A theory and challenges for coarsening in microstructure

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Cellular networks are ubiquitous in nature. Most technologically useful materials arise as polycrystalline microstructures, composed of a myriad of small crystallites, the grains, separated by interfaces, the grain boundaries. The energetics and connectivity of the network of boundaries are implicated in many properties across all scales of use. Coarsening is governed primarily by the attempt of the system to decrease the interfacial energy subject to spatial constraints. The recently discovered grain boundary character distribution (GBCD) shows that festures of the configuration texture, and more generally, the boundary network is ordered. We discuss a theory for the evolution of this statistic which bridges mesoscopic scales. It gives rise to many interesting questions and challenges: we still have much to learn about these very ancient questions.

Interfaces in Discrete Environments

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We will discuss some results for interfaces in discrete environment, their pattern formation and dynamics. The discreteness can come from numerical discretization or physical models such as spin systems.

A degenerate Ising model for atomistic simulation of crystal-melt interfaces

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We consider an Ising-type model for a solid-liquid interface. While the standard Ising model admits only second-order phase transitions as one increases temperature, making it a poor choice for modeling the solid-liquid phase transition, a simple modification of the model introduces a first-order phase transition. This is accomplished by weighting one of the two "spin" states more heavily in the partition function, representing the larger entropy of the liquid phase. This model is combined with micro-canonical Monte-Carlo techniques to simulate systems with solid-liquid phase coexistence. The model will first be illustrated in two dimensions using a simple square lattice before presenting results for the face centered cubic lattice and further generalization to partially melted nano-cluster.

Continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries

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We present a continuum framework for dislocation structure, energy and dynamics of dislocation arrays and low angle grain boundaries which may be nonplanar and nonequilibrium. In our continuum framework, we define a dislocation density potential function on the dislocation array surface or grain boundary to describe the orientation dependent continuous distribution of dislocation in a very simple and accurate way. The continuum formulations of energy and dynamics include the long-range interaction of constituent dislocations, local line tension effect of dislocations and the cooperative motion of dislocations, which are derived from the discrete dislocation model. The continuum framework recovers the classical Read-Shockley energy formula when the long-range elastic fields are canceled out. Applications of our continuum framework are presented for dislocation structures on static nonplanar low angle grain boundaries and misfitting interfaces.

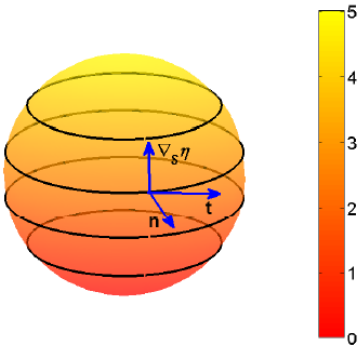

Figure 1: Representation of an array of dislocation loops on a spherical surface using the dislocation density potential function η. The color bar shows the values of η.

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Analysis of force-based multiscale method

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The force based multiscale method that couples together physical models on different scales offer great flexibility for designing consistent multiscale schemes. In this talk, we will study the stability and convergence properties of these schemes. Our result identifies the stability condition for atomistic-to-continuum hybrid method in general dimensions.

Multiscale analysis of non-linear dislocation models

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The discrete, generalized Frenkel-Kontorova (FK) model treats a dislocation line as a chain of nodes, sitting in a periodic lattice potential, interacting through an arbitrarily non-local harmonic force. As the FK model supports a kink mechanism with analytical limits, it has found wide employment since the late 1920s[1].

Despite this popularity, there are very few rigorous results on the transport properties of the FK chain, arguably the main quantities of interest for the dis- location community. In my talk, I will outline a way to derive exact bounds on the transport properties of the FK chain through the novel application of multiscale analysis to the adjont Fokker-Planck equation[2].

It is found that the free energy barrier is always a lower bound to the true finite temperature migration barrier for this general and popular system, an important result for the large community working on such problems. Numerical simulation confirms the analysis, whilst limiting cases provide a connection the results of transition state theory. The application of these techniques to other problems in crystal plasticity will be discussed.

[1] L.Prandtl, J. Appl. Math. Mech. 8, 85 (1928)
[2] T. D. Swinburne, Phys. Rev. E, 88, 012135 (2013)

A parameter identification problem for random heterogeneous materials

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This work is concerned by transport phenomena in porous media, modeled by the Darcy equation. We consider heterogeneous materials, the properties of which are modeled by a random stationary permeability. Based on experimental results, the conductivity, at the microscopic scale, is supposed to be distributed according to a Weibull probability law, the parameters of which are yet unknown. In this work [1], we discuss the identification of the parameters of this microscopic model on the basis of some observed quantities at the macroscopic scale, including the effective (homogenized) permeability.

This is joint work with W. Minvielle, A. Obliger and M. Simon.

[1] F. Legoll, W. Minvielle, A. Obliger and M. Simon, arXiv preprint 1402.0982.

Homogenization of heat diffusion in a cracked medium

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We consider the propagation of heat through a periodic cracked medium, exposed to an incoming energy flux. We assume that the cracks are orthogonal to the surface of the material, where an incoming heat flux is applied. The cracks are supposed to be of depth 1, of small width $\alpha\varepsilon$, ε being the period of the medium and $\alpha \in [0,1)$ is a fixed parameter related to the width of the crack.

Physically, the exchange surface between the medium and the energy source may be greatly modified by the fractures. This may have a significant impact on the energy balance of the considered system. In many situations, the intricacies of the cracked medium are such that it is almost impossible to carry out a direct calculation. Besides, many spatial scales may be involved simultaneously. Full numerical simulations of such multi-scaled media become hence infeasible. That is why we look for an average approach that could capture the effects of cracks in a homogenizedmedium. Themodel presented here is simple enough to be coupled to standard FEM codes. The physical idea behind the model is to treat the flux enhancement induced by the crack as a volume source term in the homogenized energy equation. We show this can be rigorously justified by homogenization theory.

The considered linear diffusion problem reads $\partial_t u_e - \Delta u_e = 0$ with Neumann boundary conditions imposed on the surface of the cracked domain Ω_ε.

We find that, in the limit $\varepsilon \longrightarrow 0, u_e$ is well approximated by the solution of a limit equation of the form $-\Delta u + \partial_t u = \alpha\chi(x)$ where χ is the indicator function of the cracked zone; u evolves in a homogenized domain where the crack is not described anymore. A full mathematical proof as well as numerical illustrations are presented.

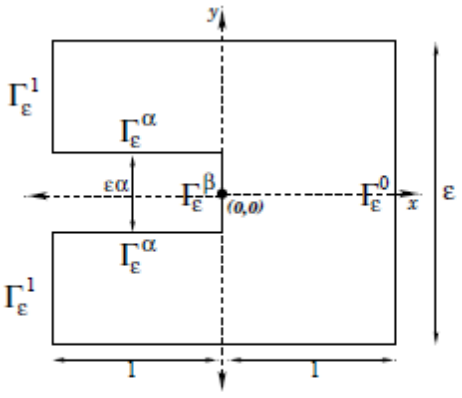

Figure 1: Ω_ε

[1] X Blanc, B-E Peigney, Homogeneization of heat diffusion in a cracked medium, SIAM MMS, 2013, submitted. Preprint on Arxiv at: http://arxiv.org/abs/1305.6071

Multiscale modeling of spin transfer torques in ferromagnetic multilayers

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UCSB

Ferromagnetic multilayers are essential building units for data storage and manipulation. Recent experiments reveal that the existence of a spin current makes ease of magnetization switching and magnetic domain-wall motion. Starting from quantum mechanics, we derive models at different scales for spin dynamics, which is coupled to magnetization dynamics described by Landau-Lifshitz-Gilbert equation. In the hydrodynamic regime, our model recovers the model derived from linear response theory under the assumption of weak spin-magnetization coupling. Quantitative comparison of our model and experimental data will also be presented.