

Development Allocation Committee for NCSA Award Report

Submission dates starting from April 10 and ending July 28, 2004

Principal Investigator: N. R. Aluru
Institution: Univ of Illinois, Urbana
Proposal Number: ECS040008
Proposal Type: New
Proposal Title: Large Scale Molecular Dynamics Simulation of Electroosmotic Transport in Nanometer Channels

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

Principal Investigator: Shanker Balasubramaniam
Institution: Michigan State Univ
Proposal Number: ECS010003
Proposal Type: Renewal
Proposal Title: Development and Application of High Performance Algorithms for Transient Electromagnetic

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

Principal Investigator: Purushotham Bangalore
Institution: Univ of Alabama, Birmingham
Proposal Number: ASC040034
Proposal Type: New
Proposal Title: HOOPLA: A New Linear Algebra Benchmark for High Performance Scalable Computers

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

Principal Investigator: Martin A. Lopez Bertodano
Institution: Purdue Univ
Proposal Number: CTS040038
Proposal Type: New
Proposal Title: TWO-FLUID MODEL LES OF A BUBBLE COLUMN

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

Principal Investigator: Dorothy Bollman
Institution: Univ of Puerto Rico, Mayaguez
Proposal Number: DMS040026
Proposal Type: New
Proposal Title: Reverse Engineering Genetic Networks

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

Principal Investigator: Hector Bravo
Institution: Univ of Wisconsin, Milwaukee
Proposal Number: CTS040042
Proposal Type: New
Proposal Title: Flow Around Ellipses at Low Reynolds Numbers

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

Principal Investigator: Christopher Cartwright
Institution: Lawrence Technological Univ
Proposal Number: ASC040039
Proposal Type: New
Proposal Title: Parallel Quadtree Algorithms for Meshfree Methods

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

Principal Investigator: Junhong Chen
Institution: Univ of Wisconsin, Milwaukee
Proposal Number: CTS040033
Proposal Type: New
Proposal Title: Model of Ozone Production in the DC Corona Discharge of Humid Air

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

Principal Investigator: Joel Conte
Institution: Univ of California, San Diego

Proposal Number: MSS040023
Proposal Type: New
Proposal Title: Finite Element Response Sensitivity Analysis

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

Principal Investigator: Pedro A. Derosa
Institution: Louisiana Tech Univ
Proposal Number: MCB040038
Proposal Type: New
Proposal Title: Effects of Ultra-wide Band Radiation on Biological Systems

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

Principal Investigator: Chris Dietrich
Institution: Univ of Illinois, Urbana
Proposal Number: DEB040005
Proposal Type: New
Proposal Title: Phylogenetic Analyses of Leafhoppers (Insecta: Hemiptera: Cicadellidae)

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

Principal Investigator: Robert H. Dodds Jr.
Institution: Univ of Illinois, Urbana
Proposal Number: MSS030016
Proposal Type: Renewal
Proposal Title: Fracture Mechanics of Advanced Materials

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

Principal Investigator: Joshua A. Faber
Institution: Northwestern Univ
Proposal Number: PHY040023
Proposal Type: New
Proposal Title: Parallel Relativistic SPH Simulations of Collapsing Cores

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

Principal Investigator: Michael Falcetta
Institution: Grove City College
Proposal Number: CHE040036
Proposal Type: New
Proposal Title: Computational Studies of anions, sulfenes, and cobalt complexes

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

Principal Investigator: Miaolin Feng
Institution: Univ of Nevada, Reno
Proposal Number: MSS020010
Proposal Type: Renewal
Proposal Title: Simulation of Cyclic Plasticity of Single Phase Polycrystalline Materials

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

Principal Investigator: Robert A Fiedler
Institution: Univ of Illinois, Urbana
Proposal Number: ASC030027
Proposal Type: Renewal
Proposal Title: Development and Benchmarking of a Whole System Rocket Simulation Code

Resources(SUs) Approved:
NCSA IBM P690 6,000
NCSA Xeon Linux Supercluster 4,000

Principal Investigator: Robert J. Fowler
Institution: Rice Univ
Proposal Number: CCR040013
Proposal Type: New
Proposal Title: Software Technology for the TeraGrid

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

Principal Investigator: Jonathon Gillen
Institution: Harvard Univ

Proposal Number: PHY040028
Proposal Type: New
Proposal Title: Multiple Scattering in Dilute Atomic Samples

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

Principal Investigator: Evelyn M. Goldfield
Institution: Wayne State Univ
Proposal Number: CHE040037
Proposal Type: New
Proposal Title: Interactions of Small Molecules with Single Walled Carbon Nanotubes

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

Principal Investigator: Alan S Goldman
Institution: Rutgers the State Univ
Proposal Number: CHE040045
Proposal Type: New
Proposal Title: Quantum Chemical Investigation of Catalytic Dehydrogenation of Amines by Transition Metal Complexes

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

Principal Investigator: Robert B Haber
Institution: Univ of Illinois, Urbana
Proposal Number: MSS040026
Proposal Type: New
Proposal Title: Parallel Spacetime Discontinuous Galerkin Methods

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

Principal Investigator: Randall Hall
Institution: Louisiana State Univ
Proposal Number: CHE040046
Proposal Type: New
Proposal Title: Molecular Dynamics Simulations of Natural and Synthetic Beta-Sheet Polypeptides

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

Principal Investigator: Thomas J. Hanratty
Institution: Univ of Illinois, Urbana
Proposal Number: CTS030039
Proposal Type: Renewal
Proposal Title: Wall Turbulence

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

Principal Investigator: Gerald Hoffman
Institution: Edinboro Univ of Pennsylvania
Proposal Number: CHE040050
Proposal Type: Renewal
Proposal Title: Ab Initio Investigation of Noble Gas Dihalides

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

Principal Investigator: Jennifer C. Hou
Institution: Univ of Illinois, Urbana
Proposal Number: NCR030001
Proposal Type: Renewal
Proposal Title: A Component-Based Software Environment for Simulating and Synthesizing Network Protocols in Large-Scale Networks

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

Principal Investigator: K. Jimmy Hsia
Institution: Univ of Illinois, Urbana
Proposal Number: DMR030040
Proposal Type: Renewal
Proposal Title: Molecular Dynamics Simulations of Collapse of Carbon Nanotubes

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

Principal Investigator: Hyonseok Hwang
Institution: Northwestern Univ

Proposal Number: MCB040052
Proposal Type: New
Proposal Title: Calculation of Potential of Mean Force of Ions in the Cyclic Peptide Nanotubes

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

Principal Investigator: Anthony Jacobi
Institution: Univ of Illinois, Urbana
Proposal Number: CTS040037
Proposal Type: New
Proposal Title: Air-Side Heat Transfer Research on Highly Interrupted Fin Surfaces

Resources(SUs) Approved:
NCSA IBM P690 7,500

Principal Investigator: Timothy Jenkins
Institution: Syracuse Univ
Proposal Number: CHE040017
Proposal Type: New
Proposal Title: Low Vibrational Frequency Calculations On Biotin, Cysteine, and Serine

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

Principal Investigator: Nicholas Jones
Institution: Univ of Illinois, Urbana
Proposal Number: CTS040034
Proposal Type: New
Proposal Title: Three Dimensional Simulation of the Flow Around the Square Cylinder

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

Principal Investigator: Renu Joseph
Institution: Univ of Maryland, College Park
Proposal Number: ATM040017
Proposal Type: New
Proposal Title: Stationary Wave Changes and Teleconnection Dynamics in the Warmed Climate Scenarios As Represented in the CMIP II Models

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

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

Resources(SUs) Approved:
NCSA IBM P690 2,000

Principal Investigator: Naod Kebede
Institution: Edinboro Univ of Pennsylvania
Proposal Number: CHE040056
Proposal Type: New
Proposal Title: Quantum Chemical Study of Oxynitrenes

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

Principal Investigator: Athol Kemball
Institution: Univ of Illinois, Urbana
Proposal Number: AST030025
Proposal Type: Renewal
Proposal Title: Fidelity Assessment of Astronomical Pipeline Images

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

Principal Investigator: Susan W. Kieffer
Institution: Univ of Illinois, Urbana
Proposal Number: BCS040013
Proposal Type: New
Proposal Title: Numerical Modelling of Explosive Volcanic Eruptions

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

Principal Investigator: Jeongnim Kim
Institution: Univ of Illinois, Urbana
Proposal Number: DMR040033
Proposal Type: New
Proposal Title: Development of Electronic Structure Toolkits

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

Principal Investigator: Viatcheslav Kokoouline
Institution: University of Central Florida
Proposal Number: PHY040022
Proposal Type: New
Proposal Title: Three-body Resonances in Degenerate Quantum Gases

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

Principal Investigator: Timothy Korter
Institution: Syracuse Univ
Proposal Number: CHE040041
Proposal Type: New
Proposal Title: Vibrational Anharmonicity in Solution Phase Molecular Clusters

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

Principal Investigator: Praveen Kumar
Institution: Univ of Illinois, Urbana
Proposal Number: EAR040006
Proposal Type: New
Proposal Title: Analysis of Mositure Recycling using a coupled Land Surface/Regional Climate Model

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

Principal Investigator: Andy LiWang
Institution: Texas A & M Univ
Proposal Number: MCB040043
Proposal Type: New
Proposal Title: Stereoelectronic Nature of Trans-Hydrogen Bond Deuterium Isotope Effects

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

Principal Investigator: Mingyu Lu
Institution: Univ of Illinois , Urbana
Proposal Number: ECS040006
Proposal Type: New
Proposal Title: Development of a Parallel Plane Wave Time Domain (PWTB) Accelerated Solver for the Design of
Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 10,000

Principal Investigator: Qiang Lu
Institution: Univ of California, Irvine
Proposal Number: MCB030023
Proposal Type: Renewal
Proposal Title: The molecular Dynamics Study of Cancer Gaudian Protein:p53
Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 10,000

Principal Investigator: Glenn R. Luecke
Institution: Iowa State Univ
Proposal Number: ASC040033
Proposal Type: New
Proposal Title: NAS Parallel Benchmarks
Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 10,000

Principal Investigator: G. Kumar Mahinthakumar
Institution: North Carolina State Univ, Raleigh
Proposal Number: BCS030004
Proposal Type: Renewal
Proposal Title: Investigation of Parallel Hybrid Optimization Strategies for Solving Groundwater Inverse and Optimization Problems
Resources(SUs) Approved:
NCSA IBM P690 6,000
NCSA Xeon Linux Supercluster 4,000

Principal Investigator: Claudio Margulis
Institution: Univ of Iowa
Proposal Number: CHE030055
Proposal Type: Renewal
Proposal Title: Theoretical and Computational Study of the Interaction of Proteins (Lectins) with Sugars Relevant in

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

Principal Investigator: Pedro Marronetti
Institution: Univ of Illinois, Urbana
Proposal Number: PHY020007
Proposal Type: Renewal
Proposal Title: Neutron Star Binaries

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

Principal Investigator: Jose Martinez
Institution: Cornell Univ
Proposal Number: CCR040017
Proposal Type: New
Proposal Title: Checkpointed Processor Architectures

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

Principal Investigator: Moshe Matalon
Institution: Northwestern Univ
Proposal Number: CTS040040
Proposal Type: New
Proposal Title: A Computational Study of the Nonlinear Dynamics of Hydrodynamically Unstable Premixed Flame

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

Principal Investigator: Sally McKee
Institution: Cornell Univ
Proposal Number: CCR040019
Proposal Type: New
Proposal Title: Toward Autonomous Computing Platforms: System-Wide Hardware/Software Performance Monitoring and Adaptation

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

Principal Investigator: Celso L. Mendes
Institution: Univ of Illinois, Urbana

Proposal Number: CCR040015
Proposal Type: New
Proposal Title: Porting of Pablo Tools

Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 9,000

Principal Investigator: Dmitri Migas
Institution: Univ of Louisville
Proposal Number: DMR040039
Proposal Type: New
Proposal Title: Structural and electronic properties of Si nanowires

Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 9,000

Principal Investigator: Gerald Nelson
Institution: Univ of Illinois, Urbana
Proposal Number: DEB040006
Proposal Type: New
Proposal Title: Modelling Global Land Use: A Spatial Economic Analysis

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

Principal Investigator: Timothy Newman
Institution: Univ of Alabama, Huntsville
Proposal Number: ASC040040
Proposal Type: New
Proposal Title: Out-of-core Isosurface Extraction

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

Principal Investigator: David Nicol
Institution: Univ of Illinois, Urbana
Proposal Number: NCR040001
Proposal Type: New
Proposal Title: Large-Scale Network Simulation

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

Principal Investigator: Richard O'Shaughnessy
Institution: Northwestern Univ
Proposal Number: AST040018
Proposal Type: New
Proposal Title: Exploring the Dependence of Binary Black Hole Merger Rate on Stellar Evolution Parameters

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

Principal Investigator: David A. Padua
Institution: Univ of Illinois, Urbana
Proposal Number: CCR040020
Proposal Type: New
Proposal Title: A Parallel MATLAB Extension Based on Hierarchically Tiled Arrays

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

Principal Investigator: Kara Peters
Institution: North Carolina State Univ, Raleigh
Proposal Number: MSS040027
Proposal Type: New
Proposal Title: Design and Optimization of Minimally Invasive Polymer Sensors for Structural Applications

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

Principal Investigator: John Popovics
Institution: Univ of Illinois, Urbana
Proposal Number: MSS040024
Proposal Type: New
Proposal Title: Time Domain Method for Non-Destructive Determination of Concrete Pavement Thickness

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

Principal Investigator: Avijit Purkayastha
Institution: Univ of Texas, Austin

Proposal Number: CCR040016
Proposal Type: New
Proposal Title: Optimized Collective Communication

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

Principal Investigator: Umberto Ravaioli
Institution: Univ of Illinois, Urbana
Proposal Number: ECS040007
Proposal Type: New
Proposal Title: Parallel Simulation of Terahertz Detectors

Resources(SUs) Approved:
NCSA Xeon Linux Supercluster 9,000

Principal Investigator: John Rogers
Institution: Univ of Illinois, Urbana
Proposal Number: DMR040048
Proposal Type: New
Proposal Title: Microfluidic Fabrication Systems

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

Principal Investigator: Kausik Sarkar
Institution: Univ of Delaware
Proposal Number: CTS040041
Proposal Type: New
Proposal Title: Parallel Computation of Drop Dynamics and Rheology in Concentrated Emulsions

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

Principal Investigator: Kevin Schmidt
Institution: Arizona State Univ
Proposal Number: PHY020009
Proposal Type: Renewal
Proposal Title: Pairing Studies with Quantum Monte Carlo

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

Principal Investigator: Sameer Shende
Institution: Univ of Oregon
Proposal Number: ASC020029
Proposal Type: Renewal
Proposal Title: Evaluating Performance Tool Scalability and Applicability on High-end Parallel Systems

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

Principal Investigator: Jonathan E. Stevens
Institution: University of Detroit Mercy
Proposal Number: CHE040055
Proposal Type: New
Proposal Title: Mechanism of reactions of $\text{CH}_3\text{C}(\text{O})\text{O}_2$ and $\text{C}_x\text{F}_{2x+1}\text{C}(\text{O})\text{O}_2$ ($x=1,2,3,4$) with HO_2

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

Principal Investigator: Sergey Stolbov
Institution: Kansas State Univ
Proposal Number: DMR010003
Proposal Type: Renewal
Proposal Title: First Principles Study of Reactivity of Metal Surfaces.

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

Principal Investigator: Jason Tumlinson
Institution: Univ of Chicago
Proposal Number: AST040023
Proposal Type: New
Proposal Title: Interstellar Processes at Low Metallicity

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

Principal Investigator: Blair Tuttle
Institution: Pennsylvania State Univ

Proposal Number: DMR030010
Proposal Type: Renewal
Proposal Title: Simulations of Electronic Materials

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

Principal Investigator: Mark Voit
Institution: Michigan State Univ
Proposal Number: AST040021
Proposal Type: New
Proposal Title: Entropy Production in Clusters of Galaxies

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

Principal Investigator: Grover Waldrop
Institution: Louisiana State Univ
Proposal Number: MCB040041
Proposal Type: New
Proposal Title: Computational Studies of Reaction Mechanisms of Carbon Dioxide Activation in Acetyl-CoA Carboxylase

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

Principal Investigator: Junmei Wang
Institution: Univ of California, San Francisco
Proposal Number: MCB000017
Proposal Type: Renewal
Proposal Title: Development of a General a Polarizable AMBER Force Field

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

Principal Investigator: Richard Wirtz
Institution: Univ of Nevada, Reno
Proposal Number: CTS040039
Proposal Type: New
Proposal Title: Structurally Efficient Anisotropic Organized Reticulated Structures For Cooling Of Electronics And

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

Principal Investigator: Tian-xiang Xiang
Institution: Univ of Kentucky
Proposal Number: MCB040035
Proposal Type: New
Proposal Title: Computer Simulation of Partition Coefficients and Related Conformation Changes for Small Peptides
Resources(SUs) Approved:
NCSA IBM P690 10,000

Principal Investigator: Dmitry Yandulov
Institution: Stanford Univ
Proposal Number: CHE040040
Proposal Type: New
Proposal Title: Computational Studies of Transition Metal-Catalyzed Fluorination of Organic Substrates
Resources(SUs) Approved:
NCSA IBM P690 3,000

Principal Investigator: Tao Ye
Institution: Univ of Michigan
Proposal Number: BIO030007
Proposal Type: Renewal
Proposal Title: Direct Simulation of Bubble-Induced Blood Vessel Deformation in Gas Embolotherapy
Resources(SUs) Approved:
NCSA IBM P690 10,000

Principal Investigator: Jian Zhang
Institution: Univ of Illinois, Urbana
Proposal Number: BCS040014
Proposal Type: New
Proposal Title: Advanced Simulation Tools for Soil-Structure Interaction Analysis
Resources(SUs) Approved:
NCSA IBM P690 10,000

Principal Investigator: Yong Zhang
Institution: Univ of Illinois, Urbana

Proposal Number: MCB040040
Proposal Type: New
Proposal Title: Ab initio Studies on ^{31}P NMR Chemical Shifts of Biomimetic Pentacoordinate Oxyphosphoranes

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