

Argonne Leadership Computing Facility – 2008 INCITE Projects

Computational Proteomics

Computational Protein Structure Prediction and Protein Design

David Baker, University of Washington
Blue Gene Hours: 12,000,000

Nuclear Physics

Computational Nuclear Structure

David Dean, Oak Ridge National Laboratory
Blue Gene Hours: 10,000,000

Life Sciences

Large-Scale Simulations of Cardiac Electrical Activity

Jeffrey Fox, Gene Network Sciences
Blue Gene Hours: 846,720

Materials Science

Modeling the Rheological Properties of Concrete

William George, National Institute of Standards and Technology
Blue Gene Hours: 750,000

Astrophysics

Study of Buoyancy-Driven Turbulent Nuclear Burning and Validation of Type Ia Supernova Models

Don Lamb, ASC/Alliance Flash Center, University of Chicago
Blue Gene Hours: 21,000,000

Chemical Sciences

Molecular Simulation of Complex Chemical Systems

Christopher Mundy, Pacific Northwest National Laboratory
Blue Gene Hours: 750,000

Computer Sciences

Blue Gene/P Plan 9 Measurements on Large-Scale Systems

Ronald Minnich, Sandia National Laboratories
Blue Gene Hours: 1,000,000

Combustion

Massively Parallel Simulation of Combustion in Gas Turbines

Thierry Poinsot, European Center for Research and Advanced Training in Scientific Computation
Blue Gene Hours: 4,000,000

Nuclear Energy

Predictions of Thermal Striping in Sodium Cooled Reactors

Andrew Siegel, Argonne National Laboratory
Blue Gene Hours: 5,000,000

Lattice Gauge Theory

Lattice QCD

Robert Sugar, University of California, Santa Barbara
Blue Gene Hours: 19,600,000

Fusion Energy (Plasma Physics)

High Resolution Global Simulation of Plasma Microturbulence

William Tang, Princeton Plasma Physics Laboratory

Blue Gene Hours: 2,000,000

Climate Research

Climate-Science Computational End Station Development and Grand Challenge Team

Warren Washington, National Center for Atmospheric Research

Blue Gene Hours: 1,000,000

Materials Science

Kinetics and Thermodynamics of Metal and Complex Hydride Nanoparticles

Christopher Wolverton, Northwestern University

Blue Gene Hours: 1,000,000

Chemical Sciences

Molecular Simulations of Surfactant Assisted Aqueous Foam Formations

Kelly Anderson, Procter and Gamble

Blue Gene Hours: 4,000,000

Engineering Physics

High Fidelity LES Simulations of an Aircraft Engine Combustor to Improve Emissions and Operability

Peter Bradley, Pratt and Whitney

Blue Gene Hours: 1,377,000

Applied Mathematics

Reactor Core Hydrodynamics

Paul Fischer, Argonne National Laboratory

Blue Gene Hours: 14,000,000

Physical Chemistry

Water in Confined States

Giulia Galli, University of California

Blue Gene Hours: 6,000,000

Life Sciences

Gating Mechanism of Membrane Proteins

Benoit Roux, Argonne National Laboratory and The University of Chicago

Blue Gene Hours: 1,500,000

Life Sciences

Simulation and Modeling of Synuclein-based 'Protofibril Structures' as a Means of Understanding the Molecular Basis of Parkinson's Disease

Igor Tsigelny, University of California, San Diego

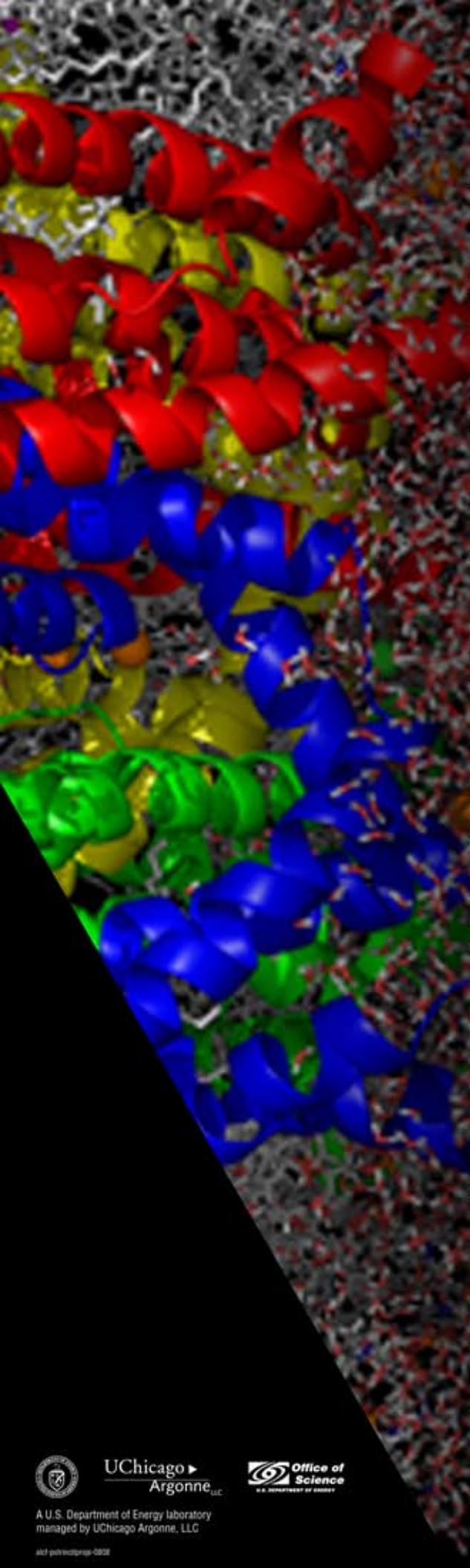
Blue Gene Hours: 1,200,000

Computer Sciences

Performance Evaluation and Analysis Consortium End Station

Patrick Worley, Oak Ridge National Laboratory

Blue Gene Hours: 4,000,000



UChicago
Argonne LLC



A U.S. Department of Energy laboratory
managed by UChicago Argonne, LLC

ALCF-PRIMER2008-0001