Advanced Developments for Surface and Interface Dynamics - Analysis and Computation 18w5033

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1 Overview of the workshop themes

This workshop focused on advanced topics involving interfaces, thin domains around them and free boundary problems. These geometric objects are governed by nonlocal, singular or anisotropic motion laws. A particular topic was the partial differential equations (PDEs for short) defined in thin domains around moving interfaces. Effective numerical algorithms for simulating these problems was another leading theme of the workshop.

Some of the top specialists in analysis and numerical methods came to discuss recent advances in above mentioned problems and to present the state of the art both in analysis and numerical computations. The goal was to improve our understanding of the surface and interface dynamics. Below we present the overview of the presentations.

Nonlocal, anisotropic and degenerate diffusions equations The following groups of topics have been discussed during the workshop.

- PDE with singular diffusivity. Among the typical examples are total variation flows for denoising images or anisotropic curvature flows with very strong anisotropy such as crystalline curvatures. These flows describe motion of free surfaces. In these problems motion of surfaces is determined by nonlocal quantities which cannot be written in an explicit way. Even these relatively accessible problems analysis are nontrivial and have been studied for many years. However, if one considers more realistic problems like crystal growth models with general Wulff shape having facets, multi-grain problems or higher order problems involving crystalline mean curvature, mathematical tools are still limited.

  One method to treat these problems is the theory of viscosity solutions, whose scope of applicability is widening. It is based on comparison principle, hence it is restricted to formally 2nd order problems.

  The variational approach presents possibilities of developing another set of methods. But these methods have limitations since they require special structure of the variational models.

  Of course, there is a diffuse interface approach represented by use of reaction diffusion equations. However, the relation to sharp interface approach given above is often not clear, especially for multi-grain problems in materials science.

- Stefan problem with fractional time derivatives. Although the fractional diffusion equations have been studied, the problem of Caputo fractional time derivative is less developed and even simple questions, e.g. concerning existence of solutions, are outstanding. The nonlinear theory that is capable of handling this kind of free boundary problems (e.g. for the position of the head of fluvial sediments) is yet to be developed.

- Modeling and simulating crystal growth. This topic encompasses large networks of grains of different orientations, with grain boundaries moving according to certain notion of curvature.

Numerical algorithms The methodologies discussed in this workshop encompass non-parametric sharp interface models, such as level set methods or the closest point methods, and diffuse interface methods involving phase field approximation. However, the challenges presented in the problems discussed above require non-trivial mathematical formulations before one can apply the standard methodologies and careful numerical approximations in some cases to derive well-conditioned discrete systems.

Topics that have been discussed in this workshop include:

- Generalization of ℓ_1 optimization, augmentation and splitting based approaches for efficient accurate computation of singular diffusion problems.

- Numerical methods for PDEs on manifolds or thin domains around them. There has been significant development in numerical algorithms for PDEs or integral equations on implicitly or non-parametrically defined surfaces. These methods transform equations defined on surfaces into ones defined in thin tubular neighborhoods of the surfaces, and have great potential in dealing with data in the form of point clouds (e.g. surfaces sampled by a finite point set and values of data given on the point set).

- Numerical methods for simulating large network of interfaces and junctions. The leading question is: How to compute junctions under anisotropic motion laws?

2 Recent Developments and Open Problems

PDEs with singular diffusivity. Progress has been made in several directions within this area. For example, the level-set method is extended to crystalline mean curvature flow in an arbitrary dimensional Euclidean space. Two approaches are presented, one is by A. Chambolle and the other is by N. Požár.

The first method is based on the signed distance function and it applies to a class of evolution problems where the velocity of the interface depends on crystalline mean curvature linearly. In paper [2] the following problem is studied $V = \gamma H_\gamma$, where γ is the surface energy density and H_γ is the anisotropic mean curvature of the surface. The advantage of the approach used by Chambolle is that it applies to a general interfacial energy, see [3].

The second approach is based on the theory of viscosity solutions. It applies when the speed of the interface depends monotonically on the curvature but so far it is restricted to a purely crystalline energy. However, the applicability of both approaches is still limited to the second order problems, because they depend on the comparison principle, see [9], [10].

Several lectures on the recent development of a few versions of the total variation flow were presented during this workshop. One of them was the presentation by P. Mucha, who discussed the anisotropic total variation flow with the ℓ_1 norm anisotropy. Another one was the talk of M. Muszkieta, in which results on the higher order total variation flow with several numerical computations were given.

I. Kim addressed a surprisingly difficult but easy to state problem of preserving the star shape property of sets by the mean curvature flow. This problem remains open.

Stefan problem with fractional time derivative. V. Voller presented an array of problems arising in engineering which fall into the broadly understood anomalous diffusion. This area is rich with problems waiting for rigorous analysis. One of them was studied by T. Namba. He presented an extension of the notion of viscosity solutions to equations with Caputo time fractional derivatives.

Modeling and simulating crystal growth. D.Margetis and J.-G.Liu presented recent development on modeling crystal growth by a high order partial differential equation with exponential nonlinearities. They also offered the analysis of such a high order model, see [13].

S.Esedoglu presented a novel variational formulation for large network of grains with boundaries modeled by different anisotropic interface energies. Based on the new variational formulation, threshold dynamics algorithms with judiciously chosen, averaging kernels are developed. The approach to formulate variational principles and the related algorithms that uses threshold dynamics lead to a wide range of applications involving multiphase problems, see [5], [6].

Numerical algorithms Developments of new algorithms for surface partial differential equations were presented in this workshop. They require extensions of the surface PDEs into a thin tubular neighborhood of evolving smooth surfaces. B. Stinner and K. Decklenick presented algorithms that use a phase field formulation. J. Chu and C. Kublik talked about methods that use an extension approach preserving certain properties of the given equations and integrals. C. Kublik also discussed new work in computing integrals on Lipschitz surfaces, see [4], [12]. A graduate student K. Taguchi gave a new numerical scheme for constrained total variation flow, [18].

Even if we witness progress in several directions, still special variational structure is necessary for advancing studies of these problems.

Other related topics José Mazon presented a development of the theory of harmonic functions and the diffusion equations on graph and metric spaces without any obvious differential or linear structure. This seems to be a new exciting direction. We will present it in more details below.

Juan Manfredi talked about the integral formulas for solutions to the p-Laplace equations. This topic is linked to the stochastic game theory. More details are given below.

3 Presentation Highlights

We present below ten lectures lectures which are representative of the Workshops main themes.

Mazón: Heat Flow on Metric Random Walk Spaces

The speaker presented results, in the context of "metric random walk spaces", see [16], on

- Ergodicity
- Functional Inequalities and Curvature (such as Poincaré inequality, its relation to isoperimetric inequality, Bakry-Emery curvature)
- Transport inequalities

A random walk m on X is a family of probability measures m_x such that

1. they depend measurably on x;
2. each measure m_x has finite first moment (with respect to the distance).

A metric random walk space is a Polish space equipped with such a random walk. One also has the detailed balance condition,

$$dm_x(y)d\nu(x) = dm_y(x)d\nu(y).$$

Example: in R^N we take a $J \geq 0$ with total mass 1, then we set

$$m_x^J(A) = \int_A J(x-y)dx,$$

where dx is the Lebesgue measure.

Ollivier-Ricci curvature. In Riemannian geometry, positive Ricci curvature is characterized by the fact that "small balls are closer, in the 1-Wasserstein distance, than their centers are". In the framework of metric random walk spaces, inspired by this, Y. Ollivier (JFA 2009) introduces the concept of *coarse Ricci curvature* changing the ball by the measures m_x.

First, we recall the Monge-Kantorovich problem and the Wasserstein distance.

Definition: Take $x, y \in X$, the Ollivier-Ricci curvature of (X, d, m) along (x, y) is defined as

$$\kappa_m(x, y) := 1 - \frac{W_1^d(m_x, m_y)}{d(x, y)},$$

where W_1^d is the 1-Wasserstein distance with respect to the metric d.

The Heat Flow. Let (X, d, m) be a metric random walk space with invariant measure ν for m. For a function $u : X \to \mathbb{R}$ its nonlocal gradient is

$$\nabla u(x, y) = u(y) - u(x),$$

it is a function in $X \times X$. Likewise we define the m-divergence of a function in $X \times X$

The averaging operator is

$$M_m f(x) := \int_X f(y) dm_x(y)$$

and the m-Laplace operator $M_m - I$. If the invariant measure ν is reversible, the following integration by parts formula is straightforward

$$\int_X f(x)\Delta_m g(x)\, d\nu(x) = -\frac{1}{2}\int_{X\times X} (f(y) - f(x))(g(y) - g(x))\, dm_x(y)\, d\nu(x).$$

This gives rise to a symmetric form, $\mathcal{E}_m$.

Theorem: Let (X, d, m) be a metric random walk space with invariant and reversible measure ν for m. Then $-\Delta_m$ is a non-negative self-adjoint operator in $L^2(X, \nu)$ with associated closed symmetric form $\mathcal{E}_m$, which is Markovian.

The associated continuous semigroup T_t^m solves the associated heat equation.

Infinite speed of propagation and ergodicity The infinite speed of propagation of the heat flow $e^{t\Delta_m}$, i.e.,

$$e^{t\Delta_m} u_0 > 0 \text{ for all } t > 0$$

occurs, whenever $0 \leq u_0 \in L^2(X, \nu)$ and $u_0 \neq 0$.

Consider $\Omega = (-\infty, 0] \cup [\frac{1}{2}, +\infty) \times \mathbb{R}^{N-1}$ and the metric random walk space $(\Omega, d, m^{J,\Omega})$, where d is the Euclidean distance and $J(x) = |B_1|^{-1}\chi_{B_1}$. This space has Ollivier-Ricci curvature κ, which is negative.

We now introduce the *m-total variation function*,

$$\frac{1}{2}\int_X \int_X |u(y) - u(x)| dm_x(y) d\nu(x).$$

Therefore, we define the concept of m-perimeter of a ν-measurable subset $E \subset X$ as the m-total variation of the indicator function of E. In the particular case of a graph, this gives the classical definition of a set.

Theorem: If (X, d, m) is a metric random walk space with invariant and reversible measure ν, and $\nu(X) < \infty$, then the following facts are equivalent:

1) Δ_m is ergodic;

2) $\Delta_m \chi_D = 0$ implies χ_D is constant;

3) $P_m(D) > 0$ for every set such that $0 < \nu(D) < \nu(X)$.

Functional inequalities and curvature Let us assume ν is a probability measure. We define the mean and the variance of a function f. Then, we define the spectral gap.
Definition: We say (m, ν) satisfies a Poincaré inequality if there is a $\lambda > 0$ such that

$$\lambda \text{Var}_\nu(f) \leq \mathcal{H}_m(f).$$

There is an example of an infinite, weighted linear graph, which does not satisfy the Poincaré inequality.

Remark: Ollivier showed a Poincaré inequality under certain assumptions on the Ricci-Ollivier curvature. The Poincaré inequality at the level of sets implies the following isoperimetric inequality

$$\min\{\nu(D), 1 - \nu(D)\} \leq \frac{2}{\lambda} P_m(D).$$

Question: P. Rybka asked about the motivation for studying these problems?

Question: What about Lévy processes? Some cases are covered, but not all: the integrability at infinity becomes an issue – e.g. the process corresponding to the standard fractional Laplacian in $\mathbb{R}^d$ is covered by the theory.

Manfredi – A discrete stochastic interpretation of the dominative p-Laplacian

Dominative p-Laplacian is defined by

$$\mathcal{L}_p u(x) = \frac{1}{p}(\lambda_1 + \ldots + \lambda_{N-1}) + (p-1)/p\lambda_N,$$

where $\lambda_1 \leq \ldots \leq \lambda_N$ are the eigenvalues of $D^2 u(x)$. The speaker discussed the relationship between $\mathcal{L}_p$ and the regular p-Laplacian, which the topic of a recent paper, [15].

The ordinary p-Laplacian $\Delta_p^h u$ is given by the formula $\text{div}(|\nabla u|^{p-2}\nabla u) = |\nabla u|^{p-2}\Delta_p^h u$. It is is not difficult to show, (Brustad, 2017), that $\Delta_p^h u \leq p\mathcal{L}_p u$ with equality for radial functions.

Mean values

$$MV_q(v, B_\varepsilon(x)) = \frac{1}{q-1}\frac{1}{|B_\varepsilon|}\int_{B_\varepsilon(x)} v(y)dy + \frac{q-2}{q-1}\sup_\sigma \frac{v(x+\varepsilon\sigma(x)) + v(x-\varepsilon\sigma(x))}{2},$$

where σ is what is called a strategy, $q = (p + 4n + 6/2N + 4)$. What is important is to know this for $p = 2$ and for $p \to \infty$

If $\mathcal{L}_p v(x)$, we have the asymptotic mean value property

$$v(x) = MV_q(v, B_\varepsilon(x)) + o(\varepsilon).$$

Fix $x_0 \in \Omega$ and a strategy σ. We will consider a discrete process

$$x_0, x_1, \ldots$$

defined as follows: If $x_0 \in \Gamma_\varepsilon$, we set $x_1 = x_0$ and stop. Otherwise, $B_\varepsilon(x_0) \subset X$. In the latter case, we move one step according to the following rules:
- with probability $1/(q-1)$ select $x_1 \in B_\varepsilon(x_0)$ at random;
- with probability $(q-2)/2(q-1)$ select $x_1 = x_0 + \varepsilon\sigma(x_0)$;
- with probability $(q-2)/2(q-1)$ $x_1 = x_0 - \varepsilon\sigma(x_0)$.

Then, we consider the pay off function associated to the strategy σ,

$$u_\varepsilon^\sigma(x) = E_\sigma^{x_0}[F(x_{\tau_\sigma})],$$

which we call the ε-stochastic solution.

Theorem: Stochastic solution = mean value solution.

"The interesting thing (to me) is that one can actually prove that something satisfies the dynamic programming principle."

One uses the idea of Barles-Souganidis from 1991, exploiting the upper and lower semicontinuous envelopes.

Question by R.Choksi: What was the original motivation of Brustad?
Manfredi: It may have come from the motivation of explaining that result about the sum of p-superharmonic radial functions, the original proofs of which were quite complicated.

Stinner: On a diffuse interface approach to PDEs on surfaces and networks

This is a recent work, performed with the following applications in mind: cluster formation in different situations (cell clusters, foam and bubble clusters, grain boundaries).

These problems led to PDEs on those interfaces. Triple junctions are an important issue. Our approach is a phase field method. We shall describe these interfaces by thin layers. The phase field methodology boils down to the introduction of a bulk phase field $\varphi(t) : \Omega \to \mathbb{R}$, going from 1 to -1 on a strip of size that can be shown to be $\sim \varepsilon$. We look at

$$F^\varepsilon = \int_\Omega \tilde{K}_w(\frac{\varepsilon}{2}|\nabla\varphi|^2 + \frac{1}{\varepsilon}W(\varphi)) \text{ as } \varepsilon \to 0.$$

Example: PDE on an evolving surface $\Gamma(t)$, with material velocity $v(t) : \Gamma(t) \to \mathbb{R}^n$

$$\partial_t^\bullet c + c\nabla_\Gamma \cdot v = D^{(\Gamma)}\Delta_\Gamma c + r(c) \text{ on } \Gamma(t),$$

where $\partial_t^\bullet$ is the material derivative.

Idea: smoothing using the phase field with some $\delta_\varepsilon(\varepsilon_\varepsilon) \to \delta_\Gamma$ as $\varepsilon \to 0$. Rigorous convergence analysis as $\varepsilon \to 0$ ($\{\delta_\varepsilon\}_\varepsilon$ given): Elliot - S 2008, Abels - Lam - S 2015, Burger-Elvetun-Schlottbom 2016, Miura 2017.

PDEs on bubble clusters Domains $\Omega^{(i)}(t)$ separated by interfaces $\Gamma^{(i,j)}(t)$ meeting at triple junctions $T^{(,j,k)}(t)$ transported by a continuous solenoidal velocity field v. Species densities: $c^{(i,j)}, \Gamma^{i,j}$. The speaker presented definitions of "Energy", "Chemical potentials" for the system. The potentials drive the evolution of the system.

We approximate the resulting equations in distributional forms with a phase field. Phase variable $\varphi^{(i)}$ for phase i. A constraint: they add up to 1.

A key assumption: along the layer between i and j only φ^i and φ^j are present.

Phase field Ansatz

$$\delta_{\Gamma^{i,j}} \sim \delta_{i,j} = C_\delta \frac{1}{\varepsilon}(\varphi^i, \varphi^j)^2,$$

$$\tau_{T^{i,j,k}} = C_\tau \frac{1}{\varepsilon^2}(\varphi^i\varphi^j\varphi^k)^2.$$

In practice: the phase fields themselves solve PDEs that depend on the surfaces. One must also bear in mind additional conditions in practical applications such as Young's law. This becomes a problem, because we may need this information to calibrate C_τ (the exact form of C_τ may depend on extra modeling assumptions involving higher order terms).

Question: Can you do quadruple junctions?
Answer: No, conceptually probably you could set them up. In the applications I am interested in, they are not stable, so you do not see them.

Question: For the computations, did you do a moving mesh?
Answer: No, we used an adaptive algorithm concentrating in an ϵ neighborhood of the interface.

Kublik: Applications of distance functions to motions of curves in the plane, and integration over interfaces and unstructured point sets

We are working on a general framework for integrating over interfaces which are implicitly defined. The first part of the talk discussed an MBO (Merriman-Bence-Osher) scheme for two-dimensional area preserving motion by curvature. The normal velocity is

$$v_N = \kappa - \bar{\kappa},$$

where $\bar{\kappa}$ is the average of the curvature on the curve, when if the curve is simply connected. Otherwise, a modified expression is necessary which depends on the number of "holes". A similar thresholding scheme can be used here – the modification arising in the diffusion step.

In the second half of the talk, the speaker discussed a simple, efficient, scheme for computing such boundary integrals. The context is that the boundary is not defined by an specific parametrization (e.g. boundaries evolving in time, with possible changes in the topology). The presented strategy is to derive a volume integral around a tubular neighbor of the interface that is identical to the given integral along the interface. The idea is to approximate the integral over Γ, via an integral over Γ_η, where Γ_η is a properly chosen nearby surface Γ_η is given by a level set of the distance function,

$$\int_\Gamma v(z) dS(z) = \int_{\Gamma_\eta} v(P_\Gamma(y)) J_\eta dS_\eta(y),$$

where $P_\Gamma(y)$ is the closest point mapping to Γ. We have that J_η is a polynomial in η $J_\eta = 1 + \eta\kappa$ in 2D (similar formula in 3D). Then, averaging and using the co-area formula, we obtain a volume integral representation of the surface integral, (K-Tanushev-Tsai, 2013). The Jacobian $J(x)$ can be computed from the singular values of the Jacobian matrix of the closest point mapping P_Γ. This offers additional convenience for computation of J and interpreting it, especially for manifolds with boundaries.

The speaker further discussed: (i) how integration along curves with corners and surfaces with creases could be computed accurately by the proposed methodology, but with more elaborate averaging kernels, and (ii) analysis of the algorithm when applied to analyze finite point set that are sampled from manifolds of different Hausdorff dimensions.

Kim: Volume preserving mean curvature flow with start-shaped sets

The speaker considers motion with normal velocity given by,

$$V = -\kappa + \bar{\lambda}_t \text{ on } \Gamma_t = \partial\Omega_t$$

with λ_t such that $\int_{\Gamma_t} V = 0$, so the volume is preserved. Ω_t is assumed to have smooth boundaries and

$$\lambda_t = \frac{1}{\text{Per}(\Omega_t)} \int_{\Gamma_t} \kappa d\sigma.$$

This motion converges exponentially to the sphere (smooth, convex flow). Studies of existence of solutions but uniqueness is open.

Most people care about convex sets and the flow is known to preserve convexity. Also, the curve can undergo topological changes in finite time.

Question: Are there other geometries that are preserved by the flow (other than convexity)? The star-shapedness is expected to be preserved.

The speaker then introduced a strong version of star-shapedness, called ρ-reflection. It turns out that this property is preserved by the motion. To study the flow, we need a notion of weak solution because the flow may develop singularities. The speaker uses two techniques:

1. Notion of a viscosity solution to enable barrier arguments;
2. Variational approach to obtain energy estimates.

The flow considered is the gradient flow for Per(F), the perimeter of the set F, over sets of fixed volume (say 1). The speaker uses minimizing movement to construct the flow. This requires minimizing

$$\text{Per}(F) + \frac{1}{h}\tilde{d}^2(F, E),$$

where E is the set from the previous set and F the current one.
Discrete scheme. Approximate energy:

$$\text{Per}(E) + \frac{1}{\delta}(|F| - 1)^2 + \frac{1}{h}\tilde{d}^2(F, E).$$

When you minimize it, you get a discrete flow $\Omega_t^{\delta,h}$ that converges to the δ-flow with normal velocity,

$$V = -\kappa + \lambda_\delta(|F|), \quad \lambda_\delta(s) = \frac{2}{\delta}(s - 1).$$

This is the δ-flow Ω_t^δ. Now, the speaker uses a modified viscosity-type argument to show that the strong star-shapedness property is preserved. She needs to investigate the convergence of the δ flow.

Result: $\Omega_t^{\delta,h} \to \Omega_t^\delta$ as $h \to 0$ and $\Omega_t^\delta \to \Omega_t$ as $\delta \to 0$. Regularity of δ-flow: the boundary of Ω_t^δ can be locally represented by a Lipschitz graph.

Last result: Assume Ω_t is star-shaped, smooth, preserves volume over time. Then Ω_t is the unique solution of the motion with normal velocity,

$$V = -\kappa + \bar{\lambda}_t,$$

and Ω_t converges exponentially fast to a unit ball. More details can be found in [11].

Chu: Numerical methods for energy minimization problems on surfaces

We look at an energy defined on a surface Γ of the form

$$I_\Gamma(u) = \int_\Gamma F(u, \nabla_\Gamma u) ds.$$

We take an ϵ-neighborhood of Γ and write $\bar{u}(x) = u(P_\Gamma(x))$, $\frac{\partial \bar{u}}{\partial n} = 0$ (constant extension along the normals). We want to construct an integral formulation $I_{\Gamma_\epsilon}(\bar{u})$, such that

$$I_{\Gamma_\epsilon}(\bar{u}) = I_\Gamma(u), \quad \forall u.$$

Questions: Is the minimizer of $I_{T_\epsilon}(\bar{u})$ equivalent to the minimizer of $I_\Gamma(u)$? The answer is yes.

We derive

$$I_{\Gamma_\epsilon}(v) = \int_{T_\epsilon} \tilde{F}(v, \nabla v) dx,$$

where T_ϵ is a tubular neighborhood around Γ.
Question: Is $\bar{\nabla_\Gamma} u(z) = \nabla \bar{u}(z), \forall\, z \in T_\epsilon$? No, this is only true when $z \in \Gamma$. In fact we have

$$\bar{\nabla_\Gamma} u(z) = A(z) \nabla \bar{u}(z),$$

where $A = (1 - \eta\kappa_1)\tau_1 \otimes \tau_1 + (1 - \eta\kappa_2)\tau_2 \otimes \tau_2 + \delta n \otimes n$. η corresponds to the η level set. There is an extra dimension in the normal direction which gives us a free parameter δ (because the normal derivative is 0).
Question: Choice of δ? δ plays a different role for elliptic than for hyperbolic equations. $\delta > 0$ preserves ellipticity of elliptic equation. $\delta = 0$ is for hyperbolic equation.

Construct an identical volume integral,

$$I_\Gamma(u) = \int_\Gamma F(u, \nabla_\Gamma u) ds = I_{\Gamma_\epsilon}(v) = \frac{1}{2\epsilon} \int_{T_\epsilon} \tilde{F}(x, v, \nabla v) dx.$$

The speaker discussed the boundary (of the tube) treatment: project boundary point ($d = \epsilon$ or $d = -\epsilon$) to any point along the normal inside the tube. He also studied the instability (he has a model problem for that). This instability was previously studied by Kreiss, but the speaker studied this for manifolds. He uses the Fourier transform in space and the Laplace transform in time. He studies the existence of unstable modes. For δ large, there is an instability so it is necessary to have small δ.

The speaker discussed a stabilization strategy: add another term to the PDE (already done by Kreiss). He discretizes the integral first (direct method). Looks at obstacle problems and TV-denoising on a torus.
Question asked by a member of the audience: can you solve Maxwell's equation with this method?

Margetis: On the mathematical modeling of crystal facets

The speaker presents a PDE approach with a touch of discreteness in the modeling.

Classical relaxation by surface diffusion Region Ω_t with moving boundary, $\Gamma_t = \partial\Omega_t$, with velocity

$$v_n = -\text{div}_\Gamma J,$$

where J - the surface flux is given by

$$J = -\nabla_\Gamma \mu$$

and μ is the chemical potential.

This model has to be revised in the presence of line defects (steps) and facets (at low temperatures).

Multiple scales Typically, micro- (atomic scale), mesoscale (about 25 nm), macroscale (20 μm). The last two scales are subject of the talk.

How is macroscale facet evolution linked to the step motion? To address this question, one needs to consider 1) PDE away from facets, 2) boundary conditions. Typically for the step flow away from facets, one uses the BCF model. Near a facet, one needs to consider the discrete nature of the problem.

Adatom diffusion On the i-th terrace,

$$J_i = -D_s \nabla \rho_i, \qquad D_s \Delta \rho_i + F = \frac{\partial \rho_i}{\partial t} \approx 0.$$

and Robin-type boundary conditions at bonding step edges. Here, $\rho_i^{eq} = \rho_s e^{\mu_i/T}$ is the Gibbs-Thomson relation, $\mu_i(s,t)$ is the step chemical potential.

- Step motion and continuum limit (heuristics in 1D): Step velocity leads to $\partial_{\bar{t}} h = -\partial_x J$, where

  $$J = \frac{D_s}{1 + \frac{2D_s}{q\alpha}|\partial_x h|} \partial_x \rho^{eq}$$

  attachment/detachment at bonding steps leads to "Fick's law" for surface diffusion.

- Chemical potential near equilibrium leads to energy $E(h)$.

- Force dipole-dipole interaction model (nearest neighbor).

- Relaxation PDE in 2+1 dimensions, outside facets yields a 4-th order parabolic-like PDE for h. PDE for height profile.

How does the full (nonlinear) Gibbs-Thomson relation affect facet evolution?

$$\partial_t h = \Delta \exp\left[-\beta \text{div}\left(\frac{\nabla h}{|\nabla h|} + g|\nabla h|\nabla h\right)\right],$$

here $\beta = T^{-1}$, $g \geq 0$.

In 1+1 dimensions:

$$\partial_t h = \partial_{xx} \exp[-\partial_x \frac{\partial_x h}{|\partial_x h|}].$$

We neglect $|\partial_x h|\partial_x h$ in the exponent (of facets $\partial_x h = 0$).

The speaker then discussed some further analysis of the newly derived model: the appropriate boundary conditions at facets. The discussion led to free boundary problems. More details can be found in [14].

Liu: Dynamics of a degenerate PDE model of epitaxial crystal growth

This talk complements Dionisios Margetis lecture.

Epitaxial growth is an important physical process for forming solid films or other nano-structures. It occurs as atoms, deposited from above, adsorb and diffuse on a crystal surface. Modeling the rates that atoms hop and break bonds leads in the continuum limit to a degenerate 4th order PDE that involve exponential nonlinearity and the p-Laplacian with $p = 1$, for example. The lecturer discussed a number of analytical results for such models, some of which involving subgradient dynamics for Radon measure solutions.

Particularly noteworthy was how the author dealt with exponentials of singular measures.

Voller: Anomalous infiltration into Heterogeneous Porous media: Simulation and fractional calculus models

Sub-diffusive behavior was demonstrated in some physical systems and with fractional derivative the same behavior can be observed. This motivated that fractional derivatives can be used to model such systems. Problems, where obstacles were considered and the volume of fluid method was used to study how flows go through these obstacles. Two one dimensional measures for the progress of filling was found which gave good agreement with experimental data. The two measures: 1) S: the one dimensional representative front, and 2) F: an effective filling length, the infiltration depth were related to physical parameters such as porosity and the obstacle pattern. The talk was based on [1], [7] and [19].

Questions: fine structures such as fingers? Neglected here but for viscous fluids, no fingering, one still observe sub diffusion.

Does the shape of the obstacles affect the model with the fractional derivative?

Namba: Well-posedness of fully nonlinear PDEs with Caputo time fractional derivatives

Caputo time fractional derivatives were motivated for modeling anomalous diffusion that is observed in heterogeneous media ($\partial_t^\alpha u = \Delta u$). In the talk the notion of viscosity solutions were extended to equations with Caputo time fractional derivatives. Perron's method and comparison principle were used to construct sub and super-solution and to establish the unique existence of viscosity solutions for the initial value problem with Caputo time fractional derivatives. Continuous dependence of the solution on the fraction of the time derivative was also addressed. The talk is based on the following papers, [8], [17].

Questions: Do Caputo time fractional derivatives make sense also for functions that have jumps? Yes!

4 Scientific Progress Made

There were talks on different models and numerical algorithms for treating junctions and grain boundary motions. Discussions on how to extend surface PDEs into thin domains around interfaces for numerical computation were held. There were lectures on very novel high order PDEs for modeling the dynamics of facets in crystal growth. There were discussion about different nonlocal equations, connection to random walks, and relation between local and non-local diffusions in different domains.

5 Outcome of the Meeting

Specialists from many disciplines and background took part in the meeting. As a result exchanging ideas from distant area of the Science was facilitated. Indeed, the participants praised the choice of speakers, which conveyed new ideas and viewpoints. This is why one of the outcomes of the meeting was the transfer of knowledge among specialists.

Another outcome, which will turn out to be material, is the meeting of old collaborators, working on joint projects. We expect that the discussions held during the meeting will result in new projects leading to publications.

References

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