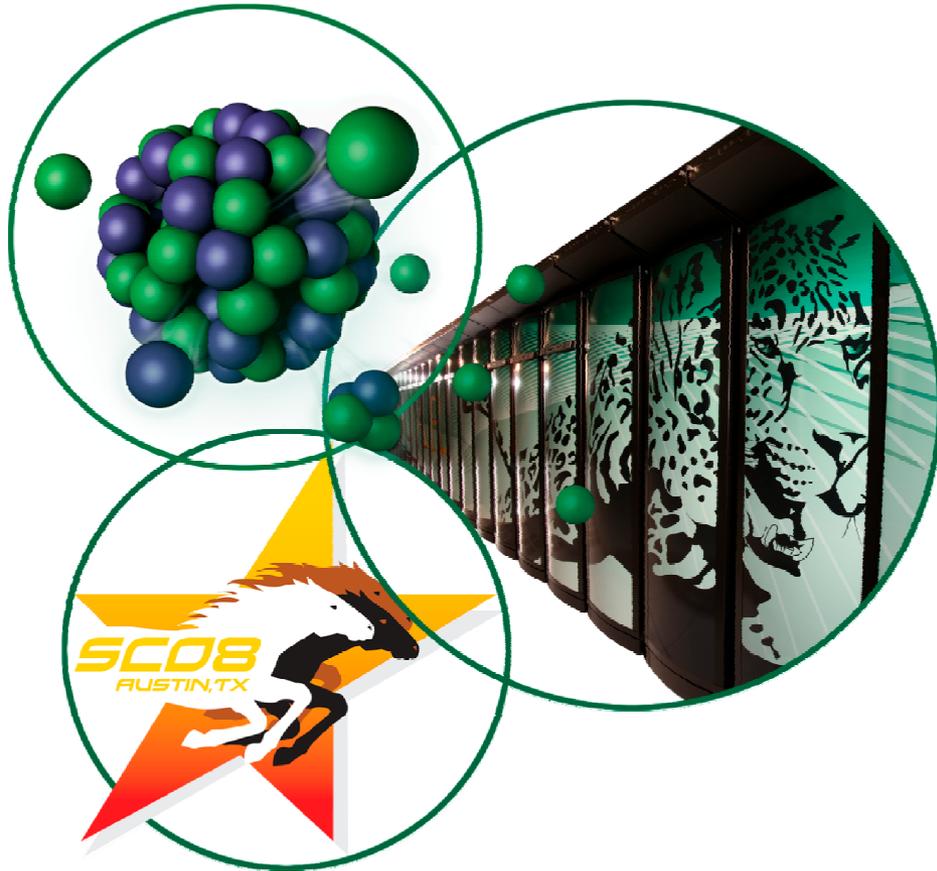


NSF and NICS Allocations

Presented by

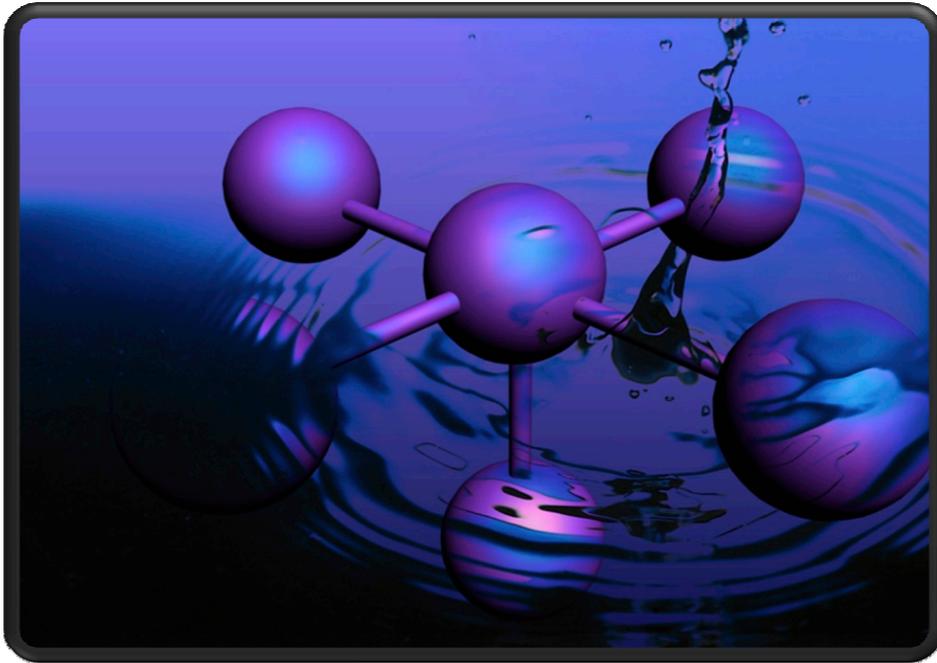
Phil Andrews

Project Director
National Institute for Computational Sciences



Lattice QCD calculations of Hadron physics

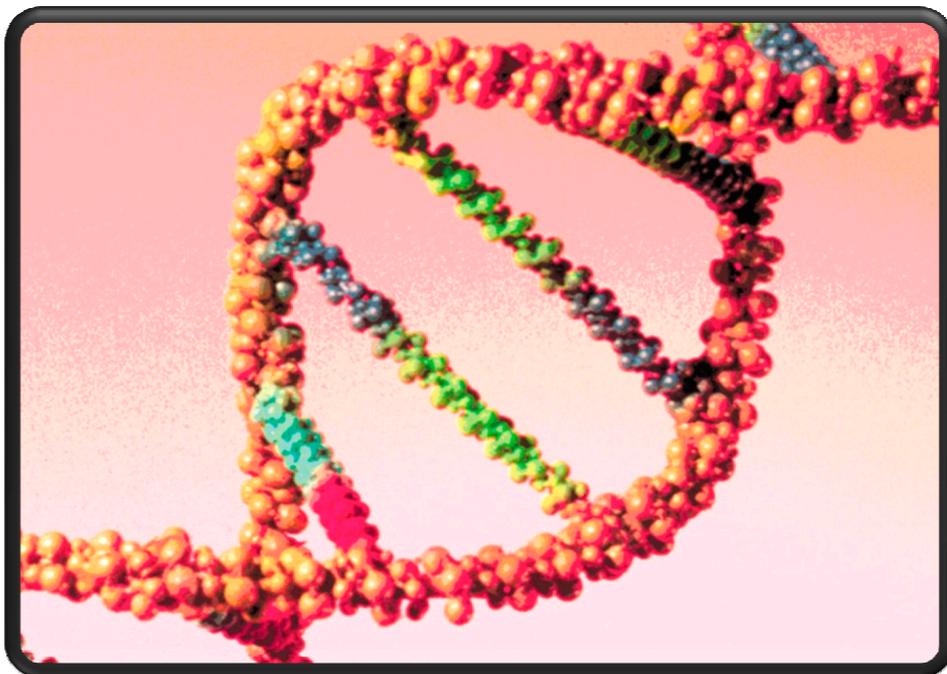
Nuclear physics



PI: Keh-Fei Liu
Co-PI: Terrence Draper
University of Kentucky
2,500,000 hours

Computer simulations of biomolecular structure and dynamics

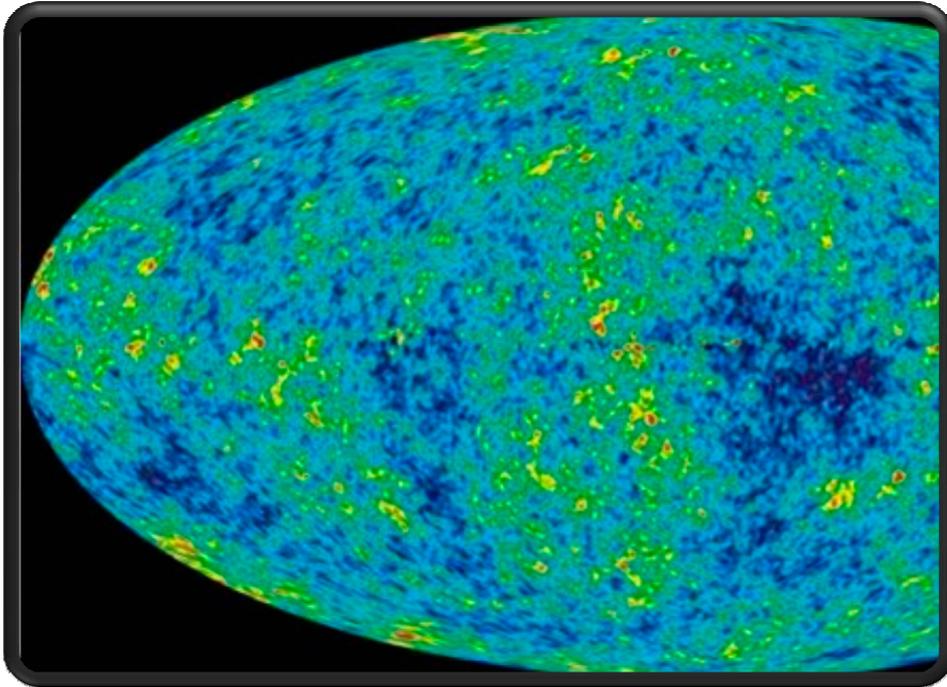
Biology



PI: Carlos Simmerling
SUNY Stony Brook
3,587,800 hours

Nonlinear evolution of the universe

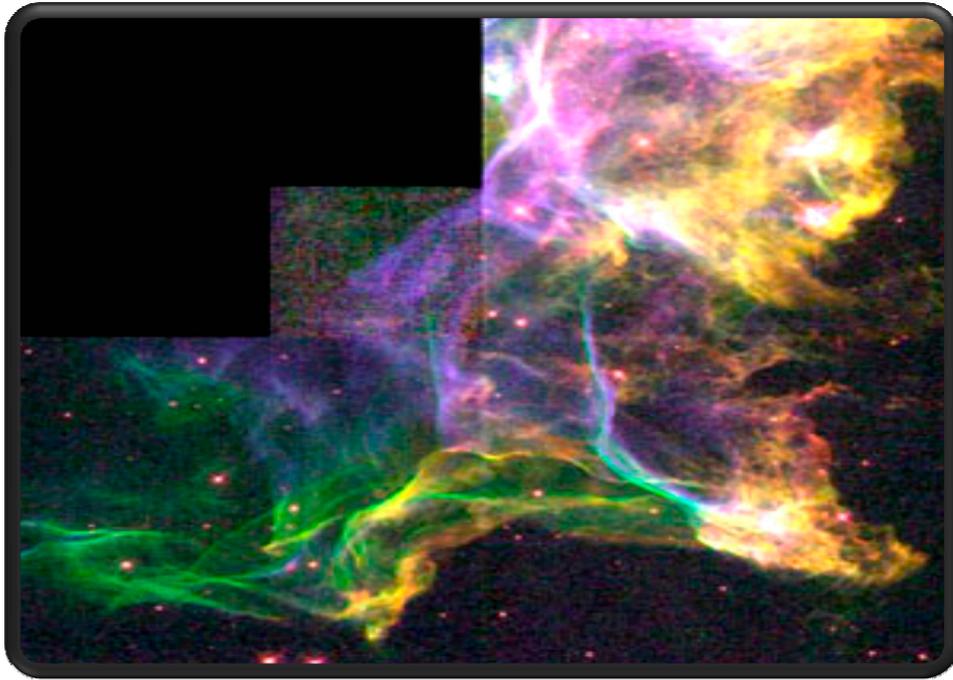
Astrophysics



PI: Renyue Cen
Co-PI: Jeremiah P. Ostriker
Princeton University
100,000 hours

Intermittency in interstellar turbulence

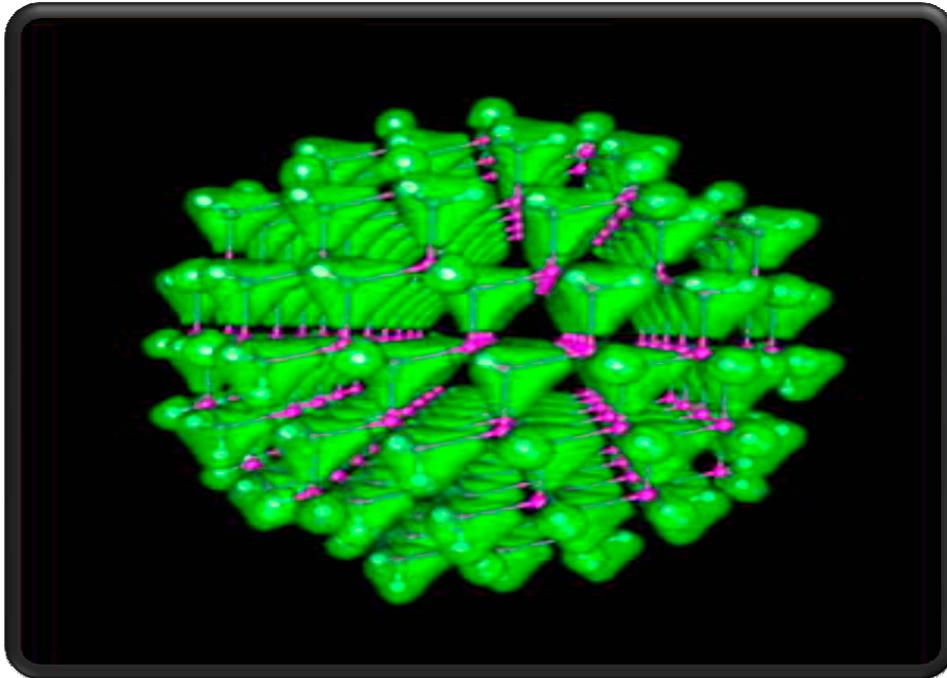
Astrophysics



PI: Alexei Kritsuk
University of California–San Diego
300,000 hours

First principles simulations of semiconductor nanostructures

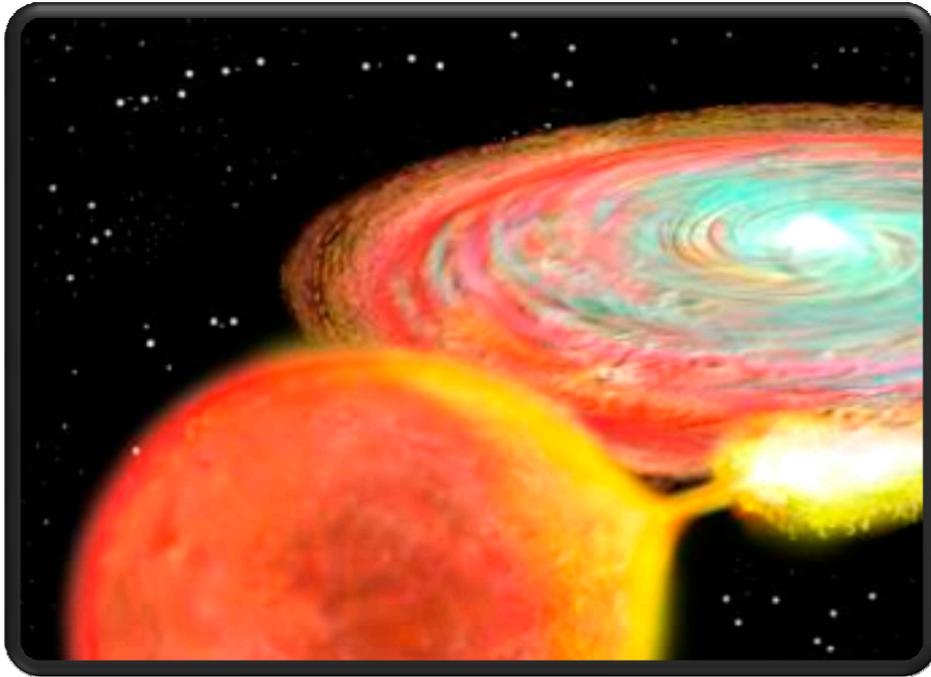
Materials science



PI: Giulia Galli
University of California–Davis
200,000 hours

Astrophysical applications of numerical relativity: Coalescing binary systems and stellar collapse

Astrophysics



PI: Erik Schnetter
Co-PIs: Peter Diener, Gabrielle Allen, Harry E. Seidel, Luciano Rezzolla, Manuel Tiglio, Christian Ott
Louisiana State University
150,000 hours

Local models of interior magnetohydrodynamics

Astrophysics



PI: Nicholas Brummell
University of California–Santa Cruz
100,000 hours

Turbulence simulations towards the petascale: Intermittency, mixing, reaction, and stratification

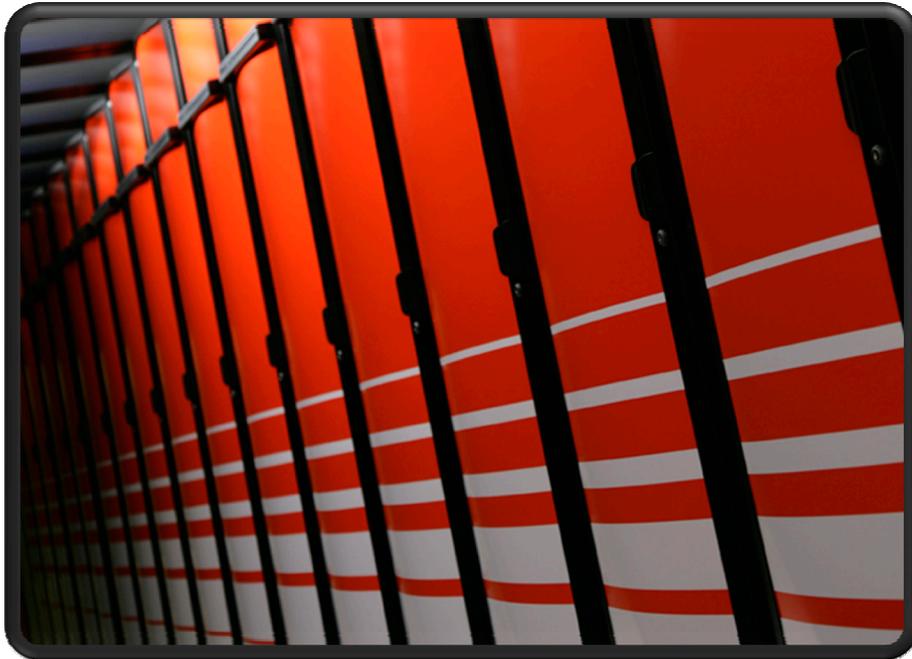
Turbulence



PI: Pui-kuen Yeung
Co-PIs: Katepallii
Sreenivasan, Stephen Pope,
Robert Moser, James J. Riley
Georgia Institute of Technology
12,000,000 hours

Atomic detail investigations of the structural and dynamic properties of biological systems

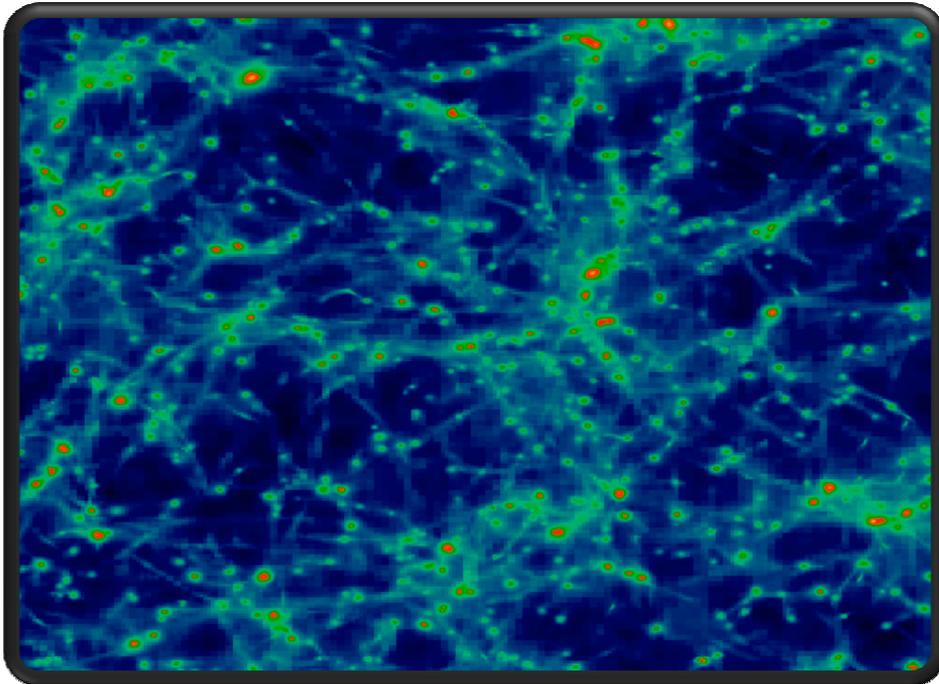
Biology



PI: Alexander MacKerell
University of Maryland, Baltimore County
250,000 hours

Projects in astrophysical and cosmological structure formation

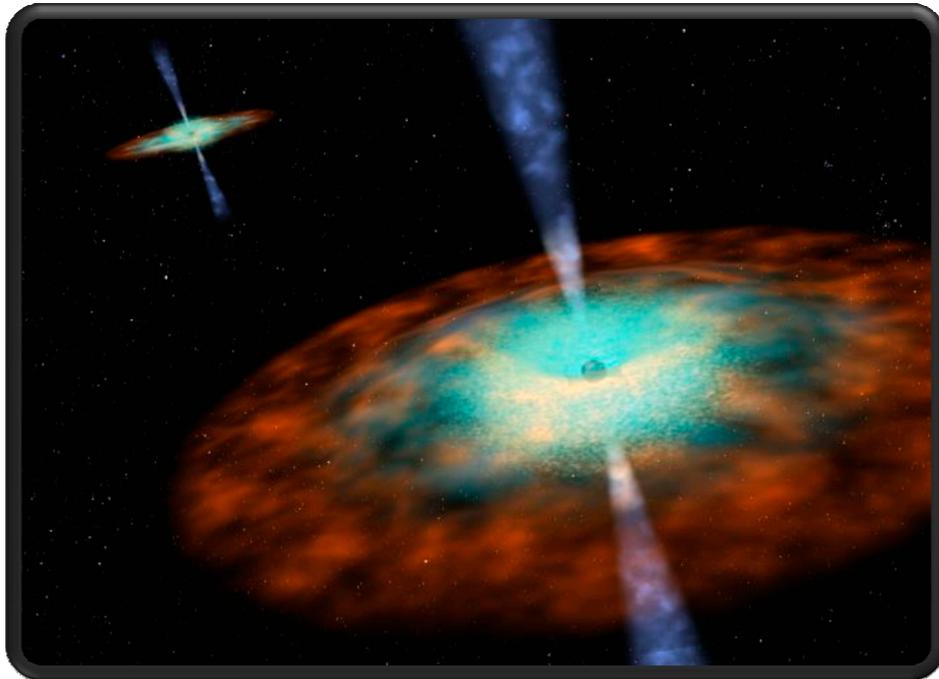
Astrophysics



PI: Michael L. Norman
University of California–San Diego
5,560,000 hours

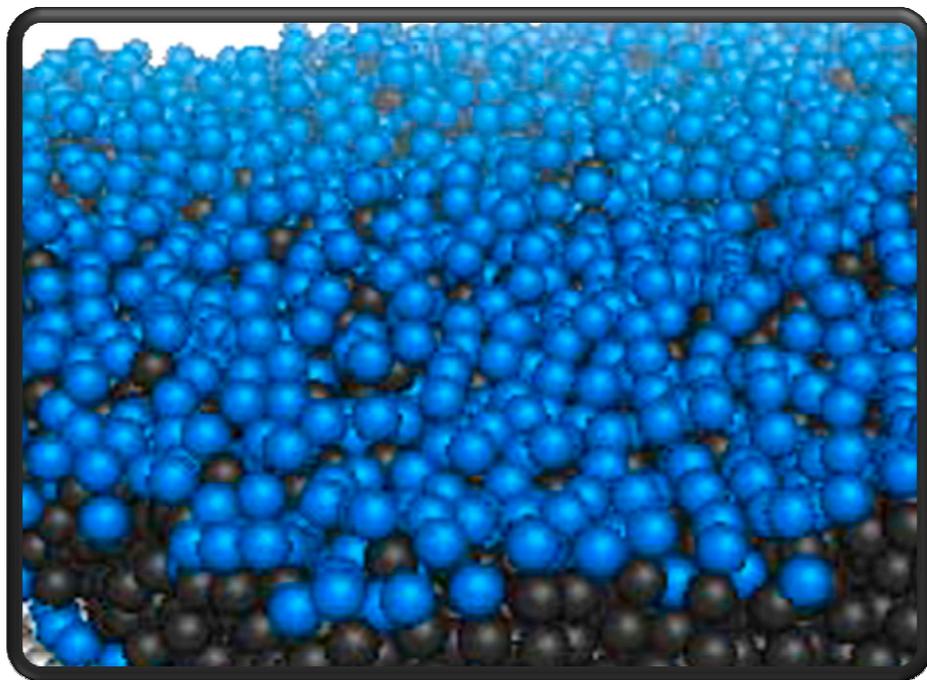
Numerical simulations of binary black hole systems

Astrophysics



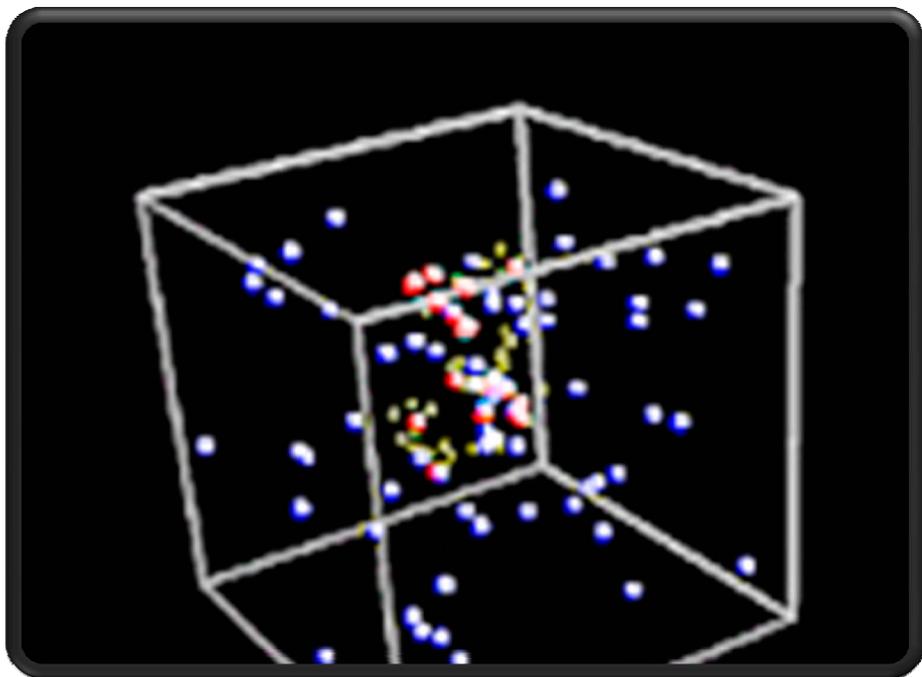
PI: Pablo Laguna
Co-PIs: Deirdre Shoemaker,
Frank Herrmann, Ian Hinder
Pennsylvania State University
50,000 hours

Multiscale modeling of biomembranes



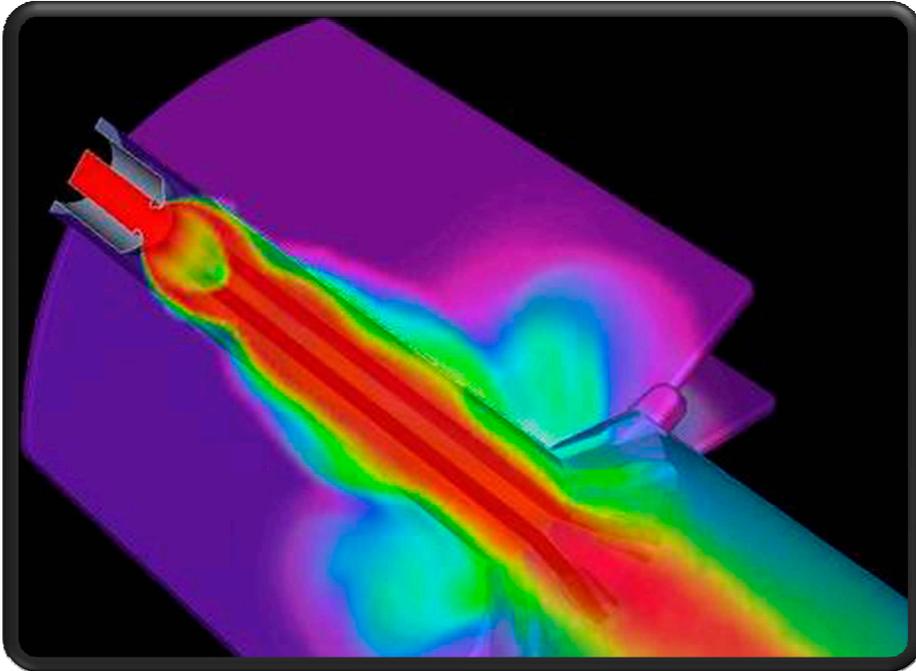
PI: Roland Faller
University of California–Davis
200,000 hours

Macromolecular and cell simulations



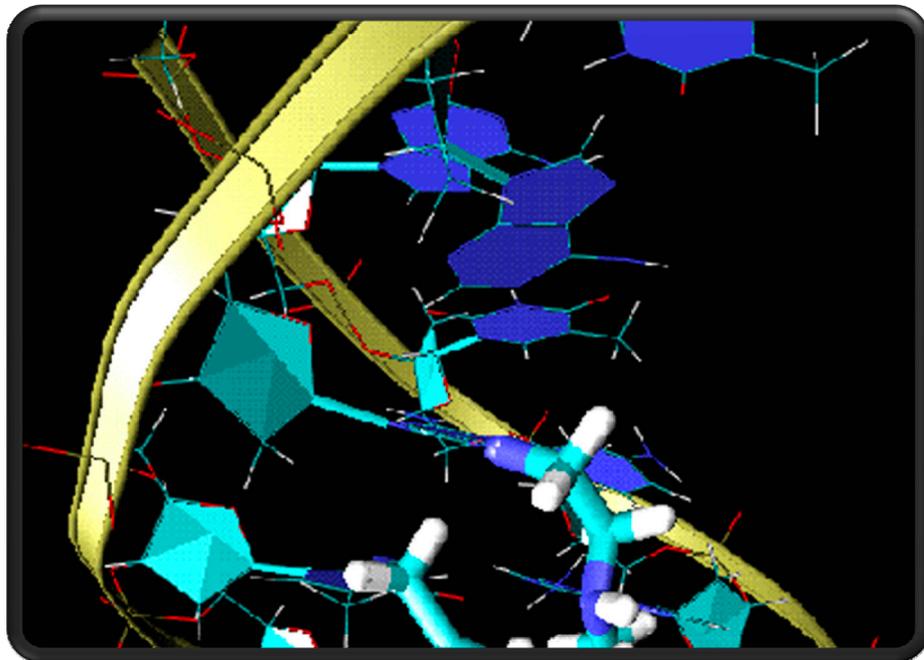
PI: Thomas Kepler
Duke University
400,000 hours

Programming and runtime techniques with Charm++ and AMPI



PI: Celso Mendes
University of Illinois–Urbana-Champaign
145,000 hours

Molecular dynamics simulations of semistructured biomolecules



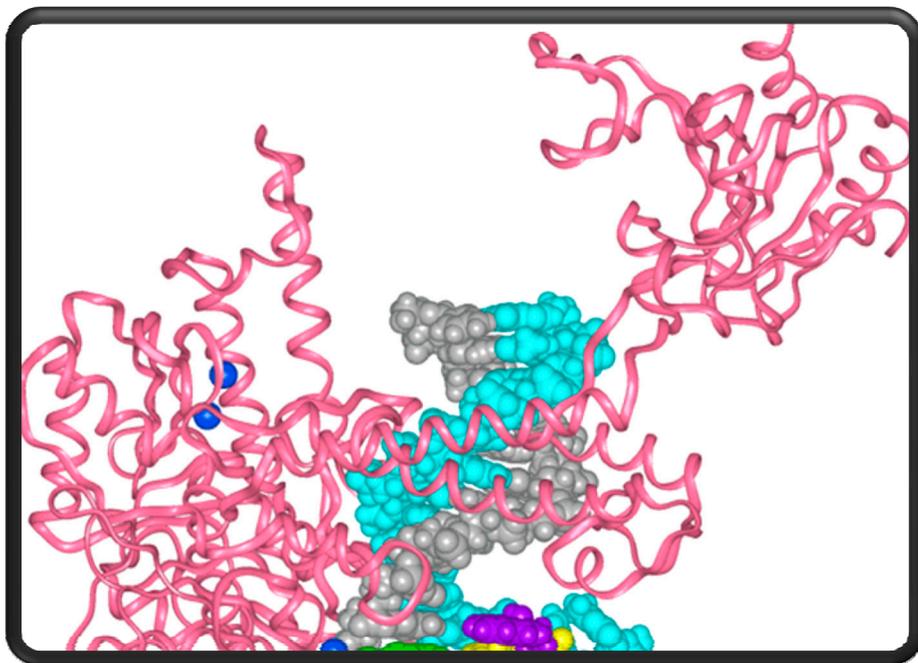
PI: Michael Colvin
University of California–Merced
250,000 hours

A framework for performance modeling and prediction



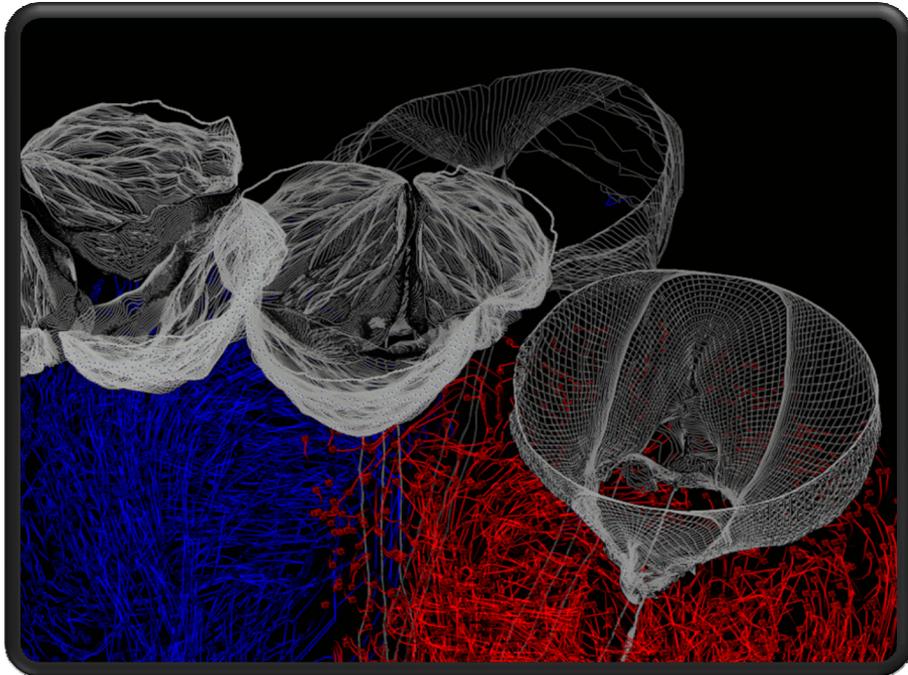
PI: Allan Snavely
University of California–San Diego
67,840 hours

Structural study of DNA adducts derived from tumorigenic metabolites of benzo[a]pyrene



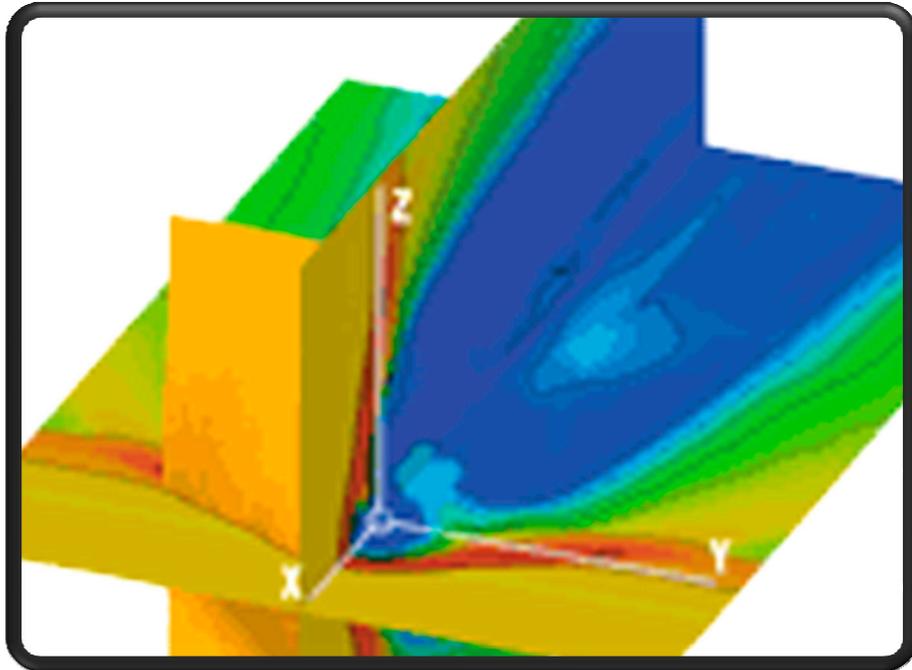
PI: Suse Broyde
New York University
50,000 hours

Simulations of cardiac fluid dynamics



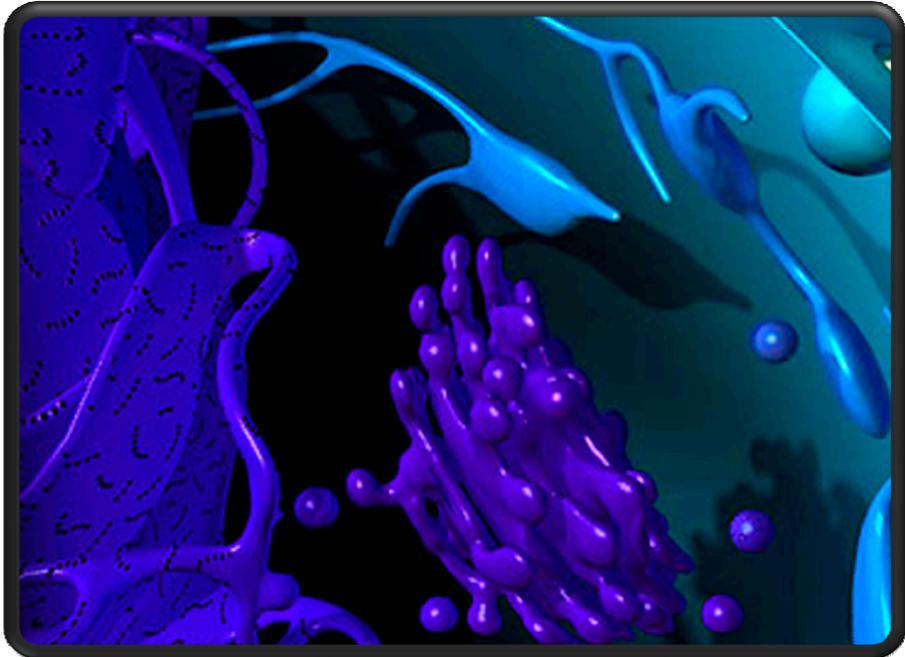
PI: Boyce Griffith
New York University
50,000 hours

Simulating the inner magnetospheric environment



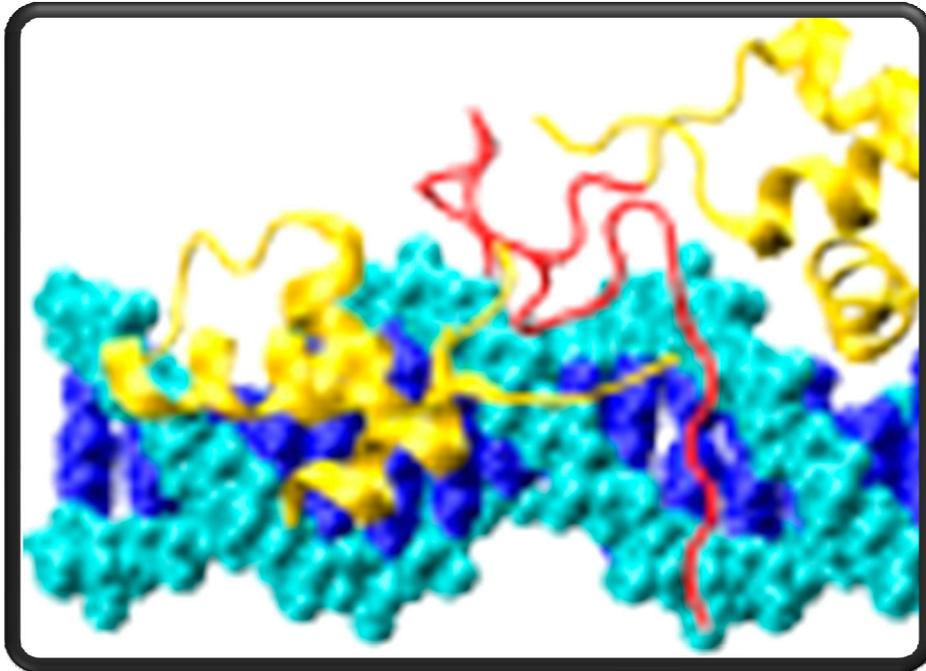
PI: Mostafa El-Alaoui
University of California–Los Angeles
250,000 hours

Reciprocal BLAST analysis of the UniProt Knowledgebase



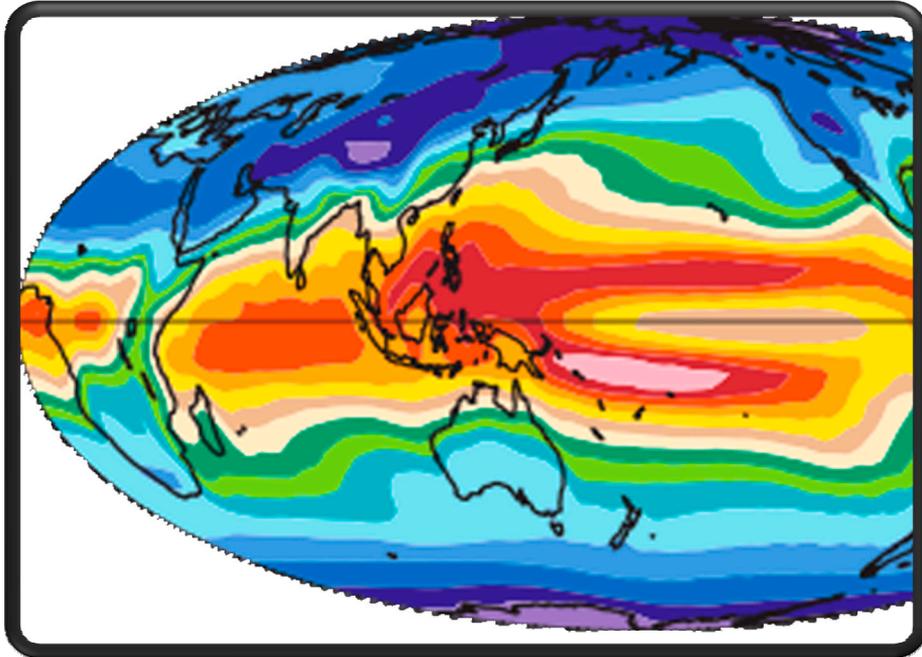
PI: Cathy Wu
Georgetown University
250,000 hours

Simulations of sequence-specific DNA-binding proteins



PI: Arjan van der Vaart
Arizona State University
87,500 hours

Climate modeling



PI: Peter Gent
National Center for Atmospheric Research
5,000,000 hours

Contact

Phil Andrews

**Project Director
National Institute for Computational Sciences
andrewspl@ornl.gov**