



2012 INCITE Projects

at the Argonne Leadership Computing Facility

Biological Sciences

Protein-Ligand Interaction Simulations and Analysis

T. Andrew Binkowski, Argonne National Laboratory

Allocation: 10 Million Hours

Multiscale Blood Flow Simulations

George Karniadakis, Brown University

Allocation: 50 Million Hours

Chemistry

Towards Breakthroughs in Protein Structure Calculation and Design

David Baker, University of Washington

Allocation: 33 Million Hours

Simulations of Deflagration-to-Detonation Transition in Reactive Gases

Alexei Khokhlov, The University of Chicago

Allocation: 20 Million Hours

Energetic Aspects of CO₂ Absorption by Ionic Liquids from Quantum Monte Carlo

William Lester, Jr., UC Berkeley

Allocation: 4 Million Hours

Large-Eddy Simulation of Two-Phase Flow Combustion in Gas Turbines

Thierry Poinso, European Center for Research and Advanced Training in Scientific Computation

Allocation: 10 Million Hours

Potential Energy Surfaces for Simulating Complex Chemical Processes

Donald Truhlar, University of Minnesota

Allocation: 15 Million Hours

Computer Science

Scalable System Software for Performance and Productivity

Ewing Lusk, Argonne National Laboratory

Allocation: 5 Million Hours

Fault-Oblivious Exascale Computing Environment

Ronald Minnich, Sandia National Laboratories

Allocation: 10 Million Hours

Performance Evaluation and Analysis Consortium End Station

Patrick H. Worley, Oak Ridge National Laboratory

Allocation: 10 Million Hours

Earth Science

CyberShake 3.0: Physics-Based Probabilistic Seismic Hazard Analysis

Thomas Jordan, Southern California Earthquake Center

Allocation: 2 Million Hours

Large-Eddy Simulations of Contrail-to-Cirrus Transition

Roberto Paoli, CERFACS

Allocation: 20 Million Hours

Climate-Science Computational Development Team: The Climate End Station II

Warren Washington, National Center for Atmospheric Research

Allocation: 30 Million Hours

Energy Technologies

Optimization of Complex Energy System Under Uncertainty

Mihai Anitescu, Argonne National Laboratory

Allocation: 10 Million Hours



Advanced Reactor Thermal Hydraulic Modeling

Paul Fischer, Argonne National Laboratory

Allocation: 25 Million Hours

Atomistic Adaptive Ensemble Calculations of Eutectics of Molten Salt Mixtures

Saivenkataraman Jayaraman, Sandia National Laboratories

Allocation: 10 Million Hours

Enabling Green Energy and Propulsion Systems via Direct Noise Computation

Umesh Paliath, GE Global Research

Allocation: 45 Million Hours

Engineering

Direct Simulation of Fully Resolved Vaporizing Droplets in a Turbulent Flow

Said Elghobashi, University of California—Irvine

Allocation: 20 Million Hours

Stochastic (w^*) Convergence for Turbulent Combustion

James Glimm, Stony Brook University

Allocation: 35 Million Hours

Adaptive Detached Eddy Simulation of a Vertical Tail with Active Flow Control

Kenneth Jansen, University of Colorado—Boulder

Allocation: 40 Million Hours

Turbulent Multi-Material Mixing in the Richtmyer-Meshkov Instability

Sanjiva Lele, Stanford University

Allocation: 20 Million Hours

Materials Science

Vibrational Spectroscopy of Liquid Mixtures and Solid/Liquid Interfaces

Giulia Galli, University of California—Davis

Allocation: 25 Million Hours

High-Fidelity Simulation of Complex Suspension Flow for Practical Rheometry

William George, National Institute of Standards and Technology

Allocation: 22 Million Hours

Probing the Non-Scalable Nano Regime in Catalytic Nanoparticles with Electronic Structure Calculations

Jeffrey Greeley, Argonne National Laboratory

Allocation: 10 Million Hours

Petascale Simulations of Stress Corrosion Cracking

Priya Vashishta, University of Southern California

Allocation: 45 Million Hours

Multiscale Modeling of Energy Storage Materials

Gregory Voth, The University of Chicago and Argonne National Laboratory

Allocation: 25 Million Hours

Physics

Simulations of Laser-Plasma Interactions in Targets for the National Ignition Facility and Beyond

Denise Hinkel, Lawrence Livermore National Laboratory

Allocation: 63 Million Hours

Toward Exascale Computing of Type Ia and Ib, c Supernovae: Verification and Validation of Current Models

Donald Lamb, The University of Chicago

Allocation: 40 Million Hours

Lattice QCD

Paul Mackenzie, Fermi National Accelerator Laboratory

Allocation: 50 Million Hours

Petascale Simulations of Inhomogeneous Alfvén Turbulence in the Solar Wind

Jean Perez, University of New Hampshire

Allocation: 10 Million Hours

Nuclear Structure and Nuclear Reactions

James Vary, Iowa State University

Allocation: 18 Million Hours