

U.S. Department of Energy



Office of Science

Advanced Scientific Computing Research Program

Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Update

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August 14, 2007



Background

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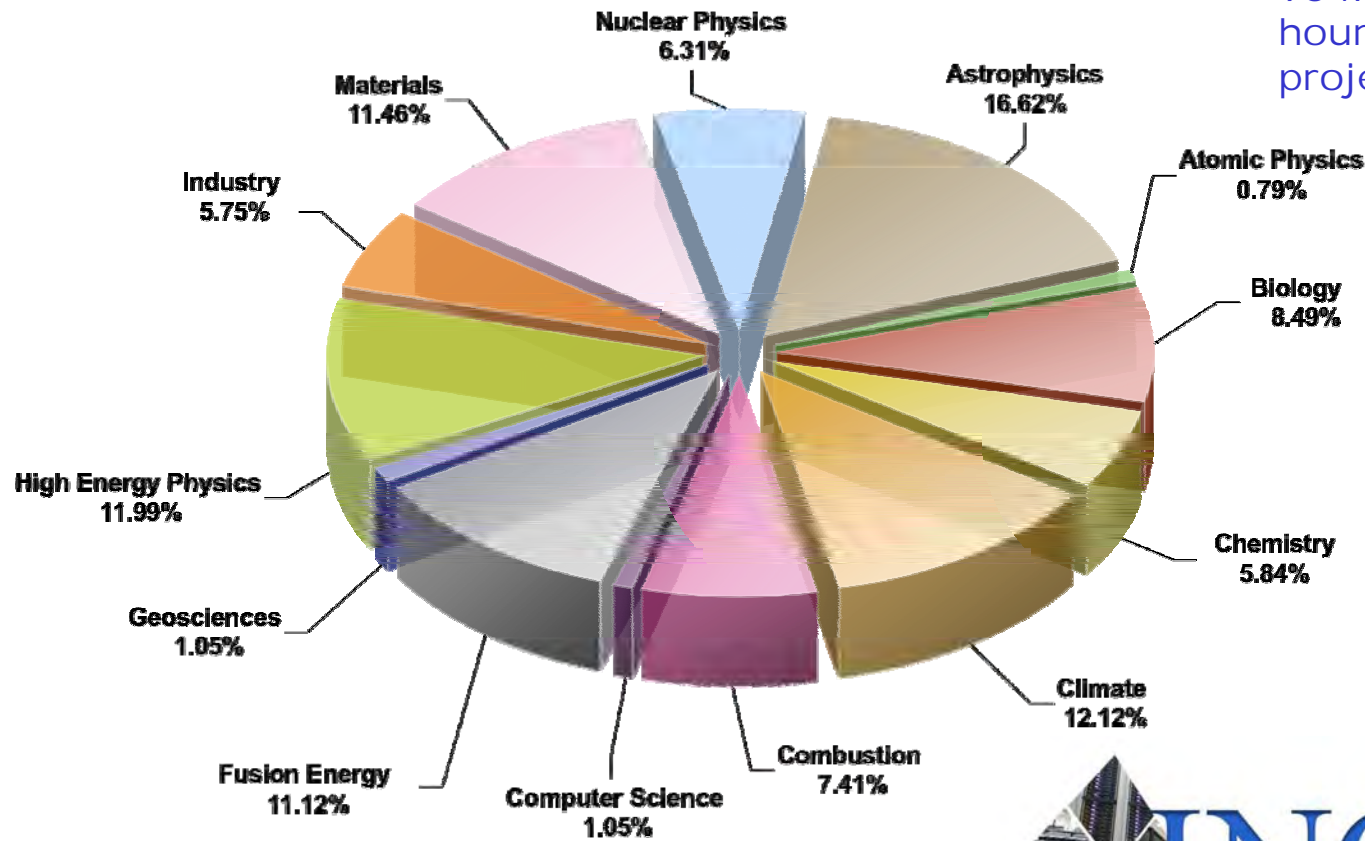
- Provides Office of Science computing resources to a small number of computationally intensive research projects of large scale, that can make high-impact scientific advances through the use of a large allocation of computer time and data storage
- Open to national and international researchers, including industry
- No requirement of DOE Office of Science funding
- Peer and computational reviews
- Initiated at National Energy Scientific Computing Center (NERSC) at LBNL in 2004
- Expanded in 2006, includes portions of Office of Science high performance computing (HPC) resources at ANL, LBNL, ORNL and PNNL
- 80% of resources at Leadership Computing Facilities at ANL and ORNL are allocated through INCITE program



2007 INCITE Allocations by Disciplines

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95 Million processor hours allocate to 45 projects



Factsheets available at <http://www.science.doe.gov/ascr/incite>



Climate Scientists on Cloud 9 (or 3.5)

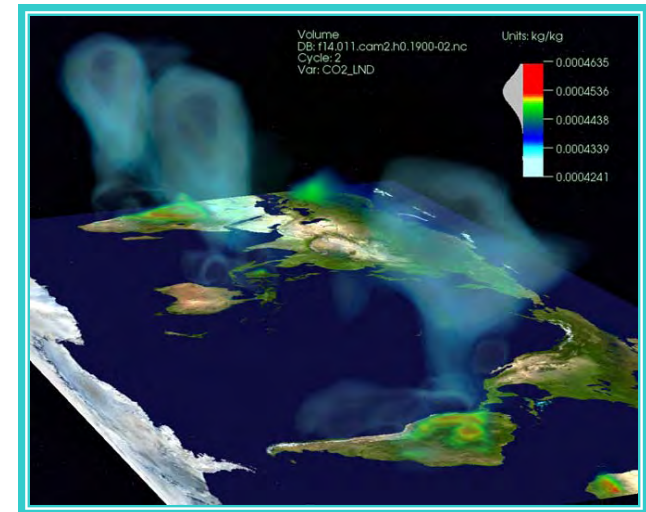
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- **First-ever control runs of CCSM 3.5 at groundbreaking speed**

“[On Jaguar,] we got 100-year runs in three days. This was a significant upgrade of how we do science with this model. 40 years per day was out of our dreams.”

Peter Gent of NCAR, Chairman of CCSM Scientific Steering Committee, during keynote at CCSM Workshop, June 19, 2007

- **Major improvements in CCSM 3.5**
 - Arctic and Antarctic sea ice: Will the Arctic be ice free in summer of 2050?
 - Surface hydrology of land, critical for predictions of drought
- **Positioned to test full carbon-nitrogen cycle**



Simulated time evolution of the atmospheric CO₂ concentration originating from the land's surface

“The most impressive new result in ten years.”

**Peter Gent, NCAR, on
El Niño/Southern Oscillation**

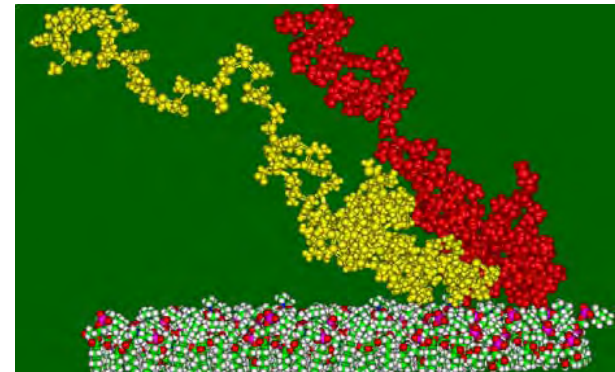
INCITE PI: Warren Washington, National Center for Atmospheric Research



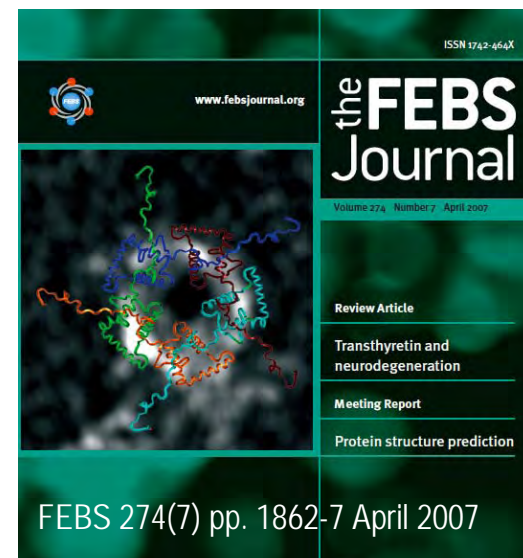
Modeling of Protofibril Structures Provides Insight into Molecular Basis of Parkinson's Disease

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- 2007 INCITE Project at ALCF
- PI: Igor Tsigelny, UCSD
- Parkinson's Disease is the 2nd most common adult neurological disease
- Increased aggregation of *alpha-synuclein* protein is thought to lead to harmful pore-like structures in human membranes
- UCSD - SDSC team used molecular modeling and molecular dynamics simulations in combination with biochemical and ultrastructural analysis to show that *alpha-synuclein* can lead to the formation of pore-like structures on membranes
- Used NAMD and MAPAS on Blue Gene/L at ALCF and SDSC



Above - formation of alpha-synuclein dimer on a membrane, aggregating toward the pentamer pore structure - below.



Early INCITE Successes for 2007

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- PI: Don Lamb, University of Chicago's Center for Astrophysical Thermonuclear Flashes
- First 3-dimensional detonation of white dwarf
- NERSC support for
 - Tuning the FLASH code for memory use to correct an error condition
 - Tuning and debugging the global tropospheric circulation analysis code
 - Adding multi-level parallelism to bundle several associated parallel jobs

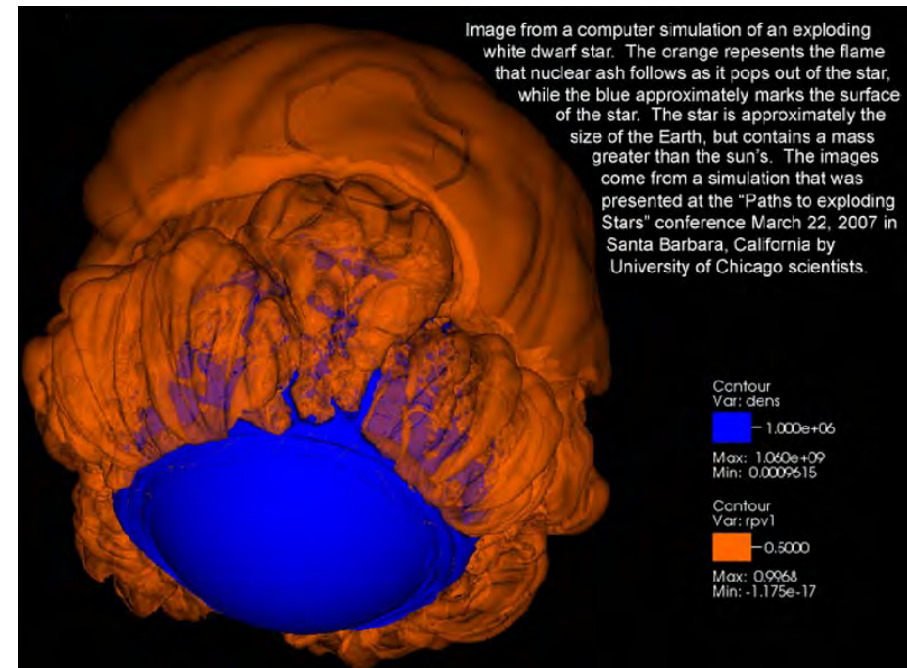


Image courtesy of Cal Jordan/University of Chicago Flash Team

"We could not have asked for better or more support than we got from the folks at NERSC, in helping us to get on the NERSC machines quickly, in giving the job special status, and in helping us meet the challenges of running a large job on Bassi."

Don Lamb, University of Chicago's Center for Astrophysical Thermonuclear Flashes



Timeline for 2008 Awards

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- RFP for new proposal released: May 16, 2007
- Solicitation closed : August 10, 2007
- Renewal proposals due : September 5, 2007
- Computational Readiness review: August-September, 2007
- Panel Reviews: October 15-19, 2007
- Awards Announced: December, 2007
- Allocations start: January, 2008