

# Towards Macroscopic Plasticity from Microscopic Discrete Dislocation Dynamics

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Dislocations are topological line defects in the crystalline structure of a lattice. They carry a vectorial charge with units of length and magnitude at the Angstrom scale. Being defects in the lattice structure, they induce high localized stresses in the body. Their motion in huge numbers produces permanent deformation of macroscopic solids (i.e. ductility) of the order of doubling or halving their dimensions; time scale separations between the speed of motion of a single defect and some types of quasi-static macroscopic plastic deformations can be of the order of twelve orders of magnitude. Moreover, their interactions, through their stress fields, impede their motion. Understanding and describing the collective dynamics of dislocations leading to macroscopic plasticity is a holy grail of solid mechanics. We will describe a setting where we develop a macroscopic model by filtering a microscopic pde model and then attempt to develop the constitutive response of emergent quantities at the macroscopic scale by averaging a discrete-dislocation version of the microscopic model (much like vortex dynamics) based on theory for slow-fast dynamics developed by Artstein-Kevrekidis-Slemrod-Titi.

This is joint work with Xiaohan Zhang (currently post-doc at Stanford).

# Merging Shil'nikov and Hopf via Pulse Trains: Can We Regard Excitability and Oscillations as Two Sides of the Same (Universality Class) Coin?

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Dissipative nonlinear waves arise in many systems that comprise non-equilibrium properties, such as action potentials, calcium waves, Belousov--Zhabotinsky chemical reaction, and electrochemical oscillations. Two variable Reaction--Diffusion models are frequently employed to scrutinize the generic features of these spatiotemporal behaviors and to distinguish between two universality classes: Oscillations that arise through a linear Hopf instability and excitability which gives rise upon nonlinear localized perturbations, to pulses via homoclinic (often Shil'nikov) connections to a rest state. However, an extension to a three variable model allows formation of finite pulse trains under the same choice of parameters and thus blurs the distinction between the above universality classes. Moreover, biological and chemical systems tend to be highly noisy and comprise many reacting and diffusing subsets, making it difficult experimentally to distinguish between excitable and phase waves. Consequently, using a prototypical three-variable FitzHugh-Nagumo model, bifurcation theory, and numerical continuation methods, we trace the origin of finite and infinite pulse trains to nonlinear traveling and standing waves that organize in the vicinity of the subcritical finite wavenumber Hopf-Shil'nikov instability. Using these novel insights, we also demonstrate how in isotropic media it is possible to generate spiral waves via a single spatially localized perturbation. In particular, these results are expected to shed light on biological experiment that seek to determine the origin of nonlinear waves, such as cellular actin waves, vasomotion, and cardiac arrhythmia.

# Fluids, Solids, Geometry, Turbulence

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In a recent series of papers DeLellis et al have used Gromov's theory of convex integration to produce turbulent like solutions to inviscid multi-d fluid mechanics.

In this talk i will show how a simple direct approach will yield similar results by-passing Gromov's theory and using only Nash's  $C^1$  isometric embedding theorem.

Furthermore the new applies to elastodynamics as well.

The admissibility of such solutions relates to work of Bardos, Titi, Wiedemann, and separately Rom-Kedar and I will comment on this as well.

The work is joint with Amit Acharya ( CMU), G-Q Chen (Oxford), D. Wang ( Pittsburgh).

# Projection Methods for Feasibility Problems

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Projection methods are iterative algorithms that use projections onto sets while relying on the general principle that when a family of sets is present, then projections onto the given individual sets are easier to perform than projections onto other sets (intersections, image sets under some transformation, etc.) that are derived from the given individual sets.

Their robustness, low computational effort and their ability to handle huge-size problems make them very useful for many convex real-world problems such as Image Reconstruction (IR) and Intensity-Modulated Radiation Therapy (IMRT) Treatment Planning.

Over the past decade, some projection methods have proven very effective also in some non-convex and discrete settings such as Sudoku.

# Continuum Models for Highly Concentrated Solution and Ionic Liquids: an Inverse Problem

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Differential capacitance data is one of the most widely used experimental quantities for characterizing the structure of electrolyte solutions near charged interfaces. Many studies have attempted to fit differential capacitance data to generalized Poisson-Boltzmann models, particularly to account for finite-volume, ion-crowding effects.

In this work we consider the inverse problem, deriving generalized Poisson-Boltzmann models which recover prescribed differential capacitance data. We introduce a closed method for the derivation of such models by computing their free energy. The method is demonstrated by considering differential capacitance data from common models, as well as from experimental data.

We further use the above method to reveal the limitations of the generalized Poisson-Boltzmann framework for modeling highly concentrated solutions. In particular, contrary to the common approach, we show that it is inappropriate to model ionic liquids using a generalized Poisson-Boltzmann framework. Instead, we suggest a novel continuum model for electrolyte solutions which is valid for highly concentrated solutions, as well as for ionic liquids, and identify the bifurcation point at which the PNP framework ceases to qualitatively describe concentrated electrolyte solutions.

This is a joint work with Keith Promislow, Michigan State University, Doron Elad, Technion, and Arik Yochelis, BGU.

# A High-Order Compact Scheme for Navier-Stokes Equations in Complex Geometry

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We present a high-order finite difference scheme for Navier-Stokes equations in complex geometry. The scheme is an extension of a fourth-order scheme for Navier-Stokes equations in streamfunction formulation on a rectangular domain [1]. The discretization offered here contains two types of interior points. The first is regular interior points, where all eight neighboring points of a grid point are inside the domain and not too close to the boundary. In this case a fourth-order compact scheme on a rectangle element is used. The second is interior points where at least one of the closest eight neighbors is outside the computational domain or too close to the boundary. In the second case we design discrete operators which approximate spatial derivatives of the streamfunction on irregular meshes, using discretizations of pure derivatives in  $x$ ,  $y$  and along the diagonals of the element. Numerical results indicate fourth-order convergence rates for the Navier-Stokes equations in streamfunction formulation.

[1] M. Ben-Artzi, J.-P. Croisille and D. Fishelov, "Navier-Stokes Equations in planar domains", Imperial College Press, 2013.

# Resilience of Complex Networks

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Resilience is a system's ability to cope with change, or to bounce back after stress. The loss of resilience in a natural system occurs when the stress exceeds a certain threshold, beyond which the system loses its ability to bounce back and retain proper functionality. For instance, when the loss of trees in a forest (deforestation) crosses a tipping point and the forest turns barren, or when the load on the electrical power grid becomes too high and a massive power failure emerges. The challenge is that most complex systems are multidimensional, disordered and described by nonlinear dynamics - characteristics that firmly avoid analytical treatment. We address this challenge here by showing how to map a complex system into an effective one dimensional equation, exposing the universal patterns of resilience exhibited by diverse systems, from ecological to technological systems. Along the way we will understand why systems lose resilience all of a sudden, learn how to predict such resilience loss and show how to fortify a system to become more resilient.

# Community Detection Using Local Graph Diffusions

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In community detection problems, one seeks to identify sets of nodes in a network that are both internally cohesive and well separated from the rest of the graph. Such sets are then referred to as communities or clusters. In one important variant, the goal is to build a community around a given seed node or set of seed nodes. That is, the algorithm is given, as an input, a node (or nodes) in the graph, and the goal is to find a cluster in which it is a member.

One popular technique for identifying communities using seed nodes is to use local graph diffusions. The general framework is as follows. Using the seed, a diffusion vector is computed. The diffusion vector is reweighted based on the degrees, and the nodes are sorted according to their magnitude in the reweighted diffusion vector. The community is found by making a sweep over the nodes according to their rank, selecting the prefix that minimizes (or maximizes) some scoring function. If the number of seeds is small, most of the entries in the diffusion vectors tend to be tiny, in which case a sparse approximation is viable (the exact diffusion vector is generally dense), and this allows algorithms that work even on massive graphs. Algorithms that find sparse approximations to diffusion vectors are local graph diffusion algorithms.

In the talk, I will discuss the use of local graph diffusion algorithms for community detection. In particular, I will present an efficient local algorithm for approximating a graph diffusion that generalizes both the celebrated personalized PageRank and its recent competitor/companion - the heat kernel. The algorithm is based on writing the diffusion vector as the solution of an initial value problem, and then using a waveform relaxation approach to approximate the solution.