

Small Allocations Committee for NCSA Award Report

October 01-December 31, 2002

Principal Investigator: Kiran Boggavarapu
Institution: Washington State Univ
Proposal Number: DMR030013
Proposal Type: New
Proposal Title: Magic Numbers in Metal-encapsulated Gold clusters

Resources(SUs):	Approved
NCSA SGI Origin2000	5,000
NCSA IA32 Linux Supercluster	2,500
NCSA IA64 Linux Supercluster	2,500

Principal Investigator: John Robert Burger
Institution: California State Univ, Northridge
Proposal Number: CCR030006
Proposal Type: New
Proposal Title: Quantum Parallelism Simulation

Resources(SUs):	Approved
NCSA SGI Origin2000	10,000

Principal Investigator: Kirk Cameron
Institution: Univ of South Carolina
Proposal Number: ASC030009
Proposal Type: New
Proposal Title: Latency-Based Performance Analysis of Large-Scale Scientific Applications

Resources(SUs):	Approved
NCSA SGI Origin2000	2,000
NCSA IA32 Linux Supercluster	4,000
NCSA IA64 Linux Supercluster	4,000

Principal Investigator: Jian Cao
Institution: Northwestern Univ
Proposal Number: DDM030003
Proposal Type: New
Proposal Title: Wrinkling Prediction

Resources(SUs): **Approved**
NCSA SGI Origin2000 5,000

Principal Investigator: Xuelei Chen
Institution: Univ of California, Santa Barbara
Proposal Number: AST030007
Proposal Type: New
Proposal Title: Simulations in Cosmology and Galaxy Formation Theory

Resources(SUs): **Approved**
NCSA SGI Origin2000 5,000

Principal Investigator: Leon Chua
Institution: Univ of California, Berkeley
Proposal Number: MIP030002
Proposal Type: New
Proposal Title: Analysis of All Universal CNN Von Neumann Templates

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Edward J. Cording
Institution: Univ of Illinois, Urbana
Proposal Number: MSS010003
Proposal Type: Renewal
Proposal Title: Analysis of Ground Movements and Building Response around Deep Excavations in Sand

Resources(SUs): **Approved**
NCSA SGI Origin2000 5,000

Principal Investigator: Thomas R. Cundari
Institution: Univ of North Texas
Proposal Number: CHE030008
Proposal Type: New
Proposal Title: Thermochemistry of Transition Metal Complexes

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Hans De Sterck
Institution: Univ of Colorado, Boulder
Proposal Number: MCB020011
Proposal Type: Renewal
Proposal Title: Taskspaces Framework For Scientific Computing on Computational Grids

Resources(SUs): **Approved**
NCSA SGI Origin2000 5,000
NCSA IA32 Linux Supercluster 5,000

Principal Investigator: Gary DeBoer
Institution: LeTourneau University
Proposal Number: CHE020016
Proposal Type: Renewal
Proposal Title: Carbon Nanotube Precursors

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Jeff Derby
Institution: University of Minnesota, Twin Cities
Proposal Number: CTS030008
Proposal Type: New
Proposal Title: Materials Processing Fundamentals: Large-Scale Simulation of Crystal Growth Processes

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Michael Falcetta
Institution: Roberts Wesleyan College
Proposal Number: CHE000054
Proposal Type: Renewal
Proposal Title: Computational Studies of Temporary Anions

Resources(SUs): **Approved**
NCSA SGI Origin2000 8,000

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: Valentin Gogonea
Institution: Cleveland State Univ
Proposal Number: CHE030010
Proposal Type: New
Proposal Title: OPLS Parameters for Sulfonium ion from ab Initio Calculations

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Shannon Hackett
Institution: Field Museum
Proposal Number: DEB030002
Proposal Type: New
Proposal Title: Early Bird

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: James Hammonds
Institution: CUNY City College
Proposal Number: CTS030011
Proposal Type: New
Proposal Title: Thermal Radiation in Inhomogeneous Microspaces

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Richard T. Hart
Institution: Tulane Univ of Louisiana
Proposal Number: BCS020003
Proposal Type: Renewal
Proposal Title: Super Computing in Biomedical Engineering

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: William L. Hase
Institution: Wayne State Univ
Proposal Number: CTS030004
Proposal Type: New
Proposal Title: Dynamics of O(3P) Reactions with Gaseous, Liquid, and Solid Hydrocarbons

Resources(SUs): **Approved**
NCSA SGI Origin2000 5,000
NCSA IA32 Linux Supercluster 5,000

Principal Investigator: Aimo Hinkkanen
Institution: Univ of Illinois, Urbana
Proposal Number: DMS030003
Proposal Type: New
Proposal Title: Computational Complex Dynamics

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

Principal Investigator: Dominic Holland
Institution: Univ of California, San Diego
Proposal Number: DMR030004
Proposal Type: New
Proposal Title: Code Development for Atomic Dynamics

Resources(SUs): **Approved**
NCSA SGI Origin2000 1,000

Principal Investigator: Jennifer C. Hou
Institution: Univ of Illinois, Urbana
Proposal Number: NCR030001
Proposal Type: New
Proposal Title: On the Scalability of JavaSim for Extremeley Large-Scale Network Simulation

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

Principal Investigator: Shuanghong Huo
Institution: Clark Univ
Proposal Number: CHE020001
Proposal Type: Renewal
Proposal Title: Protein-Protein and Protein-Ligand Interaction

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Andrey G. Kalinichev
Institution: Univ of Illinois, Urbana
Proposal Number: CHE030005
Proposal Type: New
Proposal Title: Molecular Dynamics Simulations of the Adsorption of Bacterial Aginate onto Polyamide Membrane Materials

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

Principal Investigator: Klod Kokini
Institution: Purdue Univ
Proposal Number: MSS030001
Proposal Type: New
Proposal Title: The Effect of Surface Crack Morphology to the Interfacial Thermal Fracture of the Thermal Barrier Coatings

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Susan M. Larson
Institution: Univ of Illinois, Urbana
Proposal Number: ATM030003
Proposal Type: New
Proposal Title: Future Ozone Concentrations: Effects of Climate and Emissions Changes

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Pierre LeBreton
Institution: Univ of Illinois, Chicago
Proposal Number: MCB020019
Proposal Type: Renewal
Proposal Title: Transition States for DNA Alkylating Reactions

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Christopher Lehmann
Institution: Univ of Illinois, Urbana
Proposal Number: ATM030001
Proposal Type: New
Proposal Title: Modeling of Atmospheric Deposition in the National Atmospheric Deposition Program

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: William Lineberger
Institution: Univ of Colorado, Boulder
Proposal Number: CHE030009
Proposal Type: New
Proposal Title: Femtosecond Dynamics of Gas-Phase Copper-Solvent Clusters

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Ning Liu
Institution: Univ of Illinois, Urbana
Proposal Number: ASC030003
Proposal Type: New
Proposal Title: Development of a Parallel Plane Wave Time Domain (PWTD) Algorithm

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

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

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Donald Morton
Institution: University of Montana
Proposal Number: CCR030004
Proposal Type: New
Proposal Title: Parallel Genetic Ensemble Feature Selection

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Tom Murphy
Institution: Contra Costa College
Proposal Number: ASC030013
Proposal Type: New
Proposal Title: High Performance Computing Curriculum

Resources(SUs):	Approved
NCSA SGI Origin2000	1,000
NCSA IA32 Linux Supercluster	6,000
NCSA IA64 Linux Supercluster	3,000

Principal Investigator: Klara Nahrstedt
Institution: Univ of Illinois, Urbana
Proposal Number: MIP030001
Proposal Type: New
Proposal Title: Resource Discovery in Grid Systems

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

Principal Investigator: Fady Najjar
Institution: Univ of Illinois, Urbana
Proposal Number: CTS030010
Proposal Type: New
Proposal Title: Benchmarks of Rocfluid -MP on IA-64 Platforms

Resources(SUs):	Approved
NCSA IA64 Linux Supercluster	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 SGI Origin2000	10,000

Principal Investigator: Abby Parrill
Institution: University of Memphis
Proposal Number: MCB030015
Proposal Type: New
Proposal Title: Evaluation of Pi-Stacking Involvement in Immunosuppressant Activity

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

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

Resources(SUs): **Approved**
NCSA IA 32 Linux Supercluster 10,000

Principal Investigator: Padma Raghavan
Institution: Pennsylvania State Univ
Proposal Number: ASC030002
Proposal Type: New
Proposal Title: Performance Analysis of Robust Limited-Memory Hybrid Sparse Solvers

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

Principal Investigator: Huseyin Sehitoglu
Institution: Univ of Illinois, Urbana
Proposal Number: MSS010014
Proposal Type: Renewal
Proposal Title: Contact Analysis of Fatigue Crack Surfaces

Resources(SUs): **Approved**
NCSA SGI Origin2000 8,000

Principal Investigator: Alexandre Silva Lopes
Institution: Univ of Maryland, College Park
Proposal Number: CCR030001
Proposal Type: New
Proposal Title: Parallel Simulation of Fluid Flows

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

Principal Investigator: Chris Sontag
Institution: Space Telescope Sci Inst
Proposal Number: CCR030008
Proposal Type: New
Proposal Title: OPUS Pipeline Processing at NCSA

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

Principal Investigator: Robert F. Stein
Institution: Michigan State Univ
Proposal Number: AST030016
Proposal Type: New
Proposal Title: Supergranulation Scale Magneto-Convection

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Jonathan E. Stevens
Institution: University of Detroit Mercy
Proposal Number: CHE020020
Proposal Type: Renewal
Proposal Title: Mechansim of Reactions of Fluoprinated Iodoalkanes

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Sergey Stolbov
Institution: Kansas State Univ
Proposal Number: DMR010003
Proposal Type: Renewal
Proposal Title: First Principles Studies of Chemisorption on the Stepped Metal Surfaces.

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: K. Subramani
Institution: West Virginia Univ
Proposal Number: ASC030012
Proposal Type: New
Proposal Title: Distributed Dispatching of Hard Real-Time Systems

Resources(SUs): **Approved**
NCSA SGI Origin2000 3,000

Principal Investigator: Haihong Sun
Institution: Univ of Illinois, Urbana
Proposal Number: CHE030006
Proposal Type: New
Proposal Title: Protein Structure via Quantum Chemistry and NMR

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Xian-He Sun
Institution: Illinois Institute of Technology
Proposal Number: ASC020004
Proposal Type: Renewal
Proposal Title: Adaptive Wavelet Element Method for Highly Parallel Computations

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

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

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

Principal Investigator: Warren Warren
Institution: Princeton Univ
Proposal Number: CHE030011
Proposal Type: New
Proposal Title: Numerical Simulations of NMR Spectra and MR Images

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Richard L. Weaver
Institution: Univ of Illinois, Urbana
Proposal Number: MSS000011
Proposal Type: Renewal
Proposal Title: High Precision Numerical Modeling of Guided Waves in Rails

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Yong Zhang
Institution: Univ of Illinois, Urbana
Proposal Number: MCB030008
Proposal Type: New
Proposal Title: Density Functional Studies on Paramagnetic Metalloproteins and Model Compounds

Resources(SUs): **Approved**
NCSA SGI Origin2000 10,000

Principal Investigator: Xu Zhou
Institution: Univ of Vermont
Proposal Number: CTS030014
Proposal Type: New
Proposal Title: Large-eddy Simulation of Planar Reactive Buoyant Jets

Resources(SUs):	Approved
NCSA SGI Origin2000	2,000
NCSA IA32 Linux Supercluster	8,000

Principal Investigator: Jingzhi Zhu
Institution: Pennsylvania State Univ
Proposal Number: DMR030007
Proposal Type: New
Proposal Title: Phase Field Simulations of Microstructural Evolution in Ni-base Superalloys

Resources(SUs):	Approved
NCSA SGI Origin2000	5,000
NCSA IA64 Linux Supercluster	5,000