Nonconvexity, Nonlocality and Incompatibility: From Materials to Biology

Conference in honor of Lev Truskinovsky’s 60th birthday

Organizing committee:
Anna Vainchtein (University of Pittsburgh)
Yury Grabovsky (Temple University)
Pierre Recho (CNRS, Liphy, Grenoble)
Giovanni Zanzotto (University of Padua)

University of Pittsburgh, May 5-7, 2017
Overview

The conference aims to facilitate exchange of ideas and establish new connections between researchers from different fields working on problems in materials science and biology that involve nonconvex nonlocal interactions and incompatibility, as well as other closely related issues. Conference topics include plasticity and phase transitions in crystals, nucleation and evolution of defects and microstructures in crystal lattices, self-organized criticality and avalanches, crystallization, wrinkling, rupture processes in earthquakes, morphogenesis, cell motility, growth and remodeling of biological tissues, mechanics of muscles and protein motors. Mathematical studies of such problems involve multiscale variational methods and homogenization, stochastic analysis, differential geometry and analysis of nonlinear partial, functional and lattice differential equations.

The conference is sponsored by the Mathematics Research Center at the University of Pittsburgh and partially supported by the Institute for Mathematics and its Applications through its Participating Institution Program.
## Contents

### Overview

### Abstracts

<table>
<thead>
<tr>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>A New Class of Pattern-Forming Equations in Continuum Mechanics</td>
<td>1</td>
</tr>
<tr>
<td>Amit Acharya</td>
<td></td>
</tr>
<tr>
<td>Towards Modeling Longitudinally Propagating Shear Bands: Rajat Arora</td>
<td>1</td>
</tr>
<tr>
<td>The Non-Linear Mechanics of Slender Deformable Bodies</td>
<td>2</td>
</tr>
<tr>
<td>Basile Audoly</td>
<td></td>
</tr>
<tr>
<td>Crystal Plasticity on a Small Time Scale, Slip Avalanches, Acoustic</td>
<td>2</td>
</tr>
<tr>
<td>Emission and The Stress-Strain Curve: Victor L. Berdichevsky</td>
<td></td>
</tr>
<tr>
<td>Sympathy for the Devil: Andrea Braides</td>
<td>2</td>
</tr>
<tr>
<td>Morphomechanics of Bacterial Biofilms: Ana Carpio</td>
<td>3</td>
</tr>
<tr>
<td>Mechanical Modeling of Active and Passive Force Generation in Skeletal Muscles: Matthieu Caruel</td>
<td>3</td>
</tr>
<tr>
<td>Essential Role of Non-Essential Multifield Approximations in Lattice Dynamics: Miquel Charlotte</td>
<td>4</td>
</tr>
<tr>
<td>Computing Singularly Perturbed Differential Equations and Plasticity</td>
<td>4</td>
</tr>
<tr>
<td>Without Constitutive Assumptions: Sabysachi Chatterjee</td>
<td></td>
</tr>
<tr>
<td>Compatibility in Frames and Lattices: Andrej Cherkaev</td>
<td>5</td>
</tr>
<tr>
<td>Design of 3d Objects Using Stress Relaxation in 2d Thin-Films: The</td>
<td>5</td>
</tr>
<tr>
<td>Interplay Between Geometry and Mechanics: Alexandre Danescu</td>
<td></td>
</tr>
<tr>
<td>Biological and Bio-Inspired Locomotion at Small Scales: Antonio DeSimone</td>
<td>6</td>
</tr>
<tr>
<td>Incompatibility in Multi-Walled Nanotube Composites: Marcelo Epstein</td>
<td>6</td>
</tr>
<tr>
<td>Registry Effects in Carbon Nanostructures: Malena Espanol</td>
<td>6</td>
</tr>
<tr>
<td>Epitaxially Strained Elastic Films: Quantum Dots and Dislocations: Irene Fonseca</td>
<td>7</td>
</tr>
<tr>
<td>A Generalized Continuum with Internal Corner and Surface Contact</td>
<td>7</td>
</tr>
<tr>
<td>Interactions: Roger Fosdick</td>
<td></td>
</tr>
<tr>
<td>Dissipation Potentials and a Gradient-Regularization of a Granular Flow: Joe Goddard</td>
<td>8</td>
</tr>
<tr>
<td>Model: Robert Kohn</td>
<td>9</td>
</tr>
<tr>
<td>Zig-zag Microstructures Mixing Two Variants of Martensite:</td>
<td>9</td>
</tr>
<tr>
<td>Robert Kohn</td>
<td></td>
</tr>
<tr>
<td>Modeling Recrystallization by Means of Non-Convex Energy Minimization: Khanh Chau Le</td>
<td>9</td>
</tr>
<tr>
<td>A Model of Controlled Growth: Marta Lewicka</td>
<td>9</td>
</tr>
<tr>
<td>An Epidemic Model with Nonlocal Diffusion on Networks: Elisabeth Logak</td>
<td>10</td>
</tr>
<tr>
<td>Non-Euclidean Elasticity and Asymptotic Rigidity of Manifolds: Cy Maor</td>
<td>10</td>
</tr>
<tr>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>Boundary Behavior and Confinement of Dislocations Inside a Crystal</td>
<td>10</td>
</tr>
<tr>
<td>Marco Morandotti</td>
<td></td>
</tr>
<tr>
<td>Modelling Avalanches in Solids (Francisco Perez-Reche)</td>
<td>11</td>
</tr>
<tr>
<td>A Predictive Model for Soft Materials With Unfolding Domains: From</td>
<td>11</td>
</tr>
<tr>
<td>Macromolecules to Macroscopic Material Behavior (Giuseppe Puglisi)</td>
<td></td>
</tr>
<tr>
<td>Statistical Mechanics and Electrostatics in DNA Phase Transitions</td>
<td>12</td>
</tr>
<tr>
<td>Prashant K Purohit</td>
<td></td>
</tr>
<tr>
<td>Stability of Frictional Travelling Waves (Thibaut Putelat)</td>
<td>13</td>
</tr>
<tr>
<td>Plates with Incompatible Prestrain of Higher Order (Diego Ricciotti)</td>
<td>13</td>
</tr>
<tr>
<td>Thermo-Hydro-Mechanical Processes Stabilizing Antarctic Ice Stream</td>
<td>14</td>
</tr>
<tr>
<td>Margins (James R. Rice)</td>
<td></td>
</tr>
<tr>
<td>Can Cells Use Phase Transitions to See Each Other in Fibrous Darkness?</td>
<td>14</td>
</tr>
<tr>
<td>Algorithm for Studying Flow-Induced Phase Transitions in Nematic</td>
<td>15</td>
</tr>
<tr>
<td>Crystals (Shawn Ryan)</td>
<td></td>
</tr>
<tr>
<td>The Global Geometric Viewpoint of Continuum Mechanics: An Overview</td>
<td>15</td>
</tr>
<tr>
<td>of some Applications (Reuven Segev)</td>
<td></td>
</tr>
<tr>
<td>Mean-Field Limits for Ginzburg-Landau Vortices (Sylvia Serfaty)</td>
<td>16</td>
</tr>
<tr>
<td>Stability Analysis and Applications of the Rate, State, Temperature</td>
<td>16</td>
</tr>
<tr>
<td>and Pore Pressure Friction (Rstpfl) Model for Earthquake and Landslides</td>
<td></td>
</tr>
<tr>
<td>Phenomena (Arun Kumar Singh)</td>
<td>17</td>
</tr>
<tr>
<td>Optimal Wall-To-Wall Transport by Incompressible Flows (Ian Tobasco)</td>
<td>17</td>
</tr>
<tr>
<td>New Statistical Parameters for Grain Growth (Pawan Vedanti)</td>
<td>17</td>
</tr>
<tr>
<td>Nonlinear Mechanics of Surface Growth for Cylindrical and Spherical Elastic Bodies (Arash Yavari)</td>
<td>18</td>
</tr>
<tr>
<td>Surface Elasticity in Steigmann-Ogden Form in Modeling of Fracture (Anna Zemlyanova)</td>
<td>18</td>
</tr>
<tr>
<td>Relevance and Applications of Generalized Disclination Theory in Defect Mechanics (Chiqun Zhang)</td>
<td>19</td>
</tr>
<tr>
<td>Printing Non-Euclidean Solids (Giuseppe Zurlo)</td>
<td>19</td>
</tr>
</tbody>
</table>

**Author Index**
Abstracts

A New Class of Pattern-Forming Equations in Continuum Mechanics

Amit Acharya
Carnegie Mellon University

A pde model of non-singular line defect dynamics arising from the strong interaction of incompatibility, nonlocality, and nonconvexity in continuum mechanics will be described. A new class of pattern-forming pde emerge, that may be loosely considered as a ‘multiplicative mixture’ of reaction diffusion and (manifestly) wave-propagative effects. As some examples, the interaction and annihilation of a nematic disclination (alternatively a screw dislocation) dipole and the splitting of a strength 1 into two strength 1/2 defects, and their subsequent repulsive interaction, will be discussed, all within a completely deterministic setting.

Towards Modeling Longitudinally Propagating Shear Bands

Rajat Arora
Carnegie Mellon University

Dynamic adiabatic shear bands are narrow, localized zones of large plastic deformation which are widely observed in metals and metallic alloys under intense dynamic loading. Because of its impact on materials under extreme conditions, it has been of immense interest for the scientific community and several experiments have been performed to explore the phenomenon of shear band formation in materials. Conventional elasto-viscoplastic theories by themselves are incapable of modeling shear band dynamics as they do not have the kinematical feature necessary for the longitudinal propagation of shear bands due to plastic flow. The objective of this presentation is to propose an appropriate model that overcomes this fundamental limitation of conventional theories and develop a validated mechanics based massively parallel computational tool to model dynamic propagation of shear bands.

We present computational results of various aspects of a full finite deformation model of mesoscale dislocation dynamics (a first in the literature) before moving on to results of longitudinal shear band propagation through essentially the motion of its tip. This is a unique feature enabled by the theory.
The Non-Linear Mechanics of Slender Deformable Bodies
Basile Audoly
CNRS and Ecole polytechnique

We discuss some challenges arising in the mechanics of slender (quasi-1D) deformable bodies, such as a thin thread of polymer, curly hair, or a carpenter’s tape for example. Slender bodies can exhibit a number of complex and intriguing behaviors that are accessible through simple experiments. The analysis of slender bodies exposes one to many of the fundamental concepts of 3D non-linear mechanics, albeit in a simpler setting where explicit analytical solutions and fast numerical methods can be proposed. Based on examples, we review some problems arising in the analysis of deformable bodies, including the derivation of accurate 1D mechanical models by dimensional reduction, the solution of non-linear 1D models by analytical or numerical methods, and the analysis of material or geometrical instabilities.

Crystal Plasticity on a Small Time Scale, Slip Avalanches, Acoustic Emission and The Stress-Strain Curve
Victor L. Berdichevsky
Wayne State University

It is commonly accepted that work hardening, slip avalanches and acoustic emission rise from the same mycelium, an extremely complex energy relief in dislocation phase space. It was argued recently (Berdichevsky 2017) that this complexity possesses a quite special structure: phase space splits into a family of equipolarization subspaces; each subspace contains a finite number of states which the system can occupy, and the phase trajectory goes from an admissible state of one subspace to an admissible state of another subspace. Such a simple picture clarifies the structure of plasticity thermodynamics and yields the existence of new thermodynamic parameters, dislocation polarizations and entropy of microstructure, and the links between statistics of slip avalanches, acoustic emission and the rate of work hardening.

Sympathy for the Devil
Andrea Braides
University of Rome Tor Vergata

In two recent inspiring papers Novak and Truskinovsky study a ”devil’s staircase” phenomenon in some simple discrete systems. We revisit those examples as a non-linear homogenization process. That process can be adapted to treat some continuum analogs. Comparing the continuum with the discrete, some diabolic features are seemingly lost (but reappear in the details).
Morphomechanics of Bacterial Biofilms

Ana Carpio
Complutense University of Madrid

From microbial colonies to tissues, multicellular organisms arise through the interaction of cell processes and macroscopic forces. Bacterial communities provide model systems for exploring such interaction. Biofilms are bacterial aggregates encased in a self-produced polymeric matrix which spread on moist habitats. Their shape depends on environmental factors. Whereas filamentary structures proliferate in flows, wrinkled sheets are observed on air/solid interfaces. We are able to reproduce both types of shapes through plate and rod models that incorporate rates and stresses determined by the cellular activity, as well as environmental constraints.

Mechanical Modeling of Active and Passive Force Generation in Skeletal Muscles

Matthieu Caruel
Université Paris-Est Créteil

We present an overview of recent attempts to complement the chemistry-centered microscopic models of skeletal muscles by purely mechanical models. The force generation phenomena of interest can be divided into two classes and their mechanisms are usually modeled in different ways. Models in the first class deal with fast force recovery, which is believed to be a passive process. It can be viewed as a collective folding phenomenon in a system of interacting bi-stable units and is modeled by equilibrium statistical mechanics and Langevin kinetics. Models in the second class deal with active force generation taking place at slower time scales, requiring an energy input provided by ATP hydrolysis. The underlying mechanisms operate far from equilibrium and are usually represented by stochastic models with broken time reversal symmetry, non-potentiality and/or correlated noise. The mechanical approach reinforces an alternative biochemical perspective that phenomena involved in slow (active) and fast (passive) force generation are, tightly intertwined and cannot be fully understood if separated.
Essential Role of Non-Essential Multifield Approximations in Lattice Dynamics

Miguel Charlotte
Université de Toulouse

Relevant scales of length and time in lattice dynamics depend on both, the structure of atomic interactions and the nature of the observed phenomenon. In this work we are interested in building such a mesoscale description of dynamics in a mass-spring system which will be capable of capturing atomically fast and localized phenomena that cannot be handled correctly by the classical quasi-continuum theories relying on a single displacement field. Our approach is based on a nonessential multilattice description of a chain with nearest neighbor interactions and its multi-field long wavelength approximations. The outcome is a non-classical multifield continuum elastodynamics with nontrivial inertia whose complexity depends on the level of frequencies intended to be captured. The advantage of the multi-field approach is that we can deal in the same framework with both continuum and anticontinuum phenomena.

Computing Singularly Perturbed Differential Equations and Plasticity Without Constitutive Assumptions

Sabyasachi Chatterjee
Carnegie Mellon University

Obtaining coarse response of a system of ordinary differential equations (ODE) containing rapidly oscillatory response without detailed information on the evolution of the original (fine) variables is an interesting, but challenging task. For a given autonomous system of ODE, we consider developing practical models for determining the slow/coarse behavior of the ODE system which reflect a measurement of the underlying dynamics. We study equations with and without apriori split into slow and fast components. When there is a vast separation of the time-scales of the coarse and the fine dynamics, computing the ordinary differential equation takes a lot of computing time and is not practical. The goal of our study is to suggest efficient computational tools that help revealing the limit behavior of such systems. We define coarse variables using modern mathematical tools like Young Measure and Practical Time Averaging (PTA) which incorporates many rigorous ideas. The computational algorithm reveals an approximation of the limit dynamics which is an approximation of the full solution. We also discuss how to determine the fine initial conditions which ensures a correct coarse response.

Finally we apply this theory to develop a macroscopic model to compute the plastic strength and study the microstructure of crystalline materials at the meso-macro scale from the underlying motion of crystal defects. We couple an exact, non-closed partial differential equation based theory (Mesoscale Field Dislocation Mechanics, MFDM) representing the evolution of space-time averaged dislocation dynamics, that contains well-defined place-holders for microscopic dislocation dynamics based input. These inputs are prescribed by a carefully designed coupling.
on the slow time-scale of meso-macro response, with time-averaged response of fast, local Discrete Dislocation dynamics (DD) simulations. The rationale behind adopting such a coupled PDE-ODE approach instead of a completely DD based approach is primarily the vast separation in time-scales between plasticity applications that operate at quasi-static loading rates and the fundamental time scale of dislocation motion as embodied in DD which makes it impractical to reach appreciable applied strain using DD alone. The developed model will be truly material microstructure-sensitive that does not involve postulating constitutive assumptions beyond those embodied in DD methodology and macroscopic elastic response.

---

**Compatibility in Frames and Lattices**

Andrej Cherkaev  
University of Utah

We derive compatibility conditions in lattices and frames that bond the lengths of the rods, and prove the continuous limit of these conditions. The results are applied to description of the state of partially damaged lattices.

Joint work with Predrag Krolika and Andrejs Treibergs

---

**Design of 3d Objects Using Stress Relaxation in 2d Thin-Films: The Interplay Between Geometry and Mechanics**

Alexandre Danescu  
Lyon Institute of Nanotechnology

It is well-known that a free pre-stressed elastic material change its shape so as to “relax” its total energy. Depending on the pre-stress distribution, the relaxation process deforms simple straight segments into rolls, curls, etc. In an attempt to cover more complex three-dimensional geometries we address and solve the general question concerning the relaxation of an arbitrary planar curve. We illustrate our theoretical results by the design and fabrication of several three-dimensional spherical objects using pre-stressed semiconductor multilayers. The multilayered stacks are fabricated by molecular beam epitaxy (MBE), a growth method that allows very accurate control of the composition, lattice mismatch and thickness. We explore the validity of our results for semiconductor films with thickness between 70 and 400 nm and illustrate geometrical incompatibilities between the planar and spherical geometries. Following the analogy between classical crystals and photonic crystals, we address the design and fabrication of the more exotic objects like “single-wall photonic nano-tubes”. We discuss the limitations of the method as well as several open questions.
Biological and Bio-Inspired Locomotion at Small Scales
Antonio DeSimone
SISSA

Locomotion at the micrometer scale is at the root of many fundamental processes in Biology. These include the immune system response, the migration of metastatic tumour cells, and sperm cells successfully swimming their way by beating a flagellum until they reach and fertilise an egg cell. Besides their biological interest, motile cells provide a template for the bio-inspired design of micrometer-scale, self-sufficient machines capable of executing controlled motion.

We will report on some of our recent studies on swimming micro-motility, discussing general principles first, and then a concrete case study.

Incompatibility in Multi-Walled Nanotube Composites
Marcelo Epstein
University of Calgary

A modeling paradigm for continuous distributions of defects in multi-walled nanotube composites is proposed in terms of differential forms. A necessary and sufficient condition for a defect-free composite is derived and, concomitantly, a measure of defect density is proposed. Mathematically, this condition ensures the consistency of an over-determined system of partial differential equations. Physically, the condition expresses the fact that each multi-layered nanotube can find mutually coherent nanotubes in its neighborhood. Several examples of defect-free arrangements are presented and discussed.

Registry Effects in Carbon Nanostructures
Malena Espanol
The University of Akron

A graphene sheet is a single-atom thick macromolecule of carbon atoms arranged in a hexagonal lattice. The phenomena addressed by our work include pattern formation and localized wrinkling driven by lattice and orientation mismatches between a graphene sheet and its supporting substrate, moire patterns in bilayer graphene, and polygonization and faceting in multi-walled carbon nanotubes. In this talk, we present atomistic-to-continuum models that retain lattice registry effects to describe weak van der Waals interactions in carbon nanostructures.
Epitaxially Strained Elastic Films: Quantum Dots and Dislocations
Irene Fonseca
Carnegie Mellon University

The formation and assembly patterns of quantum dots play a central role on the optoelectronic properties of semiconductors. We will address quasistatic equilibria and regularity of islands (quantum dots), and using De Giorgi’s minimizing movements we will obtain short time existence for a surface diffusion evolution equation with curvature regularization in the context of epitaxially strained films. A variational model for the nucleation of misfit dislocations will be analyzed.

A Generalized Continuum with Internal Corner and Surface Contact Interactions
Roger Fosdick
University of Minnesota

In classical continuum mechanics the admissible contact interaction that takes place between adjacent parts of a body is surfacial and it is assumed to act as a force per unit area (surface traction) on an oriented surface which separates these parts. As a well-known generalization of this, the surfacial interaction may include the action of a couple measured per unit area (surface-couple traction). A lesser known generalization of a possible contact interaction between the adjacent parts of a body supposes that on the edge of an arbitrary part there is a force measured per unit length (edge traction) due to contact of the edge with the adjacent material of the body. Of course, other types of contact interactions between adjacent parts of a body can be imagined such as an edge-couple traction which acts on edges and is measured per unit length, or a corner force which acts at the corner of an arbitrary part due to the surrounding material that is in contact with it. In this talk, to be explicit, only surface, surface-couple and edge traction interactions will be allowed to act. Such a fundamental change in the way the parts of a body may interact due to contact is a broad generalization of classical ideas in continuum mechanics and it may be expected to affect cornerstone elements of the theory. In particular, the stress theorem of Cauchy, which concludes that the surface traction is given by a linear function (stress tensor) evaluated on the oriented unit normal to a surface, is no longer valid. We follow the point of view that the arbitrary parts of a body—those parts that are supposed to satisfy the balance of mass, together with the balance of linear and angular momentum—must now be distinguished as volumes, surfaces and edges which support contact interactions. That is, we consider that not only volume parts have a structure in the sense that they respond as an entity to changes of shape, but also surface and edge parts, considered as parts of a body, have their own structure and that they also respond as identifiable entities to changes of shape and form. For simplicity, we assume that volume parts carry a specific mass density measured per unit volume, and that surface and edge parts do not carry the intrinsic property of a specific mass density.
In this talk, the balances of mass and linear and angular momentum are applied to the arbitrary parts of a continuum which supports internal edge and surface contact interactions. A generalized form of Cauchy’s stress theorem is derived which shows that the surface traction on an oriented surface depends in a specific way on both the oriented unit normal as well as the curvature of the surface. An explicit form of the surface-couple traction which acts on every oriented surface is obtained. Two fields in the continuum, which may be called stress and hyperstress fields, are shown to exist and their role in representing the surface traction and the surface-couple traction is identified. Finally, the field equations and the power theorem for this theory are exhibited. In the absence of internal edge and surface-couple traction interactions, classical continuum mechanics prevails.

Dissipation Potentials and a Gradient-Regularization of a Granular Flow Model

Joe Goddard

University of California, San Diego

This talk deals with the Hadamard instability, reported recently by Barker et al. (2015, J. Fluid Mech., 779, 794-818), of the so-called mu(I) model of dense rapidly-sheared granular flow. The present work presents a more comprehensive study of the linear stability of simple shearing flow, with account taken of wave-vector stretching by the base flow. The latter leads to asymptotic stabilization of the initial instability found by Barker et al.. We also explore the stabilizing effects of higher velocity gradients in an enhanced-continuum model based on a dissipation potential and the dissipative analog of the Van der Waals-Cahn-Hilliard equation of equilibrium thermodynamics. This model involves a dissipative hyper-stress, as the analog of the elastic Korteweg stress, with surface viscosity representing the analog of elastic surface tension. We also present a model of shear bands resulting from the combined effects of wave-vector stretching and short-wavelength cut-off provided by the enhanced-continuum model.

Apart from the theoretical interest, the present work may suggest stratagems for the numerical simulation of continuum field equations involving the mu(I) rheology and variants.
Zig-zag Microstructures Mixing Two Variants of Martensite

Robert Kohn
Courant Institute, NYU

When two stress-free variants of martensite mix by twinning, the volume fraction can vary only in the direction normal to the twin plane. In some settings, applied loads require the volume fraction to vary along the twin plane. Such loads induced stress and make the twin boundaries tilt, leading to formation of what have been called “zig-zag microstructures.” I will discuss recent joint work with Alex Misiats and Stefan Mueller, concerning the modeling of this class of microstructures via minimization of elastic plus surface energy.

Modeling Recrystallization by Means of Non-Convex Energy Minimization

Khanh Chau Le
Ruhr University Bochum

The present paper considers the formation of grain boundaries during severe plastic deformations. Within the continuum dislocation theory (CDT) we reduce this to the non-convex variational problems of energy minimization. We interpret the grain boundary as surfaces of weak discontinuity in placement but strong discontinuity in plastic slip. The set of governing equations and jump conditions are derived for the energy minimizers admitting such surfaces of discontinuity from the variational principle. By constructing energy minimizing sequences having piecewise constant plastic and elastic deformation in two examples of ductile single crystals deforming in plane strain simple shear or uniaxial compression, it is shown that the formation of lamellae structure with grain boundaries is energetically preferable. The number of lamellae is estimated by minimizing the energy of grain boundaries plus the energy of boundary layers. The model taking the energy dissipation into account will also be considered.

A Model of Controlled Growth

Marta Lewicka
University of Pittsburgh

We consider a free boundary problem for a system of PDEs, modeling the growth of a biological tissue. A morphogen, controlling volume growth, is produced by specific cells and then diffused and absorbed throughout the domain. The geometric shape of the growing tissue is determined by the instantaneous minimization of an elastic deformation energy, subject to a constraint on the volumetric growth. For an initial domain with C2, boundary, our main result establishes the local existence and uniqueness of a classical solution, up to a rigid motion.

This is a joint work with Alberto Bressan.
An Epidemic Model with Nonlocal Diffusion on Networks
Elisabeth Logak
Université de Cergy-Pontoise

We consider a SIS system with nonlocal diffusion which is the continuous version of a discrete model for the propagation of epidemics on a metapopulation network. Under the assumption of limited transmission, we prove the global existence of a unique solution for any diffusion coefficients. We investigate the existence of an endemic equilibrium and prove its linear stability, which corresponds to the loss of stability of the disease-free equilibrium. In the case of equal diffusion coefficients, we reduce the system to a Fisher-type equation with nonlocal diffusion, which allows us to study the large time behaviour of the solutions. We show large time convergence to either the disease-free or the endemic equilibrium. Joint work with Isabelle Passat.

Non-Euclidean Elasticity and Asymptotic Rigidity of Manifolds
Cy Maor
University of Toronto

Liouville’s rigidity theorem (1850) states that a map $f : \Omega \subset \mathbb{R}^d \to \mathbb{R}^d$ that satisfies $Df \in SO(d)$ is an affine map. Reshetnyak (1967) generalized this result and showed that if a sequence $f_n$ satisfies $Df_n \to SO(d)$ in $L^p$, then $f_n$ converges to an affine map.

In this talk I will discuss generalizations of these theorems to mappings between manifolds and describe how these rigidity questions arise in the theory of elasticity of pre-stressed materials (non-Euclidean elasticity). Based on a joint work with Asaf Shachar and Raz Kupferman.

Boundary Behavior and Confinement of Dislocations Inside a Crystal
Marco Morandotti
Technical University of Munich

We study the behavior of screw dislocations near the boundary. Our aim is to elucidate a variety of qualitative features of this model for the dynamics of dislocations. It is commonly observed in numerical simulations that dislocations are attracted to free boundaries and that dislocations of opposite signs attract. By contrast, we show how it is possible to confine screw dislocations inside a crystal which undergoes an anti-plane shear deformation by prescribing an external strain. By means of Gamma-convergence, we prove that it is energetically favourable for one single dislocation to remain confined inside the crystal instead of migrating to the boundary. The results are extended to the case of many dislocations. These results are contained in joint works with Thomas Hudson, Ilaria Lucardesi, Riccardo Scala, and Davide Zucco.
Solids subject to continuous changes of temperature or mechanical load often exhibit discontinuous avalanche-like responses. For instance, such dynamics have been observed during plastic deformation, fracture, domain switching in ferroic materials or martensitic phase transitions. The statistical analysis of avalanches reveals a very complex scenario with a distinctive and ubiquitous lack of characteristic scales. In this talk, I will focus on the mathematical models developed in collaboration with Lev Truskinovsky and Giovanni Zanzotto to study avalanches in both thermally and mechanically driven martensitic transformations. The starting point of our models is a continuum description of crystal deformations at mesoscopic scales. Such description is then reduced to (pseudo-)spin models of the random field type with athermal dynamics. The resulting models establish a conceptual bridge between structural phase transformations in solids and the statistical mechanics of disordered systems. I will review some of the predictions and explanations provided by our framework. These include: (i) The prediction of a driving-induced crossover from classical criticality to self-organized criticality in mechanically driven martensites and (ii) a recent explanation of the origin of scale-free intermittency in thermally driven martensites.


Giuseppe Puglisi
Politecnico di Bari

We deduce a general multiscale approach for the mechanical behavior of macromolecular soft materials undergoing strain-induced unfolding. Starting from a (statistically based) energetic analysis of the macromolecules unfolding, we obtain a three-dimensional continuum model that, based on a limited number of experimental macromolecular parameters, including the persistence and contour length, describes the complex macroscopic behavior observed in soft materials. The comparison with our experimental cyclic tests on spider silk and keratin fibers (human, cow, and rabbit hair) shows that our model is robust and reproduces with surprising accuracy the mechanical behavior of protein materials undergoing damage and residual stretches.
Statistical Mechanics and Electrostatics in DNA Phase Transitions
Prashant K Purohit
University of Pennsylvania

Experimental studies on single molecules of DNA have reported a rich variety of structural transitions including coexistence of three phases, in a torsionally con-strained molecule. A comprehensive knowledge of these structural transitions is useful for unraveling the in vivo and in vitro behavior of DNA. Our objective is to understand the structural transitions in a torsionally constrained DNA molecule when it is pulled using optical or magnetic tweezers. We use foundational concepts from the Zimm-Bragg helix-coil transition theory and merge them with ideas from the theory of fluctuating elastic rods to model the mechanics of DNA. We also account for the electrostatic interactions between the ions and the negatively charged phosphate backbone of DNA. Using our model, we calculate the force and torque corresponding to the over-stretching transition characterized by a 70% jump in the contour length of the molecule and examine the effect of salt concentration on this transition. We also deduce conditions under which the co-existence of B-, S- and P-DNA is possible. We examine how the cooperativity parameter for each transition affects the force-extension curve or torque-rotation curve. We attempt to rationalize the non-monotonic dependence of external work done on the ion concentration by connecting it to the electrostatic dependence of the interfacial energy between two phases of DNA. We also present a theoretical model to study the overstretching transition with the possibility that the overstretched state is a mixture of two phases: a structure with portions of inner strand separation (melted or M-DNA), and an extended phase that retains the basepair structure (S-DNA). We model the double-stranded DNA as a chain composed of n segments of length l, where the transition is studied by means of a Landau quartic potential with statistical fluctuations. By analyzing the different values of l corresponding to a wide spectrum of experiments, we find that for a range of temperatures and ionic conditions, the overstretched form is likely to be a mix of M-DNA and S-DNA. For a transition close to a pure S-DNA state, where the change in extension is close to 1.7 times the original B-DNA length, we find l is 25 basepairs regardless of temperature and ionic concentration. Our model is fully analytical, yet it accurately reproduces the force-extension curves, as well as the transient kinetic behavior, seen in DNA overstretching experiments.
Stability of Frictional Travelling Waves
Thibaut Putelat
University of Bristol

Inhomogeneous frictional sliding along regional contact between solid bodies such as earthquakes is ubiquitous and characterized by multiple spatiotemporal scales. A comprehensive understanding of the physical mechanisms and mathematical ingredients that underlie the diversity of the frictional slip patterns that has been reported over the years is still lacking. Based on recent advances in the nonlinear dynamics of distributed frictional rupture of a thin elastic slab, we shall discuss a possible origin of such patterns described as travelling waves of slip or stick occurring between sliding interfaces. Under rate-and-state friction, we find a plethora of solutions, including propagating wavetrains, pulses and fronts, can arise from homoclinic or heteroclinic bifurcations as the applied shear stress is varied. The key ingredient of the mathematical model is that the friction law should present a non-monotonic velocity-dependent steady-state characteristics. We stress that such localized solutions exist only along specific lines in parameter space, giving stress-velocity relations that we compute and which separate domains of generic travelling fronts and wavetrains of various types. A special emphasis on the stability of such localized slip patterns will be given, in particular with respect to the effect of contact stiffness.

Plates with Incompatible Prestrain of Higher Order
Diego Ricciotti
University of Pittsburgh

We study the effective elastic behaviour of incompatibly prestrained thin plates, characterized by a Riemannian metric $G$ on the reference configuration. We assume the incompatible elastic energy $E^h$ has scaling of order less than $h^2$ in terms of the plate’s thickness $h$. We show that the Γ-limit of the scaled functionals $h^{-4}E^h$ consists of a von Karman-like energy and prove that in the scaling regime $E^h \sim h^\beta, \beta > 2$, there is no other non trivial limiting theory.
Thermo-Hydro-Mechanical Processes Stabilizing Antarctic Ice Stream Margins

James R. Rice
Harvard University

Flow of the Western Antarctic Ice Sheet is distinctly heterogeneous in a vast region bordering the Ross Sea, where the sheet is of order 1 km thick. Broad streaks of ice, called "ice streams", having horizontal width ranging up to several 10s of km, slide over their bed (which was seafloor in the last inter-glacial period) at $> 100$ m/yr, whereas they are bordered laterally by stagnant ridges flowing at $< 10$ m/yr. Issues addressed, in studies with coworkers Thibaut Perol, John Platt and Jenny Suckale, are those of why this morphology forms, and what it mean for the overall rate of ice loss. We show how shear heating of the ice, consequent formation of temperate ice zones producing melt as they deform, and subglacial hydrological processes associated with Rothlisberger channels, can select the shear margin location, leading to a smooth transition from a slipping to a locked bed.

Can Cells Use Phase Transitions to See Each Other in Fibrous Darkness?

Phoebus Rosakis
University of Crete

Biological cells are known to die if they cannot sense other cells in their vicinity. Experiments on fibroblasts embedded in a fibrous extracellular matrix (ECM) have shown that these cells locate each other using not only chemical signals, but also mechanical fields, such as displacement or stress, a process known as mechanosensing. The cells induce deformations in the ECM by contracting themselves by as much as 50%. Apparently they do this so that other cells can detect the resulting strain fields in the ECM, using what are essentially microscopic strain gages at focal adhesions where the cell membrane attaches to the matrix.

It is noteworthy that cell contraction causes the appearance of so-called tethers, or thin bands in the ECM joining neighboring cells. Within tethers, the density of the ECM is much higher than outside.

This is suggestive of a phase transition, which in turn points to an underlying material instability. We observe that the ECM consists of fibrin, a spaghetti-like fibrous network. Individual fibers can resist tension, but buckle under compression.
Algorithm for Studying Flow-Induced Phase Transitions in Nematic Liquid Crystals

Shawn Ryan
Cleveland State University

In this work, we propose a new method for studying vorticity driven dynamics in a liquid crystal arising from torques due to an externally imposed shear flow or other sources of torque. Here a spatially homogeneous liquid crystal system governed by a Smoluchowski equation for the orientational probability density function is investigated. To analyze the PDE model, we develop a novel direct computational algorithm based on a Voronoi cell-based finite volume scheme. This method has the capability of describing abrupt changes in the density function, using fluxes through cell boundaries. We first validate our approach by capturing prior results from Maier-Saupe theory illustrating phase transitions in the system due to nematic interactions. We then investigate the coupling of an external flow field with the Smoluchowski equation describing the full orientational and translational dynamics of the system.

The Global Geometric Viewpoint of Continuum Mechanics: An Overview of some Applications

Reuven Segev
Ben-Gurion University of the Negev

The talk will overview some applications of notions from global geometric analysis in the formulation of continuum mechanics and classical field theory. A central role will be played by the configuration space of the continuous system—an infinite dimensional manifold. Viewing generalized forces as elements of the cotangent bundle of the configuration space, stress theory follows naturally from a representation theorem for the corresponding linear functionals. Properties of optimal stress fields and estimations of the load capacities of perfectly plastic bodies also follow from an analogous analysis. As the global geometric analysis is applicable in the case where both the body manifold and the space manifold are not provided with a Riemannian metric, it is naturally applicable for the description of fields associated with the material structure of bodies, such as distributions of dislocations and defects. Finally, the global geometric viewpoint is general enough to include p-form, pre-metric electrodynamics as a special case.
Mean-Field Limits for Ginzburg-Landau Vortices
Sylvia Serfaty
New York University

Ginzburg-Landau type equations are models for superconductivity, superfluidity, Bose-Einstein condensation. A crucial feature is the presence of quantized vortices, which are topological zeroes of the complex-valued solutions. This talk will review some results on the derivation of effective models to describe the statics and dynamics of these vortices, with particular attention to the situation where the number of vortices blows up with the parameters of the problem. In particular we will present new results on the derivation of mean field limits for the dynamics of many vortices starting from the parabolic Ginzburg-Landau equation or the Gross-Pitaevskii (= Schrodinger Ginzburg-Landau) equation, as well as results and questions on the situation with random environment.

Stability Analysis and Applications of the Rate, State, Temperature and Pore Pressure Friction (RSTPF) Model for Earthquake and Landslides Phenomena
Arun Kumar Singh
Visvesvaraya National Institute of Technology Nagpur India

In recent times, the rate and state friction (RSF) model has found wide spread applications in the study of earthquake phenomena and rock slope instability. According to the RSF model, friction of rock surfaces depend on slip rate and history of sliding surfaces. Nevertheless, the original RSF model has been modified considering the complexity and scale of the sliding phenomena in nature. For instance, Segall and Rice (1995, 1996) have used modified the RSF constitutive laws to take into account the role of pore pressure and shear heating at the sliding interface. Chester and coworkers (1992, 1994) have also proposed the modified RSF equation considering the role of temperature at the sliding interface. Upon combining these two modifications, we propose the rate, state, temperature and pore pressure friction (RSTPF) model. Using spring-mass sliding system, linear stability analysis showed that critical stiffness increases with coefficient of thermal pressurization. But hydraulic diffusivity have dilatancy decreases critical stiffness of the sliding system. This friction model is also used for predicting time of failure of a planar rock slope and the results are justified in the light of Vaiont slope failure. It is also shown that aging law results in longer time of failure of a rock than corresponding to the slip law. At end, we also discuss the practical issues faced during the implementation of the proposed model.

References:

**Optimal Wall-To-Wall Transport by Incompressible Flows**

Ian Tobasco  
University of Michigan

The wall-to-wall optimal transport problem asks for the design of an incompressible flow between parallel walls that most efficiently transports heat from one wall to the other, given a prescribed flow intensity budget. In the energy-constrained case, with a given kinetic energy budget, optimal designs are known to be convection rolls in the large energy limit. In the enstrophy-constrained case, numerical studies performed by P. Hassanzadeh, G. Chini, and C. Doering, and also by A. Souza in his PhD thesis, indicate a much more complicated flow structure is favorable in the large enstrophy limit. In particular, these authors observe the presence of recirculation zones near the walls whose existence is left unexplained. In this poster, we present a useful reformulation of the wall-to-wall optimal transport problem inspired by related questions in homogenization theory. This leads to an unexpected connection between the wall-to-wall problem and questions from the study of energy-driven pattern formation in materials science. We demonstrate this connection with a few key examples. The result is a new multiple-scales construction for the enstrophy-driven wall-to-wall problem which goes beyond the complexity observed in the numerical studies, and achieves the optimal rate of transport in the large enstrophy limit up to possible logarithmic corrections. We also briefly discuss implications for the problem of finding the best a priori upper bounds on the rate of heat transport in turbulent Rayleigh-Bernard convection. This is joint work with C. Doering.

**New Statistical Parameters for Grain Growth**

Pawan Vedanti  
Wayne State University

A statistical model containing two new characteristics of grain structure in pure metals and alloys is suggested. Non-equiaxed geometry of grains and grain structure are described by these characteristics. The probability distribution of grain sizes is obtained in terms of these parameters. It describes the previously obtained experimental data reasonably well. Evolution of grain size distribution and the above mentioned parameters have been studied during recrystallization and grain growth in AZ31b magnesium alloy.
Nonlinear Mechanics of Surface Growth for Cylindrical and Spherical Elastic Bodies

Arash Yavari
Georgia Institute of Technology

We formulate the initial-boundary value problems of accreting cylindrical and spherical nonlinear elastic solids in a geometric framework. It is assumed that the body grows as a result of addition of new (stress-free or pre-stressed) material on part of its boundary. We construct Riemannian material manifolds for a growing body with metrics explicitly depending on the history of applied external loads and deformation during accretion and the growth velocity. We numerically solve the governing equilibrium equations in the case of neo-Hookean solids and compare the accretion and residual stresses with those calculated using the linear mechanics of surface growth.

Surface Elasticity in Steigmann-Ogden Form in Modeling of Fracture

Anna Zemlyanova
Kansas State University

A problem of a straight mixed mode non-interface fracture in an infinite plane is treated analytically with the help of complex analysis techniques. The surfaces of the fracture are subjected to surface elasticity in the form proposed by Steigmann and Ogden. The boundary conditions on the banks of the fracture connect the stresses and the derivatives of the displacements. The mechanical problem is reduced to two systems of singular integro-differential equations which are further reduced to the systems of equations with logarithmic singularities. It is shown that modeling of the fracture with the Steigmann-Ogden elasticity produces the stress and strain fields which are bounded at the crack tips. The existence and uniqueness of the solution for almost all the values of the parameters is proved. Additionally, it is shown that introduction of the surface mechanics into the modeling of fracture leads to the size-dependent equations. A numerical scheme of the solution of the systems of singular integro-differential equations is suggested, and the numerical results are presented for different values of the mechanical and the geometric parameters.
Relevance and Applications of Generalized Disclination Theory in Defect Mechanics

Chiqun Zhang
Carnegie Mellon University

We utilize a theory of generalized disclination (g.disclination) mechanics introduced recently that goes beyond treating standard translational and rotational Volterra defects (dislocations and disclinations) in a continuously distributed approach; it is capable of treating the kinematics and dynamics of terminating lines of elastic inverse distortion (strain + rotation) discontinuities. In this work, the utility of g.disclinations in materials science is discussed within the physical context of modeling interfacial and bulk line defects like defected grain and phase boundaries, dislocations and disclinations. An explicit formula for the displacement jump of a single localized composite defect line in terms of given g.disclination and dislocation strengths is deduced based on the Weingarten theorem for g.disclination theory at finite deformation. The Burgers vector for a g.disclination dipole at finite deformation is also derived. A numerical method based on the least squares method is developed to solve for stress and energy density fields of the g.disclination system. Problems of small and finite deformation theory are considered. The fields of a single disclination, a single dislocation, a tilt grain boundary, an incoherent grain boundary with disconnections, a star disclination and a disclination loop (with twist and wedge segments) are approximated. It is demonstrated that while the far-field topological identity of a dislocation of appropriate strength and a disclination-dipole plus a slip dislocation comprising a disconnection are the same, the latter microstructure is energetically favorable. This underscores the complementary importance of all of topology, geometry, and energetics (plus kinetics) in understanding defect mechanics. It is established that finite element computations of fields of interfacial and bulk line defects can be achieved in a systematic and routine manner, hopefully enabling the study of intricate defect microstructures in the scientific understanding and predictive design of materials.

Printing Non-Euclidean Solids

Giuseppe Zurlo
National University of Ireland, Galway

Non-Euclidean, geometrically frustrated solids are ubiquitous in biology, but how they acquire a particular incompatibility is not usually known. In many cases these solids grow through surface deposition of mass and here we use the mechanics of incompatible surface growth to show that the distributed pre-stress, developing during such deposition, can be fine-tuned to ensure a target behavior of the system in physiological conditions. As illustrations, we present explicit 3D printing protocols for arteries, guaranteeing stress uniformity under inhomogeneous loading, and for explosive plants, allowing them to completely release their residual elastic energy with a single cut.
Author Index

Acharya
  Amit , 1
Arora
  Rajat , 1
Audoly
  Basile, 2
Berdichevsky
  Victor, 2
Braides
  Andrea, 2
Carpio
  Ana, 3
Caruel
  Matthieu, 3
Charlotte
  Miguel, 4
Chatterjee
  Sabyasachi, 4
Cherkaev
  Andrej, 5
Danescu
  Alexandre , 5
DeSimone
  Antonio, 6
Epstein
  Marcelo , 6
Espanol
  Malena , 6
Fonseca
  Irene, 7
Fosdick
  Roger, 7
Goddard
  Joe, 8
Kohn
  Robert, 9
Le
  Khanh Chau , 9
Lewicka
  Marta, 9
Logak
  Elisabeth, 10
Maor
  Cy, 10
Morandotti
  Marco, 10
Perez-Reche
  Francisco , 11
Puglisi
  Giuseppe, 11
Purohit
  Prashant , 12
Putelat
  Thibaut, 13
Ricciotti
  Diego , 13
Rice
  James, 14
Rosakis
  Phoebus, 14
Ryan
  Shawn, 15
Segev
  Reuven , 15
Serfaty
  Sylvia, 16
Singh
  Arun Kumar, 16

Tobasco
  Ian, 17

Vedanti
  Pawan, 17

Yavari

Arash, 18

Zemlyanova
  Anna, 18

Zhang
  Chiqun, 19

Zurlo
  Giuseppe, 19