offer a systematic physical approach for investigating complex multiphase systems such as near-critical interfacial behavior, phase separation under shear, and microstructure evolution during solidifications. 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 with the addition of the energy equation that constitutes a phase field model for binary fluids with variable mobility, viscosity and thermal diffusivity. The numerical method is a time-split scheme that combines a novel semi-implicit discretization for the convective Cahn-Hilliard equation with state-of-the-art high-resolution CFD 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. The capabilities of the method are demonstrated with several examples including phase separation with and without, shear in two and three dimensions, isothermal and adiabatic turbulent phase separation. 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, involving strings.

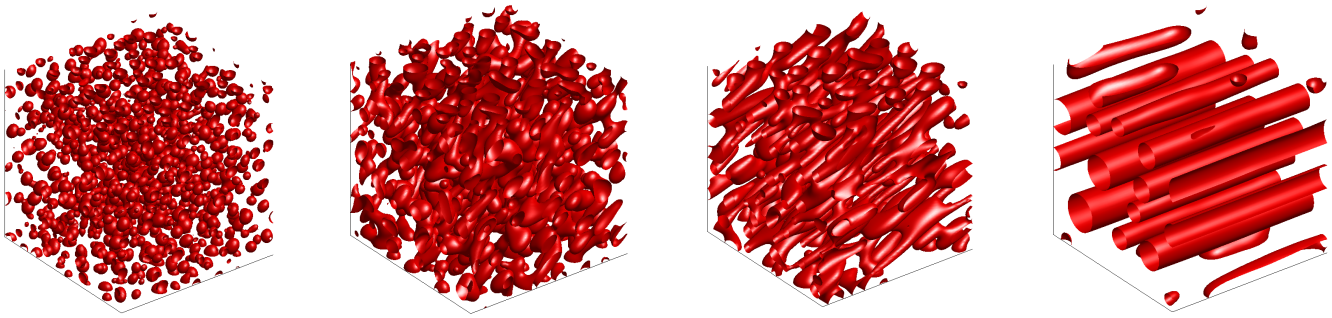

Figure 1: 3D spinodal decomposition in a channel under shear

References

[1] V. E. Badalassi, H. D. Ceniceros and S. Banerjee, "Computation of Multiphase Systems with Phase Field Models", *Journal of Computational Physics*, accepted for publication, 2003.