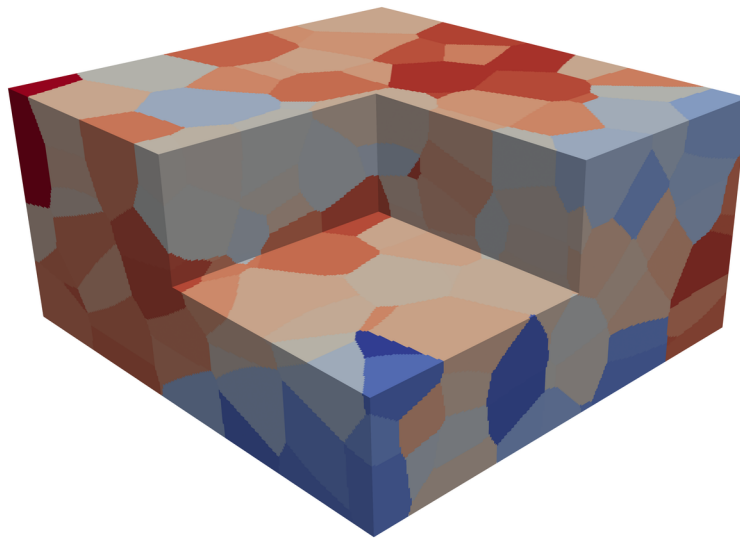


Frontiers of Mathematical and Computational Aspects of Materials Science

Carnegie Mellon University
October 12–14, 2026
Singleton Room, Roberts Hall

The conference brings together researchers working on the mathematical and computational aspects of materials science for the discussion and exchange of ideas. It is held in honor of David Kinderlehrer. Funding for junior participants, and an opportunity for them to present their work in a poster session and lightning talks, have been available. The conference is supported by the NSF, the Center for Nonlinear Analysis, the Department of Materials Science and Engineering, the Department of Mathematical Sciences and the Mellon College of Science.



Local Information



Two paths from the hotel to the conference venue are shown. The walk is about 0.8 miles long.

Food options for lunch.

1. **S. Craig Street.** A short walk from Roberts Hall, with the largest concentration of options: *Ali Baba* (Syrian, 404 S. Craig St.), *Union Grill* (American, 413 S. Craig St.), *Sushi Fuku* (sushi and poke bowls, 415 S. Craig St.), *EatUnique* (café and sandwiches, 305 S. Craig St.), *Grapow* (Asian street food, 411 S. Craig St.) and *Pepper Space* (Sichuan, 4609 Forbes Ave. at S. Craig St.).
2. **The Porch at Schenley** (American bistro), Schenley Plaza.
3. **University Center** (various options), on campus.
4. **Hunan Express** (Chinese).

Program

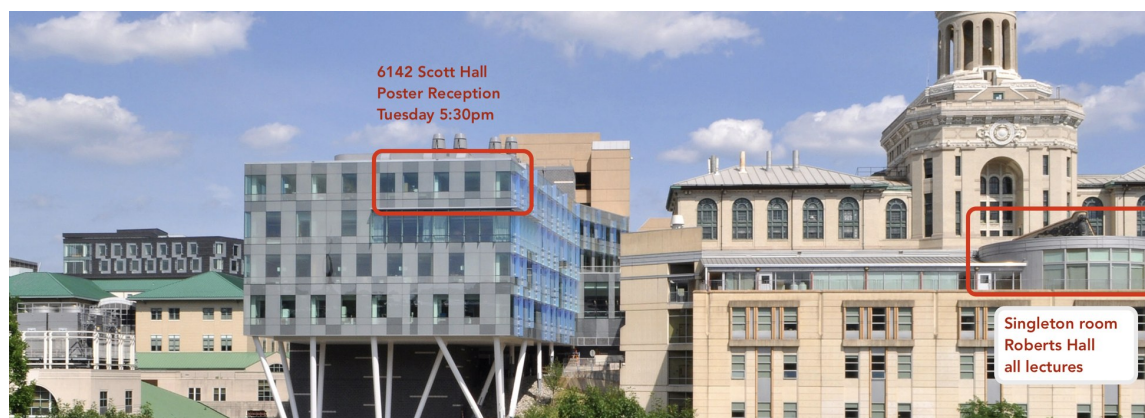
Monday, October 12

Time	Session Details
08:20–09:00	Registration and Breakfast
09:00–09:10	Opening Remarks
09:10–09:50	John Ball <i>Compatibility of microstructures in polycrystals</i>
09:50–10:30	Felix Otto <i>Capillarity-driven thin viscous films with thermal noise</i>
10:30–11:00	Coffee Break
11:00–11:40	Tony Rollett <i>Grains, Tails and Ears</i>
11:40–12:20	Kaushik Bhattacharya <i>Learning from experiments</i>
12:20–2:30	Lunch
2:30–3:10	Amanda Krause <i>The Search for Accurate Predictors of Grain Growth</i>
3:10–3:50	Gero Friesecke <i>Mass splitting in the generalized Euler equations and non-Monge solutions in multi-marginal optimal transport</i>
3:50–4:20	Coffee Break
4:20–5:00	Mitchell Luskin <i>From Structural to Electronic Phase Transitions</i>
5:00–5:40	Russell Schwab <i>On free boundary problems and nonlinear fractional heat equations</i>

Tuesday, October 13

Time	Session Details
08:20–09:00	Breakfast
09:00–09:40	Henri Berestycki <i>Range Expansion by Growth and Congestion</i>
09:40–10:20	Ian Tobasco <i>Derivation of the Flamant solution for a nonlinear elastic wedge</i>
10:20–11:00	Michel Chipot <i>On some class of nonlinear nonlocal problems</i>
11:00–11:30	Coffee Break
11:30–12:10	Richard James <i>An unusual rolling/unrolling phenomenon in nanoscale films with links to the rigidity inequality</i>
12:10–12:50	Gregory Rohrer <i>Microstructure evolution in networks containing flat boundaries</i>
12:50–2:30	Lunch
2:30–3:10	Yekaterina Epshteyn <i>Multiscale Modeling, Simulation, and Analysis of Microstructure Evolution in Polycrystalline Materials</i>
3:10–3:50	Qiang Du <i>Heterogeneously localized nonlocal operators with applications to semi-supervised learning</i>
3:50–4:20	Coffee Break
4:20–5:20	Lightning Talks
5:30–7:30	Poster Reception — 6142 Scott Hall

After the lightning talks, walk to **6142 Scott Hall** for the poster reception.



Wednesday, October 14

Time	Session Details
08:20–09:00	Breakfast
09:00–09:40	Lia Bronsard <i>On a partitioning problem inspired by triblock copolymers</i>
09:40–10:20	Andrea Braides <i>Asymptotic behaviour of fractional Sobolev spaces on thin films</i>
10:20–10:50	Coffee Break
10:50–11:30	Jeff Rickman <i>Point Process Models of Nucleation and Growth Phenomena in Materials Science</i>
11:30–12:10	Chun Liu <i>Active Fluids and Applications in Complex Fluids</i>
12:10–2:00	Lunch
2:00–2:40	Maria Emelianenko <i>Towards Robust Data-Driven Multiscale Modeling of Microstructure–Property Relations</i>
2:40–3:20	Adrian Tudorascu <i>Sticky particle solutions as energy minimizers for the pressureless Euler system</i>
3:20–3:50	Coffee Break
3:50–4:30	Marshall Slemrod <i>The least action principle and new admissibility criteria for initial value problems</i>
4:30–4:40	Closing Remarks

Abstracts

Monday, October 12

09:10–09:50

John Ball Heriot-Watt University and Maxwell Institute for Mathematical Sciences, Edinburgh

Compatibility of microstructures in polycrystals

The talk concerns martensitic microstructures in polycrystals, focussing on their compatibility across grain boundaries. Using a computer-assisted proof it is shown that for cubic-to-tetragonal transformations it is not in general possible to achieve compatibility when the grain boundary separates two simple laminates of zero energy, thus explaining why higher-order laminates are typically observed. The Taylor set of deformation gradients is defined and studied, this set having the property that any deformation whose gradient belongs to it corresponds to a zero-energy microstructure for the polycrystal independent of grain geometry and grain rotations. New upper bounds for the Taylor set are proved for cubic-to-tetragonal and cubic-to-orthorhombic transformations, generalizing those of Bhattacharya and Kohn for the geometrically linearized theory. This is joint work with Myrto Galanopoulou.

09:50–10:30

Felix Otto Max Planck Institute for Mathematics in the Sciences, Leipzig

Capillarity-driven thin viscous films with thermal noise

David Kinderlehrer taught me an intuition for thermal noise, and the pragmatic use of tools to describe it mathematically – I don't think that I would have ever learned this from a standard course in probability.

The themes of the talk are geometric concepts in the high-dimensional setting of a discretization of an over-damped continuum model driven by thermal noise, as given by the fluctuation-dissipation principle.

The topic is specific: We consider the evolution of the height of a liquid film on a planar solid substrate, driven by capillarity and limited by viscosity, yielding a height-dependent mobility. Any spatial discretization of this singular stochastic PDE relies on a choice of a numerical mobility, and leads to a large system of stochastic ODEs. The latter requires a non-obvious counter term that diverges as the grid size goes to zero, and which does not vanish when passing to the Stratonovich formulation. The counter term can be derived from the informal gradient flow structure via the corresponding Fokker–Planck equation; it ensures a Riemannian covariance property, and amounts to a Wick renormalization.

This is joint work with B. Gess, R. Gvalani, F. Kunick, and – in progress – M. Sauerbrey.

11:00–11:40

Tony Rollett Carnegie Mellon University

Grains, Tails and Ears

A shared enthusiasm has been the challenge of understanding grain growth in polycrystalline solids. Supported by a wide range of collaborations, this has touched on many different aspects from equilibrium at triple lines, to size distributions, to abnormal coarsening, etc. Starting with a re-working of Hillert's adaptation of LSW theory and showing that it does, in fact, admit the possibility of abnormal grain growth confirmed by Potts model simulations, continuing with analysis of the effects of anisotropic energy and mobility, then extreme value statistics to quantify Barmak's "tail and an ear" and recently a machine-learning-informed analysis of both normal and abnormal grain growth, this area has offered a cornucopia of puzzles. David Kinderlehrer's mathematical contributions dwarf these applications to materials science, but this speaker has deeply appreciated the interdisciplinarity of his insights over the decades.

11:40–12:20

Kaushik Bhattacharya California Institute of Technology

Learning from experiments

I will discuss problems in the Calculus of Variations that arise when we seek to determine properties of materials from experiments. These are often described as indirect inverse problems. Material properties are characterized in terms of intensive quantities like (fields/strains and current/stresses) while experiments typically measure extensive quantities (potential/displacements and flow/force), often on the boundary. Obtaining the material properties from these experiments requires us to infer the intensive quantities, but these depend on the material properties through partial differential equations. Classically, experimental configurations are designed to readily infer intensive quantities from the extensive measurements by creating uniform states. Unfortunately, this yields limited information, grossly insufficient for engineering needs. A variety of new optical, X-ray and other methods enable full-field observation of complex states, but require us to solve the indirect inverse problem. A further complication is the complexity of the physics of these experimental techniques. All of these lead to interesting problems in the Calculus of Variations. I will discuss some principles, and demonstrate them with selected examples.

2:30–3:10

Amanda Krause Carnegie Mellon University

The Search for Accurate Predictors of Grain Growth

Grain growth is a fundamental behavior in materials processing that dictates the final microstructure and, thus, performance. Established grain growth models still fail to predict commonly observed, albeit irregular, behaviors like abnormal grain growth, in which a small fraction of grains grow faster than their neighbors. Our recent experimental observations using 3D X-ray diffraction microscopy methods reveal that curvature, the commonly assumed driving force for grain growth, is not a predictor of grain boundary velocity or direction of motion. Thus, the driving forces for grain growth must be re-examined to develop predictive models for both normal and abnormal

grain growth. In this talk, I will compare experimental observations of growth in real polycrystals with Monte Carlo Potts simulations and analytical models to interrogate the role of grain boundary energy anisotropy in microstructure evolution. Then, I will describe how machine learning models can capture the underlying behavior of an evolving Markov decision process and “teach” it to maximize the “rewards” regarding the agreement between prediction and experimental observations. I will demonstrate how our model emulates grain growth trained by either Monte Carlo Potts grain growth simulations or real experimental data. The accuracy of our short- and long-term predictions will be evaluated, and the limits of this approach will be discussed.

3:10–3:50

Gero Friesecke Technical University of Munich

Mass splitting in the generalized Euler equations and non-Monge solutions in multi-marginal optimal transport

Brenier, building on earlier work by Arnold, introduced a celebrated variational formulation of the incompressible Euler equations of fluid dynamics. This formulation, after time discretization, is a prototype example of multi-marginal optimal transport, yet the question whether it exhibits mass-splitting (or equivalently, whether there exist solutions which are not of Monge form) has remained open. In this talk – after introducing Arnold’s and Brenier’s formulations of Euler and explaining the connection to optimal transport – we resolve this question by giving a mass-splitting example in one spatial dimension. Moreover we present a corresponding very simple fully discrete example of mass-splitting which reveals a transparent underlying mechanism. Reference: arXiv:2601.02616

4:20–5:00

Mitchell Luskin University of Minnesota

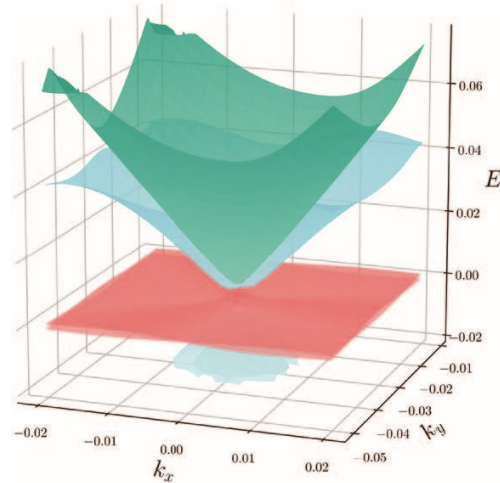
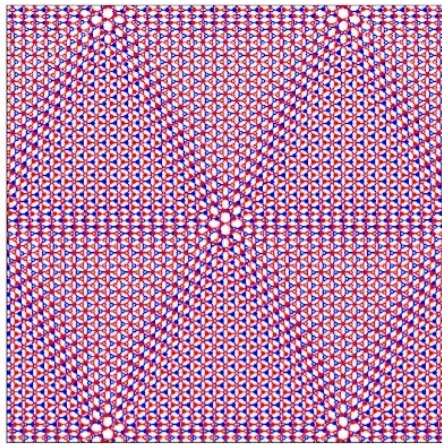
From Structural to Electronic Phase Transitions

A small relative rotation between two-dimensional lattices produces nearly periodic “moiré” patterns on a superlattice scale much larger than that of the underlying lattices. Moiré materials provide a new setting for the mathematical study of symmetry-breaking phase transitions in electronic wave functions, with connections to the theory of structural phase transitions developed by Ericksen, Kinderlehrer, Ball, and James.

We use mathematical techniques for waves in inhomogeneous media to derive effective models for electron dynamics in twisted bilayer graphene. In particular, we identify a regime in which the Bistritzer–MacDonald continuum model emerges from the underlying atomistic description. This regime occurs near the first magic angle, where the electron group velocity becomes very small and electron–electron interactions become comparable to or larger than the kinetic energy. These strong correlations give rise to a rich variety of electronic phases, including superconducting and Mott-insulating states.

In this talk, we will present recent rigorous results extending our analysis to incorporate structural relaxation and electron–electron interactions. We will discuss how these effects lead to effective mathematical models for symmetry-breaking electronic phases and how the resulting framework

can be used to analyze phase transitions in moiré materials.



5:00–5:40

Russell Schwab Michigan State University

On free boundary problems and nonlinear fractional heat equations

The dynamics for the interface in many free boundary problems is driven by the normal derivative of a corresponding pressure function, and often the free boundary is the boundary of the positivity set of this unknown pressure, which evolves in time. Two well-known examples of these types of models are called the Hele-Shaw equation and the one-phase Muskat problem. In this talk we will describe the set-up of some of these free boundaries and show how, in many situations, their solution becomes equivalent to solving a nonlinear fractional heat equation (in one fewer space variable), which opens up the original model to a whole different set of tools for analysis (Hamilton-Jacobi-Bellman equations).

Tuesday, October 13

09:00–09:40

Henri Berestycki University of Maryland and EHESS Paris

Range Expansion by Growth and Congestion

Motivated by the range expansion of immotile cell colonies, we introduce a nonlinear nonlocal model in which spatial expansion results solely from growth and competition for space. In a singular congestion limit, the model converges to a nonlocal free-boundary problem that describes the evolution of saturated regions where growth is arrested owing to contact inhibition. After discussing the motivation and introducing a general model, I will present the derivation of this singular limit and discuss its main mathematical properties. The resulting framework provides a new perspective on invasion phenomena driven by growth and congestion. I report here on joint work with Antoine Mellet and Gabi Steinbach.

09:40–10:20

Ian Tobasco University of Michigan

Derivation of the Flamant solution for a nonlinear elastic wedge

Mechanical metamaterials such as ones based on origami and kirigami achieve bulk shape change through coordinated rearrangements of their panels. Typically, bar-and-hinge models are used to model this behavior, while in reality the underlying material is a continuum. For instance, origami is made by folding paper, while kirigami is made by cutting holes from a rubber sheet. Motivated by kirigami, we study the response of a truncated nonlinear elastic wedge in a double limit where both the truncation length and scale of the applied forces tend to zero. We prove that the classical Flamant solution (stress $\sim 1/r$) governs the leading-order response of the wedge. Since the linear elastic stress blows up at the tip of the wedge, the choice of nonlinearity plays a key role. We show that the Flamant solution is correct for models with at least quadratic growth at infinity; the case of quadratic growth is borderline, as we also explain. This is joint work with Paul Plucinsky (USC) and Dominik Engl (KU Eichstätt-Ingolstadt).

10:20–11:00

Michel Chipot University of Zurich

On some class of nonlinear nonlocal problems

The goal of this talk is to study Dirichlet problems of the type

$$-\Delta u + g\left(\int_{\Omega} F(u)\right)f(u) = 0,$$

where F denotes a primitive of f . Diverse techniques are presented depending on the shape of f or g . These problems are nonlinear and nonlocal, and thus they experience very different behaviours depending on the data.

11:30–12:10

Richard James University of Minnesota

An unusual rolling/unrolling phenomenon in nanoscale films with links to the rigidity inequality

Freestanding single crystal films of nanoscale thickness are now being produced in lots of materials, due to the development of a lift-off technology. This involves growing the film epitaxially on an interlayer that later can be dissolved by adding a drop of water. When this is done with Barium Titanate (BTO), the film spontaneously cracks into an array of little rectangles. Then, without provocation, the little rectangles spontaneously roll up into perfect little cylinders. After that, some of them spontaneously unroll, and then roll up again. We present an explanation of these phenomena, and notice an unexpected connection to the optimal constant for the rigidity inequality. Joint work with Kalpesh Jaykar, Sooho Choo and Bharat Jalan.

12:10–12:50

Gregory Rohrer Carnegie Mellon University

Microstructure evolution in networks containing flat boundaries

Recent studies of grain growth in polycrystals have been able to quantify grain boundary migration rates in a variety of materials. One of the principal findings has been that grain boundary curvature is not a good predictor of the direction or speed of grain boundary migration, overturning what was considered a governing principle of microstructure evolution. Another surprising result is that the fastest observed grain boundaries are also those with zero curvature. This presentation will focus on the mechanism for, and the impact of, the migration of flat, singular grain boundaries. When there is a cusp in the energy of a grain boundary as a function of orientation, the Herring equilibrium condition becomes an inequality and the dihedral angle of the grain boundary can take a range of values. Simulated migration under the weighted mean curvature driving force can lead to unexpected behavior that contradicts conventional grain growth theory. These results are compared to experimental observations to determine the impact of singularities in the grain boundary energy function on grain boundary migration.

2:30–3:10

Yekaterina Epshteyn University of Utah

Multiscale Modeling, Simulation, and Analysis of Microstructure Evolution in Polycrystalline Materials

In this talk, we will present recent perspectives on mathematical modeling, numerical simulation, and mathematical analysis of the evolution of the grain boundary network in polycrystalline microstructures. This evolution is a very complex, multiscale, and multiphysics process.

Our efforts support the solutions of the central problems in materials science, the design of technologies delivering an arrangement of grains that produces a desired set of material properties. Relevant recent experiments, along with current and future research, will be discussed as well.

Most technologically useful materials—spanning the length scale from meters to nanometers, from aircraft to microprocessors—are polycrystalline. Polycrystals are composed of small monocrystalline grains that are separated by grain boundaries of crystallites with different lattice orientations. The changes in the grain and grain boundary structure of polycrystalline materials highly influence their properties, including, but not limited to, electrical, mechanical, optical, and thermal.

A method by which the grain structure can be engineered in polycrystalline materials is through grain growth (coarsening) of a starting structure. The evolution of the grain/grain boundary structure and associated grain growth involve, for example, the dynamics of grain boundaries, triple junctions in 2D (triple curves/lines and quadruple points in 3D), and the dynamics of lattice misorientations. Therefore, grain growth can be regarded as the anisotropic evolution of a large cellular network and can be described by a set of deterministic local evolution laws (nonlinear ODEs/PDEs) for the growth of individual grains combined with stochastic models for the interaction between them.

3:10–3:50

Qiang Du Columbia University

Heterogeneously localized nonlocal operators with applications to semi-supervised learning

We present heterogeneous localization techniques for formulating nonlocal integral models on a finite domain with local boundary conditions. We discuss, in particular, applications to the seamless coupling of local and nonlocal models and to the development of well-defined nonlocal models for semi-supervised learning with low labeling rates. The latter also provides analytical bridges linking discrete learning models and PDE-based local continuum models.

Wednesday, October 14

09:00–09:40

Lia Bronsard McMaster University

On a partitioning problem inspired by triblock copolymers

I will introduce a new partitioning problem that arises in the study of triblock copolymers in certain limiting regimes. I will present the appropriate setting for this new geometrical problem, some solutions as well as answers to some conjectures based on analytical and numerical results. This is joint work with Stan Alama, Silas Vriend, Mike Novack, Matthieu Dolbeault, Thanh Huynh and Dominik Stantejsky.

09:40–10:20

Andrea Braides SISSA

Asymptotic behaviour of fractional Sobolev spaces on thin films

The asymptotic behaviour of Gagliardo H^s seminorms on thin films of thickness tending to 0 is studied, showing that the behaviour is different in the low-integrability regime ($s < 1/2$) and in the high-integrability regime ($s > 1/2$). In both cases, there exists a critical scaling (depending on s) for which the limit is dimensionally reduced. In the case $s > 1/2$ the scaling highlights a combined effect of the geometrical dimensions and the relevant range of interactions in the Gagliardo seminorms, and the limit is an H^1 seminorm. Moreover, in the light of the results by Bourgain, Brezis and Mironescu (BBM) and Maz'ya and Shaposhnikova (MS), we study the asymptotic behaviour as $s \rightarrow 1$ and $s \rightarrow 0$. In the case $s \rightarrow 1$ the asymptotic behaviour highlights a separation of scales and a compatibility with the BBM result. In the case $s \rightarrow 0$ the scaling is purely geometrical and leads to an $H^{1/2}$ seminorm, differently from the MS result. The proofs rely on two different approaches to dimension-reduction compactness. If time allows, I will compare this analysis with dimension reduction for some functionals studied by Brezis and Nguyen. Work in collaboration with A. Pinamonti and M. Solci.

10:50–11:30

Jeff Rickman Department of Materials Science and Engineering and Department of Physics, Lehigh University

Point Process Models of Nucleation and Growth Phenomena in Materials Science

I will describe the use of various point process models to describe the kinetics of first-order phase transitions and associated microstructural evolution. More specifically, beginning with the Sekimoto formalism, I will outline the calculation of non-equilibrium, n -point correlation functions that embody both homogeneous and heterogeneous nucleation and growth kinetics, with particular application to polycrystalline thin films. The impact of spatial interactions among nuclei on the evolution of transitions will also be explored. Finally, I will summarize applications of this formalism to related problems, such as electrodeposition and nucleation in special geometries, and discuss point processes that exhibit hyperuniform behavior.

11:30–12:10

Chun Liu Illinois Institute of Technology

Active Fluids and Applications in Complex Fluids

I plan to present a general theory for active fluids which are capable of converting chemical energy into various types of mechanical energy. This is an extension of the classical energetic variational approaches for mechanical systems. The methods will cover a wide range of both chemical reaction kinetics and mechanical processes. Moreover, the framework is naturally consistent with the principles of thermodynamics.

2:00–2:40

Maria Emelianenko George Mason University

Towards Robust Data-Driven Multiscale Modeling of Microstructure–Property Relations

This talk will present a perspective on microstructure modeling in polycrystals, with a focus on connecting mesoscopic characteristics to mechanical response. Advances in computational materials modeling over recent decades, including mathematical theory, large-scale simulations, and experimental techniques, have highlighted statistical features of grain boundary networks as an important factor in microstructure–property relationships. A key challenge is to identify descriptors that are appropriate for a given materials application and to develop robust multiscale models capable of capturing the key aspects of material behavior.

Different statistical patterns can emerge when comparing two- and three-dimensional material structures, while models often struggle to capture the full complexity of physical phenomena. In this talk, I will discuss recent work carried out in collaboration with materials scientists, focusing on entropic descriptors and stochastic grain growth models. These approaches provide a framework for exploring some of the challenges involved in developing robust data-driven models of microstructure–property relationships.

2:40–3:20

Adrian Tudorascu West Virginia University

Sticky particle solutions as energy minimizers for the pressureless Euler system

Sticky Particles (SP) solutions to the Pressureless Euler system were introduced by Zeldovich in 1970 to describe large-scale formations in the universe by accretion of matter. Since then, a significant amount of work has been dedicated to studying various quantitative and qualitative properties of such solutions. In this talk we will discuss a new criterion for singling out SP solutions as the unique kinetic energy minimizers among particle solutions to the system.

3:50–4:30

Marshall Slemrod University of Wisconsin–Madison

The least action principle and new admissibility criteria for initial value problems

This talk is based on joint work with Heiko Gimperlein, Michael Grinfeld and Robin J. Knops, and addresses the use of two available admissibility criteria for weak solutions for the Euler equations of compressible fluid dynamics in dimension $n > 1$. Specifically, the talk compares results of Dafermos's entropy rate criteria and our action rate admissibility criteria for the Riemann initial value problems in two space dimensions when the “wild” solutions of C. De Lellis and L. Székelyhidi occur.