Office of Science
U.S. DEPARTMENT OF ENERGY

INCITE
Advancing America's Science and Industrial Competitiveness

What Researchers Are Saying About The INCITE Awards

Since the INCITE Program was launched in 2003, the number of processor-hours requested for projects has far exceeded the availability of DOE supercomputing resources. For example, the total number of processor hours requested for 2006 was 95 million hours, and INCITE was able to award 18 million hours on supercomputers at four facilities. In 2007, with the addition of even larger systems, INCITE will award 95 million processor hours to 45 projects, out of a total of 184 million hours of requested time.

This high level of interest in INCITE reflects both the growing role of high performance computing in all fields of science and engineering, and the attraction of being able to run applications on DOE's leading-edge supercomputers, which are some of the most powerful systems in the world.

Researchers who have received INCITE awards in the past, as well as those selected to receive allocations for 2007, provided the following comments about the value of being given access to DOE's supercomputers and the expertise of technical staff at the computing centers.

2007

High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability, Peter Bradley, Pratt & Whitney, Connecticut
"The INCITE partnership gives Pratt & Whitney access to world-leading computers to enable development of cutting-edge modeling and simulation capabilities used in design of fuel-efficient and environmentally friendly engines for commercial aircraft. These capabilities will also be applicable to military products in the defense of the Nation. While Pratt & Whitney fields supercomputing resources of its own, the Department of Energy through its mission, scientists, and infrastructure is uniquely qualified to operate and enable a supercomputing resource beyond the practical

capabilities of a large industrial company. In an ever-expanding global economy where technology leadership is critical to competitiveness, INCITE provides American industry with an engine for technological and competitive growth."

Molecular Simulations of Surfactant Assisted Aqueous Foam Formation, Kelly Anderson, Procter and Gamble, Ohio
"P&G embraces Open Innovation and collaboration; this partnership reflects that. This grant allows us to perform computer simulations, at an unprecedented scale, on the dissolving of soap, and forming of suds. The resulting approach should help us formulate products faster and more efficiently. That means the consumer wins by getting better products sooner, and at better value, than would have been possible using traditional methods."

CAE Simulation of Full Vehicle Windnoise and Other CFD Phenomena, Paul Bennis, Fluent Inc. (in partnership with General Motors), New Hampshire
"We believe there is the best opportunity for significant design analysis productivity improvements through the use of HPC. Due to the extremely large capital cost required, this has been traditionally difficult to justify, and thus never attempted. The INCITE award provides the opportunity to realize the potential productivity improvements and allows a factual and more quantitative analysis of the HPC benefits.

"There are three primary areas for competitive advantage. The first opportunity is to develop and demonstrate true high fidelity virtual prototypes which directly lead to more innovative designs and products by utilizing HPC. The second area of competitive advantage is also a direct result of the use of HPC, as it freely permits a large reduction in the need for physical testing, and therefore improves quality dramatically. At the same, because of shorter time cycles, less physical setup time, it overall lowers the total cost of product development, which is significant."

Development and Correlations of Large Scale Computational Tools for Flight Vehicles, Moeljo Hong, The Boeing Co., Washington
"To be competitive in today's marketplace Boeing must bring new airplanes to market in less time, at less cost, and with no additional risk. New tools and processes are required to meet these challenges. Many of these tools and processes are numerically based and require new, high-performance computers that are often first available through our national labs. Boeing relies on partnerships such as INCITE to be able to access these computers in order to do this proof-of-concept development and validation. Boeing will use the 2007 INCITE allocation award to demonstrate the predictive accuracy of our CFD-based processes. Once this has been successfully completed Boeing then makes the investment in hardware so that these new tools and processes can be used to design new products."

Real-Time Ray-Tracing, Evan Smyth, DreamWorks Animation, California
"Perhaps the most valuable dimension of public-private partnerships such as the INCITE program is that they afford industry the opportunity to explore ideas that would be too speculative to otherwise pursue. The computing resources available as part of this

program are some of the most powerful supercomputers in the world. To have this kind of resource available allows us to experiment with next generation HPC architectures that help keep us on the leading edge of technology, and ultimately, computer-generated movie making.

"We are using this grant to explore efficient distributed algorithms and techniques that we will apply in our production environment to significantly shorten iteration times for our artists. On a personal level, it has been immensely valuable to be able to interact and collaborate with the many top-tier scientists and engineers in the Department of Energy."

Study of the Gravitationally Confined Detonation Mechanism for Type Ia Supernovae, Don Lamb, University of Chicago, Illinois
"The INCITE award will make it possible for us to do huge computer simulations whose goal is to pin down the explosion mechanism for Type Ia supernovae, which astronomers use to measure distances in the universe. A better understanding of these supernovae will enable astronomers to learn more about the properties of dark energy -- something that DOE and NASA have identified as a science priority."

Gating Mechanism of Membrane Proteins, Benoit Roux, University of Chicago, Illinois
"The award will enable us to simulate fully atomistic models o voltage-activated potassium channels in a dynamical lipid membrane environment. These simulations will advance our understanding of how these proteins are able to alter their conformation in response to changes in the cellular potential to act as a molecular switch."

High-Fidelity Numerical Simulations of Turbulent Combustion - Fundamental Science Towards Predictive Models, Jacqueline Chen, Sandia National Laboratories, California, (also 2005 INCITE awardee)
"The DOE INCITE program has made an enormous difference in the level of detail that scientists are able to observe of turbulent combustion environments representative of aircraft and automotive engines used for transportation. For example, through terascale and petascale computing on Leadership Class machines at ORNL and NERSC, it is now possible to glean insight into detailed chemistry-turbulence interactions associated with stabilizing a lifted auto-igniting flame in a diesel engine environment, or to understand how a flame reignites once it is locally extinguished by excessive mixing rates. The answers to these and other important questions directly affect the fuel-efficiency and emissions of automobiles and airplanes."

Petascale Particle-in-Cell Simulations of Plasma Based Accelerators, Warren Mori, University of California, Los Angeles,
"Large accelerators are the principal tool used to discover and probe the fundamental particles of nature and their size is now reaching more than 10 kilometers in length using existing acceleration methods. This INCITE award will allow us to study — in unprecedented detail using sophisticated computer models — the physics of plasma-

based acceleration in order to determine if it could be used to reduce the size of the largest accelerators from 10's of kilometers to 10 meters in length."

Linear Scale Electronic Structure Calculations for Nanostructures, Lin-Wang Wang, Lawrence Berkeley National Laboratory, California
"This INCITE award will allow us to calculate the internal electric fields and their effects on the electronic and optical properties of nanostructures consisting of hundreds of thousands of atoms. It will help us to design better nanoscience applications ranging from single electron devices to solar cells."

Via Lactea: A Billion Particle Simulation of the Milky Way's Dark Matter Halo, **Piero Madau, University of California, Santa Cruz**
"This project will study in unprecedented detail the formation and evolution of the dark matter halo that envelopes the Milky Way galaxy. The simulation will start at about 50 million years after the Big Bang and calculate the interactions of one billion particles of dark matter over 13.7 billion years of cosmological time to produce a halo on the same scale as the Milky Way's. It seeks to increase our understanding of the nature of the dark matter that accounts for more than 80 percent of the matter in the universe, and of the processes that make galaxy halos clumpy, i.e., teeming with gravitationally bound substructure on all resolved mass scales."

Bose-Einstein condensation vs. quantum localization in quantum magnets, Tommaso Roscilde, Max-Planck Institute for Quantum Optics, Germany
"The INCITE computational grant will provide us with the fundamental tool to formulate accurate predictions on the behavior of complex magnetic materials exhibiting quantum mechanics at the macroscopic scale. In a joint effort with experimentalists, we aim to reveal novel phases of doped quantum magnets at very low temperature. This would represent a significant achievement in the area of quantum engineering of complex materials."

Three-Dimensional Particle-in-Cell Simulations for Fast Ignition, Chuang Ren, University of Rochester, New York
"This award will allow us to perform some of the largest ever 3D particle-in-cell simulations for fast ignition, a new scheme to achieve fusion as a long-term, environmentally friendly energy source for humanity. This work will be an important part of the integrated research within the DOE Fusion Science Center for Extreme States of Matter and Fast Ignition Physics to assess the potential of this new fusion concept and the results will have impact on fast ignition experiments now planned at the Laboratory for Laser Energetics of the University of Rochester and other facilities."

High Power Electromagnetic Wave Heating in the ITER Burning Plasma, Fred Jaeger, Oak Ridge National Laboratory, Tennessee
"The next step toward fusion as a practical energy source will be the construction of ITER, a device capable of producing self-sustained fusion reactions, i.e., "burning" plasma. This award will allow simulations of the high power electromagnetic waves that will heat and control the burning plasma in ITER."

Numerical relativity simulations of binary black holes and gravitational radiation, Joan Centrella, NASA Goddard Space Flight Center, Maryland
"Binary black hole mergers are the strongest sources of gravitational radiation, producing more energy in the burst than is in the combined starlight in the visible universe. Our INCITE award will allow us to carry out high resolution studies of these mergers and to calculate the waveforms that will be observed by gravitational wave detectors such as LISA and LIGO."

Direct Numerical Simulation of Turbulent Flame Quenching by Fine Water Droplets, Hong Im, University of Michigan
"The INCITE award will allow us to conduct high-fidelity simulations of turbulent combustion at unprecedented physical length and time scales. The high quality simulation data will enable fundamental science discovery as well as cross-validation against experimental measurements through worldwide collaborative activities."

Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture, Phani Nukala, Oak Ridge National Laboratory, Tennessee
"Through our INCITE grant, we would like to understand physics of fracture in quasi-brittle materials such as concrete and ceramics. Specifically, we are interested in understanding the precursors of catastrophic fracture so that we can develop a prognostic methodology to forecast an impending material systems failure. Our INCITE allocation would enable us to develop scaling laws that reveal these signatures of an impending system failure."

Reactor Core Hydrodynamics, Paul Fischer, Argonne National Laboratory, Illinois
"Advanced burner reactors (ABRs) are a central element of DOE's proposed Global Nuclear Energy Partnership (GNEP). By reducing radioactive wastes, ABRs can effectively increase the storage capacity of geological repositories up to one-hundredfold. To increase the economic viability of GNEP, ABRs will also be energy producers. With this INCITE award, researchers will conduct large-eddy simulations of the thermal-hydraulics that governs the ABR peak temperature, which is critical to the economy and safety of the reactor."

Coherent Control of Light in Nanoscale, Tamar Seideman, Northwestern University, Illinois
"The interaction of light with noble metal nanoparticles and with arrays thereof has inspired scientists for several centuries and continues to offer new and fascinating questions for fundamental research. Historically, noble metal particles of sub-diffraction size found applications in the staining of glass windows and ceramic pottery. Today, such particles are widely researched for applications ranging from novel sensors and medical diagnostics to enhanced solar cells and nonlinear light sources to single-molecule spectroscopy and 3D atom probe technology. Techniques of fabricating metal nanoparticle arrays are well developed, as are also methods of computing their optical properties. An open question, however, is how to size, shape and arrange the particles so as to yield a desired optical property or make a desired photonic device.

"We have developed a numerical approach wherein optimal control theory is applied as a numerical design tool, to make nanophotonics with desired functionality. The approach is being applied in collaboration with experimental groups to optimize solar cells and to develop a novel light detector. The method is numerically challenging and, although our highly parallelized codes make the solution very efficient, its application to realistic problems relies on the availability of advanced computing resources. The INCITE award will enable us to make significant contributions to the challenging problem of understanding, modeling, and manipulating nanoscale photonic devices, with a rich variety of applications in science and technology."

Performance Evaluation and Analysis Consortium End Station, Patrick Worley, Oak Ridge National Laboratory, Tennessee
"The Performance Evaluation and Analysis Consortium will investigate the performance characteristics of the computer systems in the National Leadership Computing Facility and develop performance tools and methodologies for these systems. These data and tools will enable the computational scientists and system administrators to use the leadership class computer systems more effectively and help them prepare to use the next generation petascale systems, accelerating the achievement of the INCITE science goals."

The 20th Century Reanalysis Project, Gil Compo, University of Colorado
"The INCITE award will allow us to produce the first-ever dataset of global weather maps for the period 1892-2007. Our dataset will be used to study climatic variations and trends that could not previously be addressed observationally, such as the U.S. "Dust Bowl" of the 1930s, Arctic warming in the 1920s to 1940s, and trends in severe winter storms."

Eulerian and Lagrangian Studies of Turbulent Transport in the Global Ocean, Synte Peacock, University of Chicago, Illinois
"Access to the Center for Computational Science's Cray XT3 under our INCITE award will allow us to complete the first-ever century timescale simulation of the global ocean that explicitly resolves the processes that give rise to turbulent eddies. The results of the simulation will provide us with a far more detailed and quantitative understanding than currently exists concerning the role of fine-scale features in the time-mean ocean flow and small-scale turbulent eddies in dispersing trace gases such as carbon dioxide. The results will also help us improve parameterizations of these processes in next-generation Earth system models, which will be used for future climate projections"

2006

Interaction of ETG and ITG/TEM Gyrokinetic Turbulence, Ronald E. Waltz, General Atomics, California
"The INCITE computer time award for doing coupled ITG/TEM-ETG gyrokinetic turbulence simulations allowed us to attack a high Reynolds number problem that would have been thought impossible a few years ago. Previously, the large ion-scale tokamak plasma turbulence was treated separately from the small scale electron turbulence. The

INCITE award allows us to understand where and when the large and small scales need to be coupled and where such expensive simulations were unnecessary."

Molecular Dynamics Simulations of Molecular Motors, Martin Karplus, Harvard University, Massachusetts
"With the INCITE grant, we have made important progress in our studies of two molecular machines, F1 ATPase and DNA polymerase, each of which requires on the order of 180,000 atoms for a fully solvated molecular dynamics simulation. The XT3 supercomputer at Oak Ridge has made possible a large number of multi nanosecond simulations, which we have used to aid in dissecting the mechanism of both systems. These nanomachines play an essential role in living cells. An understanding of how they function provides important elements in the fundamental description of biological organization, the development, of drugs for diseases like cancer, and the technology of nanomachines."

Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture, Phani Nukala, Oak Ridge National Laboratory, Tennessee
"Using our 2006 INCITE award, we have simulated fracture of the largest-ever 3-D lattice systems. For the first time, these simulations confirmed and explained the anomalous scaling observed in fracture experiments, a result which could only be achieved by simulating very large systems. These large scale simulations, possible only through INCITE allocation, have been instrumental in advancing the current understanding of physics of how materials fracture."

Computational Spectroscopy of Aqueous Solutions, Giulia Galli, University of California, Davis
"The main goal of our project is to provide a fundamental understanding of the properties of water from first principles, and to resolve long standing controversies on this ubiquitous liquid at ambient conditions and confined into small channels. The properties we are studying are relevant to problems in materials science, biology and chemistry and thus the relevance and impact of our results can be extremely important and broad, if the project is successful. When attempting to solve challenging problems using computational tools, especially in the presence of controversial and contradicting experimental results, the only way to possibly succeed is to have dedicated time to carry out cutting edge, thorough studies at a sustained pace. This is exactly what INCITE grants provide us with."

High Resolution Protein Struction Prediction, David Baker, University of Washington/Howard Hughes Medical Institute
"Predicting high resolution three dimensional structures of proteins is an extremely computationally intensive problem. Before the availability of the INCITE resources, the quality of predictions were limited by our in-house computing power. The massive increase in computing power through the DOE INCITE project has led to a dramatic improvement in the quality of our predictions. This has truly redefined the state of the art of computational protein science. Availability of high resolution protein structure models will have a direct positive impact on structure-based drug design, protein engineering, understanding molecular mechanisms of protein activity etc."

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/SDSC,
"This important finding could lead to new therapies for Parkinson's Disease by developing and modeling drugs that block alpha-synuclein aggregation and block and inhibit the abnormal calcium transport in the pores."

Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates Lawrence Pratt, Fisk University, Tennessee
"My research is mostly computational chemistry of organolithium compounds. We use ab initio and DFT methods to study the aggregation state, mixed aggregate formation, solvent effects, and reactions of lithium carbenoids, lithium enolates, lithium dialkylamides, and alkyllithiums. Before receiving the INCITE award, most of the work was performed on PC workstations. This severely limited the job throughput and in some cases even limited the kinds of calculations that could be performed. The award has more than doubled my research productivity, resulting in two publications for 2006 and three papers accepted for publication in 2007 to date. Several more projects are nearing completion in 2007."

Particle-in-Cell Simulation of Laser Wakefield Particle Acceleration, Cameron Geddes, Lawrence Berkeley National Laboratory, California
"INCITE 2006 simulations at NERSC yielded full scale explicit particle models of laser-driven plasma wakefield particle accelerator experiments, advancing understanding of beam formation and evolution in new devices that offer next-generation compact, ultrafast particle and radiation sources for science and medicine. Nonlinear interaction of the laser and plasma necessitates numerical simulation of these accelerators, and INCITE allowed large three-dimensional simulations as well as modeling of a series of two-dimensional cases to evaluate accelerator optimization. These simulations provide information crucial to development of laser driven accelerators, whose compactness may enable applications from next-generation particle physics to new medical radiation sources, and to advancing U.S. leadership in this emerging field."

2005

Magneto-Rotational Instability and Turbulent Angular Momentum Transport (Fausto Cattaneo, University of Chicago, Illinois

"With the help of NERSC staff, we were able to tune our software for Seaborg's hardware and realize a performance improvement which made additional simulations possible."

Molecular Dynameomics, Valerie Daggett, University of Washington, National Institutes of Health

"We are quite satisfied with our experience at NERSC and have made significant progress towards our goal of performing molecular dynamics simulations of the first 150 most populated folds of protein fold space."

2004

Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers, William Lester, Lawrence Berkeley National Laboratory and UC Berkeley, California

"The INCITE Award has made possible major advances in understanding the electronic properties of large molecules. In particular, the computations carried out on the molecules bacteriochlorophyll and spheroidene that play a crucial role in photoprotection in purple bacteria, are a benchmark against which to measure the adequacy of computational approaches including the popular density functional theory (DFT) method."

Thermonuclear Supernovae: Stellar Explosions in Three Dimensions, Tomasz Plewa, University of Chicago, Illinois

"None of this would have been possible without INCITE. These simulations are so computationally intensive that they do require hundreds of thousands of CPU hours per computational run. Computing centers typically do not give so much computing time to one project. So, the scale of INCITE grants was essential."

Fluid Turbulence and Mixing at High Reynolds Number, P. K. Yeung, Georgia Institute of Technology, Georgia

"INCITE has, through a large CPU allocation combined with strategic consultant support and favorable system policies, enabled the use of as many as 8 billion grid points to probe deeply into a subject which, even after a century of efforts, is still known as the 'last unsolved problem in physics.' Our successes with the INCITE program have drawn attention in both the science and supercomputing communities, and created a very broad range of opportunities for the future."