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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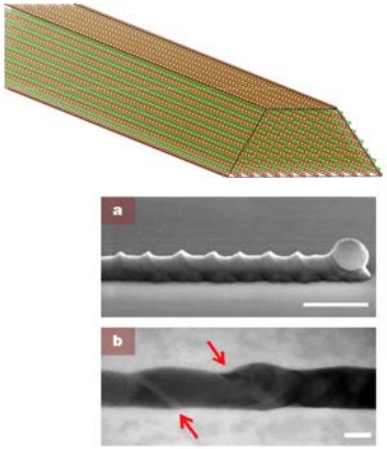

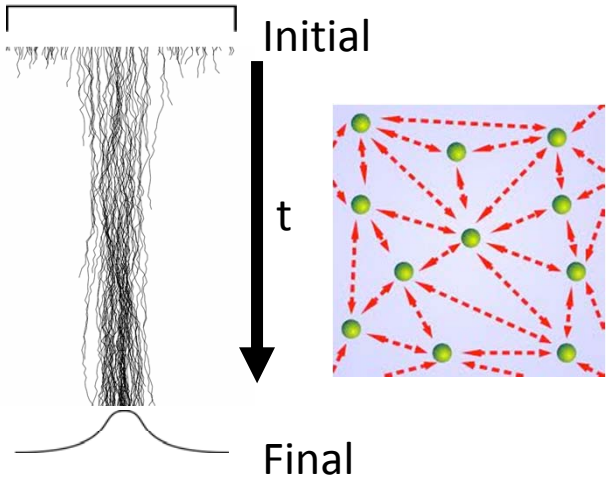

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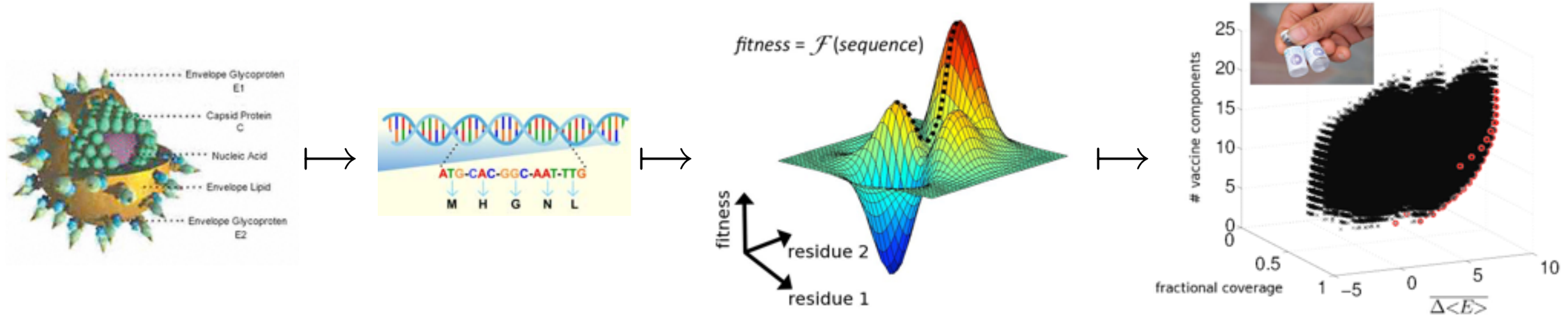
Computational Design of Hepatitis C Vaccines

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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