Using Accelerator Hardware to Improve Subresolution Modeling in Astrophysical Simulations

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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)
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