Mathematics of Multiscale and Multiphysics Phenomena in Materials Science, 24w5159

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June 16 - 21, 2024

1 Overview of the Field in the Context of the Meeting

Mathematical aspects of multiscale/multiphysics phenomena in various areas of materials science has recently emerged into a thriving interdisciplinary field. Many particular examples (examples well represented in the workshop) are Polycrystals and Materials Microstructures; Smart Materials and Materials with Unusual Properties; and Complex Fluids and Biomaterial.

Technological progress is frequently a consequence of cutting edge advances in the understanding of materials and their design. Both rigorous mathematical techniques and computer simulations play a crucial role in the study and design of new materials - from batteries to biomaterials and shape memory alloys. New scientific questions, as well as innovative mathematical methods and computational tools have emerged from the study of multiscale/multiphysics phenomena in materials such as composites, polycrystals, biomaterials, nano-structures, as well as shape memory alloys, to name a few.

The workshop focused on topics that span ideas from deterministic and stochastic modeling of materials, discrete and continuum description, multiscale analysis to numerical methods, data analysis and machine learning techniques with applications to modeling of microstructural properties of materials and their effects on macroscopic properties, the optimization of structured materials, the study of dynamics of metastable structures, as well as understanding and modeling of complex fluids.

One example of an important multiscale/multiphysics problem in materials science is the understanding of the evolution of grain boundaries in polycrystalline materials. Cellular networks are ubiquitous in nature. They display behavior on many different length and time scales and are usually metastable. Most technologically useful materials are polycrystalline microstructures composed of small monocrystalline grains separated by grain boundaries. Grains and grain boundaries play an important role in determining the properties of materials across multiple scales. The control of polycrystalline microstructures through processing is necessary for enhancement of materials properties, such as mechanical, thermal, magnetic, optical and electrical properties. Thus, one of the essential goals in engineering of polycrystals is to create technologies capable of manufacturing an arrangement of grains and grain boundaries that deliver a desired set of materials properties. One method by which the grain structure can be altered is through annealing. During annealing, larger grains grow, smaller grains shrink and the polycrystalline microstructure evolves to reduce the total grain boundary energy, a mechanism known as “grain growth/coarsening”.

Experimental, computational and analytical studies of grain growth have a long history and an extensive literature, see for example [1-19] (non exhaustive list). However, there are still many open questions related

to the understanding of the evolution of materials microstructure. One important example of this is the discovery and analysis of the processes by which certain distributions emerge during coarsening from the initial populations of grains. Therefore, to address current challenges in the field, and at the same time to develop predictive and prescriptive theories, numerical simulations and experiments of grain growth will require new insights from mathematicians, statisticians, computational scientists, data scientists and materials scientists.

Another related example of an important multiscale/multiphysics problem in materials science is smart materials and materials with unusual properties, e.g., [20-27], to name a few. For example, the development (via optimization process) of macroscopic systems with specific materials properties and the design of composite materials (microstructures) for optimal performance are important parts of the variational questions.

As a last example, an active and vibrant area pertains to complex fluids and biomaterials. Complex fluids can be defined broadly as soft matter with internal microstructures whose evolution affects the macroscopic dynamics of the materials [28]. Examples include polymer solutions and melts, liquid crystals [32, 38], gels, micellar solutions, ferrofluids [36], and biological matter such as the cytoskeleton, plasma membranes, and soft tissues. It is the interaction between the (microscopic) elastic properties and the (macroscopic) fluid motions that give not only complicated rheological phenomena but also formidable challenges in analysis and numerical simulations of the materials [34]. The mathematical tools developed in complex fluids have also seen applications in solids, and biological materials, such as the central nervous system and skeletal muscles [35]. Almost all biological activities involve electrodynamics and mechanics [37, 29]. The dynamics of ions transport on cell and tissue level and the corresponding effect in the mechanical response is another example of a very complex multiscale/multiphysics problem. For instance, the understanding of muscle contraction will involve multiscale coupling between mechanics, chemical reactions, and charge transport. To understand the selectivity of membrane-borne ion channels, one needs to take into account the steric effect at the atomic scale [31, 33, 30].

2 Presentations: Common Themes, Highlights, and Description of the Talks

The workshop was a great success and brought together established and junior researchers, including students (even a local high school student attended selected talks at the workshop) and postdocs in different but closely connected areas of materials science. Over the five days, the workshop featured an impressive forum of lectures and discussions on the state-of-the-art ideas and developments in the field of multiscale and multiphysics aspects of materials science problems. Moreover, the workshop presented a special poster session which allowed postdocs and graduate students to take a more active part in the event and showcase their work to a highly diverse audience, including distinguished researchers, as well as junior peers. Further, the workshop had a productive working session and a panel discussion where participants discussed and exchanged ideas on several important questions: a) Perspectives on current fundamental questions and challenges in their respective areas, as well as ideas on possible approaches to tackle them; b) Successes and challenges of cross-disciplinary work: for example, one topic that was considered was the improvement of communication skills (reduction of scientific language barriers) among, e.g. mathematicians, materials scientists, and engineers; c) Training the next-generation applied mathematics workforce: as a part of the conversation, we exchanged ideas about interdisciplinary training which includes close interactions/collaboration among mathematicians, materials scientists, and engineers, as well as the important questions of increasing diversity and broadening participation within the field. d) Current and new funding opportunities were discussed as a part of the working session.

The workshop began on Monday wherein two fundamental common themes/topics emerged: **The Role of Nonlocal Modelling** and **The Incorporation of Machine Learning.** Common to most of the related talks was the importance of multi-scale modelling and model reduction.

The conference began with a talk of **Qiang Du** who emphasized that nonlocality is a generic feature of model reduction (upscaling, course graining, ...). The local models we are so accustomed to are often the results of further assumptions, simplifications. There are many challenges to nonlocal modelling but the talk

focused on the important issue to address bounded domains and the proper mathematical formulation near or at the domain boundary. The results were presented on a different possibilities for imposing suitable local or nonlocal boundary conditions to complement nonlocal interactions prescribed in the interior of the domain.

Tadele Mengesha continued on the theme of nonlocality with a focus on the peridynamic model of continuum mechanics. He considered a class of nonconvex energy functionals fundamental to the bond-based peridynamic mode. He showed how variational analysis can be used to investigate the consistency of the effective behavior of these nonlocal nonconvex functionals with established classical and peridynamic models in two different regimes (small displacement and vanishing nonlocality).

Guosheng Fu's presentation focused on a topic of Lagrangian schemes for compressible fluids. The lecture discussed mathematical framework for modeling compressible fluid flows using energy-based variational principles. The talk covered the development of high-order spatial and temporal discretization methods that ensure conservation of mass, momentum, energy, and entropy stability. Additionally, numerical results were provided to validate the effectiveness of the proposed schemes, with future plans to extend the approach to address more complex systems and mesh distortion issues.

Lia Bronsard discussed new results on nonlocal isoperimetric problems resulting from three interacting phases. The lecture first addressed the pure isoperimetric problem for three phases and results depending on the relative strengths of the surface tensions were presented. Starting with 2D, the full nonlocal problem and results on the many different structures for the minimizers, ranging from a lattice of isolated simple droplets of each minority species to double-bubbles or core-shells were discussed. The geometry of these minimizers depends on the relative strengths of the coefficients of the interaction terms. While the original motivation was from phase separation of triblock copolymers, it was also discussed in the lecture of how the results lead to a new type of partitioning problem in geometry.

In the afternoon, we heard from three speakers on different (though related) uses of **Machine Learning (ML)** ideas in materials science.

Kaushik Bhattacharya began the afternoon with a lecture on the use of neural operators in multi-scale modelling. Material science involves physics at multiple length and time scales: electronic, atomistic, domains, defects etc. Experiments give much insight but he stressed that *we rarely measure what we actually need*. The lecture introduced the notion of a neural operator as a controlled approximation to operators mapping one function space to another. With examples stemming from plasticity to elasticity, he showed how these tools from ML can be used to transfer information between scales, and learn and give meaning to internal variables. In a certain sense, these tools can be viewed as a surrogate for constitutive relations in continuum mechanics.

Christoph Ortner discussed the integration of ML techniques in many body interactions for materials and molecules. He noted that increasingly, this integration into the traditional modelling ecosystem has replaced decades-old ad hoc approximations (for example, in constitutive laws, reinforcing a theme of the previous talk). On the other hand, pure machine learning approaches are rarely successful, hence fundamental is the need for the integration of domain knowledge. He discussed a class of hybrid ML models for the atomistic scale which resulted in reduced-order (coarse-grained) interatomic potentials. He argued that systematic coarse-graining leads to many-body interaction which can be efficiently parameterized. In doing so, he presented a systematic, interpretable, canonical framework to construct equivariant many-body interaction models for general particle systems. He ended with the broader and ambitious goal of producing hybrid-ML potentials for the entire periodic table.

Hector Ceniceros addressed the integration of ML into the self consistency field theory (SCFT) for soft materials. The SCFT has proven to be a powerful tool for numerical simulations in phase separation of block copolymers and other soft matter systems. Indeed, historically it has produced the most accurate (with regard to experiments) phase diagram for diblock copolymers. However, SCFT simulations are computationally very costly, and hence numerically exploring the vast possibilities of phases diagram is impractical. In this

talk, Ceniceros presented new approaches to aid SCFT simulations via ML. He showed how the design of specific architectures of convolutional neural networks and generative adversarial networks can accelerate the exploration of parameter space, and effectively predict polymer structures. Moreover he discussed how such integration can aid in the inverse design problem.

On the second day, a third fundamental common theme/topic emerged: **Grain Growth in Polycrystalline Materials**

David Srolovitz began the morning with a lecture on Grain Boundary (GB) Migration Mechanism-Based Description of Microstructure Evolution. He began by discussing curvature-based models, highlighting well-known results in materials science - the von Neumann-Mullins law and Mullins equation. The curvature-flow picture of grain growth is widely used, however he noted that *it may not be the only/or primary mechanism for real materials*. The motion of GB creates stress and discrete time steps at internal interfaces in crystalline materials also have a dislocation character. Srolovitz showed both MD and experimental evidence for these defects, and explored their basic features in GB motion. He then introduced a continuum model with applications to front tracking and phase field methods. In this model, force is not simply curvature alone, but includes the effects of the shear stress projection jump in the chemical potential. One conclusion is that the GB motion during microstructure evolution gives rise to grain rotation, and cyclic annealing or stressing can accelerate the grain growth.

Masashi Mizuno continued on the theme that curvature alone is insufficient to describe real GB motion, and presented the results of a new model for GB motion which includes dynamic lattice misorientations (e.g., possibility of grain rotation) and triple junction drag. Disappearance events of grain boundaries, the so-called critical events, are among the main difficulties in analyzing/modeling the grain growth. To overcome this difficulty, a new macroscopic model for the grain boundary character distribution (GBCD), an empirical distribution of the relative length (in 2D) (or area (in 3D)) of grain boundaries with a given lattice misorientation and normal-*a leading metric to characterize texture of the boundary network in polycrystalline materials* was introduced and studied. Moreover, the discussed model was carefully validated against known results and previous studies of the GBCD.

Emanuel (Menachem) Lazar discussed modelling the atomistic structure of grain boundaries in realistic systems. Decades of careful work have resulted in broad and deep understanding of the atomistic structure of grain boundaries. Conventional approaches, however, are often limited to special kinds of grain boundaries in special kinds of systems. He argued that the Voronoi cell topology can be used as a building block for the GBs. The distributions of these building blocks can then be used as a way of characterizing the GB distribution. Based upon these ideas, he presented a new statistical structural description of grain boundaries suitable for studying realistic systems such as those described by thermodynamic ensembles.

Next, **Arkadz Kirshtein** gave a lecture on thermodynamically consistent phase-field-micromechanics model of solid-state sintering. The model was validated and was used to simulate the microstructure evolution of polycrystalline powder particles, in order to gain better understanding in the mechanisms governing crystallite growth.

The afternoon session began with lectures by **experimentalists** in the field.

Katayun Barmak discussed recent experimental studies in grain structure, grain growth, and evolution of the grain boundary network. She stressed that a grand challenge problem in engineering of polycrystals is to develop prescriptive process technologies capable of producing an arrangement of grains that gives rise to a desired set of materials properties. To develop a predictive and prescriptive theory, an investigation of a broad range of statistical measures of microstructure is needed. These can only be obtained via close interaction and integration of experiments, simulations, data analytics, mathematical modelling and theory development. She then presented the advantages (and some disadvantages) of the use of thin films as the experimental platform. Historically, GB detection has been done manually with the eye norm. She discussed how recent

hardware and software advances have removed bottlenecks to large scale ex situ and in situ data acquisition via (1) automated grain boundary segmentation in micrographs via convolution neural networks (in particular the U-Net), (2) low thermal mass microelectromechanical systems and (3) integrated hardware-software drift correction and data management solutions. In regard to (1), it was reported that U-Net (+ post-processing) gives statistically similar results to hand-tracing. On the other hand, while doing a good job at detecting triple junctions, more accuracy is needed. In conclusion, these innovations have rendered thin films a key integrated experimental platform for current and future grain growth studies.

Ashwin Shahani continued on the importance the combination of experiment (*seeing is believing*) and modelling. He presented a talk on the dynamics of strain-energy-driven grain growth. He employed synchrotron high-energy x-ray diffraction microscopy (HEDM) to map in 3D and time the heterogeneous microstructure over three orders-in-magnitude of length-scale. He also used phase field simulations to bridge the spatiotemporal gaps in the HEDM study and proposed a mechanism of strain-energy-driven growth. The joint experiments and simulations revealed a significant diversity in grain shapes, sizes, and dislocation densities that are generated over the course of the non-isothermal anneal. His efforts highlight a complexity in the microstructural dynamics brought about by stored strain energy, not predicted by conventional theories nor metallographic analyses

The workshop was not limited to the above three timely themes. Various important and timely topics in the mathematics of material science were discussed during the workshop.

Later in the afternoon, both **Yuliya Gorb** and **Yury Grabovsky** provided new insights into the study of composite materials in their lectures.

Yuliya Gorb presented new rigorous results in periodic homogenization of heterogeneous composite materials. Several composite models were discussed and the effective or homogenized response for these composites were presented. This entails PDEs whose coefficients depend on the composite's geometry, the periodicity of the original microstructure, and the coefficients characterizing the initial heterogeneous material.

Yury Grabovsky gave a lecture on the derivation of thermodynamically consistent constitutive laws for thermoelectric composites. In particular, these thermodynamically consistent constitutive laws retain their form under homogenization.

Amit Acharya spoke on finite deformation mesoscale field dislocation mechanics with a model of dislocation mechanics based upon (crystal)plasticity of unrestricted geometric and material nonlinearity. This model, when exercised on a sufficiently fine scale, can rigorously predict fields of arbitrary dislocation distributions in finite bodies of arbitrary anisotropy. When exercised at larger scales of resolution adequate for meso/macro scale structural response, the model can make predictions up to finite strains of size and rate-dependent mechanical behaviour, texture, and mesoscale dislocation microstructure evolution in polycrystalline aggregates and single crystals. He ended by noting that the model raises significant and challenging mathematical questions.

Wednesday started with a lecture by **Irene Fonseca,** titled *"From Phase Separation in Heterogeneous Media to Learning Training Schemes for Image Denoising"*. What do these two themes have in common? In the lecture, it was shown that both are treated variationally, both deal with energies of different dimensionalities, and both involve tools from geometric measure theory. The talk focused on heterogeneous media. Working within the gradient theory of phase transitions, she addressed cases where the potential and the wells depend on the spatial position. With fixed wells and in the critical case, where the scale of the small heterogeneities is of the same order of the scale governing the phase transition, the interaction between homogenization and the phase transitions process lead to an anisotropic interfacial energy. The supercritical case lead to an isotropic interfacial energy. In the subcritical case with moving wells, where the heterogeneities of the material are of a larger scale than that of the diffuse interface between different phases, it was

observed that there is no macroscopic phase separation and thermal fluctuations play a role in the formation of nanodomains. The lecture concluded by establishing an important new relationship with image processing.

Michael Novack continued the theme of the calculus of variations with certain novel modifications of the classical Plateau problem for modelling 3D features in films/foams.

Raghavendra Venkatraman gave a lecture on the mathematical analysis of resonators made from "Epsilon-near-zero" materials (a material whose dielectric permittivity is near zero at the frequency at which the device operates). He presented theorems on the complex analytic dependence of the resonance on the near-zero permittivity. In the 2D Transverse Magnetic setting, the leading order behavior of the resonance turned out to be independent of the geometry of the ENZ shell, but only its area. However, the leading order correction depended on shell-geometry and was investigated via a shape optimization problem that optimizes the quality of the resonance. A convex relaxation resulted in a free boundary problem of Alt-Caffarelli type. The talk also addressed a more complex 3D setting.

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Mitchell Luskin presented a lecture on the stacking of multilayered two-dimensional heterostructures and the effects on their electronic properties. This is a challenging problem from a theoretical perspective and an intriguing avenue for manipulating physical properties. Luskin derived a continuum model to compute the mechanical relaxation for an arbitrary number of layers by parametrizing the displacement by the local configuration (disregistry) rather than real space, thus bypassing the need for the standard supercell approximation and giving a true aperiodic atomistic configuration. The displacement of a heterostructure of p layers is not generally periodic in real 2D space for $p > 2$, but the displacement is periodic on a $2(p-1)$-dimensional torus as a function of its disregistry. The regularity of the displacement was shown to have a major effect on electronic properties.

Pierre Degond started the last day of lectures with the role of *conservation* in passing between the Doi-Onsager and Ericksen-Leslie models for liquid crystals. He showed that suitable generalized conservation relations (generalized collision invariants) hold and make a classical method (the moment method) applicable. This leads to a much better understanding of the structural properties of the Doi-Onsager model and opens the new way to rigorous convergence proofs that would require less regularity than an alternate method (the Hilbert method).

Miranda Holmes-Cerfon presented new results on the dynamics of particles with ligand-receptor contacts. Ligand-receptor contacts are one way to glue objects together (either at the nanoscale or microscale) wherein short sticky hair-like ligands stick to receptors on another surface. These interactions are common in biology and are also useful in materials science. Via both modelling and experimental efforts, her lecture focused on how such particles move with an aim of understanding their coarse-grained dynamics.

Carme Calderer gave lecture on the analytical work on the debonding of a gel membrane from a rigid substrate. She presented a novel model for the debonding of a thin elastic film from a rigid substrate when subject to gravity and exposed to a liquid environment. The model combines nonlinear elasticity with the classical work by Flory and Rehner, together with the variational description of fracture. Analytical results were presented for both the fully bonded and partially bonded cases. In particular, the energy release rate leading to debonding was calculated as was the maximum thickness of the film that makes it stable against swelling and debonding forces. Comparisons were made with experiments.

Will Feldman spoke on models of contact angle hysteresis. He started off with the capillary energy and presented rigorous results for a partially linearized model in the regime of small contact angle. He then discussed the origin of contact angle hysteresis of capillary drops from micro-scale surface roughness. Theoretical results for some macroscopic models were presented which described the large-scale effects of pinning.

Sergey Gusarov spoke on coupling methods of quantum chemistry and molecular simulations with molecular theory of solvation. He showed that by combining various scientific models, better results can be achieved and more efficiently. Moreover, the resulting methods are more broadly applicable. In particu-

lar, he discussed how to mix different ways of studying chemicals to better understand materials and living molecules with a focus on the molecular theory of solvation which allows one to accurately introduce the effect of environment on complex nano-, bio- or macromolecular system.

Finally, **Natasha Sharma** presented a second order numerical scheme for a sixth-order Cahn-Hilliard Type Equation. The equation stems from modelling the dynamics of phase transitions in ternary oil-water-surfactant systems. Unconditional stability and unique solvability for the scheme was shown and its numerical experiments were presented.

3 Working Session and Panel Discussion

We had a very productive long working session with the participants (both senior and junior) to discuss:

1 Perspectives on current fundamental questions and challenges in their respective areas

2 Successes and challenges of cross-disciplinary work: for example, interactions between mathematicians and materials scientists (both theoretical and experimental);

3 Training the next generation applied mathematics workforce;

4 Increasing diversity and broadening participation within the field

5 Current and new funding opportunities

To this end, there was much discussion on recent **role of machine learning**. Many senior participants chimed in and the overall consensus was that machine learning (ML) is a very useful tool which should not be overlooked. However, much work remains to be done to understand its limitations and applicability, especially in light of existing approaches and tools. Moreover, ML gives trainees instruction in techniques which will enhance their knowledge and toolbox for industrial careers. There were also discussions on the interplay between analysis, numerics, and experiments. The challenges of experimental research were discussed. It was emphasized that it should be mutual communication and interaction between mathematicians and experimental materials scientists. Both communities will benefit from it.

While the central themes of the workshop (discussed above) were reiterated, it was widely acknowledged that there are still much to be discovered in, for example, some well-studied subjects, like composite materials and the calculus of variations. Indeed, these subjects, due to the development of new techniques, are now in the position to address some important long-standing challenging problems. To the younger generation, the role of mentors was emphasized. Indeed, the community in the mathematics of materials science owes much to a handful of **Pioneers in the field** who inspired and are inspiring generations of researchers.

Current and new funding opportunities were discussed as a part of the working session/panel. In particular, Yuliya Gorb (NSF) took part in the workshop and in the working session.

The working session also focused on different EDI themes. Many ideas were exchanged, for example, the importance of supporting better work-life balance, how to provide more and better resources for child care for early career faculty, among other pressing themes that were discussed during the session. Many of the younger participants gave feedback that our very open and honest discussion was very useful and informative.

4 Titles and Abstracts of the Talks

Qiang Du Models with nonlocal interactions on bounded domains
Abstract: Nonlocal interaction arises naturally as a generic feature of model reduction for multiscale processes. Recently, there has been much interest in models associated with a finite horizon parameter that characterizes the effective range of nonlocal interactions. For such models defined on a bounded domain, an

important issue is their proper mathematical formulation near or at the domain boundary. This lecture offers an overview of related works. We discuss a few possibilities for imposing suitable local or nonlocal boundary conditions to complement nonlocal interactions prescribed in the interior of the domain. We also present recent development of the mathematical and numerical analysis of the resulting problems and applications to the coupling of different models.

Tadele Mengesha: Linearization and localization of nonlocal nonconvex functionals
Abstract: We consider a class of nonconvex energy functionals that lies in the framework of the bond-based peridynamic model of continuum mechanics. The energy densities are functions of a nonlocal strain that describes deformation based on pairwise interaction of material points. We apply variational analysis to investigate the consistency of the effective behavior of these nonlocal nonconvex functionals with established classical and peridynamic models in two different regimes. In the regime of small displacement, we show the model can be effectively described by its linearization, deriving the linearized bond-based peridynamic functional as a variational limit of nonlinear functionals. In the regime of vanishing nonlocality, the effective behavior of the nonlocal nonconvex functionals is characterized by an integral representation with quasiconvex integrand. We demonstrate that the density vanishes on matrices whose singular values are less than or equal to one. These results confirm that the localization, in the context of variational convergence, of peridynamic-type energy functionals exhibit behavior quite different from classical hyperelastic energy functionals. This is a joint work with James M. Scott.

Guosheng Fu: High-order variational Lagrangian schemes for compressible fluids
Abstract: We present high-order variational Lagrangian finite element methods for compressible fluids using a discrete energetic variational approach. Our spatial discretization is mass/momentum/energy conserving and entropy stable. Fully implicit time stepping is used for the temporal discretization, which allows for a much larger time step size for stability compared to explicit methods, especially for low-Mach number flows and/or on highly distorted meshes. Ample numerical results are presented to showcase the good performance of our proposed scheme. This is a joint work with Prof. Chun Liu from IIT.

Lia Bronsard: Patterns in tri-block copolymers: droplets, double-bubbles and core-shells
Abstract: We study the Nakazawa-Ohta ternary inhibitory system, which describes domain morphologies in a triblock copolymer as a nonlocal isoperimetric problem for three interacting phase domains. We consider global minimizers on the two-dimensional torus, in a droplet regime where some species have vanishingly small mass but the interaction strength is correspondingly large. In this limit there is splitting of the masses, and each vanishing component rescales to a minimizer of an isoperimetric problem for clusters in 2D. Depending on the relative strengths of the coefficients of the interaction terms we may see different structures for the global minimizers, ranging from a lattice of isolated simple droplets of each minority species to double-bubbles or core-shells. These results have led to a new type of partitioning problem that I will also introduce. These represent joint work with S. Alama, X. Lu, and C. Wang, as well as with M. Novack and S. Vriend.

Kaushik Bhattacharya: Multi-scale modeling and neural operators
Abstract: The behavior of materials involve physics at multiple length and time scales: electronic, atomistic, domains, defects etc. The engineering properties that we observe and exploit in application are a sum total of all these interactions. Multiscale modeling seeks to understand this complexity with a divide and conquer approach. It introduces an ordered hierarchy of scales, and postulates that the interaction is pairwise within this hierarchy. The coarser-scale controls the finer-scale and filters the details of the finer scale. Still, the practical implementation of this approach is computationally challenging. This talk introduces the notion of neural operators as controlled approximations of operators mapping one function space to another and explains how they can be used for multiscale modeling. We demonstrate the ideas with examples, and highlight the open mathematical issues.

Christoph Ortner: Systematic and Efficient Many-body Interaction for Materials and Molecules
Abstract: The integration of machine learning (ML) into the traditional modeling workflows is replacing decades-old ad hoc approximations (e.g., in constitutive laws) leading to new models that far outstrip their predecessors in accuracy and transferability. ”Pure” ML approaches are rarely successful but remarkable

results can be achieved when integrated with domain knowledge. My talk will focus on the atomistic scale where the development of reduced-order (coarse-grained) interaction laws (e.g. interatomic potentials) has made immense progress. I will outline how a combination of modelling, analysis and approximation theory tools lead to an end-to-end justification of a practical class of hybrid ML models. A key point is that systematic coarse-graining leads to many-body interaction; I will therefore also show how such interactions can be parameterized efficiently.

Hector Ceniceros: Machine Learning-enabled Self-Consistent Field Theory for Soft Materials
Abstract: Numerical simulations using self consistency field theory (SCFT) have been a powerful tool to study soft materials like polymers. However, SCFT simulations are a complex and computationally costly process and exploring the vast design space of polymers via SCFT is impractical. We will discuss in this talk our recent efforts to leverage SCFT with Machine Learning (we design specific architectures of convolutional neural networks and generative adversarial networks) to accelerate the exploration of parameter space and to effectively predict polymer structures and for the inverse design problem.

David Srolovitz: A Grain Boundary Migration Mechanism-Based Description of Microstructure Evolution
Abstract: Grain boundary (GB) migration occurs through the motion of discrete steps along the GB. Unlike at free surfaces, steps at internal interfaces in crystalline materials commonly also have dislocation character. These line defects, constrained to the interface, are disconnections; characterized by a combination of a step height and Burgers vector, dictated by (bi)crystallography. I will show both MD and experimental evidence for these defects and explore their basic features, as related to GB migration. I will then describe a continuum equation of motion and show applications of this based on front tracking and phase field methods. I will demonstrate how GB motion during microstructure evolution gives rise to grain rotation and how cyclic annealing or stressing can accelerate grain growth.

Masashi Mizuno: Recent Study for Evolution of Grain Boundaries Including Dynamic Lattice Misorientations and Triple Junction Drag
Abstract: In the 1950s, one thought that the length of grain boundaries was the main effect of the evolution of grain boundaries. Nowadays, in material science, we seek the effect of the grain boundaries' length and the lattice misorientations on the evolution. In this talk, I will explain a new mathematical model of grain boundary motion, including dynamic lattice misorientations and triple junction drag. Using the energetic variational approach, we derive a system of geometric differential equations to describe the motion of such grain boundaries. Disappearance events of grain boundaries, so-called critical events, are the main difficulty in analyzing the model. To overcome this difficulty, an empirical distribution of the relative length with a given lattice misorientation and normal, called a grain boundary character distribution(GBCD, for short), was considered. To understand the relationship between the model and the previous study of GBCD, I next explain a stochastic model of the evolution of grain boundaries. This talk is based on the joint work with Yekaterina Epshteyn (The University of Utah)and Chun Liu (Illinois Institute of Technology).

Emanuel (Menachem) Lazar: Modeling the atomistic structure of grain boundaries in realistic systems
Abstract: Although grain boundaries are easy to define in a continuum setting – they are the common boundary shared by a pair of adjacent crystals - they are extremely challenging to precisely define, or even characterize, on the atomic scale. Decades of careful work have resulted in broad and deep understanding of the atomistic structure of grain boundaries. Conventional approaches, however, are often limited to special kinds of grain boundaries in special kinds of systems. In this talk I would like to tell you about a new statistical structural description of grain boundaries suitable for studying realistic systems such as those described by thermodynamic ensembles, including ones far from their "ground states". This characterization is robust in the sense that it is primarily determined by macroscopic degrees of freedom, and is only minimally affected by thermal noise, differences in local density, the presence of defects, and other variations in microscopic degrees of freedom.

Arkadz Kirshtein: A thermodynamically consistent phase-field-micromechanics model of solid-state sintering
Abstract: Sintering, a pivotal technology in additive manufacturing, transforms ceramic and metallic pow-

ders into solid objects. To achieve products with customized properties, a deep understanding of microstructure evolution during sintering is crucial. Our approach ensures thermodynamic consistency, deriving the driving force for particle motion from the system's free energy. As a result, our proposed phase-field-micromechanics model guarantees microstructure evolution that minimizes the system's energy. We rigorously validate this model against recent theoretical benchmarks. Subsequently, we employ it to simulate the microstructure evolution of polycrystalline powder particles, shedding light on the mechanisms governing crystallite growth. Additionally, we analyze how grain boundary structure and orientation impact sintering kinetics.

Katayun Barmak: Grain structure, grain growth, and evolution of the grain boundary network in polycrystalline materials: Experimental Studies
Abstract: A grand challenge problem in engineering of polycrystals is to develop prescriptive process technologies capable of producing an arrangement of grains that provides for a desired set of materials properties. One method by which the grain structure is engineered is through grain growth or coarsening of a starting structure. During grain growth, an initially random grain boundary arrangement reaches a state that is strongly correlated to the interfacial energy density. Grain growth can be considered as the evolution of a large metastable network, and can be modeled by a set of deterministic local evolution laws for the growth of individual grains combined with stochastic models to describe their interactions. However, despite tremendous progress in formulating models of grain growth, existing descriptions do not fully account for various grain growth mechanisms, detailed grain topologies, and the effects of different time scales on microstructural evolution. Thus, to develop a predictive and prescriptive theory, an investigation of a broad range of statistical measures of microstructure is needed and must be obtained using experiments, simulations, data analytics, and mathematical modeling. This talk will focus on experimental studies that use thin metallic films as the platform. Recent hardware and software advances have removed bottlenecks to large scale ex situ and in situ data acquisition via (1) automated grain boundary segmentation in micrographs, (2) low thermal mass microelectromechanical systems and (3) integrated hardware-software drift correction and data management solutions. These innovations render thin films a key integrated experimental platform for current and future grain growth studies. The experimental advances together with advances in data analytics, simulations and theory are expected to enable microstructure by design.

Ashwin Shahani: The dynamics of strain-energy-driven grain growth
Abstract: An understanding of microstructural dynamics under non-isothermal conditions is crucial to materials design. During a so-called 'cyclic heat treatment' of shape memory alloys, dissolution of semi-coherent precipitates generates dislocations, thereby raising the stored strain energy within grains. In this work, we employ synchrotron high-energy x-ray diffraction microscopy (HEDM) to map in 3D and time the heterogeneous microstructure over three orders-in-magnitude of length-scale, including the precipitates, grains, and intra-granular dislocation densities. Correspondingly, we use phase field simulations to bridge the spatiotemporal gaps in the HEDM study and propose a mechanism of strain-energy-driven growth. The joint experiments and simulations reveal a significant diversity in grain shapes, sizes, and dislocation densities that are generated over the course of the non-isothermal anneal. Our data also reveal a new mode of grain growth, involving the macroscopic translation of grain centers over time. Broadly, our efforts highlight a complexity in the microstructural dynamics brought about by stored strain energy, not predicted by conventional theories nor metallographic analyses.

Yuliya Gorb: Recent Developments in Periodic Homogenization of Heterogeneous Composite Materials
Abstract: This talk reports on the recent findings about the rigorous periodic homogenization of four coupled PDE systems that model heterogeneous composite materials. Specifically, it focuses on the following models: (i) a suspension comprising magnetizable rigid particles in a non-conducting carrier viscous Newtonian fluid, (ii) strongly coupled magnetorheological fluid, (iii) nonlinear dielectric elastomer, and (iv) high-contrast dielectric elastomer. The effective or homogenized response for these composites, which involves PDEs whose coefficients depend on the composite's geometry, the periodicity of the original microstructure, and the coefficients characterizing the initial heterogeneous material, will be demonstrated. The corresponding cell problems, along with the key concepts for justification, will also be mentioned. Additionally, various aspects of the underlying PDEs, such as nonlinearity and high contrast, will be examined.

Yury Grabovsky: Thermodynamically consistent constitutive laws for thermoelectric composites
Abstract: Thermoelectric effects are widely used in industry. Yet, in contrast to other coupled field phenomena, such as thermoelasticity or piezoelectricity, there seems to be some confusion about the proper form of constitutive laws. In this talk I will describe thermodynamically consistent constitutive laws that retain their form under homogenization. In addition I will address the question of characterizing all subclasses of constitutive laws retaining their form under homogenization.

Amit Acharya: Finite Deformation Mesoscale Field Dislocation Mechanics
Abstract: We will describe a model of dislocation mechanics based (crystal)plasticity of unrestricted geometric and material nonlinearity that, when exercised on a sufficiently fine scale, can rigorously predict fields of arbitrary dislocation distributions in finite bodies of arbitrary anisotropy, and when exercised at larger scales of resolution adequate for meso/macro scale structural response, suitably adapting established macroscale phenomenology related to kinetics of plastic flow, makes predictions up to finite strains of size and rate-dependent mechanical behavior, texture, and mesoscale dislocation microstructure evolution in polycrystalline aggregates and single crystals. The phenomenology used to go to the mesoscale can be systematically improved as the need arises, as can the geometric fields involved along with their governing equations. The framework will be demonstrated by results with a focus on effects not predictable within linear dislocation statics or dynamics, or geometrically linear or nonlinear phenomenological plasticity theories. In particular, we will show calculations of static and dynamic finite deformation stress fields of individual dislocations, including their annihilation and the production of Mach cones in intersonic dislocation motion. At the mesoscale, we shall recover the dramatically different experimentally observed size effects in compression and shear inferred from micropillar experiments that all strain gradient plasticity models overestimate and fail to predict. Similarly, additively manufactured nanolaminates show kink banding for sufficiently small lamination widths, which is again a strict test for continuum dislocation dynamics and strain gradient plasticity models at finite strains. We will show the recovery of such predictions by our model. The model raises significant and challenging mathematical questions.

Irene Fonseca: From Phase Separation in Heterogeneous Media to Learning Training Schemes for Image Denoising
Abstract: What do these two themes have in common? Both are treated variationally, both deal with energies of different dimensionalities, and concepts of geometric measure theory prevail in both. Phase Separation in Heterogeneous Media: Modern technologies and biological systems, such as temperature-responsive polymers and lipid rafts, take advantage of engineered inclusions, or natural heterogeneities of the medium, to obtain novel composite materials with specific physical properties. To model such situations using a variational approach based on the gradient theory of phase transitions, the potential and the wells may have to depend on the spatial position, even in a discontinuous way, and different regimes should be considered. In the critical case case where the scale of the small heterogeneities is of the same order of the scale governing the phase transition and the wells are fixed, the interaction between homogenization and the phase transitions process leads to an anisotropic interfacial energy. The supercritical case for fixed wells is also addressed, now leading to an isotropic interfacial energy. In the subcritical case with moving wells, where the heterogeneities of the material are of a larger scale than that of the diffuse interface between different phases, it is observed that there is no macroscopic phase separation and that thermal fluctuations play a role in the formation of nanodomains. This is joint work with Riccardo Cristoferi (Radboud University, The Netherlands) and Likhit Ganedi (Aachen University, Germany), USA), based on previous results also obtained with Adrian Hagerty (USA) and Cristina Popovici (USA). Learning Training Schemes for Image Denoising: Due to their ability to handle discontinuous images while having a well-understood behavior, regularizations with total variation (TV) and total generalized variation (TGV) are some of the best known methods in image denoising. However, like other variational models including a fidelity term, they crucially depend on the choice of their tuning parameters. A remedy is to choose these automatically through multilevel approaches, for example by optimizing performance on noisy/clean image training pairs. Such methods with space-dependent parameters which are piecewise constant on dyadic grids are considered, with the grid itself being part of the minimization. Existence of minimizers for discontinuous parameters is established, and it is shown that box constraints for the values of the parameters lead to existence of finite optimal partitions. Improved performance on some

representative test images when compared with constant optimized parameters is demonstrated. This is joint work with Elisa Davoli (TU Wien, Austria), Jose Iglesias (U. Twente, The Netherlands) and Rita Ferreira (KAUST, Saudi Arabia).

Michael Novack: A variational model for 3D features in films/foams
Abstract: Area minimization among a suitable class of 2D surfaces is the basic variational model describing the interfaces in films/foams. In this talk we will discuss a modification of this paradigm in which surfaces are replaced with regions of small but positive volume. The model captures features of real films/foams, such as Plateau borders, that cannot be described by zero volume objects. We will also discuss the PDE approximation of this problem via the Allen-Cahn equation and its relation to Plateau's laws, which govern the possible singularities.

Raghavendra Venkatraman: Mathematical analysis of resonators made from "Epsilon-near-zero" materials
Abstract: In this talk, we consider the robustness and optimal design of a class of "geometry invariant resonant cavities" that are made from "Epsilon Near Zero" (ENZ) materials that have a core-shell structure: the shell is made from a material whose dielectric permittivity is near zero at the frequency at which the device operates, while the core is a dielectric inclusion. We'll present theorems on the complex analytic dependence of the resonance on the near-zero permittivity, in a neighborhood of zero– this demonstrates the robustness of such resonators to the presence of losses, and their broadband effects around the ENZ frequency. In the 2 dimensional Transverse Magnetic (TM) setting, the leading order behavior of the resonance turns out to be independent of the geometry of the ENZ shell, but only its area. However, the leading order correction depends on shell-geometry– we investigate the shape optimization problem that optimizes the quality of the resonance, and present a convex relaxation which is a free boundary problem of Alt-Caffarelli type. In the fully three dimensional setting, the picture is substantially richer, and we describe an interesting class of resonances that are still geometry independent at leading order, but lead to an interesting vectorial version of the classical "overdetermined problem of J. Serrin". This project represents joint work with Robert V. Kohn (Courant), inspired by discussions with Nader Engheta (UPenn).

Mitchell Luskin: Structural Relaxation of Multilayer 2D Heterostructures and its Effect on Electronic Properties
Abstract: The incommensurate stacking of multilayered two-dimensional heterostructures is a challenging problem from a theoretical perspective and an intriguing avenue for manipulating their physical properties. I will derive a continuum model to compute the mechanical relaxation for an arbitrary number of layers by parametrizing the displacement by the local configuration (disregistry) rather than real space, thus bypassing the need for the standard supercell approximation and giving a true aperiodic atomistic configuration. We note that the displacement of a heterostructure of p layers is not generally periodic in real two-dimensional space for p¿2, but the displacement is periodic on a 2(p-1) dimensional torus as a function of its disregistry. We will show that the regularity of the displacement has a major effect on electronic properties.

Pierre Degond: Passage between Doi-Onsager and Ericksen-Leslie models of liquid crystals
Abstract: In previous literature the passage from the kinetic Doi-Onsager model to the Ericksen-Leslie equations has been made using the Hilbert expansion method. Classical kinetic theory offers an alternate way to pass from kinetic to fluid equations: the moment method. However, in the case of the Doi-Onsager model, the moment method is not directly applicable, due to the lack of conservations, (or collision invariants). In this talk, I will show that suitable generalized conservation relations (aka generalized collision invariants) hold and make the moment method applicable in spite of the lack of conservation relations in the strict sense. It could lead to a better understanding of the structural properties of the Doi-Onsager model and open the way to rigourous convergence proofs that would require less regularity than the Hilbert method. This talk is based on "From kinetic to fluid models of liquid crystals by the moment method" (P. Degond, A. Frouvelle, J-G. Liu, Kinetic and Related Models 15 (2022), pp. 417-465).

Miranda Holmes-Cerfon: The dynamics of particles with ligand-receptor contacts
Abstract: One way to glue objects together at the nanoscale or microscale is by ligand-receptor interactions, where short sticky hair-like ligands stick to receptors on another surface, much like velcro on the nanoscale.

Such interactions are common in biology, such as white blood cells, virus particles, cargo in the nuclear pore complex, etc, and they are also useful in materials science, where coating colloids with single-stranded DNA creates particles with programmable interactions. In these systems, the ligand-receptor interactions not only hold particles together, but also influence their dynamics. How do such particles move? Do they "roll" on each others' surfaces, as is commonly thought? Or could they slide? And does it matter? In this talk I will introduce our modelling and experimental efforts aimed at understanding the coarse-grained dynamics of particles with ligand-receptor interactions. Our models predict these interactions can change the particles' effective diffusion by orders of magnitude. Our experiments, using DNA-coated colloids, verify this dramatic dynamical slowdown, but also show other dynamical features not yet captured by our model, which suggest new avenues for exploration.

Carme Calderer: Analysis of the debonding of a gel membrane from a rigid substrate
Abstract: We propose a model for the debonding of a thin elastic film from a rigid substrate when subject to gravity and exposed to a liquid environment. The model combines nonlinear elasticity with the classical work by Flory and Rehner, together with the variational description of fracture. The theory presented is validated by laboratory experiments. The problem is motivated from the design of the synthetic polymers that coat various medical implants, in order to estimate how thin the gel coating needs to be in order to be stable against debonding from the mechanical substrate. After analyzing the variational problem for a fully bonded film, we present that of the partially attached one, formulated as an obstacle problem. The minimization of the (inequality) constraint problem is achieved by means of the Gamma convergence approach. We calculate the energy release rate leading to debonding and derive the maximum thickness of the film that makes it stable against swelling and debonding forces. We present a finite element study to validate the theoretical prediction of the energy release rate and compare the results with the laboratory experiments.

Will Feldman: Models of contact angle hysteresis
Abstract: I will discuss the origin of contact angle hysteresis of capillary drops from micro-scale surface roughness. This will motivate discussion and theoretical results on some macroscopic toy models which can describe the large-scale effects of the pinning phenomenon.

Sergey Gusarov: Coupling methods of quantum chemistry and molecular simulations with molecular theory of solvation
Abstract: In science, different kinds of shortcuts are often used to study big problems, especially in computational modeling of matter. By combining various scientific models, better results can be achieved, work can be done more efficiently, and methods can be applied to more areas. In our research, we explore how to mix different ways of studying chemicals on computers to better understand materials and living molecules. This area is growing rapidly and contributes to various studies by providing basic knowledge and predictions. Special attention is given to molecular theory of solvation which allows us to accurately introduce the effect of environment on complex nano-, bio- or macromolecular system. The uniqueness of that approach is that it can be naturally coupled with the full range of computational chemistry approaches (QM, MM, and Coarse Grained).

Natasha Sharma: A Second Order Numerical Scheme for a Sixth-Order Cahn-Hilliard Type Equation modeling Microemulsions
Abstract: In this talk we present a second order in time approximation for a sixth-order Cahn-Hilliard type equation which models the dynamics of phase transitions in ternary oil-water-surfactant systems. For its spatial discretization, we decompose this nonlinear sixth-order parabolic equation into a mixed formulation comprising a system of three second order (in space) equations, one of which is parabolic while the other two equations are algebraic. We discuss the key properties of unconditional stability and unique solvability for our scheme and demonstrate its numerical performance through results of selected computational experiments.

4.1 Examples of Some Poster Presentations

Miguel Ayala: Validated Numerical Techniques for Geometric Analysis of Carbon Nanotubes
Henry Brown: Extrapolation of completely monotone functions.

Chi-An Chen: Lagrangian Particle Scheme for Regularized Kimura Equations
Carson Collins: Free boundary regularity for a tumor growth model
Samuel Matthews: Molecular Modeling of sII Gas Hydrate Interfacial Structures and Processes
Matthew Patrick: In situ Grain Growth Experiments: Dynamic Data Collection, Processing, & Analysis
Rawan Tarabeh: Mullins' nonlinear grooving solution

5 Bibliography

[1] C. Herring. Surface tension as a motivation for sintering. In Walter E. Kingston, editor, The Physics of Powder Metallurgy, pages 143–179. Mcgraw-Hill, New York, 1951
[2] Cyril Smith. Grain Shapes and Other Metllurgical Applications of Topology. American Society of Metals, pages 65–113, 1952
[3] William W. Mullins. Two-Dimensional Motion of Idealized Grain Boundaries. J. Appl. Phys., 27:900–904, 1956.
[4] William W. Mullins. The Effect of Grooving on Grain Boundary Motion. Acta Metall., 6:414–427, 1958.
[5] D. A. Aboav. The arrangement of cells in a polycrystal. Metallography, 3:383–390, 1970
[6] Denis Weaire. Some Remarks on the Arrangement of Grains in a Polycrystal. Metallography, 7:157–160, 1974.
[7] D. A. Aboav. The Arrangement of Cells in a Net. Metallography, 13:43–58, 1980
[8] A.D. Rollett, D.J. Srolovitz and M.P. Anderson, Simulation and theory of abnormal grain growth—anisotropic grain boundary energies and mobilities, Acta Metallurgica, Volume 37, Issue 4, Pages 1227-1240, 1989
[9] Y.G. Chen, Y. Giga, and S. Goto, Uniqueness and existence of viscosity solutions of generalized mean curvature flow equations, J. Diff. Geom., 33:749–786, 1991
[10] A. Di Carlo, M. Gurtin, and P. Podio-Guidugli. A regularized equation for anisotropic motion-by-curvature. SIAM Journal on Applied Mathematics, 52(4):1111–1119, 1992
[11] David Kinderlehrer and Chun Liu, Evolution of Grain Boundaries, Mathematical Models and Methods in Applied Sciences, Vol. 4, No. 11, 2001
[12] R. MacPherson and D. Srolovitz, The von Neumann relation generalized to coarsening of three-dimensional microstructures. Nature 446, 1053–1055, 2007
[13] K. Barmak, E. Eggeling, M. Emelianenko, Y. Epshteyn, D. Kinderlehrer, R. Sharp, and S. Ta'asan. Critical events, entropy, and the grain boundary character distribution. Phys. Rev. B, 83:134117, Apr 2011
[14] P. Bardsley, K. Barmak, E. Eggeling, Y. Epshteyn, D. Kinderlehrer, S. Ta'asan, Towards a Gradient Flow for Microstructure, Rendiconti Lincei - Matematica e Applicazioni (European Mathematical Society Publishing), 28 (2017), 777-805, 2017
[15] Gabriel Martine La Boissoni‘ere and Rustum Choksi. Atom based grain extraction and measurement of geometric properties. Modelling and Simulation in Materials Science and Engi- neering, 26(3):035001, 2018
[16] Matt Elsey and Selim Esedoglu. Threshold dynamics for anisotropic surface energies. Math. Comp., 87(312):1721–1756, 2018
[17] K. Saleme Ruiz and M. Emelianenko, "The role of topology in microstructure-property relations: a 2D DEM-based study", Modelling Simul. Mater. Sci. Eng., vol. 26, 2018
[18] Y. Epshteyn, C. Liu and M. Mizuno, Motion of grain boundaries with dynamic lattice misorientations and with triple junctions drag, SIAM Journal on Mathematical Analysis, 53(3), 3072-3097, 2021
[19] J. Klobusicky, G. Menon and R. Pego, Two-Dimensional Grain Boundary Networks: Stochastic Particle Models and Kinetic Limits, Archive for Rational Mechanics and Analysis, vol. 239, no. 1, pp. 301–355, 2021
[20] Kaushik Bhattacharya, Nikan B. Firoozye, Richard D. James, and Robert V. Kohn. Re- strictions on microstructure. Proc. Roy. Soc. Edinburgh Sect. A, 124(5):843–878, 1994
[21] K. Bhattacharya, R.V. Kohn, Symmetry, texture and the recoverable strain of shape-memory polycrystals, Acta Materialia, Volume 44, Issue 2, 1996
[22] K. Bhattacharya, Microstructure of Martensite: Why It Forms and How It Gives Rise to the Shape-Memory Effect, 2003, Oxford Series on Materials Modelling

[23] Alexander B. Watson and Mitchell Luskin , Existence of the first magic angle for the chiral model of bilayer graphene, J. Math. Phys. 62, 091502 (2021)
[24] X. Chen, I. Fonseca, M. Ravnik, V. Slastikov, C. Zannoni and A. Zarnescu, Topics in the mathematical design of materials, Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 379, 2021
[25] S. Alama, L. Bronsard, and X. Lamy, Analytical description of the Saturn-ring defect in nematic colloids, Phys Rev E, 93, 012705, 2021
[26] Zhang, X., Ren, W., Bell, E. et al. Gate-tunable Veselago interference in a bipolar graphene microcavity. Nat Commun 13, 6711 (2022)
[27] N. Gorbushin, A. Vainchtein and L. Truskinovsky. Transition fronts and their universality classes. Physical Review E, 106, 024210, 2022
[28] R. G. Larson. The Structure and Rheology of Complex Fluids. Oxford, 1995.
[29] James Keener and James Sneyd. Mathematical Physiology. Springer-Verlag, NY, 1998.
[30] M.S. Kilic, M.Z. Bazant, and A. Ajdari. Steric effects in the dynamics of electrolytes at large applied voltages. II. Modifed Poisson-Nernst-Planck equations. Phys. Rev. E 75 (2007), 021503.
[31] R.S.Eisenberg,Y.Hyon, and C.Liu. Energy Variational Analysis EnVarA of Ions in Water and Channels: Field Theory for Primitive Models of Complex Ionic Fluids. Journal of Chemical Physics 133, 104104 (2010).
[32] A Majumdar, A Zarnescu, Landau–De Gennes theory of nematic liquid crystals: The Oseen–Frank limit and beyond, Archive for rational mechanics and analysis 196 (1), 227-280, 2010.
[33] T.-L. Horng, T.-C. Lin, C. Liu, and B. Eisenberg. PNP Equations with Steric Effects: A Model of Ion Flow through Channels. J. Phys. Chem. B 116 (2012), pp. 11422–11441.
[34] S. Xu ; P. Sheng ; Chun Liu. An energetic variational approach for ion transport. Commun. Math. Sci. 12 (2014), no. 4, 779–789.
[35] C. Kuthe, R. V. Uddanwadiker, P. M. Padole, A. A. Ramteke, Mathematical model for skeletal muscle to simulate the concentric and eccentric contraction. Mol. Cell. Biomech, 12 (2015), 1-16.
[36] O. M. Tovkach, M. C. Calderer, D. Golovaty, O. Lavrentovich, and N. J. Walkington, Electro-osmosis in Nematic Liquid Crystals. PHYSICAL REVIEW E 94, 012702 (2016).
[37] A. Goriely. The mathematics and mechanics of biological growth 45, (2017). Springer.
[38] Y. Wang, G. Canevari, and A. Majumdar, Order reconstruction for nematics on squares with isotropic inclusions: A Landau–de Gennes study. SIAM J. Appl. Math., 79(4):1314–1340, 2019.