

## Small Allocations Committee for NCSA Award Report (for July-September 2003)

Submission dates starting from 7/1/2003 and ending on 9/30/2003.

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**Principal Investigator:** Robert D. Bach  
**Institution:** Univ of Delaware  
**Proposal Number:** CHE030085  
**Proposal Type:** New  
**Proposal Title:** The Mechanism of Oxygen Atom Transfer

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** S. Balachandar  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** ASC030039  
**Proposal Type:** New  
**Proposal Title:** International collaboration on Grid Computing

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000  
NCSA IA32 Linux Supercluster 5,000

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**Principal Investigator:** Alvin Bayliss  
**Institution:** Northwestern Univ  
**Proposal Number:** DMS020022  
**Proposal Type:** Renewal  
**Proposal Title:** A Model for Combustion in Strongly Stratified Environments

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Don Burgess  
**Institution:** Asbury College  
**Proposal Number:** MCB030066  
**Proposal Type:** New  
**Proposal Title:** Exploration of the Reversible Nucleotide Exchange Process in Ras Catalyzed by the Son-of-Sevenless (SOS) enzyme

**Resources(SUs):** **Approved**  
NCSA IA32 Linux Supercluster 10,000

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**Principal Investigator:** Sydney Cameron  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** BIO030009  
**Proposal Type:** New  
**Proposal Title:** Molecular Phylogenetics of Bees

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000  
NCSA IA32 Linux Supercluster 5,000  
NCSA IA64 Linux Supercluster

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**Principal Investigator:** Jian Cao  
**Institution:** Northwestern Univ  
**Proposal Number:** DDM030003  
**Proposal Type:** Renewal  
**Proposal Title:** Adaptive Enrichment Meshfree Simulation and Experimental on Wrinkling and Post-Buckling Analysis

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Kathleen Carley  
**Institution:** Carnegie-Mellon Univ  
**Proposal Number:** SES030010  
**Proposal Type:** New  
**Proposal Title:** BioWar Validation and Analysis on the TeraGrid

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Stephen Downie  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** BIO030010  
**Proposal Type:** New  
**Proposal Title:** Molecular Systematics of the Flowering Plant Family Apiaceae

**Resources(SUs):** **Approved**  
NCSA IBM P690 4,000  
NCSA IA32 Linux Supercluster 3,000  
NCSA IA64 Linux Supercluster 3,000

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**Principal Investigator:** Theodore Einstein  
**Institution:** Univ of Maryland, College Park  
**Proposal Number:** DMR030054  
**Proposal Type:** New  
**Proposal Title:** VASP Calculations on Stepped Surfaces

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Hamidreza Emamipour  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CTS020023  
**Proposal Type:** Renewal  
**Proposal Title:** Simulation of Gas Flow Patterns Through an Activated Carbon Fiber Cloth Adsorption Vessel

**Resources(SUs):** **Approved**  
NCSA IBM P690 0

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**Principal Investigator:** Alessandro Gardini  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** AST030032  
**Proposal Type:** New  
**Proposal Title:** Simulations of hot bubbles in galaxy clusters

**Resources(SUs):** **Approved**  
NCSA IBM P690 0  
NCSA Xeon Linux Supercluster 0

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**Principal Investigator:** Peter Gaspar  
**Institution:** Washington Univ  
**Proposal Number:** CHE020027  
**Proposal Type:** Renewal  
**Proposal Title:** Calculations in Support of Experimental Studies of Highly Reactive Intermediates

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Hua Guo  
**Institution:** Univ of New Mexico  
**Proposal Number:** CHE030077  
**Proposal Type:** New  
**Proposal Title:** Quantum chemical study of proton transfer in proteins

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000  
NCSA IA64 Linux Supercluster 5,000

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**Principal Investigator:** Nivedita Gupta  
**Institution:** Univ of New Hampshire  
**Proposal Number:** CTS030058  
**Proposal Type:** New  
**Proposal Title:** Deformation and Breakup of Viscous Drops in Confined Domains at Finite Reynolds Numbers

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Kenneth Harris  
**Institution:** Rutgers the State Univ  
**Proposal Number:** IBN030006  
**Proposal Type:** New  
**Proposal Title:** Computational Analysis of Neuronal Assembly Activity

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Bruce Hietbrink  
**Institution:** California State Univ, Northridge  
**Proposal Number:** CHE030021  
**Proposal Type:** Renewal  
**Proposal Title:** Theoretical Studies of Organic and Organometallic Reaction Mechanisms

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Paul Hyder  
**Institution:** Univ of Colorado, Boulder  
**Proposal Number:** ATM030012  
**Proposal Type:** New  
**Proposal Title:** Modeling Environment and Atmospheric Discovery

**Resources(SUs):** **Approved**  
NCSA IA32 Linux Supercluster 3,000  
NCSA IA64 Linux Supercluster 3,000

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**Principal Investigator:** Brian Ford Jewett  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** ATM030014  
**Proposal Type:** New  
**Proposal Title:** Ensemble Modeling of Severe Mid-latitude and Tropical Storms

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Harley Johnson  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** MSS030025  
**Proposal Type:** New  
**Proposal Title:** Deformation of 3-D Inverse FCC Photonic Crystal

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000

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**Principal Investigator:** Thomas Junk  
**Institution:** Univ of Louisiana, Monroe  
**Proposal Number:** CHE030084  
**Proposal Type:** New  
**Proposal Title:** Hydrocarbon Acidities in Superheated Aqueous Media

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** S. G. Kapoor  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** DDM030006  
**Proposal Type:** New  
**Proposal Title:** Noise Reduction in High Speed Milling

**Resources(SUs):** **Approved**  
NCSA IBM P690 4,000

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**Principal Investigator:** Dinesh Katti  
**Institution:** North Dakota State Univ  
**Proposal Number:** DMR030048  
**Proposal Type:** New  
**Proposal Title:** Simulation Based Materials Design of Biomimetic Nanocomposites

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Gaurav Khanna  
**Institution:** Univ of Massachusetts, Dartmouth  
**Proposal Number:** PHY030021  
**Proposal Type:** New  
**Proposal Title:** Studies in Black Hole Perturbation Theory

**Resources(SUs):** **Approved**  
NCSA IBM P690 1,000

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**Principal Investigator:** Yu Yu Khine  
**Institution:** Univ of Alabama, Huntsville  
**Proposal Number:** DMR020028  
**Proposal Type:** Renewal  
**Proposal Title:** Modeling of Transport Phenomena during Self-Diffusivity Experiments in Liquids with an Applied Magnetic Field

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Gregory Kobidze  
**Institution:** Michigan State Univ  
**Proposal Number:** ECS010007  
**Proposal Type:** Renewal  
**Proposal Title:** Electromagnetic Scattering from Electrically Large Objects

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** April Kontostathis  
**Institution:** Ursinus College  
**Proposal Number:** IRI030006  
**Proposal Type:** New  
**Proposal Title:** Advanced Experiments using LSI and term co-occurrence

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Witold F. Krajewski  
**Institution:** Univ of Iowa  
**Proposal Number:** ATM030017  
**Proposal Type:** New  
**Proposal Title:** Development of Simulation Tools for Automated Selection of Radar Scanning Strategies

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Piotr Krekora  
**Institution:** Illinois State Univ  
**Proposal Number:** PHY000009  
**Proposal Type:** Renewal  
**Proposal Title:** Retardation and Kinematic Relativistic Effects in Scattered Light

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Koung-Hee Leem  
**Institution:** Southern Illinois Univ, Edwardsville  
**Proposal Number:** DMS030020  
**Proposal Type:** New  
**Proposal Title:** Parallel AMG for Meshfree Discretizations

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Yong Liu  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** ASC030024  
**Proposal Type:** Renewal  
**Proposal Title:** GRID-BLAST

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Edward Lorance  
**Institution:** Vanguard Univ of Southern California  
**Proposal Number:** CHE030079  
**Proposal Type:** New  
**Proposal Title:** Iron-Sulfur-Tin Hydrogenase Complexes

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** David Lowenthal  
**Institution:** Univ of Georgia  
**Proposal Number:** NCR030006  
**Proposal Type:** New  
**Proposal Title:** CC--MPI: A Compiled Communication Capable MPI Prototype for Ethernet Switched Clusters

**Resources(SUs):** **Approved**  
NCSA IA32 Linux Supercluster 10,000

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**Principal Investigator:** Francois Lutzoni  
**Institution:** Duke Univ  
**Proposal Number:** DEB030017  
**Proposal Type:** New  
**Proposal Title:** Cyanobacteria/AFTOL

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Paul Marshall  
**Institution:** Univ of North Texas  
**Proposal Number:** CHE000015  
**Proposal Type:** Renewal  
**Proposal Title:** Radical Chemistry in Combustion

**Resources(SUs):** **Approved**  
NCSA IBM P690 8,000

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**Principal Investigator:** Alberto Martinez  
**Institution:** Univ of South Carolina  
**Proposal Number:** DMR030051  
**Proposal Type:** New  
**Proposal Title:** Crystal structure of self-assembled dilithium-phthalocyanine

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Greg McFarquhar  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** ATM030016  
**Proposal Type:** New  
**Proposal Title:** Three Dimensional Modeling Simulations of Trade Wind Cumuli in Indian Ocean

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Michael Miksis  
**Institution:** Northwestern Univ  
**Proposal Number:** DMS010008  
**Proposal Type:** Renewal  
**Proposal Title:** Dynamics of Interfaces

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Fady Najjar  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CTS030065  
**Proposal Type:** New  
**Proposal Title:** Parallelization of a Navier-Stokes Solver for Particle-Wall Interactions in Multiphase Flows

**Resources(SUs):** **Approved**  
NCSA IBM P690 0

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**Principal Investigator:** Saroj K. Nayak  
**Institution:** Rensselaer Polytechnic Institute  
**Proposal Number:** PHY030024  
**Proposal Type:** New  
**Proposal Title:** Theoretical Study of Interaction of Atoms and Small Molecules with Carbon Nanotu

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Mark Neyrinck  
**Institution:** Univ of Colorado, Boulder  
**Proposal Number:** AST010015  
**Proposal Type:** Renewal  
**Proposal Title:** Redshift Survey Galaxies From CDM N-Body Simulations

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Mark R. Nimlos  
**Institution:** Colorado School of Mines  
**Proposal Number:** CHE010026  
**Proposal Type:** Renewal  
**Proposal Title:** Electronic Structure Calculations in Renewable Energy

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Serdar Ogut  
**Institution:** Univ of Illinois, Chicago  
**Proposal Number:** DMR030053  
**Proposal Type:** New  
**Proposal Title:** Pt Clusters on TiO<sub>2</sub> (110) Surface

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Ranjit Pati  
**Institution:** Rensselaer Polytechnic Institute  
**Proposal Number:** DMR020005  
**Proposal Type:** Renewal  
**Proposal Title:** Multiscale Modeling of Nanoelectronic Devices

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Eric Patterson  
**Institution:** Truman State University  
**Proposal Number:** CHE030088  
**Proposal Type:** New  
**Proposal Title:** Ab Initio Molecular Dynamics on the Ring Opening of Phenylcarbene

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Neil Pearson  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** SES030007  
**Proposal Type:** New  
**Proposal Title:** Conditional Estimation of Diffusion Processes

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** James C. Phillips  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** MCB010023  
**Proposal Type:** Renewal  
**Proposal Title:** NAMD---Scalable Molecular Dynamics support and maintenance

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Trevor David Power  
**Institution:** University of Texas Medical Branch  
**Proposal Number:** MCB030067  
**Proposal Type:** New  
**Proposal Title:** Computational Elucidation of the Human Apurinic/Apyrimidinic Endonuclease 1-DNA Mechanism

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Mark J. Rood  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CTS030056  
**Proposal Type:** New  
**Proposal Title:** Microwave regeneration of Activated Carbon Fiber Cloth

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Nikolai Roussanov  
**Institution:** Univ of Chicago  
**Proposal Number:** CDA030003  
**Proposal Type:** New  
**Proposal Title:** Numerical Approach to Human Capital and Financial Investment,

**Resources(SUs):** **Approved**  
NCSA IBM P690 0

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**Principal Investigator:** Taher Saif  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CTS030063  
**Proposal Type:** New  
**Proposal Title:** Numerical Analysis of the Fluid Flow Between two Micro Mechanical Beams

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Vivek Sarin  
**Institution:** Texas A & M Univ  
**Proposal Number:** CCR000005  
**Proposal Type:** Renewal  
**Proposal Title:** Advanced Parallel Algorithms for Sub-Micron VLSI Design

**Resources(SUs):** **Approved**  
NCSA IBM P690 7,500  
NCSA IA64 Linux Supercluster 2,500

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**Principal Investigator:** Edmund Seebauer  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CTS010016  
**Proposal Type:** Renewal  
**Proposal Title:** Surface Diffusion during Nanolithography of Amorphous Semiconductors

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Huseyin Sehitoglu  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** MSS010014  
**Proposal Type:** Renewal  
**Proposal Title:** Modeling of Fatigue Crack Closure under Contact Loading

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Petros Sofronis  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** MSS020007  
**Proposal Type:** Renewal  
**Proposal Title:** Micromechanics of Damage in Solid Propellants

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000

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**Principal Investigator:** Petros Sofronis  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** MSS020008  
**Proposal Type:** Renewal  
**Proposal Title:** A Dislocation Mechanics Approach to the Study of Void Growth in Stressed Solids

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000

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**Principal Investigator:** Yan Solihin  
**Institution:** North Carolina State Univ, Raleigh  
**Proposal Number:** CCR030023  
**Proposal Type:** New  
**Proposal Title:** Dynamically Monitoring and Adapting Dynamically Monitoring and Adapting High-Performance Scientific Applications

<b>Resources(SUs):</b>	<b>Approved</b>
NCSA IBM P690	5,000
NCSA IA32 Linux Supercluster	5,000

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**Principal Investigator:** Jiming Song  
**Institution:** Iowa State Univ  
**Proposal Number:** ECS030008  
**Proposal Type:** New  
**Proposal Title:** Fast Electromagnetic Simulations for Interconnects

<b>Resources(SUs):</b>	<b>Approved</b>
NCSA IBM P690	2,000
NCSA IA32 Linux Supercluster	500

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**Principal Investigator:** Jonathan E. Stevens  
**Institution:** University of Detroit Mercy  
**Proposal Number:** CHE030074  
**Proposal Type:** New  
**Proposal Title:** Ultraviolet Absorption Spectrum of a Stable Organic Diradical

<b>Resources(SUs):</b>	<b>Approved</b>
NCSA IBM P690	10,000

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**Principal Investigator:** Andrew Streitwieser  
**Institution:** Univ of California, Berkeley  
**Proposal Number:** CHE030073  
**Proposal Type:** New  
**Proposal Title:** Carbon Acidity

<b>Resources(SUs):</b>	<b>Approved</b>
NCSA IBM P690	10,000

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**Principal Investigator:** Wilfred van der Donk  
**Institution:** Univ of Illinois, Urbana  
**Proposal Number:** CHE030087  
**Proposal Type:** New  
**Proposal Title:** Theoretical Studies on the Mechanism of Formation and Consumption of Vinylcobalamins Involved in the Vitamin B12-Catalyzed Reductive Dechlorination of Chlorinated Ethylenes

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Yixuan Wang  
**Institution:** Univ of South Carolina  
**Proposal Number:** CHE030082  
**Proposal Type:** New  
**Proposal Title:** Competition of Lithium Cation Affinities in Polymer Electrolyte

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Larry Weber  
**Institution:** Univ of Iowa  
**Proposal Number:** DEB030015  
**Proposal Type:** New  
**Proposal Title:** Prediction of the total dissolved gas (TDG) downstream of spillways

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Evan Williams  
**Institution:** Univ of California, Berkeley  
**Proposal Number:** CHE020062  
**Proposal Type:** Renewal  
**Proposal Title:** Structure of Hydrated Amino Acid-Cation Complexes

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Robert Williams  
**Institution:** Uniformed Services University of Health Sciences  
**Proposal Number:** DMR030057  
**Proposal Type:** New  
**Proposal Title:** Accurate Potential Functions for Proteins

**Resources(SUs):** **Approved**  
NCSA IBM P690 5,000

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**Principal Investigator:** Matt A. Wood  
**Institution:** Florida Institute of Technology  
**Proposal Number:** AST010008  
**Proposal Type:** Renewal  
**Proposal Title:** Parallelizing an SPH Accretion Disk Code

**Resources(SUs):** **Approved**  
NCSA IBM P690 10,000

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**Principal Investigator:** Judith Yang  
**Institution:** Univ of Pittsburgh  
**Proposal Number:** DMR030056  
**Proposal Type:** New  
**Proposal Title:** Simulation of the Nanoscale Oxidation Behavior

**Resources(SUs):** **Approved**  
NCSA IBM P690 6,000

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**Principal Investigator:** Kathy Yelick  
**Institution:** Univ of California, Berkeley  
**Proposal Number:** CTS030061  
**Proposal Type:** New  
**Proposal Title:** Immersed Boundary Simulations in Titanium

**Resources(SUs):** **Approved**  
NCSA IA64 Linux Supercluster 10,000

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**Principal Investigator:** Dahai Yu  
**Institution:** SUNY Stony Brook  
**Proposal Number:** DMS990000  
**Proposal Type:** Renewal  
**Proposal Title:** Numerical Investigation of Turbulent Bluff-Body Flows and Elsto-Plastic Deformations

<b>Resources(SUs):</b>	<b>Approved</b>
NCSA IBM P690	7,000
NCSA IA32 Linux Supercluster	3,000