



Tuning Nanofracturing for Energy Storage and Nanofabrication



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- **Identification of research need**

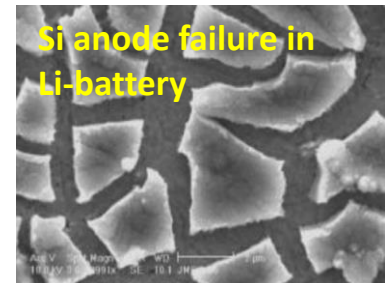
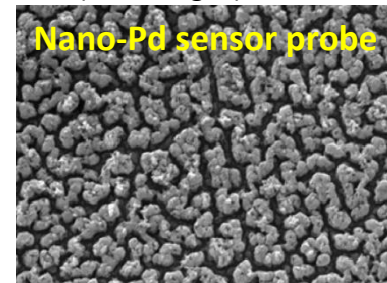
Nanostructured materials have been used in energy storage and a range of devices. Crack networks are known to form in drying media and thin films with residual tensile stress, and have been observed in several systems, including drying mud, polymer paints, aging woods, dielectric thin films, and even in monolayer of microspheres. It is expected that nano-scale facturing can be used to create ubiquitous and intriguing crack patterns to increase the performance of materials for energy storage, chemical process, environmental control applications, but it may cause the failure of materials or devices. Therefore, it is important to understand the dynamics of facturing at nanoscale and to tune/prevent nanofracturing for potential applications.



- **Objectives**

The overall objective of this project is to develop tutorial tool to understand the dynamics of nanofracturing for metal systems and tune their nanostructure for nanofabrication and energy storage applications *with the assistance of NSCA staff, facilities and funding*. The specific objectives are:

- (1) Identify numerical methods and a software platform accessible at the NSCA for this project, and develop models;
- (2) Understand nanofracturing of metal induced by electrochemical doping-dedoping
- (3) Simulate nanopatterns formed on metal surfaces and through bulk;
- (4) Correlate nanofracturing and materials/process (reaction) parameters;
- (5) Develop predictive guides to design nanopatterns for nanofabrication and physically robust metal anodes (including Si) for Li-ion batteries.

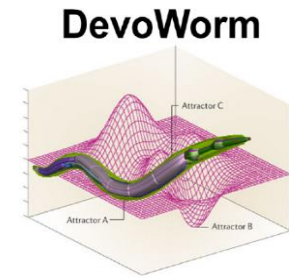


Quantifying New Variables for *C. elegans*

Integrative Biology

Bradly Alicea (<http://publish.Illinois.edu/bradly-alicea>)

Department of Crop Sciences



Goal: Move from quantification schemes for descriptive biological models to integrating these data with computational models.

AIM #1: statistical characterization of developmental processes such as recovery of organisms from dauer stage/phenotype.

AIM #2: distinguishing/defining two distinct models of development (mosaic vs. regulative development). There is a need to characterize the multivariate nature of these types of development in addition to how they correspond to evolutionary relationships.

AIM #3: identifying developmental homologies between *C. elegans* and other Nematodes.

Thematic Area: Bioinformatics and Health Sciences

* assemble long-tailed, unstructured databases from organismal-level data (NCSA's BrownDog).

* support from the OpenWorm project (whole-organismal emulation). Allows for innovation in virtual modeling.

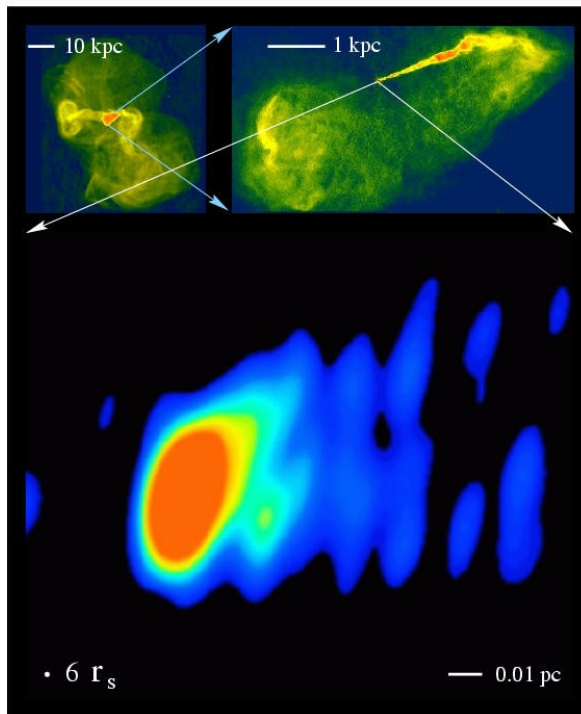
* leverage NCSA's research data service (RDS) to organize both reused data and newly-generated data. This will support replicability initiatives.

Using Accelerator Hardware to Improve Subresolution Modeling in Astrophysical Simulations

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VLBA radio image of M87 (NRAO)

Problem

- Astrophysical hydrodynamics problems involve a huge range of length and time scales
- Next generation of machines will be more unbalanced

Key idea

- Map physical scale separation onto multilevel parallel hierarchy – weak coupling over slow links

Needs

- Expertise in GPU/accelerator programming (ISL)
- Optimization within large heterogeneous HPC environment (Blue Waters)

High-Accuracy Stochastic Methods for Breakthrough Electronic Structure Calculations

Key Idea and NCSA Skills/Resources/Interests:

- Quantum Monte Carlo (QMC) methods are benchmark accuracy stochastic methods for electronic structure, and demonstrate near-linear parallelization to millions of cores. They are well-established in the physics community.
- We are interested in extending the QMC method from a physics tool to a widely applied tool for understanding real engineering materials (*e.g.* nanowires with twin plane defects, complex semiconductors, *etc.*). Current state of the art focuses on bespoke calculations, which limit systematic application to engineering problems.
- **Needed NCSA skills center on data management:** large volumes of computations will be key to overcoming the learning curve and establishing the framework for application of a new method
- We are interested in developing and maintaining a **live database of QMC results** for use by the entire international simulation community. This living data base will be a **key enabler** for developing the protocols and frameworks for the wide scale application of this method. We intend that this one-year work will form the basis for a large Illinois/NCSA proposal, which we anticipate to be of substantial interest to the US DOE.

Illinois Faculty Team:



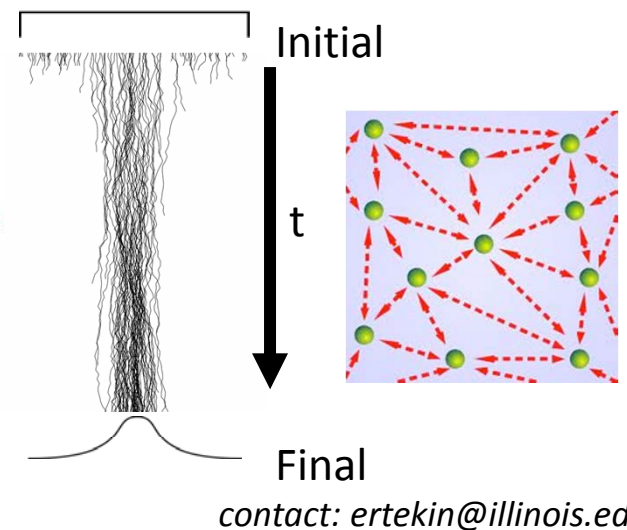
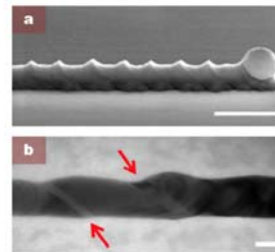
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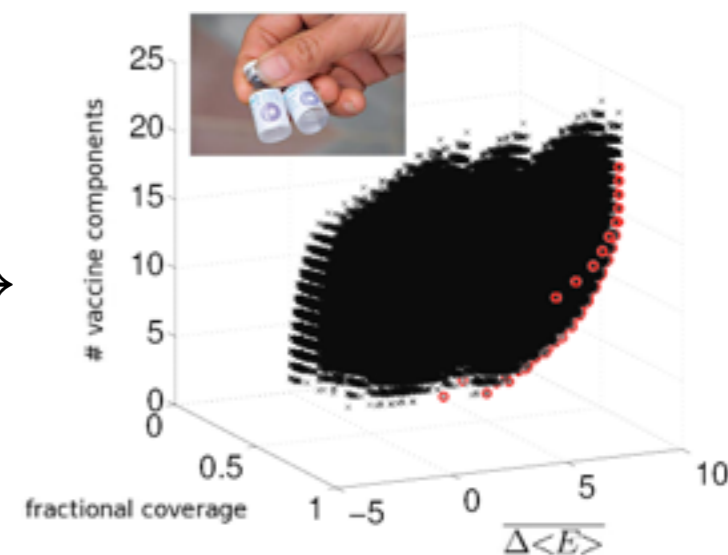
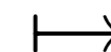
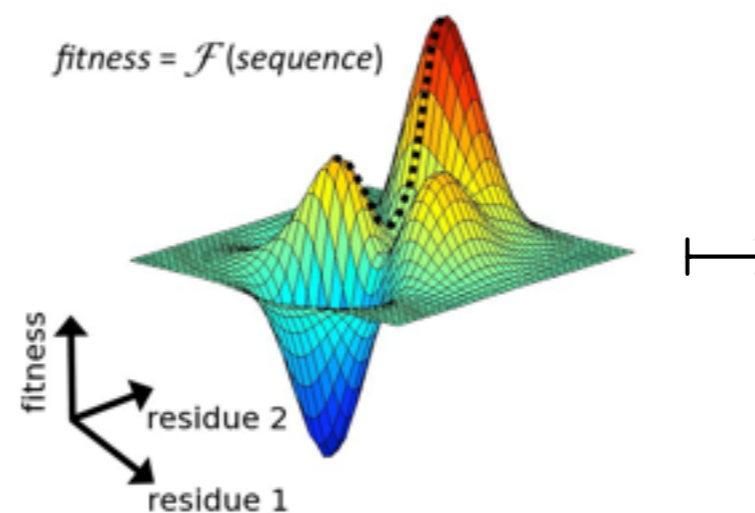
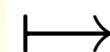
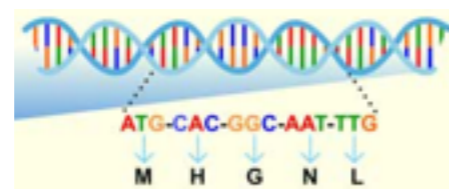
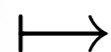
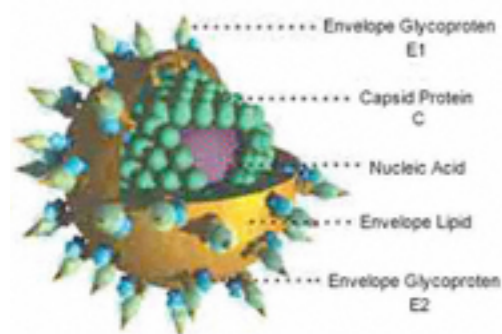
Computational Design of Hepatitis C Vaccines

Prof. Andrew Ferguson, MatSE

NCSA Thematic Area:
Biological & Health Sciences

PROJECT SYNOPSIS

- Bayesian inference of hepatitis C virus fitness landscapes from clinical sequence databases
- Fitness landscape prescribes viral replicative capacity as a function of proteome amino acid sequence
- Landscape described by a Potts spin glass Hamiltonian
- Model parameters fitted by iterative Monte Carlo fitting of model predictions to clinical data
- Quantitative landscapes reveal viral “soft spots” and guide rational vaccine design — no vaccine is yet available



PROJECT NEEDS

- Computational bottlenecks in Monte Carlo sampling limits us to single viral proteins
- Full proteome landscapes require (i) large-scale code parallelism and (ii) supercomputing infrastructure
- Codes are CPU and GPU parallelized but inexpertly and inefficiently — professional support invaluable
- Extension to full hepatitis C proteome — NCSA computing resources vital
- Success will massively accelerate discovery of viable vaccine candidates, alleviating the suffering of 170 million infected persons worldwide = 3% of global population

Constrained Optimization of Agent-based Disease Models

- I have the conceptual framework and parameters for agent-based/hybrid disease models in livestock herds
 - <http://www.aaai.org/ocs/index.php/IJCAI/IJCAI11/paper/view/3304>
- I want to work on designing these models to allow constrained optimization, ideally over multiple state spaces
 - *Allow farmers to prioritize disease-control spending*
- I need expertise in building agent-based models and interest in developing novel optimization techniques



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