

Development Allocation Committee for NCSA Award Report

Submission dates starting from September 24, 2003 and ending on April 9, 2004.

Principal Investigator: John Abraham
Institution: Purdue Univ
Proposal Number: CTS040004
Proposal Type: New
Proposal Title: Lattice Boltzmann Simulations of Liquid Breakup

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

Principal Investigator: David Angulo
Institution: DePaul Univ
Proposal Number: ASC040012
Proposal Type: New
Proposal Title: Illinois Bio-Grid Workbench

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

Principal Investigator: Aniket Bhattacharya
Institution: University of Central Florida
Proposal Number: DMR040007
Proposal Type: New
Proposal Title: Simulation Studies of Soft Condensed Matter Systems

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

Principal Investigator: Eric Blackman
Institution: Univ of Rochester
Proposal Number: PHY040015
Proposal Type: New
Proposal Title: Particle Acceleration from Poynting Flux Outflows and Application to Gamma-Ray Bursts

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

Principal Investigator: Mihaela Bojin
Institution: Univ of California, Davis
Proposal Number: CHE040006
Proposal Type: New
Proposal Title: Supramolecular Stabilization of Biologically Relevant Nonclassical Carbocations

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

Principal Investigator: Brian Borchers
Institution: New Mexico Inst of Mining and Tech
Proposal Number: DMS040023
Proposal Type: New
Proposal Title: A Parallel Implementation of a Primal--Dual Interior Point Method for SDP

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

Principal Investigator: Tyler E. Bruns
Institution: Univ of Illinois, Urbana
Proposal Number: MSS040018
Proposal Type: New
Proposal Title: Toward the systematic design of MEM devices

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

Principal Investigator: Philip H. Bucksbaum
Institution: Univ of Michigan
Proposal Number: PHY040004
Proposal Type: New
Proposal Title: Quantum Propagation Simulations on Ring-opening Reactions

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

Principal Investigator: Kirk Cameron
Institution: Univ of South Carolina
Proposal Number: ASC030009
Proposal Type: Renewal
Proposal Title: Memory-conscious, high-performance scientific applications

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

Principal Investigator: Dae-Il Choi
Institution: NASA Goddard Space Flight Center
Proposal Number: PHY040001
Proposal Type: New
Proposal Title: Simulations of the Strong Field Dynamics in Computational Relativity

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

Principal Investigator: Rodney J. Clifton
Institution: Brown Univ
Proposal Number: MSS040011
Proposal Type: New
Proposal Title: Shear Band Propagation from a Crack Subjected to Mode II or Mode III Loading

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

Principal Investigator: George Constantinescu
Institution: Univ of Iowa
Proposal Number: CTS040014
Proposal Type: New
Proposal Title: Prediction of the Unsteady Horseshoe Vortex System and Wake for the Flow Over Surface-Mounted Cylinders Using Eddy-Resolving Techniques

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

Principal Investigator: Suchuan Dong
Institution: Brown Univ
Proposal Number: CTS040028
Proposal Type: New
Proposal Title: DNS of flow past an oscillating rigid cylinder at high Reynolds numbers

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

Principal Investigator: Charles Doubleday
Institution: Columbia Univ
Proposal Number: CHE040010
Proposal Type: New
Proposal Title: Dynamics of Gas Phase Organic Reactions

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

Principal Investigator: Horacio Espinosa
Institution: Northwestern Univ
Proposal Number: MSS040002
Proposal Type: New
Proposal Title: Multiscale Modeling of Nanomaterials and Micro/Nano devices

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

Principal Investigator: Barry Friedman
Institution: Sam Houston State University
Proposal Number: DMR040011
Proposal Type: New
Proposal Title: Density Matrix Renormalization Group Studies of Quantum Hall Systems

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

Principal Investigator: Marcelo Garcia
Institution: Univ of Illinois, Urbana
Proposal Number: CTS020030
Proposal Type: Renewal
Proposal Title: Environmental Multiphase Flow Modeling

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

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 10,000 10,000

Principal Investigator: Matt Gilmore
Institution: Univ of Illinois, Urbana
Proposal Number: ATM040009
Proposal Type: New
Proposal Title: Simulations of Supercell Rear-flank Precipitation and Vorticity Generation

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

Principal Investigator: William Goddard
Institution: California Institute of Technology
Proposal Number: CHE040020
Proposal Type: New
Proposal Title: Ab initio Studies of Water Cluster Structure and Energetics

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

Principal Investigator: Paul Goldbart
Institution: Univ of Illinois, Urbana
Proposal Number: DMR040020
Proposal Type: New
Proposal Title: Electronic structure of exotic magnets

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

Principal Investigator: Indranil Gupta
Institution: Univ of Illinois, Urbana
Proposal Number: CCR040006
Proposal Type: New
Proposal Title: Experiments to study the Reliability and Scalability of Communication Protocols for Large-Scale Distributed Systems

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

Principal Investigator: Pradeep Gutta
Institution: Univ of California, Davis
Proposal Number: CHE040005
Proposal Type: New
Proposal Title: Computational Study of the Cyclisation of Farnesyl Pyrophosphate

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

Principal Investigator: Rami M. Haj-Ali
Institution: Georgia Institute of Technology
Proposal Number: MSS040007
Proposal Type: New
Proposal Title: Cohesive Fracture Modeling in Thick-Section Composites

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

Principal Investigator: Murad Hamidouche
Institution: Univ of Illinois, Urbana
Proposal Number: AST040001
Proposal Type: New
Proposal Title: Simulation of the Interstellar Scintillation and Attempt to Detect Extreme Scattering Events (ESE) in the Direction of the Pulsar B1937+21

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

Principal Investigator: David Hart
Institution: Indiana Univ
Proposal Number: DMS040002
Proposal Type: New
Proposal Title: Support for IU HPC

Resources(SUs): **Approved**
NCSA IBM P690 4,000
NCSA IA64 Linux Supercluster 2,000
NCSA Xeon Linux Supercluster 2,000

Principal Investigator: Louis Hodgson
Institution: Scripps Research Institute
Proposal Number: ASC040010
Proposal Type: New
Proposal Title: p21 Rho GTPase Activity Automatically Correlated to Cell Motility Using Digital Microscopy

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

Principal Investigator: Albert T. Hsui
Institution: Univ of Illinois, Urbana
Proposal Number: EAR040002
Proposal Type: New
Proposal Title: Origin of Surface Plate Rotation on Earth

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

Principal Investigator: Ho-Chun Huang
Institution: Univ of Illinois, Urbana
Proposal Number: ATM040006
Proposal Type: New
Proposal Title: The Continuous Development of an Air Quality Model

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

Principal Investigator: Yonggang Huang
Institution: Univ of Illinois, Urbana
Proposal Number: MSS040014
Proposal Type: New
Proposal Title: Order-N Atomic-scale Finite Element Method in Multiscale Computation

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

Principal Investigator: Gerald J. Iafrate
Institution: North Carolina State Univ, Raleigh
Proposal Number: PHY040007
Proposal Type: New
Proposal Title: Gain Mechanism in Molecular Electronic Systems

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

Principal Investigator: James Ianni
Institution: Univ of Pennsylvania
Proposal Number: CHE040031
Proposal Type: New
Proposal Title: QQSAR in the Asymmetric Lithiation/Substitution of Boc-pPyrrolidine

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

Principal Investigator: Kevin Johnson
Institution: Illinois State Natural History Survey
Proposal Number: DEB040001
Proposal Type: New
Proposal Title: Phylogenetic Relationships of Lice (Insecta: Phthiraptera)

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

Principal Investigator: S. G. Kapoor
Institution: Univ of Illinois, Urbana
Proposal Number: DDM040002
Proposal Type: New
Proposal Title: Analysis of Tool Chipping Mechanisms in Metal Cutting Process

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

Principal Investigator: Hyungson Ki
Institution: Michigan State Univ
Proposal Number: DDM040007
Proposal Type: New
Proposal Title: Numerical Simulation of Laser Hybrid Welding Process

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

Principal Investigator: Diego Klabjan
Institution: Univ of Illinois, Urbana
Proposal Number: DDM040005
Proposal Type: New
Proposal Title: Integrated Airline Planning

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

Principal Investigator: Brent Krueger
Institution: Hope College
Proposal Number: CHE010051
Proposal Type: Renewal
Proposal Title: Evaluating the accuracy of fluorescence-detected resonance energy transfer (FRET) experiments by evaluating the breakdown of the ideal dipole approximation

Resources(SUs): **Approved**
NCSA IBM P690 2,000
NCSA IA64 Linux Supercluster 8,000

Principal Investigator: Peter Kurath
Institution: Univ of Illinois, Urbana
Proposal Number: MSS040013
Proposal Type: New
Proposal Title: Evolution and Relaxation of Welding Residual Stresses

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

Principal Investigator: James LaFave
Institution: Univ of Illinois, Urbana
Proposal Number: BCS040002
Proposal Type: New
Proposal Title: Investigation of the Seismic Vulnerability of Wall Pier Supported Bridges on Priority Emergency Routes in Southern Illinois

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

Principal Investigator: Zhiling Lan
Institution: Illinois Institute of Technology
Proposal Number: CCR030012
Proposal Type: Renewal
Proposal Title: Exploring Large-scale Adaptive Applications on Distributed Terascale Facilities

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

Principal Investigator: Ronald G. Larson
Institution: Univ of Michigan
Proposal Number: DMR040025
Proposal Type: New
Proposal Title: Primitive Path Calculations in Entangled Polymers

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

Principal Investigator: Chaodi Li
Institution: Univ of Notre Dame
Proposal Number: BCS040001
Proposal Type: New
Proposal Title: Finite Element Thermal Evaluations of Femoroplasty for Osteoporitic Proximal Femur

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

Principal Investigator: Shuqing Li
Institution: Univ of Illinois, Urbana
Proposal Number: ASC040003
Proposal Type: New
Proposal Title: Development of a Parallel Time Domain Adaptive Integral Method (TD-AIM)

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

Principal Investigator: Jeff Linderoth
Institution: Lehigh Univ
Proposal Number: DDM040004
Proposal Type: New
Proposal Title: High Performance Computing for Numerical Optimization

Resources(SUs): **Approved**
NCSA IBM P690 1,000
NCSA IA64 Linux Supercluster 9,000

Principal Investigator: Erik Luijten
Institution: Univ of Illinois, Urbana
Proposal Number: DMR040022
Proposal Type: New
Proposal Title: Application of Geometric Cluster Algorithms to Colloidal Systems

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

Principal Investigator: Nancy Ma
Institution: North Carolina State Univ, Raleigh
Proposal Number: DMR030015
Proposal Type: Renewal
Proposal Title: Models of Segregation during Semiconductor Crystal Growth with Magnetic and Electric Fields

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

Principal Investigator: Patrick McDonald
Institution: Princeton Univ
Proposal Number: AST040012
Proposal Type: New
Proposal Title: Interpreting Lyman-alpha forest data from the Sloan Digital Sky Survey

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

Principal Investigator: John B. McLaughlin
Institution: Clarkson Univ
Proposal Number: CTS040020
Proposal Type: New
Proposal Title: Transport Phenomena in Multiphase Processes

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

Principal Investigator: Adrian L. Melott
Institution: Univ of Kansas
Proposal Number: AST980012
Proposal Type: Renewal
Proposal Title: The Bulls -Eye Effect, Large-Scale Structure, and the Mass Density of the Universe

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

Principal Investigator: Shelley Minter
Institution: Saint Louis Univ
Proposal Number: DMR040010
Proposal Type: New
Proposal Title: Modeling Spin and Charge Density Delocalization in Fuel Cell Catalyst Adsorbate Systems

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

Principal Investigator: David Morse
Institution: Univ of Minnesota, Minneapolis
Proposal Number: DMR040017
Proposal Type: New
Proposal Title: Computational Polymer Physics

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

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 10,000

Principal Investigator: Ty Newell
Institution: Univ of Illinois, Urbana
Proposal Number: CTS040025
Proposal Type: New
Proposal Title: Investigation of Laminar Flow in microgrooves

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

Principal Investigator: E. Irene Newhouse
Institution: Univ of New Mexico
Proposal Number: CHE020006
Proposal Type: Renewal
Proposal Title: Monte Carlo Simulations of Dendrimers in Solution

Resources(SUs): **Approved**
NCSA IBM P690 1,356

Principal Investigator: James Newhouse
Institution: Maui High Performance Computing Center
Proposal Number: CHE040029
Proposal Type: New
Proposal Title: Computational Proteomics on Extremophile Globular Proteins

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

Principal Investigator: Eve Ostriker
Institution: Univ of Maryland, College Park
Proposal Number: AST040005
Proposal Type: New
Proposal Title: 3D MHD Simulations of Structure and Evolution in the Interstellar Medium

Resources(SUs): **Approved**
NCSA IBM P690 7,000
NCSA Xeon Linux Supercluster 2,900
NCSA IA64 Linux Supercluster 100

Principal Investigator: Daniel Pack
Institution: Univ of Illinois, Urbana
Proposal Number: CTS040005
Proposal Type: New
Proposal Title: A Monte Carlo Based Model of Drug Release from Polymer Microspheres

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

Principal Investigator: R. Varkki Pallathucheril (George)
Institution: Univ of Illinois, Urbana
Proposal Number: CDA040012
Proposal Type: New
Proposal Title: Land-use Evolution and Impact Assessment Model (LEAM)

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

Principal Investigator: Dimitrios Papavassiliou
Institution: Univ of Oklahoma
Proposal Number: CTS040023
Proposal Type: Renewal
Proposal Title: RENEWAL PSN omq: COMPLEX TRANSPORT PROCESSES

Resources(SUs): NCSA IBM P690 **Approved**
9,500

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): NCSA IBM P690 **Approved**
10,000

Principal Investigator: James C. Phillips
Institution: Univ of Illinois, Urbana
Proposal Number: MCB010023
Proposal Type: Renewal
Proposal Title: NAMD Tuning and Support

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

Principal Investigator: Prasad L. Polavarapu
Institution: Vanderbilt Univ
Proposal Number: CHE040018
Proposal Type: New
Proposal Title: Quantum mechanical predictions of chiroptical properties

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

Principal Investigator: Tatyana Polenova
Institution: Univ of Delaware
Proposal Number: CHE020069
Proposal Type: Renewal
Proposal Title: Investigation of Chemical Shielding and Electric Field Gradients in Vanadium-Substituted Polyoxometalate Solids of Keggin and Wells -Dawson Families

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

Principal Investigator: Alric Rothmayer
Institution: Iowa State Univ
Proposal Number: CTS040008
Proposal Type: New
Proposal Title: Direct Numerical Simulation of Flow over Small-scale Leading Edge Surface Roughness

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

Principal Investigator: Kazuhiro Saitou
Institution: Univ of Michigan
Proposal Number: MSS040006
Proposal Type: New
Proposal Title: Design Optimization of Vehicle Structures for Crashworthiness via Equivalent Mechanism Approximations

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

Principal Investigator: Thomas Siegmund
Institution: Purdue Univ
Proposal Number: MSS040004
Proposal Type: New
Proposal Title: Numerical Simulation Fatigue Crack Growth in Multilayer Structures

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

Principal Investigator: Jean M. Standard
Institution: Illinois State Univ
Proposal Number: CHE040004
Proposal Type: New
Proposal Title: Modeling Interactions of Sulfur Oxides on Ice Surfaces

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

Principal Investigator: Robert F. Stein
Institution: Michigan State Univ
Proposal Number: AST030008
Proposal Type: Renewal
Proposal Title: Realistic Solar Magneto-Convection Simulations

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

Principal Investigator: Douglas Strout
Institution: Alabama State Univ
Proposal Number: CHE030041
Proposal Type: Renewal
Proposal Title: Thermodynamic and Kinetic Stability of High-Energy Nitrogen-Containing Molecules

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

Principal Investigator: Xian-He Sun
Institution: Illinois Institute of Technology
Proposal Number: ASC040002
Proposal Type: Renewal
Proposal Title: Adaptive Wavelet Element Method for Highly Parallel Computations

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

Principal Investigator: Christos George Takoudis
Institution: Univ of Illinois, Chicago
Proposal Number: DMR040023
Proposal Type: New
Proposal Title: DFT Studies of Micro- and Nano-Electronic Systems

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

Principal Investigator: Ezgi Taskinoglu
Institution: Rutgers the State Univ
Proposal Number: CTS040030
Proposal Type: New
Proposal Title: Numerical Simulation of Turbulence and Particle dispersion in Deep-Sea

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

Principal Investigator: Ganesh Thiagarajan
Institution: Louisiana State Univ
Proposal Number: MSS040017
Proposal Type: Renewal
Proposal Title: Fracture Simulation of Brittle and Ductile Materials using a VIB Model

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

Principal Investigator: Jeffrey Toney
Institution: Montclair State University
Proposal Number: MCB040030
Proposal Type: New
Proposal Title: Identifying Non-Peptidyl SARS Proteinase Inhibitors using Structure-Aided Design

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

Principal Investigator: Arnaud C. Trouve
Institution: Univ of Maryland, College Park
Proposal Number: CTS030003
Proposal Type: Renewal
Proposal Title: Large-Eddy Simulation of Turbulent Fire Plumes

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

Principal Investigator: George Truskey
Institution: Duke Univ
Proposal Number: BCS040006
Proposal Type: New
Proposal Title: 3D NUMERICAL SIMULATION OF RECEPTOR-MEDIATED LEUKOCYTE ADHESION TO ARTERIAL ENDOTHELIUM

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

Principal Investigator: Wilfred van der Donk
Institution: Univ of Illinois, Urbana
Proposal Number: CHE030087
Proposal Type: Renewal
Proposal Title: Theoretical Investigations into the Intermediacy of Chlorinated Vinyl Cobalamins in the Reductive Dehalogenation of Chlorinated Ethylenes

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

Principal Investigator: Jan Verschelde
Institution: Univ of Illinois, Chicago
Proposal Number: DMS040019
Proposal Type: New
Proposal Title: Parallel Polynomial Homotopy Continuation

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

Principal Investigator: Amy Walker
Institution: Washington Univ
Proposal Number: DMR040019
Proposal Type: New
Proposal Title: Computational Studies of Molecular Electronic Circuit Components

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

Principal Investigator: Donghai Wang
Institution: Hampton Univ
Proposal Number: ATM020005
Proposal Type: Renewal
Proposal Title: High-resolution Regional 4D Data Assimilation and Tropical Cirrus Cloud Modeling

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

Principal Investigator: Peng Wang
Institution: Indiana Univ
Proposal Number: ASC040004
Proposal Type: New
Proposal Title: System Evaluation

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

Principal Investigator: Richard L. Weaver
Institution: Univ of Illinois, Urbana
Proposal Number: MSS000009
Proposal Type: Renewal
Proposal Title: Guided Waves in Rails

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

Principal Investigator: Jason Weckstein
Institution: Univ of Illinois, Urbana
Proposal Number: DEB040003
Proposal Type: New
Proposal Title: Cophylogenetics of Chewing Lice (Phthiraptera) and Their Associated Avian Hosts (Aves)

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

Principal Investigator: James Whitfield
Institution: Univ of Illinois, Urbana
Proposal Number: DEB030011
Proposal Type: Renewal
Proposal Title: Phylogenetics of Braconid Parasitoid Wasps and Their Symbiotic Viruses

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

Principal Investigator: Walter M. Wilcox
Institution: Baylor Univ
Proposal Number: PHY040016
Proposal Type: New
Proposal Title: Hadron Structure, Deflation Algorithms, and Lattice QCD

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

Principal Investigator: Michael Wilde
Institution: Argonne Natl Lab
Proposal Number: PHY040008
Proposal Type: New
Proposal Title: GriPhyN Exploratory Application Porting

Resources(SUs): **Approved**
NCSA IA64 Linux Supercluster 2,000
NCSA Xeon Linux Supercluster 2,000

Principal Investigator: Allen Williams
Institution: Univ of Illinois, Urbana
Proposal Number: PHY020012
Proposal Type: Renewal
Proposal Title: Atmospheric Emissions Modeling

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

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

Principal Investigator: Kwai L. Wong
Institution: Univ of Tennessee, Knoxville
Proposal Number: ASC040013
Proposal Type: New
Proposal Title: Parallel Interoperable Computational Mechanics Simulation System

Resources(SUs):	Requested	Approved
NCSA IBM P690	1,000	1,000
NCSA IA64 Linux Supercluster	3,000	3,000
NCSA Xeon Linux Supercluster	7,000	6,000

Reviewers:
Loftis

Principal Investigator: Y. Lawrence Yao
Institution: Columbia Univ
Proposal Number: MSS040012
Proposal Type: New
Proposal Title: Three Dimensional FEM Simulation of Plastic Deformation Induced by Microscale Laser Shock Peening

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

Principal Investigator: Zhan Zhang
Institution: National Institutes of Health
Proposal Number: ASC040014
Proposal Type: New
Proposal Title: Continuum Mechanics Based Colon Straightening for Virtual Colonoscopy

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

Principal Investigator: Huimin Zhao
Institution: Univ of Illinois, Urbana
Proposal Number: MCB040001
Proposal Type: New
Proposal Title: Functional Studies of Human Estrogen Receptor Using Molecular Dynamics Simulation

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