Office of Science
U.S. DEPARTMENT OF ENERGY

INCITE
Advancing America's Science and Industrial Competitiveness

# 2004-06 INCITE Results

As one of the world's leading sponsors of scientific research, the U.S. Department of Energy in 2003 launched a major program to allocate millions of hours of dedicated supercomputing time to address some of the most challenging research problems in physics, chemistry, life sciences and energy. Called *Innovative and Novel Computational Impact on Theory and Experiment (INCITE)*, the program seeks computationally intensive large-scale research projects, with no requirement of current DOE sponsorship, that can make high-impact scientific advances through the use of a substantial allocation of computer time, technical staff support and data storage. The INCITE program specifically encouraged proposals from non-DOE researchers.

Supercomputers typically use hundreds or thousands of processors to model complex scientific processes. Using more processors allows scientists to create more detailed simulations, which are also more scientifically accurate. Large allocations such as those provided under INCITE are critical to advancing understanding in areas ranging from astrophysics to global climate change, from fusion energy to combustion.

In the first two years of the competitive program, the Department of Energy (DOE), Office of Science received and reviewed 75 proposals, requesting a total of nearly 160 million hours of processing time. About two-thirds of the proposals came from university researchers. From these proposals, three were chosen for each of the first two years and all of the projects used supercomputers at DOE's National Energy Research Scientific Computing (NERSC) Center at Lawrence Berkeley National Laboratory.

In the third year of the program, DOE expanded the INCITE call for proposals to include proposals from industry. Additional computing resources at Argonne, Oak Ridge and Pacific Northwest national laboratories were also made available. For 2006, 43 proposals were submitted, requesting over 95 million processor hours. Fifteen projects, including four from industry, were awarded a total of 18 million processor-hours.

Here is a look at some of those projects and their accomplishments to date.

# 2006

**Development and Correlations of Large Scale Computational Tools for Flight Vehicles (Moeljo Hong, The Boeing Co.)**
For decades, the aircraft industry has developed and improved mathematical models for improving the aerodynamic performance of aircraft. As supercomputers have become increasingly powerful, more accurate methods were developed, decreasing the amount of time needed to take a design from the drawing board to the runway. This project was designed to produce even faster simulation and performance improvements through the use of higher-order physics and aeroelastic modeling in designing aircraft wings. Aeroelasticity is the study of the interaction of different forces on an aircraft. In order to adapt to accommodate the effects of these forces, modern aircraft are designed with structures that are not completely rigid. Such forces can lead to vibrations and cause control surfaces to react in different ways, unless the design takes aeroelasticity into account.

**Interaction of ETG and ITG/TEM gyrokinetic turbulence (Ronald E. Waltz, General Atomics)**
Using the GYRO gyrokinetic code, the team compared fusion energy simulations of differing "computational cost" (the amount of processing time needed to complete an application). The goal is to demonstrate that for some investigations, the less expensive simulation is sufficiently accurate. This project is concluding that electron temperature gradient (ETG) is likely the dominant factor inside a tokamak transport barrier. Such insight is providing important guidance for the design and construction of the international ITER fusion energy project in France.

**Molecular Dynamics Simulations of Molecular Motors (Martin Karplus, Harvard University)**
The human body is an amazing machine, but only now are we beginning to realize the incredible depth of scale at which this machinery functions. Using an INCITE award, scientists studied the role of molecular motors in the process of life through computer simulations. The team looked at two motors, both of which play major roles in everyday biological processes. The first motor, dubbed $F_1$ATP-synthase, is responsible for the manufacture of ATP, or adenosine triphosphate, the molecule that turns food into usable energy, allowing the numerous processes necessary for life to take place. The second motor is DNA polymerase, which copies nucleic acid to make new cells and bacteria or reproducing.

**Computational Atomic and Molecular Physics for Advances in Astrophysics, Chemical Sciences and Fusion Energy Sciences (Michael Pindzola, Auburn University)**
This research team applied 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.

**Time-dependent close-coupling (TDCC) calculations:** Research into the double photoionization of molecular hydrogen found good agreement with exterior complex scaling (ECS) calculations carried out at NERSC and with synchrotron light source experiments. The preliminary ECS results have already appeared in Science, while TDCC results will be submitted to Physical Review Letters.
**Time-dependent lattice (TDL) calculations:** Calculations carried out with low-order finite difference and higher-order FFT approximations for the kinetic energy operator in Schrodinger's equation to study charge transfer in ion-ion collisions found good agreement with crossed ion beams experiments.
**Molecular dynamics (MD) calculations:** Calculations carried out for chemical sputtering, reflection, and sticking by C, D, and $D_2$ impinging on deuterated, amorphous, and crystalline carbon surfaces found excellent agreement with ion beam on surfaces experiments. Results will be published in Europhysics Letters and the Journal of Plasma Physics.
**Classical trajectory Monte Carlo (CTMC) calculations:** As part of research into atomic processes in strong magnetic fields, calculations of three body recombination in strong magnetic fields were done in support of CERN experiments to make trapped anti-hydrogen atoms, with the results to be published in the Journal of Physics.

**High Fidelity LES Simluations of an Aircraft Engine Combustor to Improve Emissions and Operability (Peter Bradley, Pratt & Whitney)**
The use of computational fluid dynamics (CFD) modeling in the design of aircraft engine combustors is continually increasing as designers strive to improved fuel efficiency and control emissions. 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 investigate asymmetric fueling effects on operability.

**Large Scale Simulations of Fracture in Disordered Media: Statistical Physics of Fracture (Phani Nukala, Oak Ridge National Laboratory)**
The statistical properties of fracture in disordered media are interesting for both practical and theoretical reasons. From a practical point of view, the main issue associated with the fracture of quasi-brittle materials (such as concrete and ceramics) is the scaling of material strength – how properties like strength scale with sample size. Additionally, understanding the acoustic emission signatures associated with the crackling noise of fracture experiments may lead to methods for predicting impending structural failure. This project will model fracture in disordered media and answer fundamental issues of the universality of scaling exponents.

**Computational Spectroscopy of Aqueous Solutions (Giulia Galli, University of California, Davis)**
Although the structure of water has been probed for more than 100 years, scientists still can't agree on its electronic structure and detailed atomic structure. Using an INCITE allocation, this team is seeking to determine the structure of water by running first principles simulations based on well-established laws of quantum mechanics. Understanding the electronic structure of water could lead to revolutionary new

discoveriers in biology, chemistry and other fields. The potential impact of these new findings on chemistry and biology, if confirmed, is so high that several years ago Science magazine has defined the understanding of water structure and electronic properties as one of the top 10 scientific topics.

**High Resolution Protein Struction Prediction (David Baker, University of Washington/Howard Hughes Medical Institute)**
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 this project 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.

**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)**
Recent studies suggest that the pathogenesis of Parkinson's Disease is related to the misfolding and abnormal accumulation of a-synuclein in neurons. Although several NMR and biochemical studies have investigated the folding abnormalities of alpha-synuclein at fibrilizition state less is known about early alterations. The molecular dynamics and docking studies conducted using an INCITE award and corresponding experiments of Dr. Tsigelny and Dr. Masliah have revealed the early folding anomalies of synuclein, suggesting that aggregates form porelike structures with channel activity.

**Reactions of Lithium Carbenoids, Lithium Enolates, and Mixed Aggregates (Lawrence Pratt, Fisk University)**
To coax the next blockbuster drug out of chemical compounds, scientists must explore how these compounds work with each other. This process of assembling the right ingredients takes years and millions of dollars, and the result can lead to life-saving medicines. Figuring out the right mix requires knowledge about the characteristics of various compounds and a dose of serendipitous discovery. This process of synthesizing compounds is the focus of an INCITE project examining how lithium enolates, lithium carbenoids and the blend of the two interact with other lithium compounds. Lithium is commonly found in portable batteries that power laptops and cell phones. In pharmacology, lithium compounds such as lithium carbonate and lithium citrate are commonly used to control mood swings.

**Particle-in-Cell Simulation of Laser Wakefield Particle Acceleration (Cameron Geddes, Lawrence Berkeley National Laboratory)**
Large scale particle in cell simulations under INCITE are advancing understanding of laser driven wakefield accelerators, whose high accelerating fields may offer more compact machines for high energy physics, and whose ultrashort electron bunches may revolutionize applications of accelerators to radiation sources and applications including chemistry and biology. Recent experiments have demonstrated high quality beams from such accelerators, with accelerating fields thousands of times greater than conventional

machines. Large scale three dimensional particle simulations done under INCITE clarify mechanisms of beam formation and evolution, and have begun to identify potential optimizations in this emerging field.

## 2005

**Direct Numerical Simulation of Turbulent Non-Premixed Combustion (Jacqueline Chen, Sandia National Laboratories)**
With terascale resources at NERSC, the team performed the first three-dimensional direct numerical simulation of a turbulent nonpremixed $H_2/CO/N_2$-air flame with detailed chemistry. This simulation, the first in a series of different Reynolds numbers, is targeted at providing insight into key outstanding issues related to modeling of turbulent nonpremixed combustion: extinction and reignition, flow and flame unsteadiness, the correlation of strain rate and scalar dissipation rate, differential diffusion of species, and turbulent mixing in a finite-rate chemical environment.

**Magneto-Rotational Instability and Turbulent Angular Momentum Transport (Fausto Cattaneo, University of Chicago)**
This project studied the forces that help newly born stars and black holes increase in size. In space, gases and other matter often form swirling accretion disks around attracting central objects such as newly formed stars. Strong magnetic fields can cause the disks to become unstable, develop turbulence and lose orbital angular momentum, thereby causing the disk material to fall onto the central object. In recent years, laboratory experiments have been developed to test many aspects of this magnetically caused instability, turbulence and angular momentum transport, but on a much smaller scale. The large-scale simulations of magnetized fluid between two concentric cylinders extends the lab experiments by several orders of magnitude and tests theories on how turbulence and angular momentum transport can develop in the astrophysical accretion disks.

**Molecular Dynameomics (Valerie Daggett, University of Washington, National Institutes of Health)**
The goal of this project was to understand the general principles of protein folding. The project combined molecular dynamics and proteomics to create an extensive repository of the molecular dynamics structures for protein folds, including the unfolding pathways. There are approximately 1,130 known, non-redundant protein folds, and prior to their INCITE award, the team had simulated about 30 of them. Using NERSC's supercomputer, the team was able to simulate proteins from the 151 most common folds, which represent about 75 percent of all known protein structures.. The group plans to use the information from these simulations to improve algorithms for predicting protein structure.

# 2004

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

This project aimed to increase understanding of the complex processes which occur during photosynthesis, the process by which plants and bacteria convert the sun's light into energy, taking in carbon dioxide and producing oxygen in the process. Lester's team focused on gaining a greater understanding of the chemistry of the photoprotective carotenoids, the molecules which detect the over-absorption of energy by the plant and "quench" the chlorophyll molecules before they can pose a danger to the plant. As a result of their INCITE award, the group improved their code so that it now runs 10 times faster and they are now able to study systems four times larger than before the INCITE grant.

**Thermonuclear Supernovae: Stellar Explosions in Three Dimensions (Tomasz Plewa, University of Chicago)**

This project was aimed at understanding the mechanism for triggering supernovae. These explosions are one of the brightest events in the universe and supernovae produce the heavy elements essential for formation of planetary systems. Yet after four decades of research, there is still no comprehensive theory does to explain this mechanism. The project team conducted for the first time the most detailed, high-resolution, three-dimensional simulations of the critical initial phase of Type Ia supernova explosions using a self-consistent physical model developed at the ASC Flash Center at the University of Chicago.

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

Although turbulence is a phenomenon that has applications in a wide range of natural and human activities, it is not well understood and is extremely difficult to model accurately on supercomputers. With improved modeling capability of fluid turbulence, scientists will gain greater insight into meteorology, astrophysics, oceanography, environmental quality, combustion and propulsion, among other research areas. Using their INCITE awrd, the team performed the largest simulation of fluid flow turbulence in the U.S., at a level of detail and within a time frame not possible otherwise, effectively re-defining the state of the art in addressing a Grand Challenge problem arising in multiple fields of science and engineering.