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Mini-Workshop: Inelastic and Non-equilibrium Material Behavior: from Atomistic Structure to Macroscopic Constitutive Relations

Organised by
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Abstract.

The workshop brought together 15 scientists, which included leaders in the fields of mathematics (partial differential equations, statistical mechanics and calculus of variations) and mechanics (continuum mechanics, computational mechanics, microstructure and material science) as well as mid- and early-career participants. We addressed the themes of modeling crystal plasticity, crystallization and fracture, and non-equilibrium thermodynamics.

Mathematics Subject Classification (2010): 74, 35, 82, 49.

Introduction by the Organisers

The workshop *Inelastic and Non-equilibrium Material Behavior: from Atomistic Structure to Macroscopic Constitutive Relations* addressed two key problems in the multiscale characterization of materials undergoing large inelastic deformations: (i) the understanding of non-equilibrium deformation of materials and nanostructures, and (ii) the atomistic-to-continuum limit of inelastic processes such as dislocation induced plasticity, crystal formation, and fracture. The diverse background of the participants made it possible to have a vibrant and open exchange of ideas in this intrinsically interdisciplinary problem of scale bridging in materials.

On the materials science side of the topic, we had presentations from areas of computation and modeling, in particular regarding the topic of objective structures and their thermodynamic behavior, phase field models for modeling phase transitions and crystallization. The mathematical topics covered included relaxation

in models for crystal plasticity, crystallization and fracture, as well as modeling thermodynamic processes far from equilibrium in both particle systems and the continuum. In all presentations we had a lively discussion that usually already started during the lecture and continued during the afternoon and evening breaks, sparking many ideas for improvements and further research and collaboration. The discussions in the mini-workshop atmosphere exceeded our expectations.

Complementary to the lectures on current research we had evening sessions where experts in the respective fields provided introductions to specialized topics. These sessions covered three areas: models for crystal plasticity, with a particular focus on kinematics derived from atomistics, the Boltzmann equation, and gradient flows. These lectures proved to be very successful and further facilitated the interdisciplinary exchange within the workshop.

In the feedback we solicited from the workshop participants, the high scientific standard and the benefits of informal structure and the small group, leading to long and in depth discussions during and after the presentations were explicitly mentioned. The more tutorials were also praised by the participants, especially their focus on open questions. This even lead to some new collaborations.

The workshop participants came from the US, Germany, and the UK, with a diverse mix of established researchers and early career scientists as well as PhD students. The excellent working and living conditions at the institute were vital for the lively and productive scientific atmosphere. The organizers thank the NSF for contributing to the travel expenses of two doctoral students and two professors from the US.

Mini-Workshop: Inelastic and Non-equilibrium Material Behavior: from Atomistic Structure to Macroscopic Constitutive Relations

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Abstracts

Objective Density Functional Theory: Ab-initio simulation schemes for Objective Structures

Amartya Banerjee
(joint work with Ryan Elliot, Richard D. James)

Objective structures are atomic/molecular configurations which generalize the notion of crystals and are such that all the constituent atoms/molecules of the structure see the same environment up to orthogonal transformations and translations. Objective structures are ubiquitously present in all of materials science, biology and nanotechnology and examples of these structures include nanotubes, buckyballs, tail sheaths and capsids of viruses, graphene sheets and molecular bilayers. Due to their association with large degrees of symmetry, objective structures are likely to be a fertile source of materials with remarkable material properties - particularly, collective material properties such as ferromagnetism and ferroelectricity. A systematic study of objective structures therefore, is likely to lead to the discovery of novel materials. At the same time, formulation of computational methods specifically designed for studying objective structures, is likely to lead to the development of novel nanomechanics simulations methodologies.

Following this line of thought, we have been developing Objective Density Functional Theory - a suite of rigorously formulated quantum mechanical theories and numerical algorithms for carrying out abinitio simulation studies of objective structures. Drawing analogies from the classical plane-wave density functional method of solid state physics, our focus has been on the development of novel spectral schemes for studying objective structures using Kohn-Sham Density Functional Theory. In this work, we first demonstrate how the equations of Kohn-Sham Density Functional Theory for objective structures admit interpretation in terms of symmetry adapted cell problems. Next, we propose a complete orthonormal basis set for discretizing these cell problems. We then discuss the significant challenges associated with the efficient solution of the discretized cell problems and our progress in addressing these challenges through a variety of numerical and algorithmic strategies.

We discuss some examples highlighting the efficiency and accuracy of our numerical methods. Finally, we present applications of our spectral schemes to the study of some problems in nano-mechanics, including the study of nano-clusters and simulations of the bending and twisting of nano-beams.

References

[1] M. Muster, *Computing certain invariants of topological spaces of dimension three*, Topology **32** (1990), 100–120.
[2] M. Muster, *Computing other invariants of topological spaces of dimension three*, Topology **32** (1990), 120–140.

Quasi-Static Brittle Damage Evolution in Elastic Materials with Multiple Damaged States

Isaac Vikram Chenchiah
(joint work with Christopher J. Larsen)

We present energetic and strain-threshold models for the quasi-static evolution of brutal brittle damage for geometrically-linear elastic materials. By allowing for anisotropic elastic moduli and multiple damaged states we present the issues for the first time in a truly elastic setting, and show that the methods developed in [Garroni, A., Larsen, C. J., Threshold-based quasi-static brittle damage evolution, Archive for Rational Mechanics and Analysis 194 (2), 585-609 (2009)] extend naturally to a class of elastic damageable materials. We show existence of solutions and that energetic evolutions are also threshold evolutions.

1. Introduction

Many irreversible phenomena in mechanics have been studied through variational models, plasticity and fracture being prominent examples. Variational formulations enable the use of the powerful tools of calculus of variations, for instance it is typically easy to show existence of global minimisers albeit perhaps only for a relaxed energy.

Mechanical phenomena have also been understood through threshold criteria. In the examples given above, plastic behaviour is triggered when stress reaches a yield surface and fracture occurs where the stress has a sufficiently large singularity. An attractive feature of these models is that these criteria are spatially local, which is physically natural, expresses engineering intuition and facilitates modelling. On the other hand it is unclear what correspondence (if any) there is between variational and threshold formulations of the same phenomenon.

In this paper we present, first, energetic (i.e., variational) and threshold models for the quasi-static evolution of brutal brittle damage in geometrically-linear elastic materials. This part of our work may be viewed as an extension to true elasticity (i.e., with vector-valued displacement fields and possibly anisotropic elastic moduli) of an earlier model [1] which was restricted to anti-plane shear (a scalar setting) with essentially scalar moduli (multiples of the identity). Moreover we allow for multiple damage processes, and thus multiple damaged states; to the best of our knowledge this is the first model to do so. For the energetic formulation we show existence of solutions under reasonable hypotheses.

These two approaches to damage are formulated independently but the question arises as to whether they are related for any given material and, if yes, how. In the second part of our work we relate these formulations for a broad class of materials. We show that energetic evolutions are also threshold evolutions, for a threshold that is related to the energetic cost of damage (i.e., the energy dissipated per unit volume due to damage). Thus energetic evolutions also have a spatially-local description.

1.1. **Notation.** We set $\mathbb{D} := \{0,1\}$. Let s be the dimension of space. Let $\Omega \subset \mathbb{R}^s$ be Lipschitz and $\mathbb{P}(\Omega) := 2^\Omega$, the set of subsets of Ω. $|\cdot|$ denotes either the Euclidean norm on $\mathbb{R}$ or the Lebesque measure on $\mathbb{R}^s$. We denote the Euclidean inner product in $\mathbb{R}^s$ by $\cdot$. For $a, b \in \mathbb{R}^s$,

$$a \otimes_s b := \frac{1}{2}(a \otimes b + b \otimes a)$$

where $a \otimes b$ is the tensor product of a and b.

Let $\mathbb{S} := \left\{M \in \mathbb{R}^{s\times s} \mid M = M^T\right\}$ be the linear space of symmetric matrices. We denote the standard inner product in $\mathbb{S}$ by $\langle\cdot,\cdot\rangle$. $\mathcal{P}$ is the set of all orthogonal projections on $\mathbb{S}$ and $\mathcal{M}$ is the set of all elastic modulli (i.e., positive-definite self-adjoint linear operators) on $\mathbb{S}$. We use the standard operator norm on $\mathcal{M}$:

$$\|\cdot\| := \sup_{\epsilon\in\mathbb{S}} \frac{\langle\cdot\epsilon,\epsilon\rangle}{\|\epsilon\|^2},$$

and the standard partial order that is defined through quadratic forms: $\forall\alpha_1,\alpha_2 \in \mathcal{M}$,

$$\alpha_1 \leqslant \alpha_2 \iff \forall\epsilon\in\mathbb{S}, \langle\alpha_1\epsilon,\epsilon\rangle \leqslant \langle\alpha_1\epsilon,\epsilon\rangle.$$

We set

$$\mathcal{M}(c_1,c_2) := \{\alpha\in\mathcal{M} \mid c_1 \leqslant \|\alpha\| \leqslant c_2\}$$

for $0 < c_1 < c_2$.

The map $e\colon H_0^1(\Omega,\mathbb{R}^s) \to L^2(\Omega,\mathbb{S})$ is defined through

$$e(\cdot) := \frac{1}{2}\left(D\cdot + D^{\cdot T}\right),$$

so $e(u)$ is the strain corresponding to the deformation u. For $\alpha \in L^\infty(\Omega,\mathcal{M}(c_1,c_2))$ and body force $f \in H^{-1}(\Omega,\mathbb{R}^s)$ by $u(\alpha,f)$ we denote the solution in $H_0^1(\Omega,\mathbb{R}^s)$ of

$$-\operatorname{div}(\alpha e(\cdot)) = f.$$

In addition we set $e(\alpha,f) := e\left(u(\alpha,f)\right) \in L^2(\Omega,\mathbb{S})$. The corresponding elastic energy is

$$\mathcal{E}(\alpha,f) := \int_\Omega \left(\frac{1}{2}\langle\alpha\ e(\alpha,f), e(\alpha,f)\rangle - f\cdot u(\alpha,f)\right)\,\mathrm{d}x.$$

Unless explicitly indicated otherwise, by $\overset{\star}{\rightharpoonup}$ we denote weak* convergence in $L^\infty(\Omega,\mathbb{R}^m)$, where m would be clear from the context.

1.2. **G-convergence and G-closures.** We recall the notion of G-convergence:

Definition 1.1 (G-convergence, $\overset{G}{\to}$)**.** *A sequence $A^n \in L^\infty(\Omega,\mathcal{M}(c_1,c_2))$ G-converges to $A \in L^\infty(\Omega,\mathcal{M}(c_1,c_2))$, $A^n \overset{G}{\to} A$, iff for every $f \in H^{-1}(\Omega,\mathbb{R}^s)$,*

$$u(A^n,f) \rightharpoonup u(A,f) \text{ weakly in } H_0^1(\Omega,\mathbb{R}^s).$$

Next we introduce two notions of G-closure. While the concept of G-closure is standard the specific notation here has been chosen to suit our purposes. Our definition of Constrained G-closures extends the corresponding definition in [1]. For these definitions we set $A_0 \in \mathcal{M}(c_1, c_2)$, $m \in \mathbb{N}$ and

$$\mathbf{A} := \{A_0\} \cup \{\Delta A_i \in \mathcal{M}(c_1, c_2) \mid i = 1, \dots, m\},$$

(viewed as a $(m+1)$-tuple) while requiring

$$A_0 - \sum_{i=1}^{m} \Delta A_i \in \mathcal{M}(c_1, c_2).$$

Definition 1.2 (G-closure, $\mathcal{G}_\cdot$)**.** *Let $\theta \in L^\infty(\Omega, [0,1]^m)$ and let $\chi^n \colon \Omega \to \mathbb{D}^m$ be such that $\chi^n \overset{\star}{\rightharpoonup} \theta$. Then the G-closure of $\mathbf{A}$, $\mathcal{G}_\theta(\mathbf{A})$, is the set of all possible G-limits of*

$$A_0 - \sum_{i=1}^{m} \chi_i^n \Delta A_i.$$

We also set

$$\mathcal{G}(\mathbf{A}) := \{\alpha \mid \exists \theta \in L^\infty(\Omega, [0,1]^m), \alpha \in \mathcal{G}_\theta(\mathbf{A})\}.$$

Definition 1.3 (Constrained G-closure)**.** *Let $\xi^n \colon \Omega \to \mathbb{D}^m$ be weak-* convergent characteristic functions on Ω. When the sequence χ in Definition 1.2 is picked such that $\chi_i^n \geqslant \xi_i^n$, $i = 1, \dots, m$, then the set of all possible G-limits of*

$$A_0 - \sum_{i=1}^{m} \chi_i^n \Delta A_i$$

is the constrained G-closure of $\mathbf{A}$ (with phase fraction θ and constraint $\{\xi\}$), $\mathcal{G}_\theta(\{\xi\}, \mathbf{A})$.

2. Damage

We consider a geometrically-linear elastic material which in the undamaged state has elastic modulus $\alpha_{\{0\}^m} \in \mathcal{M}$ (the reason for this notation will become clear in a moment) and, thus, energy density $W_{\{0\}^m} \colon \mathbb{S} \to \mathbb{R}$ given by

$$W_{\{0\}^m}(\cdot) = \frac{1}{2} \left\langle \alpha_{\{0\}^m} \, \cdot, \cdot \right\rangle.$$

This material is capable of undergoing $m \geqslant 1$ damage processes, any combination of which can occur simultaneously in both space and time. The (pointwise) damage state of the material is denoted by $d \in \mathbb{D}^m$ where

$$d_i = \begin{cases} 1 & \text{if } i\text{-damage has occurred,} \\ 0 & \text{otherwise.} \end{cases}$$

Thus, for example, $\{0\}^m$ denotes the undamaged material and $\{1\}^m$ the fully damaged material.

The i^{th} damage process ("i-damage") weakens the material by diminishing the elastic modulus by $\Delta\alpha_i \in \mathcal{M}$ where $\Delta\alpha_i \geqslant 0$. Thus, the elastic modulus and energy density corresponding to damage $d \in \mathbb{D}^m$ are

$$\alpha_d := \alpha_{\{0\}^m} - \sum_{i=1}^{m} d_i \, \Delta\alpha_i, \tag{1a}$$

$$W_d := \frac{1}{2} \langle \alpha_d \, \cdot, \cdot \rangle + kd, \tag{1b}$$

and the possible elastic moduli are

$$\boldsymbol{\alpha} = \{\alpha_d \mid d \in \mathbb{D}^m\} \subset \mathcal{M}.$$

The weakest elastic modulus corresponds to the material being damaged in all m ways; we require this to be positive-definite:

$$\alpha_{\{1\}^m} = \alpha_{\{0\}^m} - \sum_{i=1}^{m} \Delta\alpha_i > 0.$$

For convenience we set $\mathbf{M} := \{1, \ldots, m\}$.

2.1. **Two criteria for damage.** Let $i \in \mathbf{M}$.

Criterion 2.1 (Threshold criterion for damage)**.** *The i^{th} damage process is (pointwise) sensitive only to the strain ϵ and only through an orthogonal projection Λ_i on a subspace of $\mathbb{S}$: At $x \in \Omega$, i-damage occurs only if*

$$\|\Lambda_i \epsilon(x)\| > \lambda_i \tag{2}$$

for some threshold $\lambda_i > 0$. We refer to range(Λ_i) *as the i^{th} damage subspace.*

Criterion 2.2 (Energetic criterion for damage)**.** *The i^{th} damage process costs $k_i > 0$: The energy density corresponding to damage $d \in \mathbb{D}^m$ is*

$$W_d(\cdot) := \frac{1}{2} \langle \alpha_d \cdot, \cdot \rangle + d \cdot k$$

where α_d is given by (1)*.*

We explore these criteria in Sections 3.1 and 3.2 respectively. In Theorem 3.5 we explore the relationship between these formulations for materials that possesses the following property:

Property 2.3.

(1) *The damage subspaces are strain compatible: For each $i \in \mathbf{M}$,*

$$\epsilon \in \text{Range}(\Lambda_i) \implies \exists a, b \in \mathbb{R}^s \text{ such that } \epsilon = a \otimes_s b.$$

(2) *The undamaged elastic modulus is a multiple of the identity on each damage subspace: For each $i \in \mathbf{M}$,*

$$\alpha_{\{0\}^m} \Lambda_i = \beta_i \Lambda_i$$

for some (scalar) $\beta_i > 0$. (That is, the damage subspaces are eigenspaces of the undamaged elastic modulus with β_i being the corresponding positive eigenvalue.)

(3) *The elastic modulus is weakened only on the relevant damage subspace, and uniformly on the subspace: For* $i \in \mathbf{M}$*,*

$$\Delta\alpha_i = \Delta\beta_i \Lambda_i.$$

for some $\Delta\beta_i \in (0, \beta_i)$*.*

(4) *The damage subspaces are orthogonal: For* $i, j \in \mathbf{M}$ *with* $i \neq j$*,*

$$\Lambda_i \Lambda_j = 0.$$

2.2. **Notation.** In the rest of the paper we adopt the following notation:

Let $D_i \subset \Omega$, $i \in \mathbf{M}$, denote the region in which i-damage has occurred, and let χ_{D_i} be the corresponding characteristic functions. We define:

$$D := (D_1, \dots, D_m) \in \mathbb{P}(\Omega)^m,$$
$$\chi_D := (\chi_{D_1}, \dots, \chi_{D_m}).$$

By abuse of notation we set,

$$\alpha_D(x) := \alpha_{\chi_{D(x)}},$$
$$e(D, \cdot) := e(\alpha_D, \cdot).$$

Set-theoretic operations on $\mathbb{P}(\Omega)^m$ are performed component-wise, e.g., for $D, D' \in \mathbb{P}(\Omega)^m$,

$$D \cup D' = (D_1 \cup D'_1, \dots, D_m \cup D'_m),$$
$$D \cap D' = (D_1 \cap D'_1, \dots, D_m \cap D'_m),$$
$$D \setminus D' = (D_1 \setminus D'_1, \dots, D_m \setminus D'_m);$$

and likewise for set-theoretic statements on $\mathbb{P}(\Omega)^m$:

$$D \subset D' \iff D_i \subset D'_i, \quad \forall i \in \mathbf{M}.$$

3. Damage Evolution

3.1. **Threshold formulation.**

Definition 3.1 (Weak threshold evolution)**.** *Let* $f\colon [0,T] \to H^{-1}(\Omega, \mathbb{R}^s)$*. An evolution*

$$[0,T] \ni t \mapsto (A(t), \theta(t)) \in L^\infty(\Omega, \mathcal{M}(c_1, c_2)) \times [0,1]^m$$

is a weak threshold evolution with thresholds (2) *if: For every* $t \in [0,T]$ *there exists a sequence* $\{D^n(t)\} \subset \mathbb{P}(\Omega)^m$ *such that*

$$\alpha_{D^n(t)} \xrightarrow{G} A(t)$$
$$\chi_{D^n(t)} \xrightarrow{\star} \theta(t)$$

and the following hold for each $i \in \mathbf{M}$*:*

(1) Monotonicity*: The damage evolution* $t \mapsto D_i^n(t)$ *is non-decreasing.*

(2) Threshold*: For each $\delta > 0$ the sets in which there is no i-damage but the threshold is exceeded by at least δ converge in measure to the empty set:* $\forall t \in [0,T]$,

$$|U_i^n(\delta)| \to 0 \quad \text{as } n \to \infty,$$

where

$$U_i^n(\delta) := \{x \notin D_i^n(t) \mid \|\Lambda_i\ e(D^n(t), f(t))(x)\| > \lambda_i + \delta\}.$$

(3) Necessity of the damage*: For each* $\delta > 0$,

(a) *For every* $E^n \subset D_i(T)$ *with* $\liminf |E^n| > 0$ *and every sufficiently small* $\Delta\tau$, *there exists* $\tau < T - \Delta\tau$ *such that, with* $\Delta E^n \in \mathbb{P}(\Omega)^m$,

$$\Delta E_j^n := \begin{cases} E^n \cap D_i^n(\tau + \Delta\tau) \setminus D_i^n(\tau) & \text{if } j = i, \\ \emptyset & \text{if } j \neq i, \end{cases}$$

we have

$$\liminf_{n\to\infty} |V_i^n(\delta)| > 0,$$

where

$$V_i^n(\delta) := \{x \in E_i^n \mid \|\Lambda_i\ e^n(x)\| > \lambda_i - \delta\},$$
$$e^n := e(D^n(\tau + \Delta\tau) \setminus E^n, f(\tau + \Delta\tau)).$$

(b) *(Trivially satisfied if* $\int_\Omega \theta_i(x,\cdot)\,\mathrm{d}x$ *is continuous from below at* T.*) For every* $t^n \nearrow T$ *and every* $E^n \in \mathbb{P}(\Omega)^m$ *satisfying*

$$E_j^n \subset \begin{cases} D_i^n(T) \setminus D_i^n(t^n) & \text{if } j = i, \\ \emptyset, & \text{if } j \neq i, \end{cases}$$

with $\liminf |E_i^n| > 0$ *we have*

$$\liminf_{n\to\infty} |W_i^n(\delta)| > 0,$$

where

$$W_i^n(\delta) := \{x \in E_i^n \mid \|\Lambda_i\ e(D^n(T) \setminus E^n, f(T))(x)\| > \lambda_i - \delta\}.$$

3.2. **Energetic formulation.**

Definition 3.2 (Energy)**.** *The energy associated with* $\alpha \in L^\infty(\Omega, \mathcal{M}(c_1,c_2))$, $f \in H^{-1}(\Omega,\mathbb{R}^s)$ *and* $\theta \in L^\infty(\Omega,\mathbb{R}^m)$ *is*

$$\begin{aligned} \mathcal{W}(\alpha,\theta,f) &:= \mathcal{E}(\alpha,f) + \int_\Omega k\cdot\theta\,\mathrm{d}x \\ &= \int_\Omega \frac{1}{2}\langle \alpha\ e(\alpha,f), e(\alpha,f)\rangle - f\cdot u(\alpha,f) + k\cdot\theta\,\mathrm{d}x. \end{aligned} \tag{3}$$

In (3), where necessary, by f we mean the localisation of a representative of f to S, see [1, page 602] for details.

Definition 3.3 (Weak energy-minimizing evolution)**.**
Let $f \in W^{1,1}([0,T], H^{-1}(\Omega, \mathbb{R}^s))$. An evolution

$$[0,T] \ni t \mapsto (A(t), \theta(t)) \in L^\infty(\Omega, \mathcal{M}(c_1, c_2)) \times L^\infty(\Omega, \mathbb{R}^m)$$

with

$$A(t) \in \mathcal{G}_{\theta(t)}(\boldsymbol{\alpha})$$

is a weak energy-minimizing evolution if the following hold:

(1) Monotonicity*: The map $t \mapsto A(t)$ is non-increasing and for each $i \in \mathbf{M}$, the map $t \mapsto \theta_i(t)$ is non-decreasing.*

(2) Energy balance*: For every $t \in [0,T]$ the energy*

$$\mathcal{W}(t) := \mathcal{W}(A(t), \theta(t), f(t))$$

satisfies

$$\mathcal{W}(t) = \mathcal{W}(0) - \int_0^t \dot{f}(s) \cdot u(A, f)(s) \, \mathrm{d}s.$$

(3) Minimality*: There exists a sequence $\{D^n(t)\} \subset \mathbb{P}(\Omega)^m$, non-decreasing in t for each n, such that for every $t \in [0,T]$,*

$$\alpha_{D^n(t)} \overset{G}{\to} A(t),$$
$$\chi_{D^n(t)} \overset{\star}{\rightharpoonup} \theta(t)$$

and for every $(\tilde{A}, \tilde{\theta})$ such that $\tilde{A} \in \mathcal{G}_{\tilde{\theta}(t)}(\{\chi_{D^n(t)}\}, \boldsymbol{\alpha})$ we have

$$\mathcal{W}(t) \leqslant \mathcal{W}(\tilde{A}, \tilde{\theta}, f(t)).$$

We are able to show that weak energy-minimising evolutions exist and are also threshold evolutions:

Theorem 3.4. *For every $f \in W^{1,1}([0,T], H^{-1}(\Omega, \mathbb{R}^s))$, there exists a weak energy-minimising evolution.*

Theorem 3.5. *For a material satisfying Property 2.3, a weak energy-minimising evolution with damage cost $k \in \mathbb{R}^m$ is a weak threshold evolution with threshold $\lambda \in \mathbb{R}^m$ satisfying*

$$k_i = \frac{1}{2} \frac{\beta_i \, \Delta\beta_i}{\beta_i - \Delta\beta_i} \lambda_i^2, \quad i \in \mathbf{M}.$$

References

[1] Garroni, A., Larsen, C.J.: Threshold-based quasi-static brittle damage evolution. Archive for Rational Mechanics and Analysis **194**, 585–609 (2009)

Interfaces of discrete patterns

Marco Cicalese
(joint work with A. Braides)

The behavior of several physical systems is strongly influenced by phase instabilities. Roughly speaking this kind of instabilities can be thought as the spontaneous emergence of a large number of interfaces during phase separation.

In the framework of atomistic systems characterized by finitely many stable states (the case of bi-stable systems being firstly studied by Braun, Cahn, McFadden and Wheeler in [3]) we consider a class of systems presenting phase instabilities. Our interest is the description of the atomistic-to-continuum limit of these systems and in particular the macroscopic description of the instabilities in terms of "natural" continuum order parameters and energies.

As usual in this context (see [1]) we may regard atomistic systems as classical lattice spin systems whose state is described by an order parameter $u : \mathbb{Z}^n \to X$ where $X \subset \mathbb{R}$ is such that $\#X < +\infty$.

The physical systems we are interested in are driven by energies of the type:

$$E_\varepsilon(u) = \sum_{i \in \mathbb{Z}^n} \varepsilon^{n-1} \psi(\{u^{i+j}\}_{j \in \mathbb{Z}^n})$$

where $\psi : (X)^{\mathbb{Z}^n} \to [0, L]$ is the potential energy, $\varepsilon > 0$ denotes the lattice spacing of the atomistic system (a small parameter which will eventually go to zero in the so-called continuum limit) and the surface scaling ε^{n-1} is reminiscent of the fact that we want to study interfacial type phenomena.

Note that we let all the atoms of the system interact, and moreover we do not account only for pairwise interactions: any interaction between one particle and all the rest of the system is admissible.

We make the following set of hypotheses (here we denote by $\{e_1, e_2, \dots, e_n\}$ the standard basis in $\mathbb{R}^n$ and we set $Q := [-1/2, 1/2]^n$ the unitary cube in $\mathbb{R}^n$ centered at the origin):

given $h \in \mathbb{N}$, we assume that there exist $K \in \mathbb{N}$ functions $v_1, v_2, \dots, v_K : \mathbb{Z}^n \to X$ that are hQ-periodic and such that

(H1) (ground states energy) $\psi(\{z^j\}_{j \in \mathbb{Z}^n}) = 0 \Leftrightarrow z^j = v_l^j, l \in \{1, 2, \dots, K\}$,

(H2) (incompatibility of ground states) for $k \in \{1, 2, \dots, n\}$ and $l, l' \in \{1, 2, \dots, K\}$, $l \neq l'$ let $z_{k,l,l'} : \mathbb{Z}^n \to X$ be such that

$$z^i_{k,l,l'} := \begin{cases} v^i_l & \text{if } i \in hQ \cap \mathbb{Z}^n \\ v^i_{l'} & \text{if } i \in (hQ + e_k) \cap \mathbb{Z}^n. \end{cases}$$

Then there exists $i \in h(Q \cup (Q+e_k))$ and $C_{l,l'} > 0$ such that

$$\psi(\{z^{i+j}_{k,l,l'}\}_{j\in\mathbb{Z}^n}) \geq C_{l,l'}.$$

(H3) (mild non-locality) given $z, w : \mathbb{Z}^n \to X$ and $m \in \mathbb{N}$ such that $z^j = w^j$, $\forall j \in (mh)Q \cap \mathbb{Z}^n$, then

$$|\psi(\{w^j\}_{j\in\mathbb{Z}^n}) - \psi(\{z^j\}_{j\in\mathbb{Z}^n})| < c_m$$

where the constants c_m are such that $\sum_{m\in\mathbb{N}} c_m m^{n-1} < +\infty$.

Some comments are in order. Hypothesis (H1) states the existence of finitely many periodic ground states (as a side remark, note that for many real systems, since the energy is invariant under translations, the existence of one non-trivial periodic minimizer implies the existence of other periodic minimizers). By (H2) there is a non negative amount of energy the system has to spend in order to mix two different ground states. Hypothesis (H3) is crucial to our analysis: it refers to the control of the admissible non-locality of the energy at discrete level. Thanks to this hypothesis we are able to describe the continuum energy of the system as a local functional.

Under this set of assumptions we are able to prove the following theorem (as usual in this framework we assume that the energies E_ε have been appropriately extended to $E_\varepsilon : L^1_{loc}(\mathbb{R}^n) \to [0, +\infty]$).

Theorem 1. *Let u_ε be such that $\sup_\varepsilon E_\varepsilon(u_\varepsilon) \leq C < +\infty$. Then, under the assumptions $(H1)$,$(H2)$,$(H3)$, there exists $\tilde{A}_{1,\varepsilon}, \tilde{A}_{2,\varepsilon}, \dots, \tilde{A}_{K,\varepsilon} \subseteq \mathbb{Z}^n$ such that $u^i_\varepsilon = v^i_j$ for all $i \in \tilde{A}_{j,\varepsilon}$. Moreover, set $A_{j,\varepsilon} := \bigcup_{i\in\tilde{A}_{j,\varepsilon}} (\varepsilon(i+Q))$, we have that $\chi_{A_{j,\varepsilon}} \to \chi_{A_j}$ in $L^1_{loc}(\mathbb{R}^n)$ where $(A_1, A_2, \dots, A_n)$ is a partition of $\mathbb{R}^n$. In addition, we have that*

$$\Gamma\text{-}\lim_{\varepsilon\to 0} E_\varepsilon(u) = \sum_{l,l'} \int_{\partial^* A_l \cap \partial^* A_{l'}} \varphi(l, l', \nu_{l,l'})\, d\mathcal{H}^{n-1}, \tag{1}$$

where $\partial^* A_l$ denotes the reduced boundary of the set A_l, $\nu_{l,l'}$ the measure theoretic normal to the common boundary of A_l and $A_{l'}$ and $\varphi > 0$ is given by an asymptotic homogenization-type formula.

We observe that the macroscopic energy is the energy the system spends in a transition between two admissible periodic minimizers. It is proportional to the length of the transition layer. As a consequence any transition between different periodic ground-states is disfavored in the continuum limit.

As an application of the result above we may explain, using a minimal toy model, the following result of a Langmuir-Blodgett condensation experiment. When depositing hydrophobic/hydrophilic surfactant material on a Langmuir-Blodgett film, the geometry of the free surface strongly depends on the immersion-emersion time in the experiment. If the time is not too large, striped, but non uniformly striped pattern appear. On the contrary, for large enough times uniform patterns

characterize the geometry of the deposited surfactant. One possible explanation is that non-uniform stripes are metastable states, while only uniform stripes are the ground states of the system. Our result is compatible with this explanation since in our toy model uniformly striped patterns are unique periodic minimizers, while non uniform striped patterns are obtained as transitions between several periodic minimizers and thus energetically disfavored.

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A Multiscale Atomistic-to-Continuum Method for Atomic Monolayers Undergoing Bending

Kaushik Dayal
(joint work with A. Aghaei)

The framework of Objective Structures introduced by Richard D. James provides a method to systematically examine the behavior of various geometrically complex nanostructures. These nanostructures include rod-like objects as well as flat sheets. In this talk, we describe an extension of this framework to sheets that undergo bending in complex ways. We then apply the extended framework to develop a computational atomic multiscale method to understand the atomic structure of defects in these systems.

1. What are Objective Structures?

James [1] defined an objective atomic structure as a finite or infinite set of atoms in which every atom sees the same environment up to translation and rotation. Similarly, an objective molecular structure is defined as a structure with a number of identical *molecules*, each molecule consisting of a number of atoms, arranged such that *corresponding* atoms in every molecule see the same environment up to translation and rotation. We note that the molecules in an objective molecular structure need not correspond to standard physical molecules as usually understood. Bravais (multi) lattices are special cases of objective atomic (molecular) structures in which each atom (molecule) has the same environment up to translation and the rotation is trivial.

Following recent works that build on James' original formulation, e.g. [5, 4, 6, 2, 3], we can define OS equivalently in the language of group theory. The group theoretic approach enables practical calculations. Let $G = \{g_{\mathbf{0}}, g_{\mathbf{1}}, \cdots, g_{\boldsymbol{N}}\}$ be a set of isometries indexed by a multi-index. Each element of G has the form $g_{\boldsymbol{j}} = (\boldsymbol{Q_j}|\boldsymbol{c_j})$ where $\boldsymbol{Q_j} \in O(3)$ is orthogonal and $\boldsymbol{c_j} \in \mathbb{R}^3$ is a vector.

The action of an isometry on a point $\boldsymbol{x} \in \mathbb{R}^3$ is

$$g_{\boldsymbol{j}}(\boldsymbol{x}) = \boldsymbol{Q_j x} + \boldsymbol{c_j} \tag{1}$$

Composition of mappings then provides:

$$g_{\boldsymbol{i}}(g_{\boldsymbol{j}}(\boldsymbol{x})) = \boldsymbol{Q_i}\left(\boldsymbol{Q_j x} + \boldsymbol{c_j}\right) + \boldsymbol{c_i} = \boldsymbol{Q_i Q_j x} + \boldsymbol{Q_i c_j} + \boldsymbol{c_i}$$

This motivates a definition for multiplication of isometries:

$$g_{\boldsymbol{i}} g_{\boldsymbol{j}} = (\boldsymbol{Q_i Q_j} | \boldsymbol{Q_i c_j} + \boldsymbol{c_i}) \tag{2}$$

From this definition, it follows that the identity element is $g_{\boldsymbol{0}} := (\boldsymbol{I}|\boldsymbol{0})$ and the inverse of $g_{\boldsymbol{i}}$ is defined by $g_{\boldsymbol{i}}^{-1} := (\boldsymbol{Q_i^T} | -\boldsymbol{Q_i^T c_i})$.

If the set G is additionally a group with respect to the multiplication operation above, then placing an atom at each of the points given by the action of elements of G on a given point $\boldsymbol{x}_0$ gives an objective atomic structure. In addition, placing an atom of species k at each of the points given by the action of elements of G on a given set of points $\boldsymbol{x}_{0,k}$ gives an objective molecular structure.

2. Going beyond Objective Structures: quasi Objective Structures (qOS)

The OS framework defined above can be considered the analog of perfect crystals. While perfect crystals are an important first step in studying crystalline materials, defects and inhomogeneously-deformed crystals are closer to real systems. The analogs of these questions in OS can be studied using extensions of methods such as the quasi continuum method. However, this talk dealt with systems that are close to OS in a geometrical and energetic sense, yet cannot be considered as patched together with multiple OS. These structures, qOS, cannot be considered as perfect OS even locally. However, they are important to multiscale atomic modeling of lipid bilayers, graphene, and other low-dimensional materials.

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Relaxation and Gamma convergence for variational problems related to models in finite plasticity for single crystals with few slip systems

Georg Dolzmann
(joint work with S. Conti, C. Kreisbeck, S. Müller)

A time-incremental formulation of models for the plastic behaviour of single crystals in the framework of finite plasticity leads to a sequence of variational problems that need to be solved at each time step [10, 2]. Here we focus on the first time step for which the corresponding variational problem can be formulated as follows: minimize

$$I[u] = \int_\Omega W(Du)\mathrm{d}x$$

in a suitable class $\mathcal{A}$ of admissible functions with given Dirichlet boundary data. We adopt the multiplicative decomposition of the deformation gradient $F = Du$ into an elastic part F_e and a plastic part F_p, i.e., $F = F_eF_p$ and we assume that W is the sum of the elastic potential W_e, the plastic potential W_p, the dissipated energy and the contribution related to geometrically necessary dislocations [3]. More precisely, we assume that

$$W(F) = W_e(F_e) + W_p(F_p) + \mathrm{Diss}(F_p) + \delta|\mathrm{curl}(F_p)|(\Omega)\,.$$

In the following we restrict our attention to the case $n = 2$ and a bounded and open domain $\Omega \subset \mathbb{R}^2$. We also assume that $\delta = 0$, see [11] for recent results on scaling relations for the full model.

We begin our analysis for the case of rigid elasticity where

$$W_e(F_e) = \begin{cases} 0 & \text{if } F_e \in SO(2)\,, \\ \infty & \text{otherwise}\,. \end{cases}$$

Here $SO(2)$ denotes the group of all proper rotations of the plane. Moreover we assume that the slip systems are given by pairs of vectors s_i and m_i with $s_i \cdot m_i = 0$ for $i = 1, \dots, N$. For simplicity we suppose that we are given either one slip system with $(s_1, m_1) = (e_1, e_2)$ or two orthogonal slip systems with $(s_1, m_1) = (e_1, e_2)$ and $(s_2, m_2) = (e_2, e_1)$. The combination of the dissipative effects and the plastic potential is modeled by

$$W_p(F_p) + \mathrm{Diss}(F_p) = \begin{cases} |\gamma|^p & \text{if } F_p = I + \gamma s_i \otimes m_i\,,\ i \in \{1, \dots, N\}\,, \\ \infty & \text{otherwise}\,. \end{cases}$$

Here $p \geq 1$ and $p = 1$ corresponds to dissipation and $p = 2$ to linear hardening. The condensed energy is given by

$$W_{\mathrm{cond}}(F) = \inf_{F=F_eF_p} W(F) = \begin{cases} |\gamma|^p & \text{if } F = Q(I + \gamma s_i \otimes m_i)\,, \\ \infty & \text{otherwise}\,, \end{cases}$$

where $Q \in SO(2)$ and $i \in \{1, \dots, N\}$. Table 1 summarizes the relaxation results that are known in the literature. The quasiconvex hull of the density $W = W_{\mathrm{cond}}$

	number of slip systems		
exponent p	one	two (orthogonal)	three or more
$p = 1$	W^{qc}, see [8]	$W^{pc} \neq W^{rc}$, see [1]	?
$1 < p < 2$	?	?	?
$p \geq 2$	W^{qc}, see [4]	W^{qc}, see [5]	?

TABLE 1. Relaxation results with different exponents and slip systems in the literature. A question mark indicates models for which no results are available.

is denoted by W^{qc} and given by

$$W^{qc}(F) = \inf\Big\{ \int_{(0,1)^2} W(F + D\phi)\mathrm{d}x,\ \phi \in W_0^{1,\infty}((0,1)^2;\mathbb{R}^2) \Big\}\,.$$

For more information on this definition and on the related rank-one convex and polyconvex envelopes W^{rc} and W^{pc}, respectively, see [9].

It is notable that in the case of two orthogonal slip systems and dissipation $p = 1$ the polyconvex and the rank-one convex envelope are different in the region in which both slip systems are used. Moreover, the rank-one convex envelope cannot be obtained by finite lamination and requires arbitrarily large matrices.

The assumption of rigid elasticity is a quite restrictive assumption and it is an important question of whether these models can be derived by a notion of variational convergence like Γ-convergence from models with large elastic constants. For $\epsilon > 0$ we define for $q \geq 1$ the elastic model energy

$$W_e(F_e) = \frac{1}{\epsilon}\,\mathrm{dist}^q(F_e, SO(2))\,.$$

The condensed energy in the case of one slip system is given by

$$W_\epsilon(F) = W_{\mathrm{cond}}(F) = \inf_{\gamma\in\mathbb{R}} \Big[\frac{1}{\epsilon}\,\mathrm{dist}^q\big(F(I - \gamma e_1 \otimes e_2), SO(2)\big) + |\gamma|^p \Big]\,. \tag{1}$$

The key observation is the fact that the multiplicative decomposition $F = F_e F_p$ leads to nonstandard growth conditions. In order to illustrate this effect, we seek a one-parameter family of matrices F_t with $|F_t| \to \infty$ for which $W(F_t)$ can be estimated from above. We choose for $t > 0$ and $\alpha > 1$ the matrices

$$F_t = F_{t,e}F_{t,p} = \begin{pmatrix} t & 0 \\ 0 & t \end{pmatrix} \begin{pmatrix} 1 & t^{\alpha-1} \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} t & t^\alpha \\ 0 & t \end{pmatrix}\,.$$

This choice leads to an estimate of the form

$$W(F_t) \leq C\big(|F_{t,e}|^q + |F_{t,p}|^p\big) \leq C\big(|F_t|^{q/\alpha} + |F_t|^{p\alpha/(\alpha-1)}\big)\,.$$

A minimization in α leads to $\alpha = (p+q)/p$ and $W(F_t) \leq C|F_t|^{pq/(p+q)}$, that is, the energy has sublinear growth along the direction $t \mapsto F_t$ for $q < p/(p-1)$. This

observation leads to the definition of the parameter regions

$$S = \left\{p,\, q \geq 1,\, q < \frac{p}{p-1}\right\}, \quad H = \left\{p,\, q \geq 1,\, q \geq \frac{p}{p-1},\ q \leq 2p\right\}.$$

In order to state the convergence result we define the functionals

$$I_\epsilon(u) = \int_\Omega W_\epsilon(Du)\mathrm{d}x\,, \quad I_0(u) = \int_\Omega W_{CT}(Du)\mathrm{d}x \tag{2}$$

where W_{CT} is the relaxation of the elastically rigid energy with one slip system [8],

$$W_{CT}(F) = \begin{cases} \sqrt{|F|^2 - 2} & \text{if } F \in \mathcal{N}\,, \\ \infty & \text{otherwise}\,. \end{cases}$$

Here $\mathcal{N} = \{F \in \mathbb{R}^{2\times 2},\, \det F = 1,\, |Fe_1| \leq 1\}$.

Theorem [6, 5]**:** Suppose that W_ϵ is defined by (1) and I_ϵ and I_0 by (2).

(a) If $(p,q) \in S$, then $W_\epsilon^{qc} = 0$ on $\mathcal{N}$.

(b) If $(p,q) \in H$, then the functionals I_ϵ converge in the sense of Γ-convergence with respect to the $L^{pq/(p+q)}$-norm to the functional I_0. Moreover, sequences $(u_\epsilon)_{\epsilon>0}$ with uniformly bounded energies $I_\epsilon(u_\epsilon)$ are relatively compact.

The most subtle point in the proof is the verification of the nonlinear constraint $\det Du = 1$ for weak limits of subsequences u_{ϵ_k} with $\epsilon_k \to 0$ for $k \to \infty$. This is accomplished by a suitable div-curl lemma [7].

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Some energy estimates for strain gradient plasticity with cross-hardening

Patrick W. Dondl
(joint work with Keith Anguige)

Consideration is given to a non-convex variational model for a shear experiment in the framework of single-crystal linearised plasticity with infinite cross-hardening within the general framework developed in [1]. The rectangular shear sample is clamped at each end, and is subjected to a prescribed horizontal shear, modelled by an appropriate hard Dirichlet condition. In this setting we write the energy of the plastically deformed crystal as

$$E_L(u,\beta) = \int_{\Omega_L} |(\nabla u - \beta)_{\mathrm{sym}}|^2 \, dx + \sigma \int_{\Omega_L} |\operatorname{curl} \beta|,$$

neglecting dissipation or hardening. The side condition of infinite cross hardening is enforced by requiring

$$\begin{aligned}\beta(x) \in \Bigg\{ & s(x) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, s(x) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}, \\ & s(x) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, s(x) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ -1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \\ & s(x) \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, s(x) \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \Bigg\},\end{aligned}$$

for almost every $x = (x_1, x_2, x_3) \in \Omega_L$ and some coefficient $s\colon \Omega_L \to \mathbb{R}$. The admissible displacements for the minimisation problem are all functions u such that $u(\cdot, 0, \cdot) = (0,0,0)$, $u(\cdot, L, \cdot) = \gamma(1,0,0)$ for some parameter $\gamma \geq 0$, and such that (u, β) has finite energy for some β subject to the side condition above.

We ask: how much energy is required to impose such a shear, and how does it depend on the aspect ratio? Assuming that just two slip systems are active, we show that there is a critical aspect ratio, above which the energy is strictly positive, and below which it is zero. Furthermore, in the respective regimes determined by the aspect ratio, we prove energy scaling bounds, expressed in terms of the amount of prescribed shear. Explicitly, using methods from [2] and [3] we can show that

$$\begin{cases} \inf E_L = 0 & L \geq 2, \\ \frac{c_L \sigma \gamma^2}{\sigma + \sqrt{\sigma^2 + 2 c_L \gamma^2}} \leq \inf E_L \leq \min\left\{ \frac{\gamma^2}{2L}, 2\sqrt{2}\gamma\sigma \right\} & 1 \leq L < 2, \\ \frac{\gamma^2}{2L}(1-L) \leq \inf E_L \leq \min\left\{ \frac{\gamma^2}{2L}, \frac{\gamma^2}{2L}(1-L) + c_L \sigma \gamma \right\} & L < 1, \end{cases}$$

if $\sigma > 0$ and the single slip side condition is enforced, and

$$\begin{cases} \inf E_L = 0 & L \geq 1, \\ \inf E_L = \min\left\{ \frac{\gamma^2}{2L}, \frac{\gamma^2}{2L}(1-L) + c_L \sigma \gamma \right\} & L < 1, \end{cases}$$

otherwise.

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Unexpected thermodynamic properties of some exact far-from-equilibrium solutions in molecular dynamics

Richard D. James
(joint work with Kaushik Dayal, Stefan Müller)

I discuss recent results on objective molecular dynamics. The basic equations of molecular dynamics are

$$m_k \ddot{x}_k = -\frac{\partial \varphi}{\partial x_i}(x_1, \dots, x_N), \quad i = 1, \dots, N, \tag{1}$$

for $(x_1(t), \dots, x_N(t)) \in \mathbb{R}, t > 0$, subject to initial conditions, $x_i(0) = x_i^\circ$, $\dot{x}_i(0) = v_i^\circ$ and with positive masses $m_1, \dots, m_n$. The right hand side of these equations is interpreted as the force on atom i. We impose minimal structural assumptions on this force as a function of the atomic positions, but we do assume the standard invariance of atomic theory, i.e., frame-indifference (under the full orthogonal group) and permutation invariance. These assumptions are satisfied by all accepted models of atomic forces in the nonrelativistic case. A very general example is the Hellmann-Feynman force based on full quantum mechanics under the Born-Oppenheimer assumption. Classical models of atomic forces are of course also allowed.

The terminology "objective molecular dynamics" refers to a time-dependent invariant manifold of these equations generated by a discrete group of isometries. The invariant manifold has the usual meaning in nonlinear dynamics: if, in the space $\mathbb{R}^{6N}$ of positions and momenta, you start initial value problem on this manifold, the resulting solution stays on this manifold. For the discrete group of isometries, I concentrated in the lecture mostly on the case of the translation group, $x \to x + \sum_{j=1}^{3} (I + tA)\nu^j e_j$, where A is any given 3×3 matrix, e_1, e_2, e_3 are linearly independent vectors in $\mathbb{R}^3$ and $\nu = (\nu^1, \nu^2, \nu^3) \in \mathbb{Z}^3$. The time-dependence expressed by the presence of $I + tA$ is the most general allowed under the theorem that justifies the existence of this manifold. Some examples based on a general form of the helical group were also presented, with applications to the mechanical behavior of carbon nanotubes.

This manifold can be described most easily by describing a numerical method designed to simulate motions on this manifold. Consider the translation group and imagine a set of motions $x_1(t), \dots, x_M(t)$ associated to the *simulated atoms*.

In this case M is finite but $N = \infty$. The additional atoms will be called the non simulated atoms. The simulated atoms will be required to satisfy the equations of molecular dynamics with forces given by all the atoms. Let other motions be given by an instantaneous action of the translation group on the simulated atoms, i.e., define,

$$x_{\nu,i}(t) = x_i(t) + \sum_{j=1}^{3}(I + tA)\nu^j e_j, \quad i = 1, \ldots, M, \quad \nu = (\nu^1, \nu^2, \nu^3) \in \mathbb{Z}^3. \tag{2}$$

Since the non simulated atoms are simply given by the formula (2), they are not required to satisfy the equations of molecular dynamics. On the other hand, as noted above, the simulated atoms are so required, and for this purpose the formula (2) is substituted into the right hand side of (1). Then (1) becomes a finite nonautonomous system of ODEs in standard form for the simulated atoms. The basic theorem on objective molecular dynamics then says that all infinitely many non simulated atoms satisfy the equations of molecular dynamics.

This result can be reformulated as an invariant manifold of molecular dynamics. It is described by simple formulas that only depend on A. Thus, the manifold is independent of the material. It is exactly the same manifold whether the atomic forces are appropriate for water, air or steel.

In the case of the translation group just described, the simulated and non-simulated atoms fill all of space. They have a macroscopic motion that can easily be identified. It is described by the velocity field

$$v(x, t) = A(I + tA)^{-1}x. \tag{3}$$

If this velocity field is substituted into any accepted equation of continuum mechanics, e.g., Navier-Stokes fluid, nonlinear elastic or viscoelastic solid, models of complex fluids, then it is an exact solution. In this sense, the invariant manifold is perfectly inherited by continuum mechanics, despite the fact that molecular dynamics is time-reversible on this manifold, while many examples in continuum mechanics are time-irreversible on (the averaged version of) this manifold.

These solutions of the equations of molecular dynamics have a certain statistics. Consider an objective molecular dynamics solution, a point $x_0 \in \mathbb{R}^3$, and a fixed time t. Draw a ball around x_0 of radius $r > 0$. If r is sufficiently large, there will be atoms in this ball, perhaps some of these are simulated and the rest nonsimulated. Now consider a ball of the same radius centered at the point $x_0 + \sum_{j=1}^{3}(I+tA)\nu^j e_j$. By instantaneous periodicity, this ball will contain the same number of atoms as the one around x_0, but they will have different velocities. But their velocities are known explicitly by differentiating the formula (2). So, the statistics of the velocity distribution at different points are related by formulas. If we reinterpret this fact as an ansatz for the molecular density function $f(t, x, v)$ of the kinetic theory of gases, it becomes

$$f(t, x, v) = g(t, v - A(I + tA)^{-1}x). \tag{4}$$

Substitution of this ansatz into the Boltzmann equation gives an exact reduced equation:

$$\frac{\partial g}{\partial t} - \frac{\partial g}{\partial w} \cdot A(I + tA)^{-1} w = \mathbb{C}(g), \tag{5}$$

where the right hand side is the usual collisions operator operating on g. In this sense the Boltzmann equation also inherits exactly (an averaged version of) this invariant manifold. A further ansatz on this equation that brings out the time dependence of g in the case of inverse fifth power molecules further reduces this equation. There remains an equation restricting the initial datum $g(0, w)$.

With this background, we reach the main observation of my presentation. Both numerical simulations of objective molecular dynamics, and this reduced Boltzmann equation in the case of inverse fifth power molecules, reveal a rather unexpected thermodynamics. Before describing this observation, note that generally these solutions are far from equilibrium. For example, the reduced Boltzmann equation does not admit solutions as Maxwellians, unless $A = 0$. However, the simulations and the reduced Boltzmann equation exhibit relationships between macroscopic quantities similar to those of the equilibrium case. As a dramatic example, a Maxwellian density (appropriate for equilibrium) has an H-function (interpreted as minus the entropy) that yields the following relation between H the density ρ and the temperature θ:

$$H = -\log \frac{\theta^{3/2}}{\rho} + const. \tag{6}$$

For all of the solutions found of the reduced Boltzmann equation, this relation is still satisfied, despite the fact that, in some cases, all three of $H(t)$, $\theta(t)$ and $\rho(t)$ are strongly time dependent. In one case $H(t)$ tends to $-\infty$ in finite time, which is decidedly far-from-equilibrium. Numerical examples also reveal similar unexpected behavior.

Taken together, these examples suggest that there may be a "statistical mechanics" on this manifold, which would be extremely interesting to find. The "extremely" here refers to the fact that objective molecular dynamics is universal (independent of the material), and that there is widespread inheritance of this manifold in mesoscopic and macroscopic theory.

There is one caveat of this work in the case of the Boltzmann equation. This is the caveat that we have not yet given an existence theorem for the equation for the initial datum $g(0, w)$ referred to above.

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Atomistic-to-Continuum Multiscale Modeling of Materials with Long-Range Electrostatic Interactions

Jason Marshall
(joint work with Kaushik Dayal)

In this talk we present a multiscale atomistic-to-continuum method for ionic crystals with defects. Defects often play a central role in ionic and electronic solids, not only to limit reliability, but more importantly to enable the functionalities that make these materials of critical importance. Examples include solid electrolytes that conduct current through the motion of charged point defects, and complex oxide ferroelectrics that display multifunctionality through the motion of domain wall defects. Therefore, it is important to understand the structure of defects and their response to electrical and mechanical fields. A central hurdle, however, is that interactions in ionic solids include both short-range atomic interactions as well as long-range electrostatic interactions. Existing atomistic-to-continuum multiscale methods, such as the Quasicontinuum method, are applicable only when the atomic interactions are short-range. In addition, empirical reductions of quantum mechanics to density functional models are unable to capture key phenomena of interest in these materials.

To address this open problem, we develop a multiscale atomistic method to coarse-grain the long-range electrical interactions in ionic crystals with defects. In these settings, the charge density is rapidly varying, but in an almost-periodic manner. We develop the method following a two-scale approach from James and Müller [1]. The key idea is to use the polarization density field as a multiscale mediator that enables efficient coarse-graining by exploiting the almost-periodic nature of the variation. In regions far from the defect, where the crystal is close-to-perfect, the polarization field serves as a proxy that enables us to avoid accounting for the details of the charge variation. We combine this approach for long-range electrostatics with the standard Quasicontinuum method for short-range interactions to achieve an efficient multiscale atomistic-to-continuum method. As a side note, we examine an important issue that is critical to our method: namely, the dependence of the computed polarization field on the choice of unit cell. Potentially, this is fatal to our coarse-graining scheme; however, we show that consistently accounting for boundary charges leaves the continuum electrostatic fields invariant to choice of unit cell. Further details of the method are available in [2].

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Multiscale modeling of rapid crystallization of Germanium from amorphous thin films

Celia Reina

(joint work with Jaime Marian and Luis Sandoval)

Germanium is the base element in many phase-change materials, i.e. systems that can undergo reversible transformations between their crystalline and amorphous phases. They are widely used in current digital electronics and hold great promise for the next generation of non-volatile memory devices. However, the ultra fast phase transformations required for these applications can be exceedingly complex even for single component systems, and a full physical understanding of these phenomena is still lacking. In this talk we presented a study of nucleation and growth of crystalline Ge from amorphous thin films at high temperature using phase field models informed by atomistic calculations of fundamental material properties. The atomistic calculations capture the full anisotropy of the Ge crystal lattice, which results in orientation dependences for interfacial energies and mobilities. These orientation relations are then exactly recovered by the phase field model at finite thickness via a novel parametrization strategy based on invariance solutions of the Allen-Cahn equations. By means of this multiscale approach, we study the interplay between nucleation and growth and find that the relation between the mean radius of the crystallized Ge grains and the nucleation rate follows simple Avrami-type scaling laws. We argue that these can be used to cover a wide region of the nucleation rate space, hence facilitating comparison with experiments.

From Atomistic to Continuum Systems and Elasticity to Crystal Cleavage

Bernd Schmidt

(joint work with Julian Braun, Manuel Friedrich)

The relation of atomistic and continuum models in mathematical material science is an active area of current research, both from a computational and from the analytical point of view. Ultimately, the effective models in continuum mechanics should be derivable from atomistic interaction properties. The main aim of this note is to report on recent results on the rigorous derivation of the passage from atomistic systems to a continuum model in the following three set-ups:

(1) From nonlinear and atomistic to linear continuum elasticity,
(2) From nonlinear and atomistic to nonlinear continuum elasticity and
(3) From nonlinear and atomistic to cleavage laws in continuum mechanics.

1. In the first passage, which also serves to introduce the general scheme of discrete-to-continuum limits, we review an older result from [5] deriving linear elasticity theory from atomistic models by means Γ-convergence. In particular, we obtain the simultaneous limit when both the number of atoms tends to infinity (i.e., when the interatomic distances tend to zero) and the strains within the

material become infinitesimally small. We also consider boundary value problems where a part of the boundary is free.

Consider the atomistic reference configuration $\varepsilon\mathcal{L} \cap \Omega$, where $\Omega \subset \mathbb{R}^d$ (the 'macroscopic region' occupied by the material) is a Lipschitz domain, $\mathcal{L} = A\mathbb{Z}^d$, $A \in \mathbb{R}^{d\times d}$ with $\det A > 0$, a Bravais lattice (the 'atomic crystal') and $\varepsilon \ll 1$ is a small parameter (the 'interatomic distance'). Atomic deformations are mappings

$$y : \varepsilon\mathcal{L} \cap \Omega \to \mathbb{R}^d.$$

Let $x' \in \varepsilon\mathcal{L}'$ denote the centers of the unit cells $\varepsilon A(z + [0,1)^d)$, $z \in \mathbb{Z}^d$. Our main structural assumption is that the energy of a deformation $y : \varepsilon\mathcal{L} \cap \Omega \to \mathbb{R}^d$ be given as a sum of individual *cell energies* as follows.

$$E_\varepsilon(y) = \sum_{x'} W_\varepsilon(x', \bar\nabla y(x')), \quad W_\varepsilon(x', \cdot) = W_{\rm cell}(\cdot) + W_{\rm surface}(x', \cdot),$$

where the discrete gradient $\bar\nabla y(x')$ encodes all the relative displacements of the corners of the cell containing x'. For simplicity, we will neglect $W_{\rm surface}$ in the sequel. See [5] for further details. We also assume that $W_{\rm cell}$ satisfies suitable assumptions of frame-indifference, non-generacy at the identity matrix and growth at infinity.

We set

$$I_k(u) = \delta_k^{-2}\varepsilon_k^d E_\varepsilon(\mathrm{Id} + \delta_k u) = \delta_k^{-2}\varepsilon_k^d \sum_{x'} W_{\rm cell}(Z + \delta_k \bar\nabla u(x'))$$

for $u = g$ on boundary cells.

Theorem 1 (Compactness). If $I_k(u_k) \le C$, then for a subsequence

(i) (interpolations of) $u_k \to u$ in L^2 for some $u \in H^1_g(\Omega)$.
(ii) For (p. c. interpolations of) $\bar\nabla u_k$: $\bar\nabla u_k \rightharpoonup \nabla u \cdot Z$ in L^2.

Theorem 2 (Gamma-convergence). The functionals I_k Γ-converge to

$$I : H^1_g(\Omega) \to \mathbb{R}, \quad I(u) = \frac{1}{2\det A}\int_\Omega Q_{\rm cell}(e(u) \cdot Z),$$

$e(u) = \frac{1}{2}((\nabla u)^T + \nabla u)$.

Theorem 3. If $I_k(w_k) - \inf I_k \to 0$, then (after modification on non-Dirichlet boundary cells)

$$\bar\nabla u_k \to \nabla u \cdot Z \text{ strongly in } L^2, \quad u \text{ the unique minimizer of } I.$$

2. (Joint work with Julian Braun) With the notation introduced above we now consider the energy functionals

$$I_\varepsilon(y) = \varepsilon^d E_\varepsilon(y) = \varepsilon^d \sum_{x'} W_{\rm cell}(\bar\nabla y(x'))$$

for $y = g$ on boundary cells, the only assumption now being that W_{cell} satisfies p-growth assumptions from below and above:

$$c|F|^p - C \leq W_{\text{cell}}(F) \leq C|F|^p + C.$$

Theorem 4 (Gamma-convergence). *I_ε Γ-converges to the functional $I : W^{1,p}(g, \Omega; \mathbb{R}^d) \to \mathbb{R}$, defined by*

$$I(y) = \int_\Omega W_{\text{cont}}(\nabla y(x))\, dx$$

where $W_{\text{cont}} \colon \mathbb{R}^{d\times d} \to [0, \infty)$ is given by

$$W_{\text{cont}}(M) = \frac{1}{|\det A|} \lim_{N\to\infty} \frac{1}{N^d} \inf \Bigg\{ \sum_{x' \in \mathcal{L}' \cap A(0,N)^d} W_{\text{cell}}(\bar{\nabla} y(x')) : y \in \mathcal{A}_1(Mx, A(0, N)^d) \Bigg\}.$$

Theorem 5 (Compactness). *If $I_\varepsilon(y_\varepsilon) \leq C$, then for a subsequence $y_{\varepsilon_k} \rightharpoonup y$ and $\bar{\nabla} y \rightharpoonup \nabla y Z$ for some $y \in W^{1,p}_g(\Omega; \mathbb{R}^d)$.*

Remarks.

(1) This is related to homogenization results for nonlinear integral functionales of Braides and Müller ('85 and '87).
(2) Forces can be added without problems.
(3) The result can be extended to general finite range interactions.
(4) Even to multi-lattices.
(5) For pair interactions this has been shown previously by Alicandro and Cicalese, cf. [1].
(6) Under stronger (yet still reasonable) assumptions on W_{cell}, $W_{\text{cont}}(F)$ agrees with the Cauchy-Born energy $W_{\text{CB}}(F) = W_{\text{cell}}(FZ)$ for F in a neighborhood of $SO(d)$:

For the proofs of these results we refer the reader to [2].

3. (Joint work with Manuel Friedrich) In the last part of this note we consider the problem of deriving continuum cleavage laws for crystals from discrete interactions. We first consider a 2d model problem: a 2d strip with atoms on a (generically) rotated triangular lattice interacting via a NN Lennard-Jones type interactions under uniaxial stretch.

For interatomic distance ε we first find an asymptotic formula for the minimaum energy:

Theorem 6 (Cleavage law with sharp energy estimates).

$$\lim_{\varepsilon\to 0} \inf E_\varepsilon = \min \left\{ \frac{al}{\sqrt{3}} a^2 + \frac{6\alpha + 7\alpha' - 2(3\alpha - \alpha')\cos(6\phi)}{27\sqrt{3}} l\sqrt{\varepsilon} a^3, \frac{2\beta}{\gamma} \right\} + O(\varepsilon).$$

Here α, α' and β describe the response of the pair interaction potential near its equilibrium and for well separated atoms, respectively, l is a geometric factor of the domain and ϕ is the orientation angle of the lattice.

Theorem 8 (Strong convergence of minimizers). If $E_\varepsilon(\mathrm{id}+\sqrt{\varepsilon}u_\varepsilon) = \inf E_\varepsilon + O(\varepsilon)$ and $\tilde{u}_\varepsilon$ denotes the piecewise affine interpolation of u_ε, then there exist $\bar{u}_\varepsilon : (0,l)\times(0,1) \to \mathbb{R}^2$ with $|\{x : \bar{u}_\varepsilon(x) \neq \tilde{u}_\varepsilon(x)\}| = O(\varepsilon)$ such that:

(i) If $a < a_{\mathrm{crit}}$, then there is a sequence $s_\varepsilon \in \mathbb{R}$ such that

$$\|\bar{u}_\varepsilon - (0, s_\varepsilon) - \begin{pmatrix} a & 0 \\ 0 & -\frac{a}{3} \end{pmatrix} \cdot \|_{H^1(\Omega)} \to 0.$$

(ii) If $a > a_{\mathrm{crit}}$, then there exist sequences $p_\varepsilon \in (0,l)$, $s_\varepsilon, t_\varepsilon \in \mathbb{R}$ such that $(p_\varepsilon, 0) + \mathbb{R}\mathbf{v}_\gamma$ intersects both the segments $(0,l)\times\{0\}$ and $(0,l)\times\{1\}$ and, for the parts $\Omega^{(1)}$ to the left and $\Omega^{(2)}$ to the right of $(p_\varepsilon, 0) + \mathbb{R}\mathbf{v}_\gamma$ we have

$$\|\bar{u}_\varepsilon - (0, s_\varepsilon)\|_{H^1(\Omega^{(1)})} + \|\bar{u}_\varepsilon - (al, t_\varepsilon)\|_{H^1(\Omega^{(2)})} \to 0.$$

For the proofs of these results we refer the reader to [3].

We conclude by providing a version of Theorem 8 in higher dimensions when the energy again is given in terms of suitable cell energies as in the first two parts near the set of rigid motions and decouples into pair interactions between well separated subsets near infinity, cf. [4].

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Energy driven pattern formation in atomistic systems

Florian Theil

(joint work with Mark Peletier, David Bourne, Sabine Jansen, Wolfgang König, Bernd Schmidt)

We consider the crystallization problem at zero temperature and at finite temperature. Many nanoscale phenomena can be modeled by finite point configurations $Y \subset \mathbb{R}^d$, $d \in \{1,2,3\}$ which interact via a potential $V(y, Y)$ in the sense that

$V(y, Y)$ accounts for the interaction between a particle $y \in Y$ and $Y \setminus \{y\}$. The total energy of Y is given by

$$E(Y) = \sum_{y \in Y} V(y, Y). \tag{1}$$

We are mostly concerned with cases where V is invariant under the Euclidean group

$$V(Ry + t, RY + t) = V(y, Y) \text{ for all } R \in O(d), t \in \mathbb{R}^d. \tag{2}$$

An interesting example of an energy which can be expressed in the form (1) and respects (2) up to boundary effects is given by

$$E_\Lambda(Y) = \min\Big\{ 2\, c_6 \sum_{y \in Y} \mu(\{y\})^{\frac{1}{2}} + W^{(2)}(\mu, \mathcal{L}_\Lambda) \ : \ \mu \in M_+(Y) \text{ and } \mu(Y) = |\Lambda| \Big\}. \tag{3}$$

Here we assume that $Y \subset \Lambda$ is a finite set, $\Lambda \subset \mathbb{R}^2$ is open and bounded, $M_+(Y)$ is the set of non-negative Radon measures supported in Y, $c_6 = \frac{5\sqrt{3}}{54}$, the measure $\mathcal{L}_\Lambda$ denotes the Lebesgue measure restricted to Λ and

$$W^{(2)}(\mu, \nu) = \inf \left\{ \int_\Lambda |x - \phi(x)|^2 \, \mathrm{d}\nu(x) \ : \ \mu(\phi(A)) = \nu(A) \text{ for all } A \subset \Lambda \right\}$$

is the 2-Wasserstein distance between two non-negative measures μ and ν. The specific choice of the prefactor $2\, c_6$ is motivated by the simplicity of formula (4).

The first result shows that the minimum of $\frac{1}{|\Lambda|} E_\Lambda$ converges to the energy of a triangular lattice as $|\Lambda| \to \infty$.

Theorem 2 ([1]). *Let $H \subset \mathbb{R}^2$ be a regular unit hexagon centered in the origin. If E is given by by (3) then*

$$\lim_{|\Lambda| \to \infty} \inf_{Y \subset \Lambda} \frac{1}{|\Lambda|} E_\Lambda(Y) = E_H(\{0\}). \tag{4}$$

Refinements of Theorem 2 show that most points in Y are very close to the points of a triangular lattice.

Our second result concerns the case where the inverse temperature $\beta > 0$ is finite. Here we assume that $d = 1$ and

$$v(y, Y) = \sum_{y' \in Y \setminus \{y\}} v(|y - y'|),$$

where $v(r) = r^{-12} - r^{-6}$. If $\Lambda \subset \mathbb{R}$ is a bounded set such that $Y \subset \Lambda$ and $\beta \in (0, \infty)$, then the canonical Boltzmann-Gibbs probability of the configuration Y can be defined as

$$P_{\beta, \Lambda}(Y) = \frac{1}{Z(\Lambda, \beta)} \, e^{-\beta \, E(Y)}.$$

The value of the partition function $Z(\Lambda, \rho)$ is determined by the requirement that $P_{\beta, \Lambda}(\cdot)$ is a probability distribution.

To characterize the microstructure of a state Y we first define the Cauchy-Born energy density

$$W(r) = \sum_{i=1}^{\infty} v(r\,i)$$

and the numbers $a(\rho) \in [0, \frac{1}{\rho}]$, $e_0(\rho) \in \mathbb{R}$ by the equations

$$e_0(\rho) = W(a(\rho)) = \min_{a \le \frac{1}{\rho}} W(a).$$

The intuition is that $a(\rho), e_0(\rho)$ represent the asymptotic nearest neighbor distance and the bulk energy per particle in the limits $N \to \infty$ followed by $\beta \to \infty$. After these preparations we can partition Y into disjoint clusters $C_j \subset Y$, $j = 1 \dots M$ which are defined by the requirements

$$\begin{aligned} &Y = \bigcup_{j=1}^{M} C_j, \\ &\operatorname{dist}(C_j, C_k) \ge 2a \text{ if } j \ne k, \\ &\operatorname{dist}(y, C_j \setminus \{y\}) < 2a \text{ if } y \in C_j \text{ for some } j. \end{aligned}$$

The random variable

$$\nu_{\beta,\Lambda}(k) = \frac{1}{M} \#\{j \ : \ \#C_j = k\}$$

characterizes the distribution of the cluster lengths. We will show that the expectation of $\nu_{\beta,\Lambda}$ remains finite as $|\Lambda| \to \infty$ while $\rho = \#Y/|\Lambda|$ is kept fixed. The expectation diverges as $\beta \to \infty$. To this end we define

$$\begin{aligned} K(\beta, \rho) &= \left(\frac{1}{\rho} - a\right)^{-\frac{1}{2}} \left(\frac{\beta\, W''(a)}{2\pi}\right)^{1/4}, \\ p(\beta, \rho) &= K(\beta, \rho)\, e^{\frac{\beta}{2} e_0}. \end{aligned}$$

The number p, which is exponentially small in β if $\rho < \rho_0 = \frac{1}{a(0)}$, represents the leading order term, K accounts for lower order corrections. To characterize the asymptotic behavior of $\nu_{\beta,\Lambda}$ we define rescaled cluster length distribution $\tilde{\nu}_{\beta,\Lambda} \in L^1([0,\infty))$ by

$$\tilde{\nu}_{\beta,\Lambda}(x) = \frac{1}{p}\, \nu_{\beta,\Lambda}\left(\left\lfloor \frac{x}{p} \right\rfloor\right),$$

with the convention $\lfloor x \rfloor = \max\{k \in \{0, 1, \dots\} \ : \ k \le x\}$. Note that $\tilde{\nu}_{\beta,\Lambda}$ is piecewise constant.

Theorem 3 ([2]). *If $\rho < \rho_0$, then the rescaled cluster-length distribution $\tilde{\nu}_{\beta,\Lambda}$ converges to the exponential distribution as $\beta \to \infty$:*

$$\lim_{\beta\to\infty} \lim_{N\to\infty} \|\tilde{\nu}_{\beta,\Lambda} - \exp_1\| = 0$$

in probability with $\exp_1(x) = e^{-x}$.

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Nonequilibrium Processes for Current Reservoirs

Dimitrios Tsagkarogiannis
(joint work with Anna De Masi, Errico Presutti, Maria Eulalia Vares)

Stationary non equilibrium states are characterised by the presence of steady currents flowing through the system. Currents are produced by external forces and we are interested in forces acting on the boundary trying to establish a given current. We model this process considering the simple exclusion process in one space dimension with appropriate boundary mechanisms which create particles on the one side (right) and kill particles on the other (left). The system is then "unbalanced" and in the stationary measure there is a non-zero steady current of particles flowing from right to left. The system is designed to model Fick's law which relates the current to the density gradient. In statistical mechanics non-equilibrium is not as well understood as equilibrium, hence the interest from a physical viewpoint to look at systems which are stationary yet in non-equilibrium: in our case the stationary process is in fact non-reversible and the stationary measure not Gibbsian. We refer to [1], [2] and [3] for some recent reviews on the subject, see also [4] and [5].

Back to our model of current reservoirs, in the interior we consider simple exclusion process for $\eta(x) \in \{0,1\}$ for $x \in \{-N, -N+1, \dots, N-1\}$. Let f be a test function then the generator is given by

$$L_0 f(\eta) := \frac{1}{2} \sum_{x=-N}^{N-1} [f(\eta^{(x,x+1)}) - f(\eta)].$$

On the boundary intervals $I_\pm$ (see below), with $|I_\pm| = K$ for K finite, we impose a (microscopic) current ϵj with $\epsilon = 1/N$

$$L_{b,\pm} f(\eta) := \epsilon \frac{j}{2} \sum_{x \in I_\pm} D_\pm \eta(x) [f(\eta^{(x)}) - f(\eta)],$$

where

$$D_+\eta(x) = [1-\eta(x)]\eta(x+1)\eta(x+2)\dots\eta(N), \quad x \in I_+ \equiv \{N-K+1, \dots, N\}$$

and

$$D_-\eta(x) = \eta(x)[1-\eta(x-1)][1-\eta(x-2)]\dots[1-\eta(-N)],$$
$$x \in I_- \equiv \{-N, \dots, -N+K-1\}.$$

The first result [6] is that considering the density $\rho_\epsilon(x,t) := \mathbb{E}_\epsilon[\eta(x,t)]$ and the the correlation functions

$$v^\epsilon(\underline{x},t|\mu^\epsilon) := \mathbb{E}_\epsilon\Big[\prod_{i=1}^n\{\eta(x_i,t)-\rho_\epsilon(x_i,t)\}\Big], \quad \underline{x}\in\Lambda_N^{n,\neq},\ n\geq 1$$

we prove propagation of chaos, i.e., that $\exists\tau>0, c^*>0$, s.t. $\forall\beta^*>0, n\in\mathbb{Z}_+$, $\exists c_n$ s.t. $\forall\epsilon>0$

$$\sup_{\underline{x}\in\Lambda_N^{n,\neq}}|v^\epsilon(\underline{x},t|\mu^\epsilon)|\leq\begin{cases}c_n(\epsilon^{-2}t)^{-c^*n}, & t\leq\epsilon^{\beta^*}\\ c_n\epsilon^{(2-\beta^*)c^*n} & \epsilon^{\beta^*}\leq t\leq\tau\log\epsilon^{-1}\end{cases}$$

Then we prove that the hydrodynamic limit ($\epsilon\to 0$) is given by the linear heat equation with Dirichlet boundary conditions obtained by solving a non-linear equation which essentially fixes the values of the density at the boundary [7]. For any $t_1>t_0>0$ we have that

$$\lim_{\epsilon\to 0}\sup_{x\in\Lambda_N}\sup_{t_0\leq t\leq t_1}|\rho_\epsilon(x,t)-\rho(\epsilon x,t)|=0,$$

where

$$(1)\qquad \frac{\partial}{\partial t}\rho(r,t)=\frac{1}{2}\frac{\partial^2}{\partial r^2}\rho(r,t),\qquad r\in(-1,1)$$

$$(2)\qquad \frac{\partial\rho(r,t)}{\partial r}|_{r=1}=j(1-\rho(1,t)^K),\quad \frac{\partial\rho(r,t)}{\partial r}|_{r=-1}=j(1-(1-\rho(-1,t))^K).$$

In a similar fashion [7], we can also obtain the validity of Fourier law, i.e., we show that for the expected current through $x+\frac{1}{2}$, given by

$$j^{(\epsilon)}(x,t)=\frac{\epsilon^{-2}}{2}\,\mathbb{E}_\epsilon\big[\epsilon\{\eta(x,t)-\eta(x+1,t)\}\big]=-\frac{1}{2}\mathbb{E}_\epsilon\big[\frac{\eta(x+1,t)-\eta(x,t)}{\epsilon}\big],$$

we have that for $r\in(-1,1)$:

$$\lim_{\epsilon\to 0}j^{(\epsilon)}([\epsilon^{-1}r],t)=-\frac{1}{2}\,\frac{d\rho(r,t)}{dr}.$$

Then we show that the rescaled limiting density profile of the (unique) invariant measure of the process coincides with the unique stationary solution of the hydrodynamic equation, [8]. Let μ_N be the *unique* invariant measure, then

$$\lim_{N\to\infty}\max_{(x_1,..,x_k)\in\Lambda_N^{k,\neq}}\Big|\mu_N\big(\eta(x_1)\cdots\eta(x_k)\big)-\rho^*(x_1/N)\cdots\rho^*(x_k/N)\Big|=0,$$

where $\rho^*(r)$ is the unique stationary solution of the macroscopic equation (1).

Hence, after times of order N^2 the measure μ_N shrinks concentrating on a L^1-neighborhood of the limit profile ρ^*. Last, we also obtain a spectral gap estimate in the (non equilibrium) stationary process uniformly on the system size, see [9] and [10]. For any initial measure we have that

$$\|\mu_N^{(t)}-\mu_N^{\mathrm{st}}\|\leq cNe^{-bN^{-2}t}$$

where for any signed measure λ, $\|\lambda\|=\sum_\eta|\lambda(\eta)|$.

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Crystalline Order, Surface Energy Densities and Wulff Shapes: Emergence from Atomistic Models

Yuen Au Yeung

We address the question why (under suitable conditions) a large number of atoms self–arrange into macroscopic clusters of special polyhedral shapes in the limit of large particle number.

By assuming zero temperature and simplified interatomic interactions the emergence and derivation of such macroscopic clusters can be ultimately extracted from atomistic pair interactions through a coarse–graining process via Γ–convergence. This is performed for the physically relevant case of face–centred cubic configurations (see [2]) and generalises the previous 2D results in [1].

We begin by stating our model: We consider N particles $x_1, \dots, x_N$ in $\mathbb{R}^3$ with total energy

$$E(x_1, \dots, x_N) = \sum_{i \neq j} V(|x_i - x_j|). \tag{1}$$

Here, V is any short–range pair–interaction potential that attains its absolute minimum at distance $|x_i - x_j| = 1$ and that has a sufficiently narrow and deep potential well.

A key to our proof is to make use of the Eulerian viewpoint, *i.e.*, to identify N–particle configurations with probability measures μ_N necessitating in energies

extended to the space of probability measures in $\mathbb{R}^3$. The overall strategy, which was first employed in [1], is now outlined below:

(1) Associate to any N–particle configuration $\{x_1, \dots, x_N\}$ its empirical measure $\sum_{i=1}^N \delta_{x_i}$.
(2) Re–scale the empirical measure to keep the mass and the expected diameter of the support of order one as $N \to \infty$.
(3) Show that the limit measure is a constant multiple of a characteristic function of a set of finite perimeter. Identify the constant as the density of atoms per unit volume in a close–packed lattice.
(4) Derive, from atomistic energy minimisation, a Wulff–Herring type variational principle for the shape, by Gamma–convergence.
(5) Appeal to unique solubility of the Wulff–Herring type variational principle (cf. Taylor [4], Fonseca–Müller [3]) to identify the shape.

Steps one to three are established for arbitrary close–packing configurations and steps four and five are achieved by assuming face–centred cubic configurations. The fourth step requires the introduction of the surface energy density as a count of missing bonds per unit surface area in a thermodynamic limit. The first three steps are now summarised in the following theorem:

Theorem 1. *Assume E and V are given as above and let $\mathcal{L}$ be any close–packing. Let $\{x_1^{(N)}, \dots, x_N^{(N)}\} \subset \mathcal{L}$ be any sequence of connected N–particle configurations that is bounded,* i.e.*,*

$$\max_{i,j} |x_i^{(N)} - x_j^{(N)}| \leq CN^{1/3} \tag{2}$$

and that satisfies an energy bound, i.e.*,*

$$E(x_1^{(N)}, \dots, x_N^{(N)}) \leq -12N + CN^{2/3}, \tag{3}$$

for some constant C independent of N. Let μ_N be the associated sequence of re–scaled empirical measures

$$\mu_N = \frac{1}{N} \sum_{i=1}^N \delta_{N^{-1/3} x_i^{(N)}}. \tag{4}$$

Then, up to translation (that is to say, up to replacing μ_N by $\mu_N(\cdot + a_N)$ for some constant $a_N \in \mathbb{R}^3$) and passage to a subsequence, μ_N weak$*$ converges in $\mathcal{M}(\mathbb{R}^3)$ to $\mu \in \mathcal{M}(\mathbb{R}^3)$. Moreover, μ has mass one, i.e.*, $\int_{\mathbb{R}^3} \mathrm{d}\mu = 1$.*
Further, the limit measure is of the form

$$\mu = \rho \chi_E,$$

*where $\rho = \sqrt{2}$ (*i.e.*, the density of atoms per unit volume of $\mathcal{L}$) and E is a set of finite perimeter of volume ρ^{-1}.*

Next, for exact face–centred cubic minimiser the ensuing cluster has a unique shape (regular truncated octahedron):

Theorem 2. *Assume E and V are as above and let E have crystallised ground*

states, i.e., *every ground state is—after translation and rotation—a subset of the face–centred cubic lattice. Let* $\{x_1^{(N)}, \dots, x_N^{(N)}\}$ *be any minimising* N*–particle configuration of* E *of bounded diameters and of bounded energy,* i.e., *satisfying (2) and (3), and let* μ_N *be the associated re–scaled empirical measure (4).*
As $N \to \infty$*, up to translation and rotation (that is to say, up to replacing* μ_N *by* $\mu_N(R_N \cdot + a_N)$ *for some rotation* $R_N \in SO(3)$ *and some translation vector* $a_N \in \mathbb{R}^3$*)* μ_N *converges weak∗ to the limit measure*

$$\mu = \sqrt{2}\chi_W. \tag{5}$$

Here the set W *is the* c*–multiple of the regular truncated octahedron whose vertices are given by all permutations of* $(0, 2, 4)^T$*,* $(0, -2, 4)^T$*,* $(0, 2, -4)^T$*,* $(0, -2, -4)^T$*, with the constant* c *being* $\frac{\sqrt{2}}{512}$*.*

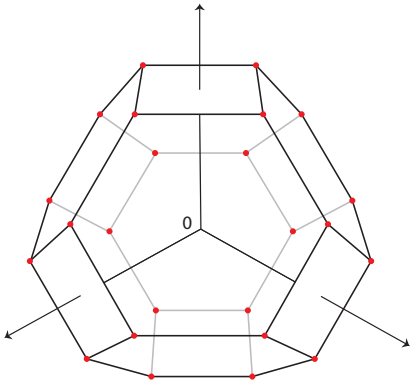

FIGURE 1. The Wulff shape for the face–centred cubic lattice is a regular truncated octahedron; its normals locally minimise the surface energy density and coincide with the directions of the 3–fold and 4–fold rotation axes. In fact, these minima give rise to the emergence of the hexagons and squares.

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From simple particle models to GENERIC

Johannes Zimmer
(joint work with S. Adams, N. Dirr, H. Duong, V. Laschos, M. A. Peletier)

One possible way to describe nonequilibrium systems is to use a framework such as GENERIC [8]. GENERIC stands for General Equation for Non-Equilibrium Reversible-Irreversible Coupling. In this setting, the evolution of a thermodynamic system in a state space Z is described by the equation

$$\partial_t z = \mathsf{L}(z)\,\mathsf{dE}(z) + \mathsf{K}(z)\,\mathsf{dS}(z), \tag{1}$$

where $\mathsf{E}, \mathsf{S}\colon Z \to \mathbb{R}$ are the energy and entropy functionals, dE, dS are appropriate derivatives (they could be Fréchet derivative or a gradient with respect to some inner product); $\mathsf{L} = \mathsf{L}(z)$ describes the conservative evolution and is an antisymmetric operator satisfying the Jacobi identity

$$\{\{\mathsf{F}_1, \mathsf{F}_2\}_\mathsf{L}, \mathsf{F}_3\}_\mathsf{L} + \{\{\mathsf{F}_2, \mathsf{F}_3\}_\mathsf{L}, \mathsf{F}_1\}_\mathsf{L} + \{\{\mathsf{F}_3, \mathsf{F}_1\}_\mathsf{L}, \mathsf{F}_2\}_\mathsf{L} = 0$$

for all functions $\mathsf{F}_i\colon Z\colon Z \to \mathbb{R},$, with Poisson bracket $\{\cdot,\cdot\}_\mathsf{L}$

$$\{\mathsf{F}, \mathsf{G}\}_\mathsf{L} := \mathsf{dF} \cdot \mathsf{L}\,\mathsf{dG},$$

$\mathsf{K} = \mathsf{K}(z)$ is symmetric and positive semidefinite [5, 8, 7]. In a nutshell, the GENERIC formulation (1) expresses the expectation that, even in nonequilibrium situations, the evolution of a thermodynamic system is governed by an energy E and an entropy S, where the former evolves conservatively and the latter is nondecreasing (the physical entropy is minus the mathematical entropy). While formulated for nonequilibrium, a setting such as GENERIC of course also suits situations near equilibrium or in local equilibrium, and we will only discuss systems without drift.

There are many facets of a possible mathematical analysis of GENERIC. Mielke has shown that GENERIC is very beneficial for mathematical modelling, giving a clear understanding how to derive thermodynamically consistent models [7]. There are two areas which are to the best of our knowledge completely open: First, there is no existence theory for a thermodynamic system using the structure of GENERIC. The evolution operators L, K are in general nonlinear. Second, there is no rigorous theory for a derivation of (1) from a microscopically conservative system (however, a systematic approach for this this passage is developed in the work of Öttinger and coworkers, e.g., [8]).

We consider the much simpler question of how to derive systems in GENERIC form from mesoscopic (stochastic) models. Two cases are discussed, diffusion as a purely entropic process and the Vlasov-Fokker-Poisson equation as a system driven by energy and entropy.

For diffusion, the (physical) entropy $\mathsf{S}(\rho) := -\int_{\mathbb{R}^n} \rho(x) \log \rho(x) dx$ is nondecreasing,

$$\frac{\partial}{\partial t}\rho(x,t) = \Delta\rho(x,t) = \operatorname{div}\left(\rho(x,t)\nabla \mathsf{dS}(\rho)\right) =: \operatorname{grad}_W \mathsf{dS}(\rho) =: \mathsf{K}\mathsf{dS}; \tag{2}$$

here $\mathsf{K}\xi = \operatorname{grad}_W \xi = \operatorname{div}(\rho(x,t)\nabla\xi)$ denotes the Wasserstein gradient and dS is the variational derivative. It is a classic result that diffusion is the many-particle limit of Brownian motion, and we show how this result can be obtained in such a way that the limit passage reveals the entropy and the Wasserstein metric directly. Namely, for the empirical measure $\rho_n := \frac{1}{n}\sum_{i=1}^n \delta_{X_i}$ associated with n Brownian particles, a large deviation result [1] states in essence

$$\mathbb{P}\big(L_n^h \approx \rho \,|\, L_n^0 \approx \rho_0\big) \approx \exp\big[-nJ_h(\rho\,;\rho_0)\big] \qquad \text{as } n \to \infty,$$

with rate function

$$J_h(\rho\,;\,\rho_0) := \inf_{q\colon\, \pi_0 q = \rho_0, \pi_1 q = \rho} H(q\,|\,q_0)$$

with

$$H(q\,|\,p) := \begin{cases} \int\limits_{\mathbb{R}\times\mathbb{R}} f(x,y)\log f(x,y)\; p(d(x,y)) & \text{if } q \ll p,\, f = \frac{dq}{dp} \\ +\infty & \text{else} \end{cases}.$$

One can then see for different classes of measures [1, 4] that J_h and the time discretisation of the variational formulation of the Wasserstein-entropy gradient flow for time step h [6] agree asymptotically in the limit $h \to 0$, in the sense of Γ-convergence.

Alternatively, given n Brownian particles and a fixed terminal time $T > 0$, one can consider the path of empirical measures $[0,T] \ni t \mapsto \rho_n(t) = \frac{1}{n}\sum_{j=1}^n \delta_{X(j)}$; then a large deviation result of Dawson and Gärtner [3] states

$$\operatorname{Prob}(\rho_n \approx \rho) \sim \exp[-nJ(\rho)], \tag{3}$$

with rate functional

$$J(\rho) := \frac{1}{2}\int_0^T \left\| \frac{\partial\rho}{\partial t} - \Delta\rho \right\|_{\rho(t),*}^2 dt, \tag{4}$$

where the norm $\|\cdot\|_{\rho(t),*}$ is associated with the Wasserstein metric. Using this connection to Wasserstein evolution and the identity $\Delta\rho = \operatorname{div}(\rho\nabla\mathsf{dS})$, the rate functional can be rewritten as

$$\mathsf{S}(\rho(T)) - \mathsf{S}(\rho(0)) + \frac{1}{2}\int_0^T \left[\left\| \frac{\partial\rho}{\partial t} \right\|_{\rho,*}^2 + \|-\mathsf{dS}\|_\rho^2 \right] dt,$$

which reveals the Wasserstein structure via the norm, and the entropy as driving force.

The Vlasov-Fokker-Poisson equation is an example of a system driven by energy and entropy. It describes the evolution of a density $\rho = \rho(p,q)$ depending on position q and momentum p,

$$\partial_t\rho = -\operatorname{div}_q\Big(\rho\frac{p}{m}\Big) + \operatorname{div}_p\rho\Big(\nabla_q V + \nabla_q\psi * \rho + \gamma\frac{p}{m}\Big) + \gamma\theta\Delta_p\rho, \tag{5}$$

which is the many particle limit of interacting Brownian particles with inertia,

$$\begin{aligned} dQ_i(t) &= \frac{P_i(t)}{m}dt, \\ dP_i(t) &= -\nabla V(Q_i(t))dt - \sum_{j=1}^{n} \nabla\psi(Q_i(t) - Q_j(t)) \\ &\quad - \frac{\gamma}{m}P_i(t)\,dt + \sqrt{2\gamma\theta}dW_i(t) \end{aligned}$$

(here Q_i and P_i are the position and momentum of particle $i = 1, \dots, n$ with mass m experiencing potential V, interaction potential ψ, drift term $-\gamma P_i dt/m$, and stochastic forcing by a Wiener measures W_i, where the W_i's are independent [5]).

Once this particle model is augmented by a heat balance to account for the exchange of energy through the heat bath, it is possible to write the Vlasov-Fokker-Poisson equation in GENERIC form [5]. To be precise, the one can add the energy balance

$$de_n = \frac{1}{n}\sum_{i=1}^{n}\left[\frac{\gamma}{m^2}P_i^2 dt - \frac{\gamma\theta d}{m}\,dt + \frac{\sqrt{2\gamma\theta}}{m}P_i dW_i\right]$$

and derive a GENERIC formulation for $(\rho, e) \in P_2(\mathbb{R}^{2d}) \times \mathbb{R}$, where P_2 are the probability measures with finite second moment. It can be shown that a large deviation principle for the Vlasov-Fokker-Poisson equation given by Budhiraja, Dupuis and Fischer [2] can be adapted to describe (up to a constant) the latter equation as minimiser of rate functional I in GENERIC form [5],

$$I(\rho) = \begin{cases} \dfrac{1}{4\gamma\theta}\displaystyle\int_0^T \left\|\partial_t\rho_t - A^{\tau}_{\rho_t}\rho_t\right\|^2_{-1,\rho_t} dt & \rho \in AC([0,T]; P(\mathbb{R}^{2d})), \rho|_{t=0} = \rho^0, \\ +\infty & \text{otherwise,} \end{cases}$$

where $A_\nu f := \frac{p}{m}\cdot\nabla_p f - \left[\nabla_q V + \nabla_q\psi * \nu + \gamma\frac{p}{m}\right]\cdot\nabla_p f + \gamma\theta\Delta_p f$.

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Epitaxially strained crystalline films: Scaling regimes and beyond

Barbara Zwicknagl
(joint work with Peter Bella, Michael Goldman, Irene Fonseca and Aldo Pratelli)

0.1. **Motivation.** We discuss variational models to describe the epitaxial deposition of a thin crystalline film on a rigid substrate when there is a mismatch between the crystal lattices. Due to this misfit, a strain is induced in the film during deposition. Experimental observations show that depending on the volume of the deposited film and the amplitude of the misfit, the film develops different morphologies. Typically, at small volumes, a flat layer is formed, while at larger volumes, compact islands arise. This pattern formation is explained as the result of a competition between the strain energy in the film and the surface energy of the film's free surface.

0.2. **Model.** Our analytical studies adopt two-dimensional continuum models introduced in the physical literature (see [1]), i.e., for fixed d, $e_0 > 0$, we consider the functional

$$F_{d,e_0}(u,h) := \int_{\Omega_h} W(\nabla u) + \int_0^1 \sqrt{1+|h'|^2} \tag{1}$$

for Lipschitz functions $h : [0,1] \to \mathbb{R}$ with $h(0) = h(1) = 0$, and $\int_0^1 h(x)\,dx = d$, and $u \in W^{1,2}(\Omega_h)$ with $u(x,0) = e_0(x,0)$, where $\Omega_h := \{(x,y) : x \in [0,1],\, 0 \le y \le h(x)\}$. Here, h is the height profile function of the deposited film, and its subgraph Ω_h is the domain occupied by the film. The first term in (1) describes the stored strain energy where W is a typical elastic energy density with p-growth, $1 < p < \infty$, typical examples for $p = 2$ being $W(M) = \operatorname{dist}^2(M, SO(2))$ or $W(M) = \frac{1}{4}|M+M^T|^2$. We study film profiles at fixed volume d, and the parameter e_0 measures the amplitude of the crystallographic misfit. Regularity and other qualitative properties of minimizers of (1) have been studied in [4, 3]

0.3. **Results.** We discuss joint work with Michael Goldman [5], in which the qualitative behavior of the minimal energy in terms of the volume d of the film and the amplitude e_0 of the misfit is studied: There are constants C_1 and $C_2 > 0$ such that for all $d > 0$ and all $e_0 > 0$,

$$C_1 \max\{1,\, d,\, e_0^{p/3} d^{2/3}\} \le \inf F_{d,e_0} \le C_2 \max\{1,\, d,\, e_0^{p/3} d^{2/3}\}.$$

Corresponding reduced asymptotic models in the sense of Γ-convergence in the various regimes are discussed. The results agree qualitatively with the experimentally observed patterns. In particular it is shown that in some regimes the formation of islands is energetically favored in the sense that properly rescaled profile functions of low energy sequences converge to sums of Dirac measures. This is in particular the case when the amplitude of the misfit large compared to the volume of the film.

The analysis makes use of the fact that the profile function h is supported on a compact interval $[0,1]$, which prevents the formation of a very thin layer, that is,

the wetting effect. We briefly discuss related results obtained in joint work with Peter Bella and Michael Goldman [6], for island formation on unbounded domains, in particular with respect to existence and nonexistence of minimizers.
In the last part, results from joint work with Irene Fonseca and Aldo Pratelli [7] are briefly discussed. Here, a fully facetted model with positive miscut angle introduced in [8] (based on [2]) is analyzed, which captures more microscopic properties of the island formation. The energy functional is given by

$$E_d(h) := \int_0^W \int_0^W \log|x-y|\,dy\,dx + \int_0^W (\sqrt{1+|h'|^2}-1)\,dx \tag{2}$$

for profile functions $h \in W^{1,\infty}(\mathbb{R})$ with $\mathrm{supp(h)} = [0,W]$, $\int_{\mathbb{R}} h(x)\,dx = d$ and $h' \in \{\tan(-\theta_m + n\theta) : \ n \in \mathcal{N}\}$ almost everywhere in their support, with some finite set $\mathcal{N} \subset \mathbb{Z}$. The second term in (2) models again the extra surface energy, and the first term is a small slope approximation of a relaxed strain energy. The angles $\theta > \theta_m > 0$ are given parameters, where the latter is the miscut angle. A positive miscut angle prevents the wetting effect, since flat profiles are not admissible due to the constraint on the slopes. Consequently, we obtain existence of minimizers for all volumes d. We discuss the relaxation of the problem with respect to uniform convergence. The limit functional turns out to be the sum of an elastic energy term and an anisotropic surface energy term. We show that all minimizers of the relaxed problem are fully facetted, i.e., $h' \in \{\tan(-\theta_m + n\theta) : \ n \in \mathcal{N}\}$ almost everywhere in their support, and we finally discuss some geometric properties of minimizers, including an analogue of the zero contact angle property.

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