2006 DOE INCITE Supercomputing Allocations

Proposal Title: "Development and Correlations of Large Scale Computational Tools for Flight Vehicles"

Principal Investigator: Moeljo Hong
Affiliation: The Boeing Company

Co-Investigators: Robert Narducci, The Boeing Company;
Stephen LeDoux, The Boeing Company;
Todd Michal, The Boeing Company

Scientific Discipline: Engineering Physics

INCITE allocation:
Site: Leadership Computing Facility at Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 200,000 processor hours

Research summary:
This project will demonstrate the benefits of higher-order physics modeling in the global design optimization cycle to wing design for aircraft, resulting in faster simulation and performance improvements. A suite of CFD tools will model unsteady vortex dominated flows, fluid-structure/flutter interaction, control surfaces, airframe effects, rotorcraft design and installation, and a SensorCraft wing.

Relevance to DOE Mission:
The proposed project will extend well-established production CFD codes to current fluid dynamic challenges in flight vehicle development. This study is connected to Office of Science Mission 7.1, "Provide the discovery-class tools required by the U.S. scientific community to answer the most challenging research questions of our era" which includes the strategy to "develop partnerships with other Federal agencies, universities and the U.S. scientific community to fully exploit the extraordinary capabilities and interdisciplinary nature of our user facilities."

Proposal Title: "Interaction of ITG/TEM and ETG gyrokinetic turbulence"

Principal Investigator: Ronald Waltz
Affiliation: General Atomics

Co-Investigators: Jeff Candy, General Atomics;
Mark Fahey, Oak Ridge National Laboratory

Scientific Discipline: Fusion Energy

INCITE allocation:

Site: Leadership Computing Facility at Oak Ridge National Laboratory
Machine: Cray X1E
Allocation: 400,000 processor hours

Research Summary:
This proposal will study the computational modeling of the interaction of turbulence on ion and electron spatial and temporal scales. These scales differ by orders of magnitude and have traditionally been treated by separate simulations. The modeling and understanding of plasma turbulence is crucial for the development of stable and efficient fusion devices.

Relevance to DOE Mission:
This proposal strongly supports the Office of Science Mission 3.2, "Develop a fundamental understanding of plasma behavior sufficient to provide a reliable predictive capability for fusion energy systems." For successful operation of the ITER tokamak, a thorough understanding of the H-mode pedestal (an edge transport barrier) is vital. The proposed project could shed new light on how short-wavelength ETC turbulence comes into play as the long-wavelength (ITG/TEM) turbulence is suppressed in the pedestal.

Proposal Title: "Molecular dynamics of molecular motors"

Principal Investigator: Martin Karplus
Affiliation: Harvard University

Co-Investigators: None

Scientific Discipline: Life Sciences

INCITE allocation:

Site: Leadership Computing Facility at Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 1,484,800 processor hours

Research Summary:
Molecular motors are nanoscale machines made of proteins that perform essential tasks in living cells. This project will perform large-scale simulations to determine how they function at an atomic level of detail, a problem that cannot be solved by experiment alone. Since errors in replication of DNA can lead to mutations detrimental to survival, it is of great interest to see how these errors are introduced. This is of fundamental importance in molecular biology with applications in understanding neuro-degenerative diseases and treating infections, including HIV.

Relevance to DOE Mission:
With the focus on nanoscale motors, this proposal has a strong connection to two of the Office of Science's missions.

- Office of Science Mission 1.2, "Lead the nanoscale science revolution, delivering the foundations and discoveries for a future built around controlled chemical processes and materials designed one atom at a time or through self-assembly"

- Office of Science Mission 2.1, "Tap the power of genomics and microbial systems for solutions to our Nation's energy and environmental challenges" and the corresponding strategy to "discover the molecular machines encoded in each microbe's genetic instructions, determining what molecular machines are present, what proteins they are made of, where they are found in cells and how they do their work."

Proposal Title: "Real-Time Ray-Tracing"

Principal Investigator: Evan Smyth
Affiliation: Dreamworks Animation

Co-Investigators: None

Scientific Discipline: Computer Science

INCITE allocation:
  Site: Leadership Computing Facility at Oak Ridge National Laboratory
  Machine: Cray XT3
  Allocation: 950,000 processor hours

Research Summary:
Work in this proposal is focused on aggressively pushing the limits of high-quality real-time ray-tracing. The PI plans to develop a real-time ray-tracing system that is designed to run on a distributed memory multi-computer comprised of a high number of multiprocessor nodes with vector processing capabilities. In addition to affecting the way films are produced, the proposed real-time, high-fidelity, ray-tracing techniques have application in other fields requiring visualization of large complex datasets.

Relevance to DOE Mission
The work in this proposal has a connection to Office of Science Mission 6.1, "Advanced scientific discovery through research in the computer science and applied mathematics to enable prediction and understanding on complex systems." Real time volume rendering is of enormous importance for scientific progress in almost all computational sciences for visualizing large 3D data sets.

Proposal Title: "Direct Numerical Simluation of Fracture, Fragmentation and Localization in Brittle and Ductile Materials"

Principal Investigator: Michael Ortiz
Affiliation: California Institute of Technology

Co-Investigators: None

Scientific Discipline: Engineering Physics

INCITE allocation:

Site: Leadership Computing Facility at Oak Ridge National Laboratory
Machine: Cray XT3
Allocation: 500,000 processor hours

Research Summary:
This project applies detailed, first principles simulations of fracture, fragmentation and strain localization in brittle and ductile solid materials. The inherent small-scale nature of these failure phenomena, dictates the use of very fine and adaptive finite-element grids for simulation. The application areas include the behavior of materials subjected to high-speed loads such as collision, impact, ballistic penetration and blast loads.

Relevance to DOE Mission:
The proposed work attacks important problems in the continuum description of the fracture of materials. It is strongly connected to the Office of Science Mission 1.1, "Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials science, chemistry, geosciences, energy geosciences, energy biosciences, and engineering."

Proposal Title: "Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences"

Principal Investigator: Michael Pindzola
Affiliation: Auburn University

Co-Investigators: Bill McCurdy, Lawrence Berkeley National Laboratory;
David Schultz, Oak Ridge National Laboratory;
Don Griffin, Rollins College;
Francis Robicheaux, Auburn University;
James Colgan, Los Alamos National Laboratory;
Nigel Badnell, Univeristy of Strathclyde;
Predrag Krstic, Oak Ridge National Laboratory;
Tom Rescigno, Lawrence Berkeley National Laborabory

Scientific Discipline: Astrophysics, Chemical Sciences, Fusion Energy

INCITE allocation:

Site: Pacific Northwest National Laboratory
Machine: HP-MPP
Allocation: 650,000 processor hours

Research Summary:
This research team will apply state-of-the-art atomic and molecular collision codes to implement time-dependent simulations relevant for numerous applications, including ultra-short laser interactions with matter, plasma diagnostics in controlled fusion experiments, X-ray astronomy, synchrotron light sources, and free-electron lasers.

Relevance to DOE Mission:
With its focus on computational atomic and molecular physics this proposal is strongly related to several goals within the Office of Science including,

- Office of Science Mission 3.2, "Develop a fundamental understanding of plasma behavior sufficient to provide a reliable predictive capability for fusion energy systems."

- Office of Science Mission 1.1, "Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials science, chemistry, geosciences, energy geosciences, energy biosciences, and engineering."

Proposal Title: "High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability"

Principal Investigator: Robert Malecki
Affiliation: Pratt & Whitney

Co-Investigators: Peter Bradley, Pratt & Whitney

Scientific Discipline: Engineering Physics

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 888,400 processor hours

Research Summary:
Future combustor design must rely more on computational fluid dynamics (CFD) modeling for emissions and operability. The goal of this study is to perform CFD simulations of gas-turbine engines to understand the impact of properly resolving turbulence scales on combustor swirler aerodynamics and to study its impact on the combusting simulation. The calculation will be extended to the full annulus to investigate asymmetric fueling effects on operability.

Relevance to DOE Mission:
Successful completion of the project will mean significant additional information in advancing the engine technology. This goal is connected to the DOE Energy Strategic Goal in that it is trying to improve energy efficiency. In addition it is related to Office of Science Mission 7.1, "Provide the discovery-class tools required by the U.S. scientific community to answer the most challenging research questions of our era" which includes the strategy to "develop partnerships with other Federal agencies, universities and the U.S. scientific community to fully exploit the extraordinary capabilities and interdisciplinary nature of our user facilities."

Proposal Title: "Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture"

Principal Investigator: Phani Nukala
Affiliation: Oak Ridge National Laboratory

Co-Investigators: Srdjan Simunovic, Oak Ridge National Laboratory

Scientific Discipline: Materials Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 1,500,000 processor hours

Research Summary:
This project will model fracture in disordered media and answer fundamental issues of the universality of scaling exponents. The PIs will perform 3D lattice simulations of interfacial fracture using a new matrix preconditioner to accelerate computation and will investigate scaling laws of fracture, avalanche precursors, universality of fracture strength distribution, size effect on the mean fracture strength, and the scaling and universality of crack surface roughness.

Relevance to DOE Mission:
The work in this proposal offers a direct means of interpreting the scaling laws associated with dynamic fracture in disorder media. It is strongly connected to the Office of Science Mission 1.1, "Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials science, chemistry, geosciences, energy geosciences, energy biosciences, and engineering."

Proposal Title: "Modeling The Response of Terrestrial Ecosystems to Climate Change and Disturbance"

Principal Investigator: David McGuire
Affiliation: University of Alaska, Fairbanks

Co-Investigators: Jeff McAllister, University of Alaska, Fairbanks

Scientific Discipline: Envirornmental Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 600,000 processor hours

Research Summary:
Simulations in this study will be performed using the Terrestrial Ecosystem Model (TEM), a framework for investigating fundamental aspects of terrestrial carbon cycle dynamics to obtain a better understanding of fundamental processes related to climate change and their dynamic interactions. These simulations provide an understanding of how anthropogenic disturbances interact with other disturbances and ecological dynamics.

Relevance to DOE Mission:
The focus on this study is to investigate fundamental aspects of terrestrial carbon cycle dynamics. The proposed simulations will help the scientific community to gain a better understanding of the

most important processes affecting the CO2 exchange between biosphere and atmosphere, and how they can be altered by climate change or other anthropogenic disturbances. This proposal has a strong connection the Office of Science Mission 2.2, “Unravel the mysteries of Earth’s changing climate and protect our living planet.”

Proposal Title: “Computational Spectroscopy of Aqueous Solutions”

Principal Investigator: Giulia Galli
Affiliation: University of California, Davis

Co-Investigators: David Prendergast, University of California, Berkeley;
Eric Schwegler, Lawrence Livermore National Laboratory;
Francois Gygi, University of Califormia, Davis;
Jeffrey Grossman, University of California, Berkeley

Scientific Discipline: Chemical Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 2,500,000 processor hours

Research Summary:
Water is present in many chemical processes and is almost ubiquitous in biology. However, after many decades of experimental and theoretical investigations, its structural and electronic properties remain controversial. In this study, the PIs propose to carry out ab-initio simulations of water and on-the-fly calculations of X-ray absorption and emission spectra to address the existing controversy on the structure of water. If confirmed, the potential impact of these new findings on chemistry and biology is so high that Science Magazine has named it as one of the 10 breakthroughs of science in 2004.

Relevance to DOE Mission:
Understanding the structural and electronic characteristics in water is important to many scientific disciplines. Particularly this proposal is strongly related to the Office of Science Mission 1.1, “Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials science, chemistry, geosciences, energy geosciences, energy biosciences, and engineering.”

Proposal Title: “High resolution protein structure prediction”

Principal Investigator: David Baker
Affiliation: University of Washington/Howard Hughes Medical Institute

Co-Investigators: None

Scientific Discipline: Life Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 5,000,000 processor hours

Research Summary:
Proteins are the workhorse molecules of all biological systems. A deep and predictive understanding of life thus requires functional portraits of all existing proteins, and these descriptions must necessarily include these molecules' high-resolution three-dimensional structures which, in turn, determine their functions. The goal of the proposed research is to compute structures for proteins, of under 150 amino acids, with atomic level resolution. The alternative, experimental determination of protein structures is slow and expensive. In addition, the rate at which protein structures are obtained lags far behind the rate at which protein sequence information is being gathered by high-throughput genomic sequencing efforts.

Relevance to DOE Mission:
With its focus on computing the structures for approximately 150 amino acids at atomic level resolutions, this proposal has a strong connection to the Office of Science Mission 2.1, "Tap the power of genomics and microbial systems for solutions to our Nation's energy and environmental challenges. Particularly this proposal will produce computational models of molecular machines at the structural level and validate these models against x-ray crystallographic studies as they are completed.

Proposal Title: "Simulation and modeling of synuclein-based 'protofibril structures' as a means of understanding the molecular basis of Parkinson's Disease"

Principal Investigator: Igor Tsigelny
Affiliation: University of California -- San Diego / SDSC

Co-Investigators: Eliezer Masliah, University of California, San Diego;
Stanley Opella, University of California, San Diego

Scientific Discipline: Life Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 16,000 processor hours

Research Summary
Parkinson's disease progression is characterized by a decrease in limb mobility over time. The loss of movement is caused by the death of dopamine producing cells in the brain, thought to be associated with defects that cause increased aggregation of alpha synucleins (aS). A key issue in treating Parkinsons disease is thus the illumination of the factors that trigger aS aggregation, and the development of strategies to prevent this phenomenon. This study will combine high-end computation with biochemical and NMR experiments to model the molecular basis for aS aggregation and to test hypotheses generated by our simulations using NMR and other biochemical techniques. By combining the theoretical findings with experimental validation, we

hope to identify key amino acid interactions that favor amyloid pore formation, and to use this information to discover new drugs.

The work described here will not only be informative in addressing the underlying molecular basis for Parkinson's disease, but will likely be instructive in identifying risk factors and therapeutic strategies for a large body of other diseases that are equally prevalent in human populations.

Relevance to DOE Mission:
This INCITE pilot study is connected to Office of Science Mission 7.1, "Provide the discovery-class tools required by the U.S. scientific community to answer the most challenging research questions of our era" which includes the strategy to "develop partnerships with other Federal agencies, universities and the U.S. scientific community to fully exploit the extraordinary capabilities and interdisciplinary nature of our user facilities."

Proposal Title: "Reactions of lithium carbenoids, lithium enolates, and mixed aggregates"

Principal Investigator: Lawrence Pratt
Affiliation: Fisk University

Co-Investigators: None

Scientific Discipline: Chemical Sciences

INCITE allocation:
Site: Argonne National Laboratory /IBM
Machine: IBM Blue Gene
Allocation: 50,000 processor hours

Research Summary:
This chemical science project will use ab initio and density functional theory (DFT) methods to investigate the structure and reactions of some important organolithium compounds. These include lithium enolates, which are among the most important reagents for forming carbon-carbon bonds in organic synthesis. Detailed reaction mechanisms for these compounds remain unknown, and may involve several reactive species. This will lead to a better understanding of the reaction pathways and to alter the reactions by way of mixed aggregates with other lithium compounds.

Relevance to DOE Mission:
With its study of the role that lithium enolates and carbenoids play in organic reactions, this INCITE Pilot study is related to the Office of Science Mission 1.1, "Advance the core disciplines of the basic energy sciences, producing transformational breakthroughs in materials science, chemistry, geosciences, energy geosciences, energy biosciences, and engineering."

Proposal Title: "Precision Cosmology using Lyman alpha Forest"

Principal Investigator: Michael Norman
Affiliation: University of California - San Diego

Co-Investigators: None

Scientific Discipline: Astrophysics

INCITE allocation:
Site: National Energy Research Scientific Computing Facility, Lawrence Berkeley National Laboratory
Machine: IBM Power 3+
Allocation: 1,000,000 processor hours

Research Summary:
A principal goal of modern cosmology is the precise measurement of cosmological parameters that describe the shape, matter-energy contents, and expansion history of our universe. Recent astronomical observations indicate important inferences about the nature of dark energy and dark matter. The examination of the absorption spectra of high redshift quasars has emerged as an important tool in this inference, since it samples matter fluctuations in the intergalactic gas. Our project will achieve greater understanding by high resolution hydrodynamical cosmological simulations of the structure of the high redshift intergalactic medium

Relevance to DOE Mission:
This proposal has a strong connection to Office of Science's Mission 4.2, "Understand the Cosmos." The scientific question addressed by the proposal relates to the most fundamental questions in the physical sciences. *What is nature of dark matter and dark energy?* Performing simulations on the proposed scale is crucial in understanding the astrophysical implications of dark energy observations.

Proposal Title: "Particle in cell simulation of laser wakefield particle acceleration"

Principal Investigator: Cameron Geddes
Affiliation: Lawrence Berkeley National Laboratory

Co-Investigators: Carl Schroeder, Lawrence Berkeley National Laboratory;
David Bruhwiler, Tech-X;
Eric Esarey, Lawrence Berkeley National Laboratory;
John Cary, University of Colorado/ Tech-X;
Wim Leemans, Lawrence Berkeley National Laboratory

Scientific Discipline: Accelerator Physics

INCITE allocation:

Site: National Energy Research Scientific Computing Facility, Lawrence Berkeley National Laboratory
Machine: IBM Power 3+
Allocation: 2,500,000 processor hours

Research Summary:
This project will perform detailed 3D models of laser driven wakefield particle accelerators (LFWAs), providing crucial understanding of the next generation of particle accelerators and ultrafast applications in chemistry and biology. These plasma based accelerators are not subject to electrical breakdown and have demonstrated accelerating gradients thousands of times those obtained in conventional accelerators. The particle-in-cell simulations proposed in this study will interpret recent experiments and assist in the planning of the next generation of accelerators.

Relevance to DOE Mission:
There is a strong connection to the Office of Science's Mission 4.1, "Explore Unification phenomena" and the specific emphasis to "pursue advanced accelerator development aimed at finding better ways to accelerate particles…" The proposed computational investigation is expected to provide substantial support for the design of laser-plasma accelerators, as alternatives to conventional particle accelerators. This investigation should also be of significant benefit for the development of new sources of intense, ultra-short-pulse coherent electromagnetic radiation for spectroscopic applications.