Emerging Interfacial Dynamics

6 January 2010 - 8 January 2010

Workshop Report

This three day workshop intended to showcase recent developments in the formation and evolution of in- terfacial structures in various media, including in elastic crystals, ferrofluids, and granular materials.

The fundamental challenge in the area is to predict, classify and compute features of structures which coexist on different length-scales. The workshop aimed to bring together experimentalists and theoreticians working in these areas, and to take advantage of recent advances in numerical techniques applied to large-scale realistic models.

There were to be six plenary talks, a number of contributed talks, a poster session and a workshop dinner. It was anticipated that travel and accommodation support will be provided for speakers and a limited number of early career researchers. The workshop was funded jointly by the Oxford Centre for Partial Differential Equations (OXPDE) and the Institute for Advanced Studies, Surrey.

The workshop was held on the 6th January - 8th January 2010. On the 5th-6th January, Guildford experienced significant snowfall causing widespread disruption in terms of transport to the University of Surrey. In particular, Gatwick and other airports were closed on the 6th January. Despite the disruption, only three speakers cancelled and we therefore decided to proceed with the workshop. The speaker cancellations allowed more space in the programme for discussions. Unfortunately, the co-organiser Jon Bevan and departmental administrator were unable to make it to the university campus.

Despite the weather, there were 12 attendees at the workshop, from the Czech Republic (1), USA (2), Germany (2), UK (7). Eight talks were presented, summarised below.

Papers

Elaine Crooks (Swansea) opened the workshop by discussing interfacial energy in a phase-transition model. This is a simple way of incorporating interfacial energy into variational solid-solid phase transition models. The widely accepted model for such phase transitions is predicated on minimizing a stored energy functional whose properties depend on the elastic material under consideration. The approach described by Crooks consists in perturbing this energy functional by adding a term involving second gradients of the deformation. Such perturbations are well-known to yield the benefit over purely elastic energy minimization of predicting a length-scale for fine-scale mixtures of phases. Crooks also discussed further consequences of such higher- gradient perturbations for interfaces between gradients lying in two distinct energy wells, and for local minimizers.

Nicolas Dirr (Bath) spoke on the motion of interfaces through random obstacles in heterogeneous media. The interface motion is modelled by a parabolic stochastic partial differential equation with a randomly varying nonlinear right hand side, representing the field of inhomogeneities in the material. The same fixed shape was assigned to each inhomogeneity; the randomness entered by making their centres and relative strengths subject to given probability laws. The model considered was related to a quenched Edwards-Wilkinson model, which describes a form of flow by mean curvature. Using the PDE Dirr then gave examples of so-called pinned interfaces, which could then be related to observed hysteresis in the physical model. Graeme Henkelman (Texas at Austin) discussed accelerated molecular dynamics simulations at surfaces. Henkelman presented the Nudged Elastic Band algorithm and the Dimer algorithm to numerically locate transition states or saddles of high-dimensional energy functionals. These methods were then applied to a carbon oxidation problem on a gold surface.

Karsten Matthies (Bath) discussed travelling waves in a quasilinear plasticity model. A reduction of a model of Field Dislocation Mechanics to a scalar problem in one spatial dimension was considered. The aim of the work was to show the existence of static and slow, rigidly moving single (or collections of) planar screw dislocation walls in this simplified setting. Two classes of drag coefficient functions were considered, namely those with linear growth near the origin and those with constant or more generally sublinear growth there. Matthies gave a pleasing mathematical characterisation of all possible equilibria of these screw wall microstructures was given. It was also shown that nontrivial travelling wave solutions existed in only one of the cases studied, corresponding to a drag coefficient function with linear growth; sublinear growth precluded such solutions.

Christof Melcher (Aachen) spoke about the motion of magnetic domain walls. The motion of a domain wall is a fundamental mechanism in the dynamics of ferromagnetic patterns. The dynamics of a magnetization distribution in a ferromagnetic material as described by the Landau-Lifshitz-Gilbert equation, is basically a damped precession of the magnetization vector about the effective field stemming from the micromagnetic energy. Melcher discussed the interplay between nonlocal stray-field interaction as an energetic force and gyromagntic precession as a dynamic force giving rise to oscillatory phenomena and an effective viscous Newtonian motion law.

Josef Otta (West Bohemia) talked about the Quasilinear Dirichlet Bistable Equation. The uniqueness results for positive solutions were shown by the Picone identity arguments and the strong maximum principle. The existence of saddle-point type solutions was proved by a standard variational method employing uniqueness of positive solutions. Otta then showed numerical experiments that illustrated the solution dependence on the equation parameters.

Bernd Schmidt (TU Munich) spoke about minimizing atomic configurations of short range pair potentials in two dimensions and its relation to crystallization in the Wulff shape. The starting point for this analysis was a study of the ground state configurations of certain atomic systems in two dimensions. As is customary in atomistic to continuum modelling the number of atoms was allowed to tend to infinity subject to suitable pair interactions. When rescaled appropriately, these configurations were shown to crystallize on a triangular lattice and to converge to a macroscopic Wulff shape which could be obtained from an anisotropic surface energy induced by the microscopic atomic lattice. This represented a significant step forward in the theory. Moreover, Schmid also gave details of how sharp estimates on the microscopic fluctuations about the limiting Wulff shape were obtained.

Aaron N. K. Yip (Purdue University) discussed analytical aspects of singular perturbation and bifurcation of transition layers. Yip began by showing that connections between diffused and sharp interfacial problems in the variational setting are well developed to a large extent by means of Gamma-convergence and also by purely analytical techniques such as asymptotic expansion and the implicit function theorem. In particular, these techniques underpin our understanding of global minimizers and non-degenerate critical points. The speaker went on to describe some results which extend the above framework to analyze the degenerate case, in particular the bifurcation of a diffused interface and its connection to the sharp interfacial limit. Examples of the Allen-Cahn Equation with parameter dependent spatial inhomogeneity were investigated.

Workshop themes

The workshop illustrated the variety of techniques available to us in furthering our understanding of and ability to model complex physical systems where the motion of interfaces plays an important role. The approaches taken by the speakers reflected this variety within the broader area of interfacial dynamics:

- talks ranged from variational analyses in the deterministic setting (Melcher, Yip, Otta) to the stochastic modelling of interface motion (Dirr, Henkelman);
- a complementary strand focussing on dynamics and travelling wave type solutions included Crooks and Matthies;
- a highly successful application of an atomistic-to-continuum method was demonstrated by Schmid.

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