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Mini-Workshop: Anisotropic Motion Laws

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Abstract. Anisotropic motion laws play a key role in many applications ranging from materials science, biophysics to image processing. All these highly diversified disciplines have made it necessary to develop common mathematical foundations and framworks to deal with anisotropy in geometric motion. The workshop brings together leading experts from various fields to address well-posedness, accuracy, and computational efficiency of the mathematical models and algorithms.

Mathematics Subject Classification (2000): 53C44, 35K55, 37E35.

Introduction by the Organisers

During the past half-centure much activity among mathematiciants, material scientists and mechaniciants has been done concerning interface problems. Besides the describing equations in the bulk phases, such problems generally result in an extra interface condition. The simplest examples of such interface equations are due to Mullins and include motion by mean curvature

$$v = -\kappa \tag{1}$$

and motion by surface diffusion

$$v = \Delta_S \kappa \tag{2}$$

with v the scalar normal velocity, κ the mean curvature of the interface and Δ_S the surface Laplacian. Due to recent technolocical trents especially in semiconductor and bio-technology towards nanometer scale applications these problems gain more and more attention. As we approach smaller and smaller scales the influence of the interface compared to the bulk phases increases and already dominates in applications such as quantum-dot formation during epitaxial growth, electromigration

of voids in metal interconnects or motion of vesicles. To provide a theoretical imput for such applications material specific parameters concerning their anisotropy have to be considered in these equations. The goal of this workshop was to deal with the arriving theoretical and numerical difficulties by considering anisotropic interface equations.

To avoid geometrical complications associated with surfaces in three-dimensional space we describe the anisotropic equations in two space dimensions. The Mullins equations now read

$$bv = -(\psi_0 + \psi_0'')\kappa \tag{3}$$

and

$$\rho^2 v = \partial_s(L\partial_s((\psi_0 + \psi_0'')\kappa) \tag{4}$$

with $b = b(\theta)$ a kinetic modulus, depending on the angle θ, $\psi_0 = \psi_0(\theta)$ the free energy density, ρ the bulk density, $L = L(\theta)$ the mobility function and ∂_s the derivative with respect to the arc length. Both equations result from a free energy of the form $E = \int_\gamma \psi_0(\theta)ds$, by assuming ψ_0 to be smooth. For $\psi_0 + \psi_0''$ nonnegative the two problems are well-posed. Under these assumptions the problems can be treated similarly to the isotropic case by considering the weighted curvature $(\psi_0 + \psi_0'')\kappa$ as an unknown.

If $\psi_0 + \psi_0''$ becomes negative for certain orientations, the equations (3) and (4) become backward parabolic. Free energy densities which lead to such ill-posdness are of relevance in thermal facetting during thin film growth. Following DiCarlo, Gurtin and Podiudugli one can deal with such anisotropies by allowing the free energy density $\psi = \psi(\theta, \partial_s\theta)$ to depend also on higher order terms. In the simplest form the free energy now reads $E = \int_\Gamma \psi_0(\theta) + \frac{\epsilon}{2}\kappa^2 ds$, with ϵ introducing a new length scale, which smears out corners in the equilibrium shape. The added Willmore term κ^2 can be viewed in a similar way as the gradient term in the Cahn-Hilliard theory. The resulting equations are

$$bv = -(\psi_0 + \psi_0'')\kappa + \epsilon(\partial_{ss}\kappa + \kappa^3) \tag{5}$$

and

$$\rho^2 v = \partial_s(L\partial_s((\psi_0 + \psi_0'')\kappa) - \epsilon(\partial_{ss}\kappa + \kappa^3)). \tag{6}$$

Only recently numerics are performed for these equations in a front-tracking, level-set and phase-field ansatz. Even if all these approaches provide reasonable results, theoretical arguments make it questionable if the added Willmore functional is enough to prevent the formation of corners during the evolution in three dimensions. Higer order term resulting from a free energy density $\psi(\theta, \partial_s\theta, \partial_{ss}\theta, \ldots)$ might be necessary to provide a smooth curvature.

A second interesting class of problem arises if ψ_0 is not smooth. In this case the geometric evolution laws can not even be written in the formulation (3) and (4) but rather have to be formulated in a way, which only contains the first derivative of ψ_0. Such anisotropies arise for crystalline materials, with facets in the equilibrium shape. Numerical approaches for geometric evolution laws with such anisotropies

have recently been considered again in a front-tracking, level-set and phase-field approach. In all approaches the idea is basically a weak formulation of the problem, which only needs the first derivative of ψ_0. Analytical results for such anisotropies are rare.

A third class of interface problems of recent interest, results from applications in surface science, where in addition to the evolution of the interface also processes, such as diffusion or decomposition on the evolving surface plays a dominant role. In addition to the evolution of the surface a PDE on the evolving surface has to be solved, which might influence its evolution. Such problems arise for example in the description of biomembranes and have only recently been proposed and numerical investigations are still rare. Theoretical results on evolution laws on evolving surfaces are still limited but definitely necessary for the development of an efficient numerical approach.

In all these classes the exact functional form of the anisotropy is not known for most materials. Only recently material specific quantities $\psi_0 + \psi_0''$ have been computed from first principles or have been derived from coarse grained atomistic models. The research on anisotropic motion laws is not restricted to mathematics, instead it is largely driven by applications. However, we believe mathematical research to play a key role in the development of the necessary theoretical and numerical approaches to deal with anisotropic motion laws and thus to be a key ingredient for many applications on nanometer length scales in materials science and biotechnology.

The focus of this workshop was to bring together the leading materials scientists, physicists and mathematicians in the field of anisotropic surface evolution. Besides the mathematical aspects of modeling, analysis and simulation of anisotropic geometric evolution laws also the connection to experimental results and ab initio computations was dealt with to drive the recent theoretical developments on anisotropic geometric evolution laws into a direction which is relevant for a large variety of applications. Ab initio calculations of material specific anisotropy functions and measurements of equilibrium shapes on a nanometer scale are only recently available and the discussion on the right functional form of the anisotropy is still controversary.

The workshop started with introductory lectures on classical isotropic geometric evolution laws, such as mean curvature flow, surface diffusion and Willmore flow in which analytical as well as numerical results have be discussed. After introducing the different sources of anisotropy in these models the main part of the workshop started with recent results on higher order evolution laws, resulting from curvature dependent surface free energies. Front tracking, phase field and level set methods were discussed for these equations. Further talks dealed with crystalline anisotropies and their analytical and numerical treatment in geometric evolution laws as well as work on evolution laws including species transport along the surface. In the last part of the workshop several applications from image processing, materials science and biophysics were discussed.