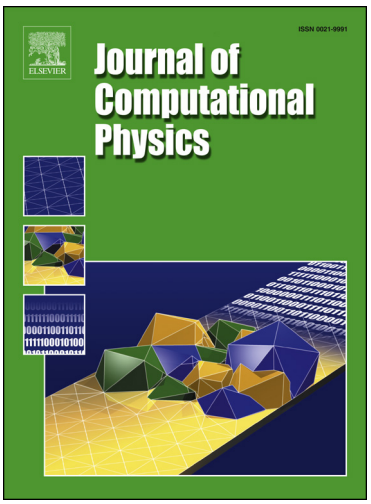
Accepted Manuscript



Computational investigation of porous media phase field formulations: Microscopic, effective macroscopic, and Langevin equations

Antonis Ververis, Markus Schmuck

PII: S0021-9991(17)30353-4
DOI: http://dx.doi.org/10.1016/j.jcp.2017.04.065
Reference: YJCPH 7331

To appear in: *Journal of Computational Physics*

Received date: 31 July 2016
Revised date: 28 February 2017
Accepted date: 26 April 2017

Please cite this article in press as: A. Ververis, M. Schmuck, Computational investigation of porous media phase field formulations: Microscopic, effective macroscopic, and Langevin equations, *J. Comput. Phys.* (2017), http://dx.doi.org/10.1016/j.jcp.2017.04.065

Computational investigation of porous media phase field formulations: microscopic, effective macroscopic, and Langevin equations

Antonis Ververis and Markus Schmuck[1]

Maxwell Institute for Mathematical Sciences and
School for Mathematical and Computer Sciences
Heriot-Watt University
Edinburgh, EH144AS

Abstract

We consider upscaled/homogenized Cahn-Hilliard/Ginzburg-Landau phase field equations as mesoscopic formulations for interfacial dynamics in strongly heterogeneous domains such as porous media. A recently derived effective macroscopic formulation, which takes systematically the pore geometry into account, is computationally validated. To this end, we compare numerical solutions obtained by fully resolving the microscopic pore-scale with solutions of the upscaled/homogenized porous media formulation. The theoretically derived convergence rate $\mathcal{O}(\epsilon^{1/4})$ is confirmed for circular pore-walls. An even better convergence of order $\mathcal{O}(\epsilon^1)$ holds for square shaped pore-walls. We also compute the homogenization error over time for different pore geometries. We find that the quality of the time evolution shows a complex interplay between pore geometry and heterogeneity. Finally, we study the coarsening of interfaces in porous media with computations of the homogenized equation and the microscopic formulation fully resolving the pore space. We recover the experimentally validated and theoretically rigorously derived coarsening rate of $\mathcal{O}(t^{1/3})$ in the periodic porous media setting. In the case of *critical quenching* and after adding thermal noise to the microscopic porous media formulation, we observe that the influence of thermal fluctuations on the coarsening rate shows after a short, expected phase of universal coarsening, a sharp transition towards a different regime.

Keywords: complex heterogeneous systems, phase transition, homogenization, upscaling, coarsening, criticality, universality, porous media, finite elements,
2010 MSC: 00-01, 99-00

1. Introduction

Over the last decades, phase field modelling has received increasing interest for theoretical and computational investigation of physical, chemical and even experimental systems inspired by the work of Cahn and Hilliard [1]. However, the idea of diffuse interface modelling seems to go back to van der Waals [2]. The variational structure based on free energies allows for thermodynamic modelling of phase transitions [3, 4] and it serves as a predictive tool in engineering of fluid mechanics [5], multiphase flow [6, 7, 8], fuel cells [9, 10], batteries [11], and porous media [12]. Since many systems and applications involve strongly heterogeneous media, we refer to these by the general term Complex Heterogeneous Multiphase Systems. From a numerical point of view, strong heterogeneities lead to computationally high dimensional systems since the mesh size $h > 0$ has to be chosen much smaller than the heterogeneity $\epsilon > 0$, i.e., $0 < h \ll \epsilon$. The heterogeneity parameter is defined by $\epsilon = \frac{\ell}{\Lambda}$ where ℓ denotes a material specific microscale, e.g., characteristic pore size, and Λ is the macroscopic size of the porous medium. As a consequence, an effective macroscopic phase field equation has been derived in [13, 14] that does not depend on such a restricting mesh constraint. In fact, a first attempt of extending the framework towards fluid flow is [15] albeit requiring specific assumptions such

[1]Corresponding author. http://www.macs.hw.ac.uk/ ms713/