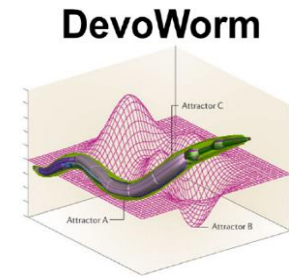


# Quantifying New Variables for *C. elegans*

## 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.

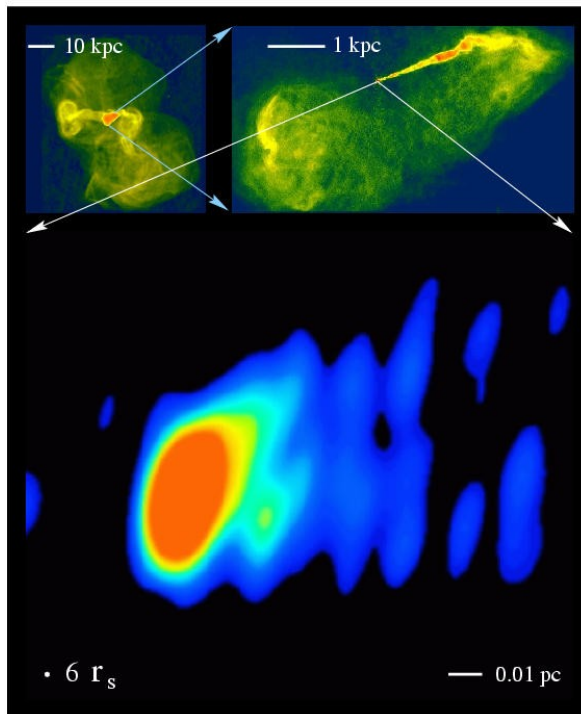
\* leverage NCSA's research data service (RDS) to organize both reused data and newly-generated data. This will support replicability initiatives.

# Using Accelerator Hardware to Improve Subresolution Modeling in Astrophysical Simulations

Paul M. Ricker

Associate Professor of Astronomy

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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:



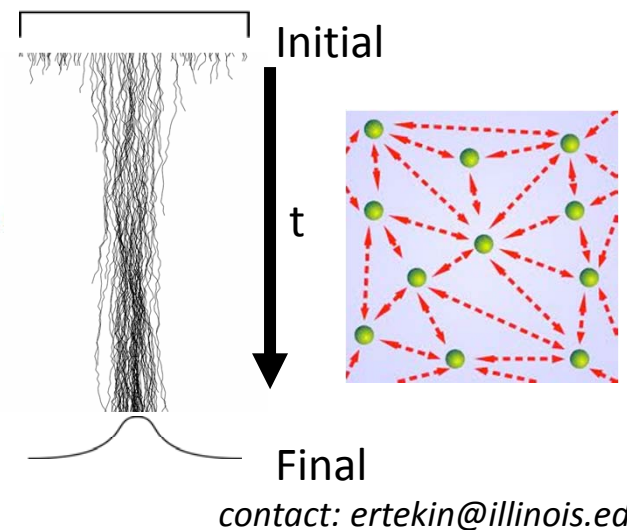
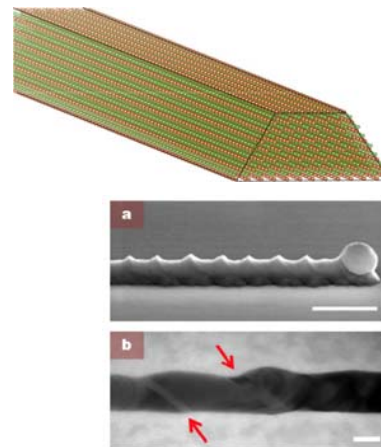
Elit Ertekin,  
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Lucas Wagner,  
Physics



Xiuling Li,  
ECE





# Andrew L Ferguson

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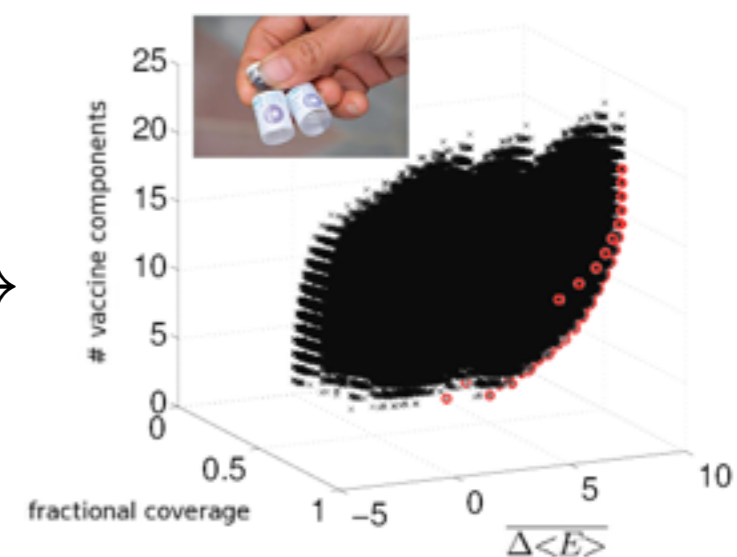
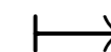
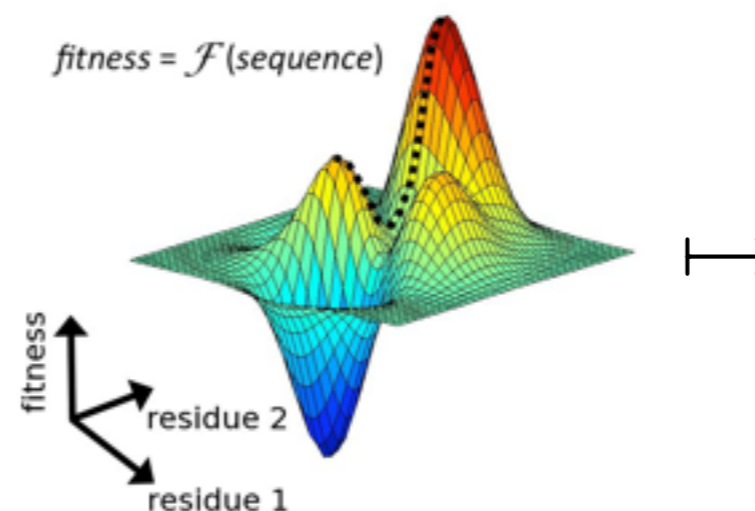
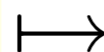
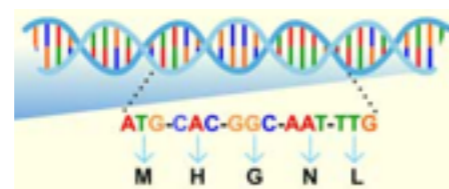
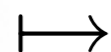
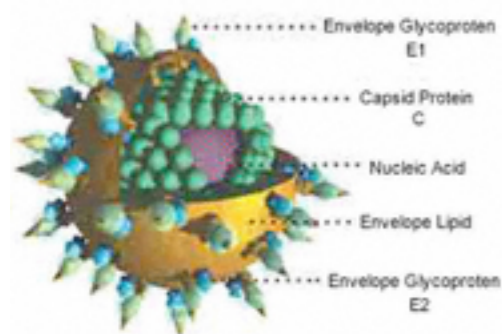
# Computational Design of Hepatitis C Vaccines

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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