

Energy stable multigrid method for local and non-local hydrodynamic models for freezing

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Abstract

In this paper we present a numerical method for hydrodynamic models that arise from time dependent density functional theories of freezing. The models take the form of compressible Navier–Stokes equations whose pressure is determined by the variational derivative of a free energy, which is a functional of the density field. We present unconditionally energy stable and mass conserving implicit finite difference methods for the models. The methods are based on a convex splitting of the free energy and that ensures that a discrete energy is non-increasing for any choice of time and space step. The methods are applicable to a large class of models, including both local and non-local free energy functionals. The theoretical basis for the numerical method is presented in a general context. The method is applied to problems using two specific free energy functionals: one local and one non-local functional. A nonlinear multigrid method is used to solve the numerical method, which is nonlinear at the implicit time step. The non-local functional, which is a convolution operator, is approximated using the Discrete Fourier Transform. Numerical simulations that confirm the stability and accuracy of the numerical method are presented.

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1. Introduction

Solid–liquid phase transitions are of great scientific interest. The equilibrium properties of this physical process are fairly well understood in the context of classical density functional theory (CDFT) of freezing [1,2]. This theory characterizes the equilibrium state of a pairwise interacting set of particles in terms of the one particle density field. The density function ρ represents the spatial distribution of particles, i.e., the probability of finding a particle at some point in space. This function at equilibrium is represented as a minimizer of a free energy, which in turn is a functional of the density. At equilibrium this function admits two forms of solutions corresponding to a homogeneous distribution known as the liquid phase and the inhomogeneous distribution known as the solid phase. The inhomogeneous distribution typically consists of peaks located on an ordered Bravais lattice representing the probable locations of

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atoms. This approach is attractive for the reason that the equilibrium solid phase carries the information about the lattice symmetries. A non-equilibrium time dependent theory that characterizes the non-equilibrium distribution has the potential to capture lattice-dependent anisotropic effects such as defect formation and microstructure evolution. Such models have many potential applications in the area of materials modeling. Consequently, the development of time dependent models has been the focus of recent research [3–10].

Given a free energy functional $\mathcal{F}[\rho]$ the simplest dynamical equations for the evolution of the density field are to use gradient dynamics on the free energy surface [3–6]. While this approach is appealing it has several shortcomings including the inability to capture the inertial effects and the effect of flow on the phase transition. Hydrodynamic coupling has been incorporated in models involving colloidal suspensions [7,8] and in models that describe the freezing of a dense hard sphere gas [10]. In all these approaches the hydrodynamic model takes the form of a compressible Navier–Stokes-like equations where the pressure (p) is defined by the equation of state $\nabla p := \rho \nabla \frac{\delta \mathcal{F}}{\delta \rho}$. This can be easily seen from a thermodynamic point of view through the Gibbs Duhem relation $dp = \rho d\mu$ where μ is the chemical potential taken to be the variational derivative of the free energy [8]. Models for hydrodynamic coupling with solid–liquid phase transitions thus take the form

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) &= 0, \\ \partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) &= -\rho \nabla \left(\frac{\delta \mathcal{F}}{\delta \rho} \right) + \gamma \nabla^2 \mathbf{u}, \end{aligned} \quad (1)$$

where $\rho(\mathbf{r}, t) : \Omega \times [0, \infty) \rightarrow \mathbb{R}^d$, $\mathbf{u}(\mathbf{r}, t) : \Omega \times [0, \infty) \rightarrow \mathbb{R}^d$, $\Omega \subset \mathbb{R}^d$, $\mathcal{F}[\rho]$ is a functional of ρ which may be local or non-local in nature, $\gamma > 0$ is a viscosity coefficient and d is the dimension of the system. It is easy to see that the model in Eq. (1) admits an energy

$$\mathcal{E}[\rho, \mathbf{u}] = \frac{1}{2} \int_{\Omega} \rho |\mathbf{u}|^2 d\mathbf{r} + \mathcal{F}[\rho], \quad (2)$$

such that

$$\frac{d\mathcal{E}}{dt} \leq 0. \quad (3)$$

The proof of Eq. (3) is presented in [Appendix A](#). The long time equilibrium for the above system corresponds to $\delta_{\rho} \mathcal{F}[\rho] = 0$, $\mathbf{u} = 0$. Thus the equilibrium properties of the system are determined by the functional $\mathcal{F}[\rho]$ which represents the free energy functional. The specific functional form of the free energy $\mathcal{F}[\rho]$ determines the theory and the phase diagram of the model. One must appeal to CDFT or a similar approximation for the specific form of the free energy.

It is worth noting that the time dynamics of the system however is much richer than a standard gradient descent model [10]. The first set of simulations using this type of model was presented in [10]. It was observed that while the total energy $\mathcal{E}[\rho, \mathbf{u}]$ and the free energy $\mathcal{F}[\rho]$ were non-increasing functions of time, the kinetic energy and the individual components of the free energy were not. However no details about the numerical method were given in [10]. Here, we present the first energy-stable method to solve such coupled systems.

The physical properties and relevance of the model lies in the free energy functional $\mathcal{F}[\rho]$ used. A large number of models for the free energy exist in literature. These models include CDFT [1,2] derived in the framework of equilibrium statistical mechanics, as well as phase field crystal (PFC) models [11], which are derived using phenomenological theories motivated by CDFT. The energy in CDFT is typically a non-local functional of the density while the energy in the PFC is a weakly non-local functional that depends only on gradients of the density. In addition, in CDFT the ideal gas part of the free energy contains a logarithm. In CDFT, the combination of the logarithmic part of the free energy with the nonlocal interaction energy induces much sharper peaks in the density field than the peaks obtained using the PFC model where the logarithmic term is replaced by a polynomial and a gradient approximation is used for the interaction energy (as described in [Appendix B](#)). Thus, the CDFT system requires a finer grid to resolve the dynamics.

These free energy models have been very popular and capture phase transitions at the atomic length scales, but on diffusion time scales, thus enabling the simulation of microstructure evolution at much longer time scales than can be captured using molecular dynamics or other stochastic approaches [11]. This makes the hydrodynamic theory considered here an extremely valuable tool in investigating non-equilibrium effects such as the effect of flow on

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