



Effective macroscopic interfacial transport equations in strongly heterogeneous environments for general homogeneous free energies

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ARTICLE INFO

Article history:

Received 14 February 2014

Received in revised form 18 March 2014

Accepted 18 March 2014

Available online 13 April 2014

Keywords:

Phase field models

Multiscale analysis

Homogenization

Porous media

Wetting

ABSTRACT

We study phase field equations in perforated domains for arbitrary free energies. These equations have found numerous applications in a wide spectrum of both science and engineering problems with homogeneous environments. Here, we focus on strongly heterogeneous materials with perforations such as porous media. To the best of our knowledge, we provide the first derivation of upscaled equations for general free energy densities. In view of the versatile applications of phase field equations, we expect that our study will lead to new modelling and computational perspectives for interfacial transport and phase transformations in strongly heterogeneous environments.

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1. Introduction: phase field formulation in heterogeneous media

Our starting point is the widely accepted diffuse-interface formulation [1] describing the dynamics of interfaces between different phases. This formulation captures different thermodynamic states of a system by a continuous macroscopic variable obtained from averaged microscopic degrees of freedom. Such a macro variable represents a locally conserved order parameter, denoted as ϕ , which defines different phases as local equilibrium limiting values of a free energy associated with the system under consideration.

Diffuse interface formulations show a high versatility which is further extended due to increasing computational power. This leads continuously to new and increasingly complex scientific and engineering applications such as more realistic descriptions for the computation of transport in porous media [2] which represents a high-dimensional multiscale problem with many numerical challenges [3]. Our main result here is the systematic and general derivation of effective macroscopic equations which reliably account for multiple phases invading strongly heterogeneous environments such as porous materials.

The physical basis of the diffuse interface formulation relies on the following class of abstract energy densities:

$$e(\phi) := \frac{1}{\lambda} F(\phi) + \frac{\lambda}{2} |\nabla \phi|^2. \quad (1)$$

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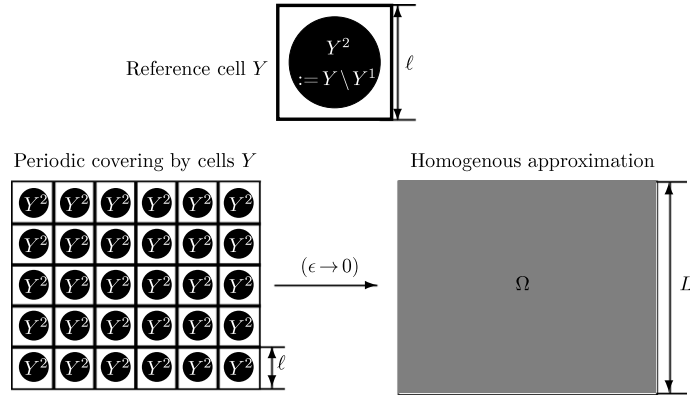


Fig. 1. **Left:** Strongly heterogeneous/perforated material as a periodic covering of reference cells $Y := [0, \ell]^d$. **Top, middle:** Definition of the reference cell $Y = Y^1 \cup Y^2$ with $\ell = 1$. **Right:** The “homogenization limit” $\epsilon := \frac{\ell}{L} \rightarrow 0$ scales the perforated domain such that perforations become invisible on the macroscale.

The free energy density F defines equilibrium phases $\phi_i, i = 1, 2, \dots, M$ as $M \in \mathbb{N}$ local minima and the gradient term $\frac{\lambda}{2} |\nabla\phi|^2$ penalizes the interfacial area between these equilibrium phases. In thermodynamic contexts, F represents the (Helmholtz) free energy density $F(\phi) := U - TS$, where U is the internal energy, T is the temperature, and S is the entropy. Popular examples include the energy of regular solutions (also known as the Flory–Huggins energy [4]). The regular solution theory plays a crucial role in many important applications such as ionic melts [5], water sorption in porous solids [6], and micellization in binary surfactant mixtures [7]. In addition, wetting phenomena, often studied using classical sharp-interface approximations, e.g. [8], are also described by phase-field equations [9–11] which have been extended to include electric fields (so-called electrowetting, e.g. [12]). This energy-functionals based framework has also been applied in image processing such as inpainting, see e.g. [13].

In a previous study [14], we focused on a specific form of the homogeneous free energy density and we recently extended it towards Stokes flow [15]. Here, we provide an upscaling for H^{-1} -gradient flows of arbitrary free energy densities based on a Taylor expansion of the free energy density at the effective upscaled solution. Before we can state our main result, we formulate the basic setting to study general interfacial dynamics.

(a) Homogeneous domains Ω . The total (Ginzburg–Landau/Cahn–Hilliard) energy is defined by $E(\phi) := \int_{\Omega} e(\phi) \, dx$ with density (1) on a bounded domain $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$ and $1 \leq d \leq 3$ denotes the spatial dimension. It is well accepted that thermodynamic equilibrium can be achieved by minimizing the energy E supplemented by a possible wetting boundary contribution $\int_{\partial\Omega} g(\mathbf{x}) \, dx$ for $g(\mathbf{x}) \in H^{3/2}(\partial\Omega)$. Mass conservation for this minimization can be generally achieved with a H^{-1} -gradient flow associated to $E(\phi)$, i.e.,

$$\text{(Homogeneous case)} \quad \frac{\partial}{\partial t} \phi = \operatorname{div} \left(\hat{M} \nabla \left(\frac{1}{\lambda} f(\phi) - \lambda \Delta \phi \right) \right) \quad \text{in } \Omega_T, \tag{2}$$

together with the boundary conditions $\nabla_n \phi := \mathbf{n} \cdot \nabla \phi = g(\mathbf{x})$ on $\partial\Omega_T$, and $\nabla_n \Delta \phi = 0$ on $\partial\Omega_T$, where $\Omega_T := \Omega \times]0, T[$, $\partial\Omega_T := \partial\Omega \times]0, T[$, ϕ satisfies the initial condition $\phi(\mathbf{x}, 0) = \psi(\mathbf{x})$, and $\hat{M} = \{\hat{m}_{ij}\}_{1 \leq i, j \leq d}$ denotes a mobility tensor with real and bounded elements $\hat{m}_{ij} > 0$. This equation serves as a prototype for interfacial dynamics [e.g. [16]] and phase transformation [e.g. [1]] under homogeneous Neumann boundary conditions, i.e., $g = 0$, and free energy densities F .

(b) Heterogeneous/perforated domains Ω^ϵ . Our main focus concentrates on (1) in a perforated domain $\Omega^\epsilon \subset \mathbb{R}^d$ instead of a homogeneous $\Omega \subset \mathbb{R}^d$. The parameter $\epsilon = \frac{\ell}{L} > 0$ is called heterogeneity where ℓ represents the characteristic pore size and L is the macroscopic length of the porous medium, see Fig. 1. Herewith, we can define the porous medium by a reference pore/cell $Y := [0, \ell_1] \times [0, \ell_2] \times \dots \times [0, \ell_d]$. For simplicity, we set $\ell_1 = \ell_2 = \dots = \ell_d = 1$. The pore (Ω^ϵ) and the solid phase (B^ϵ) are defined by

$$\Omega^\epsilon := \bigcup_{\mathbf{z} \in \mathbb{Z}^d} \epsilon (Y^1 + \mathbf{z}) \cap \Omega, \quad B^\epsilon := \bigcup_{\mathbf{z} \in \mathbb{Z}^d} \epsilon (Y^2 + \mathbf{z}) \cap \Omega = \Omega \setminus \Omega^\epsilon, \tag{3}$$

where the subsets $Y^1, Y^2 \subset Y$ are such that Ω^ϵ is a connected set. The set $Y^1 \subset Y$ represents the pore phase (e.g. liquid or gas phase in wetting problems), see Fig. 1. Herewith, we can rewrite (2) as the following microscopic porous media problem:

$$\text{(Micro-pore equation)} \quad \left\{ \begin{aligned} \partial_t \phi_\epsilon &= \operatorname{div} \left(\hat{M} \nabla \left(-\lambda \Delta \phi_\epsilon + \frac{1}{\lambda} f(\phi_\epsilon) \right) \right) \quad \text{in } \Omega_T^\epsilon, \end{aligned} \right. \tag{4}$$

with the boundary ($\nabla_n \phi_\epsilon := \mathbf{n} \cdot \nabla \phi_\epsilon = 0$ on $\partial\Omega_T^\epsilon$, $\nabla_n \Delta \phi_\epsilon = 0$ on $\partial\Omega_T^\epsilon$) and initial ($\phi_\epsilon(\mathbf{x}, 0) = \psi(\mathbf{x})$ on Ω^ϵ) conditions. Our main objective is the derivation of a systematic and reliable homogenized/upscaled phase field formulation valid for

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