DEVELOPMENT OF AN HPC PLATFORM FOR PLASMA-MATERIAL INTERACTIONS

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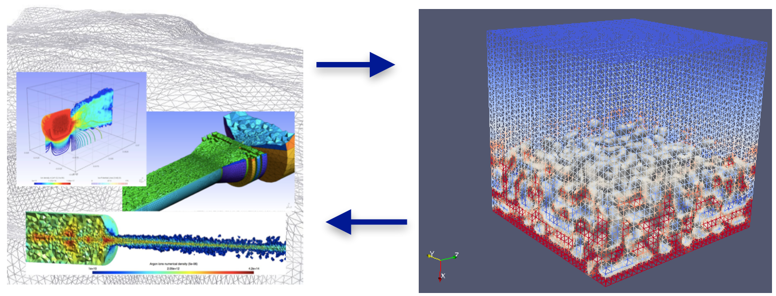
"hPIC"

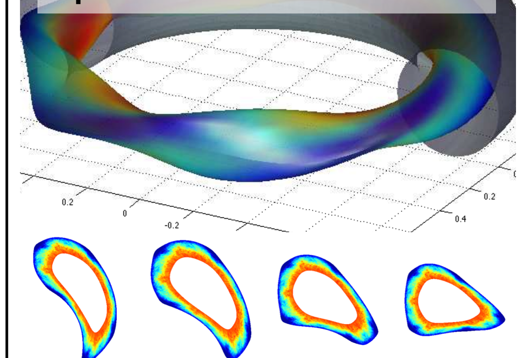
HPC platform for Plasma-Material Interactions and Nanostructuring

3D PARTICLE-IN-CELL

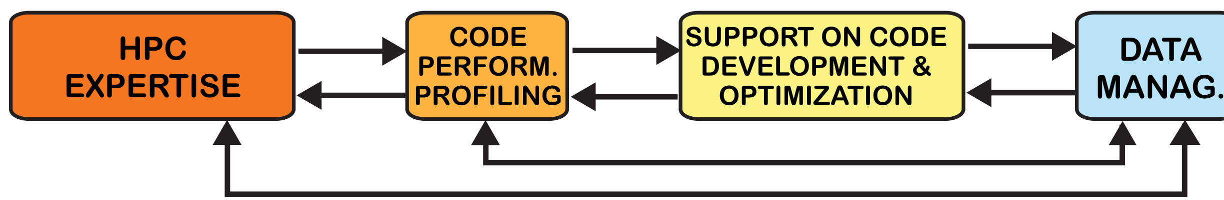
3D SURFACE MORPHOLOGY



Link with existing tools for 3D magnetized plasmas, in order to provide the first consistent description of the plasma-material interface



Proposed Role of NCSA:



THE NEED: SOLVING THE PMI PROBLEM IS THE NEXT GRAND CHALLENGE OF FUSION ENGR

- High thermal heat fluxes
- Erosion/Sputtering
- Radiation damage, etc.

BEYOND FUSION: The tendency to *nanostructuring of metals* is a problem for fusion, but a huge *opportunity* for industry!

CURRENT DOE EFFORT: LARGE PSI-SciDAC PROJECT

- I am currently one of the PI's
- Multiscale approach to the problem of Plasma-Material Interaction;
- Multiple codes coupled together
- https://collab.mcs.anl.gov/display/PSIscidac/Plasma+Surface+Interactions
- **Looking Forward**: what's the *Next Step*?

BROADER IMPACT LARGE SOCIETAL BENEFITS

- Predictive ability to modify metal surfaces using plasma processes
- Batteries, cat., etc.
- New industrial processes, patents

Acting Now is in perfect timing to prepare enough preliminary material for the next cycle of call for proposals on PMI studies

Integrated Neutron Scattering Measurements and First Principle Modeling of the Fast Dynamics of Water

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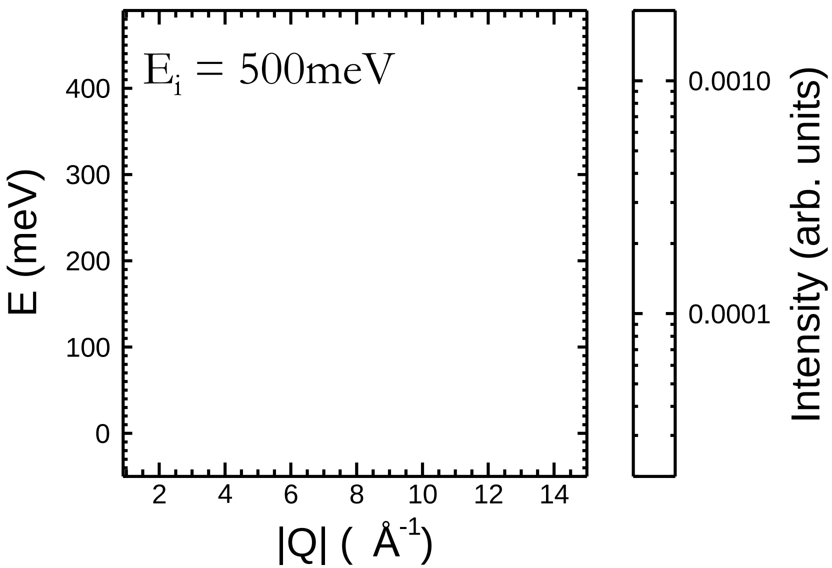
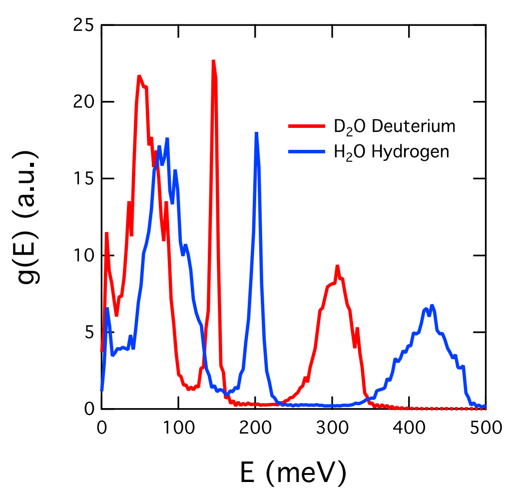
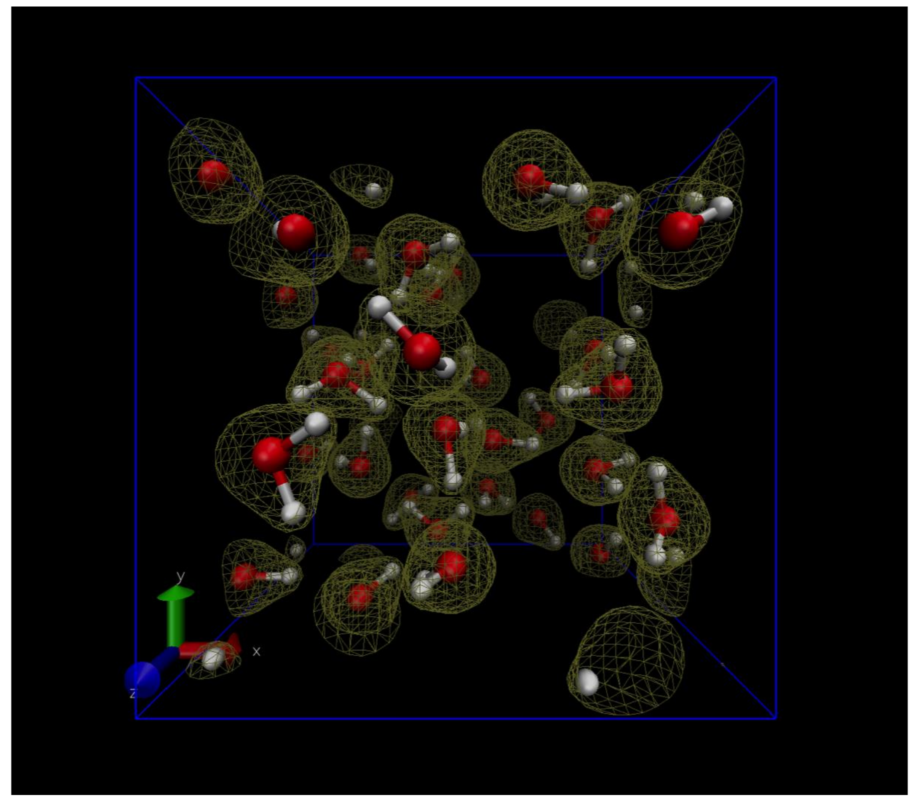
Coupled Coherent and Incoherent Inelastic Neutron Scattering Spectra of Water



AIMD Computation of the Density of States of Water

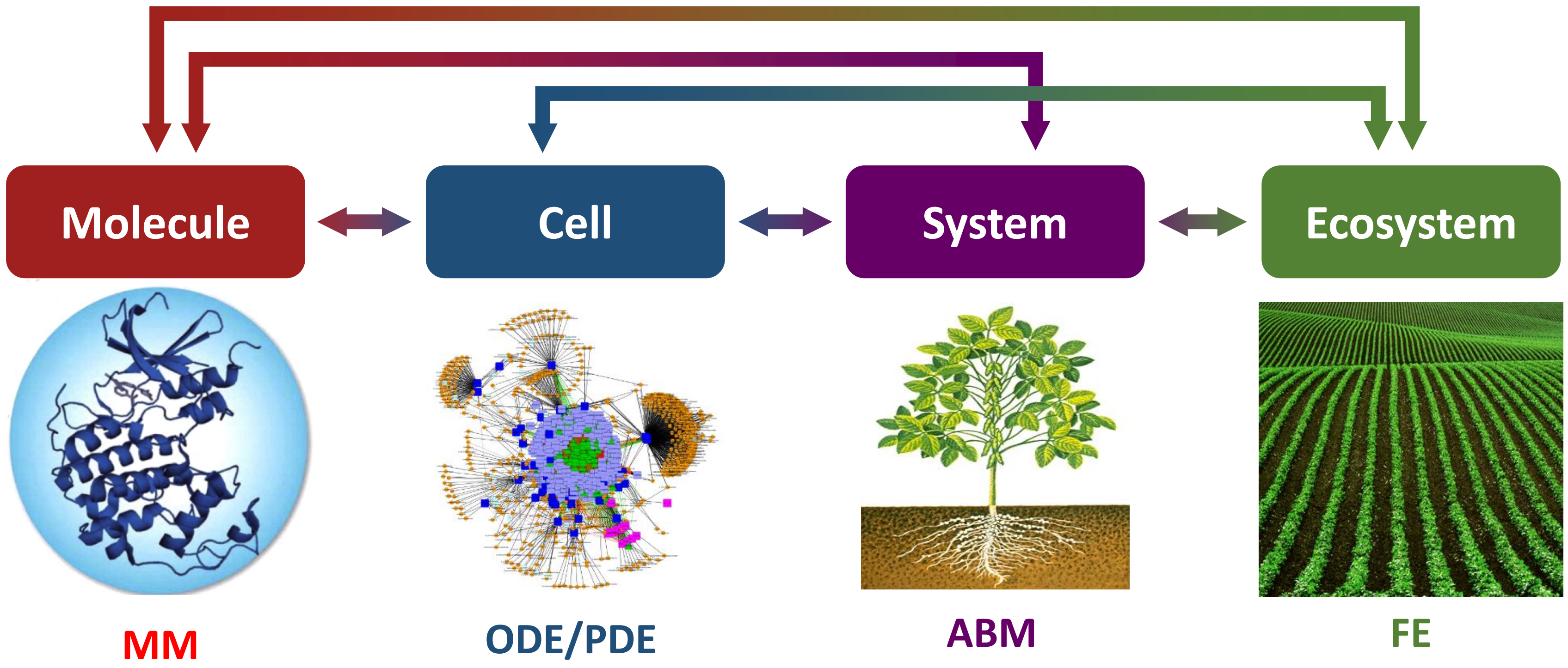




ab initio Molecular Dynamics (AIMD) Snapshot of Water

Y. Zhang, to be published.

Plants in silico: Integrative modeling to predict crop response to climate change



Plants in silico (Psi) is a multi-scale modeling platform aimed at accurately predicting plant and ecosystem response to global change. This digital representation of layered dynamic models will reach from gene networks and metabolic pathways through to cellular organization, tissue and organ development, and ultimately resource capture in dynamic competitive environments, thus allowing a mechanistic simulation of the plant or community of plants *in silico*. Modularity will be employed as a powerful approach to manage model complexity. Individual models will be broken down into less complex modules that retain an individual identity but interact with other system units. Individual modules will inform each other to ultimately enhance predictive capability of the aggregate model. *Psi* needs help from NCSA for a) data sharing, storage and management; b) data integration; and c) data visualization.

Contact: Amy Marshall-Colon, Assistant Professor Department of Plant Biology – amymc@illinois.edu
Collaborator: Steve Long, Professor Plant Biology

Alex Lipka, Assistant Professor of Biometry, Department of Crop Sciences

alipka@illinois.edu

- Ph.D. in Statistics (Purdue)
- Did a post-doc in a maize genetics lab (Cornell/USDA)
- Co-wrote a quantitative genetics R package
- Main research focus is quantitative genetics:
    - Genome-wide association studies
    - Genomic selection
    - Analyzing big data
- Interested in collaborating with NCSA to:
    - Make scripts I write more computationally efficient
    - Make scripts I write available in lower-level programming languages (e.g., C++)
    - Use clusters to perform computationally demanding jobs (e.g., search for epistasis)

Interdisciplinary Work in a Highly Technical Context:

Uncovering successful strategies and the potential costs of collaboration

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Motivation

- Interdisciplinary teams are increasingly touted as necessary for scientific progress, but research shows these teams face serious communication problems and often fail. There is a pressing need to understand how successful teams overcome these challenges.

Research Questions (extending my prior work with scientists at NCAR)

- What challenges do NCSA researchers and staff encounter as they seek to partner with individuals who have different technical expertise?
- What strategies have teams developed to surmount these difficulties?
- What costs do researchers associate with pursuing collaborative relationships?

Resources needed:

- Access to the NCSA community
- NCSA affiliates' experiences and knowledge

Proposed Methods:

- Interviews with researchers and their affiliates
- Observations of communication and work
- Network survey to reveal underlying social structures

Reducing uncertainty in ensemble prediction in ungaged basins in Illinois using multi-objective optimization

Zhenxing (Jason) Zhang, Ph.D., Hydrologist

Illinois State Water Survey, University of Illinois at Urbana-Champaign

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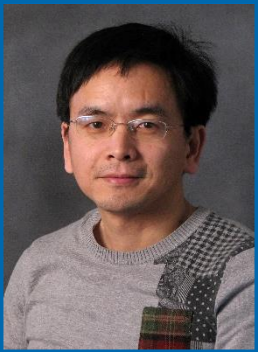
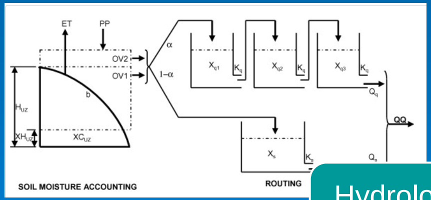


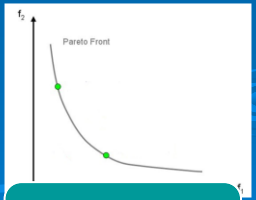
Project Idea

- ❖ Prediction in ungaged basin (PUB) is one of challenging issues facing water resources professionals.
- ❖ Use multi-objective optimization to reduce uncertainty in streamflow prediction in ungaged basins in Illinois
- ❖ Test the concept with a lumped hydrology model
- ❖ Evaluate the potential of the algorithm to run semi-distributed hydrology model for ensemble prediction in Illinois

NCSA Resources/Skills

- ❖ Expert in multi-objective optimization and/or sensitivity analysis
- ❖ High performance computation resources
- ❖ Future cooperation in high performance computation to improve ensemble prediction





Hydrology model

Multiobjective Optimization

Reducing uncertainty

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 know 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:

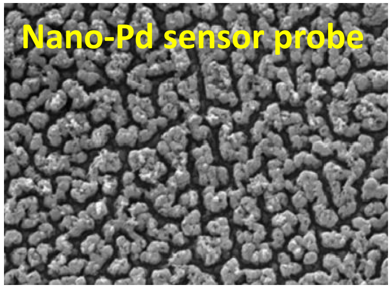
(1) Identify numerical methods and a software platform accessible at the NSCA for this project, and develop models;

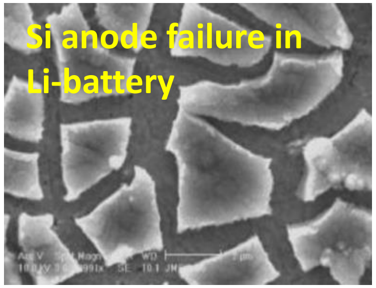
(2) Understand nanofracturing of metal induced by electrochemical doping-dedoping

(3) Simulate nanopatterns formed on metal surfaces and through bulk;

(4) Correlate nanofracturing and materials/process (reaction) parameters;

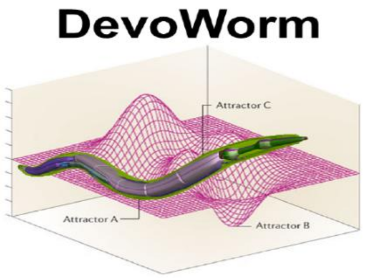
(5) Develop predictive guides to design nanopatterns for nanofabrication and physically robust metal anodes (including Si) for Li-ion batteries.





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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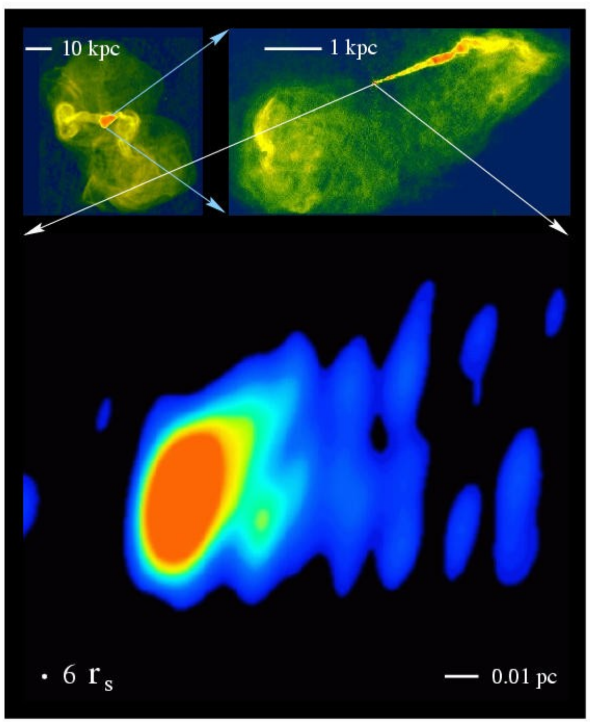


VLBA radio image of M87 (NRAO)

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:

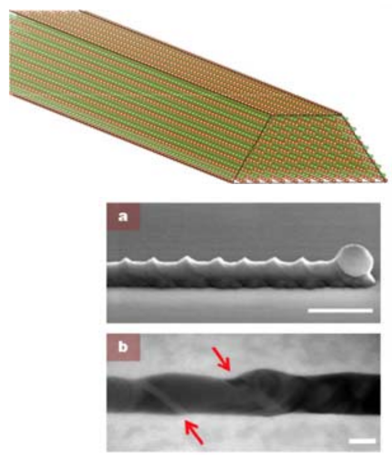
- Quantum Monte Carlo (QMC) methods are benchmark accuracy stochastic methods for electronic structure, and demonstrate near-linear parallelization to millions of cores. They are well-established in the physics community.
- We are interested in extending the QMC method from a physics tool to a widely 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.

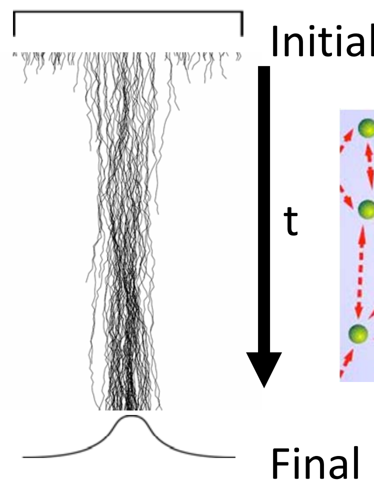
Illinois Faculty Team:

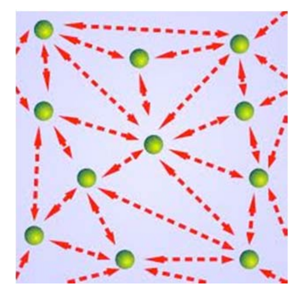
Elif Ertekin, MechSE

Lucas Wagner, Physics

Xiuling Li, ECE







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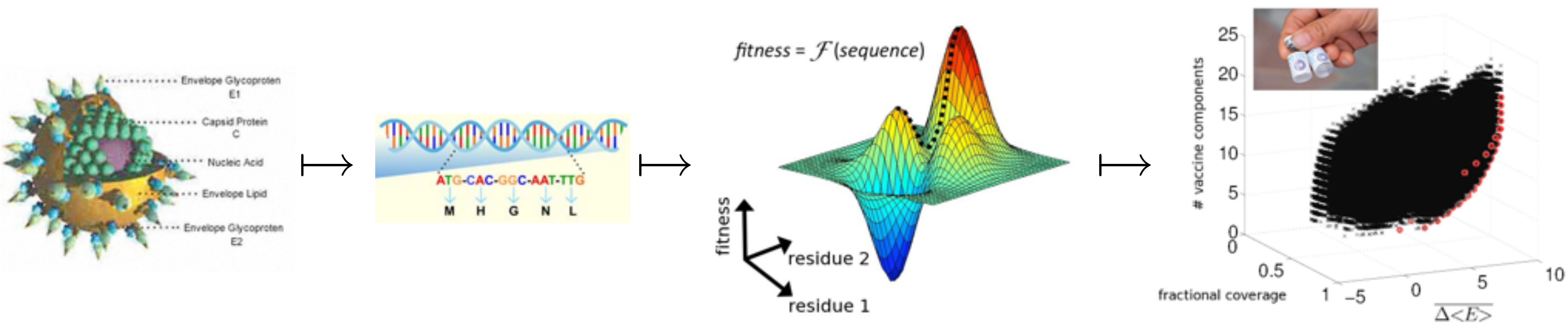
Computational Design of Hepatitis C Vaccines

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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