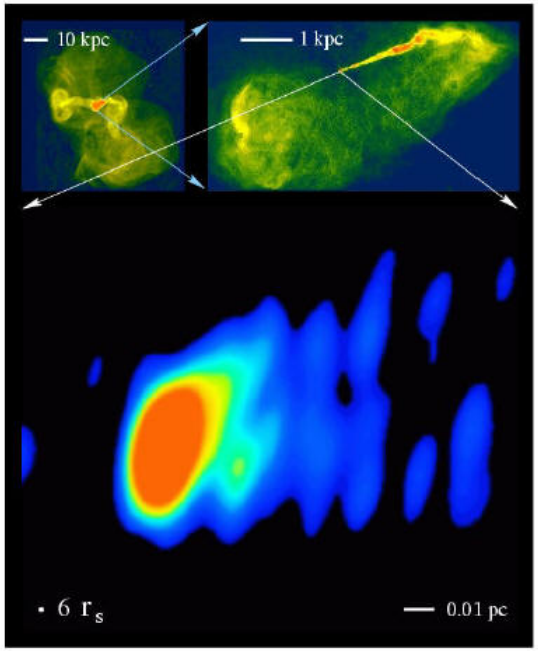
Using Accelerator Hardware to Improve Subresolution Modeling in Astrophysical Simulations

Paul M. Ricker

Associate Professor of Astronomy

pmricker@illinois.edu • http://sipapu.astro.illinois.edu/~ricker



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)

Andrew L Ferguson

Assistant Professor of Materials Science and Engineering
Affiliated Assistant Professor of Chemical and Biomolecular Engineering
Affiliated Assistant Professor of Computational Science and Engineering

204 Materials Science and Engineering Building (MC-246)
University of Illinois at Urbana-Champaign
1304 W. Green St., Urbana, IL 61801

alf@illinois.edu
http://ferguson.matse.illinois.edu

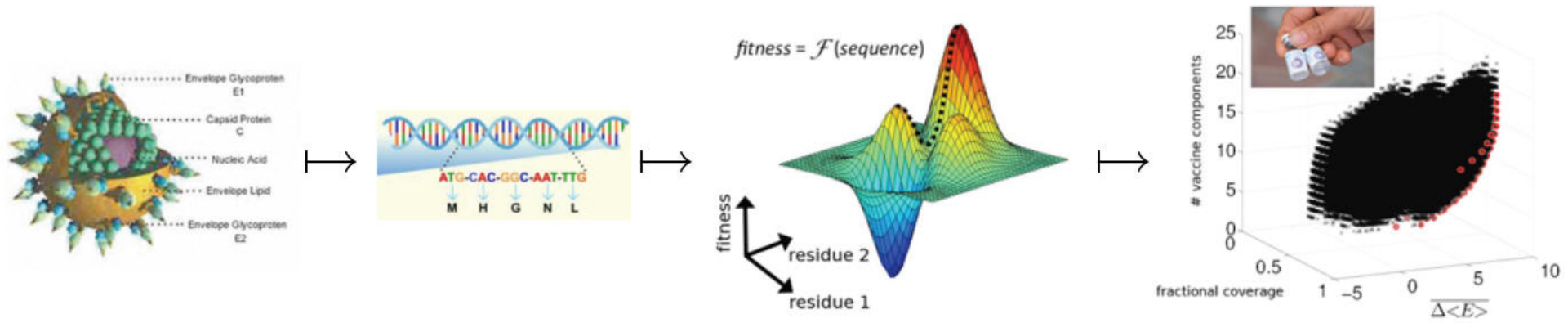
Computational Design of Hepatitis C Vaccines

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