The First Two Years of the INCITE Program: 2004 and 2005

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, genetics 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 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. Here is a look at those projects and their accomplishments to date.

2004 INCITE Awards at NERSC

In the first year, INCITE awarded three computational science projects a total of 4.9 million hours of supercomputing time at DOE’s National Energy Research Scientific Computing (NERSC) Center in Berkeley, California. The projects were selected to significantly advance our understanding of the makeup of the universe, the chemical process by which plants convert sunlight to energy while removing carbon dioxide from the atmosphere, and the turbulent forces that affect everything from weather to industrial processes.

“Thermonuclear Supernovae: Stellar Explosions in Three Dimensions,” led by Tomasz Plewa of the Center for Astrophysical Thermonuclear Flashes at the University of Chicago, was awarded 2.7 million processor hours. This project is a collaboration between scientists at the university and at DOE’s Argonne National Laboratory and aims to understand the birth of the thermonuclear explosion leading to a Type Ia supernova. These explosions are one of the brightest events in the universe and supernovae produce the heavy elements essential for formation of planetary systems.

Thermonuclear type Ia supernovae are a very important class of objects, yet after four decades of research their comprehensive theory does not yet exist. A new model for has been.

Using their INCITE allocation, the team was able to conduct for the first time the most detailed, high-resolution, three-dimensional simulations of the critical initial phase of type Ia explosions using a self-consistent physical model that was developed at the ASC Flash Center at the University of Chicago. Numerical simulations seem to agree with the type Ia supernovae model recently proposed by Plewa, Calder and Lamb (2004), and this theory may for the first time self-consistently explain these explosions. These simulations are so computationally intensive that they do require hundreds of thousands of CPU hours per computational run, so, the scale of INCITE grants was essential.

"Fluid Turbulence and Mixing at High Reynolds Number," a project led by Professor P. K. Yeung of the Georgia Institute of Technology, was allocated 1.2 million processor hours. 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.

This INCITE Award has allowed Yeung's group to perform the largest simulation of fluid flow turbulence in the US, 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. Specifically, 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". Yeung reported the results have drawn significant attention from "more than 20 leading scientists in the field have indicated a strong desire to access our database to answer questions that they have long sought to resolve."

"Quantum Monte Carlo Study of Photoprotection via Carotenoids in Photosynthetic Centers," led by William A. Lester, Jr. of DOE's Lawrence Berkeley National Laboratory and the University of California Berkeley, was awarded one million processor hours. This project aims 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. This project is important on several levels. First, plants and bacteria are the world's foremost means of "carbon sequestration," or storing carbon from the atmosphere. Additionally, photosynthesis is an example of fundamental electron chemistry and is an efficient energy transfer system – processes which are fundamental in many areas of scientific research. While commercially available photovoltaic cells in solar panels convert only 9 to 14 percent of the sunlight they absorb into electrical energy, the initial photosynthetic steps of energy and electron transfer in green plants are 97 percent efficient.

Lester's team focused on a specific aspect of this chemical process: if the plant system absorbs too much energy, a form of oxygen may be created which destroys the photosynthetic protein and eventually kills the plant. The goal was to gain 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. The group developed a linear diffusion Monte Carlo method that has high accuracy, scalability, and relative speed. The optimized Zori code now runs 10 times faster than the researchers’ original algorithm, and they are now able to study systems four times larger than those they worked on before the INCITE grant.

2005 INCITE Awards at NERSC

In December 2004, Secretary of Energy Spencer Abraham announced that 6.5 million hours of supercomputing time at NERSC had been awarded to three scientific research projects aimed at gaining greater insight into how stars and solar systems form, increasing our understanding of ways to reduce pollution and advancing our knowledge about how proteins express genetic information.

“Magneto-rotational instability and turbulent angular momentum transport,” a project led by Fausto Cattaneo, University of Chicago, was awarded 2 million processor-hours and will study the forces that help newly born stars and black holes increase in size. In space, gases and other matter often form swirling disks around attracting central objects such as newly formed stars. The presence of magnetic fields can cause the disks to become unstable and develop turbulence, thereby causing the disk material to fall onto the central object. This project carried out large-scale simulations to test theories on how turbulence can develop in such disks.

In recent years, laboratory experiments have been developed to test many aspects of this magnetically caused instability, but on a much smaller scale. The INCITE researchers collaborated with the experimentalists in the field and to develop simulations that can extend the lab experiments by several orders of magnitude.

“Direct Numerical Simulation of Turbulent Non-premixed Combustion – Fundamental Insights towards Predictive Modeling,” a research project by Jacqueline Chen and Evatt Hawkes of Sandia National Laboratories in Livermore, Calif., was awarded 2.5 million processor-hours. The researchers performed detailed three-dimensional combustion simulations of flames in which fuel and oxygen are not premixed. By better understanding the details of such flames, the researchers hope to gain insight into reducing pollutants and increasing efficiency in combustion devices. This research could have applications in such areas as jet aircraft engines, where fuel and oxidizers are not premixed for safety reasons, and in direct-injection internal combustion engines. Under certain conditions, this type of combustion can be extinguished, and this project will also try to gain a better understanding of this problem, as well as re-ignition of extinguished flames. The project seeks to develop direct numerical simulations of a turbulent nonpremixed flame that will serve as a benchmark for future theory and experiment.

“Molecular Dynameomics” by Valerie Daggett of the University of Washington was awarded 2 million processor-hours. The project combines molecular dynamics and proteomics to create an extensive repository of the molecular dynamics structures for protein folds, including the unfolding pathways. According to Daggett, there are approximately 1,130 known, non-redundant protein folds, of which her group has simulated about 30. She plans to use the information from these simulations to improve algorithms for predicting protein structure.

“Structure prediction remains one of the elusive goals of protein chemistry,” Daggett wrote in her INCITE proposal. “It is necessary to successfully predict native states of proteins, in order to translate the current deluge of genomic information into a form appropriate for better functional identification of proteins and drug design.”