

Small Allocations Committee for NCSA Award Report (January-March 2003)

Principal Investigator: Jacques Amar
Institution: Univ of Toledo
Proposal Number: DMR030025
Proposal Type: New
Proposal Title: Simulating Extended Time and Length Scales Using Parallel Kinetic Monte Carlo and Parallel Accelerated Dynamics

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

Principal Investigator: Ramesh Ande
Institution: New Mexico Inst of Mining and Tech
Proposal Number: MCB030024
Proposal Type: New
Proposal Title: Design of Novel Acetylcholinesterase Inhibitors

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

Principal Investigator: Prosenjit Bagchi
Institution: Johns Hopkins Univ
Proposal Number: CTS030023
Proposal Type: New
Proposal Title: Numerical Simulation of RBC Aggregation in Microcirculation

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

Principal Investigator: John M. Blondin
Institution: North Carolina State Univ, Raleigh
Proposal Number: AST030013
Proposal Type: New
Proposal Title: Dynamical Evolution of Accretion Disks

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

Principal Investigator: Alain Borel
Institution: Univ of Illinois, Urbana
Proposal Number: CHE020044
Proposal Type: Renewal
Proposal Title: Theoretical Study of the Electron Spin Relaxation of D and F Metal Ions

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

Principal Investigator: Weng Cho Chew
Institution: Univ of Illinois, Urbana
Proposal Number: ECS020002
Proposal Type: Renewal
Proposal Title: High Efficiency Parallel MLFMA Solver

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

Principal Investigator: Noshir Contractor
Institution: Univ of Illinois, Urbana
Proposal Number: SBE030001
Proposal Type: New
Proposal Title: p* Analysis of Large Scale Networks

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

Principal Investigator: Edward J. Cording
Institution: Univ of Illinois, Urbana
Proposal Number: MSS030007
Proposal Type: New
Proposal Title: Analysis of Ground Movements and Building Response Around Deep Excavations in Sand

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

Principal Investigator: George Deltas
Institution: Univ of Illinois, Urbana
Proposal Number: SES030005
Proposal Type: New
Proposal Title: Development of an Analytical Framework for Strategic Bidding in Competitive Electricity Markets: Modeling and Policy Analysis

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

Principal Investigator: Suhrit K. Dey
Institution: Eastern Illinois Univ
Proposal Number: ASC030022
Proposal Type: New
Proposal Title: Parallelized Predictor-Corrector Algorithm for Breast Cancer Modelling

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

Principal Investigator: J. Wayland Eheart
Institution: Univ of Illinois, Urbana
Proposal Number: SES030004
Proposal Type: New
Proposal Title: Integrated Optimization of Water Withdrawal Regulations Using Genetic Algorithms

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

Principal Investigator: Hamidreza Emamipour
Institution: Univ of Illinois, Urbana
Proposal Number: CTS020023
Proposal Type: Renewal
Proposal Title: Adsorption of Hazardous Organic Vapors from Air Streams

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

Principal Investigator: Fikret Ercal
Institution: Univ of Missouri, Rolla
Proposal Number: ASC030019
Proposal Type: New
Proposal Title: EST Clustering

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

Principal Investigator: Jonathan B. Freund
Institution: Univ of Illinois, Urbana
Proposal Number: CTS030018
Proposal Type: New
Proposal Title: Adjoint-Based Analysis of Free Shear Flow Noise

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

Principal Investigator: Les Gasser
Institution: Univ of Illinois, Urbana
Proposal Number: IRI010001
Proposal Type: Renewal
Proposal Title: Multi-Agent Simulation

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

Principal Investigator: Kirti Ghia
Institution: Univ of Cincinnati
Proposal Number: CTS030022
Proposal Type: New
Proposal Title: Simulation of Low-Pressure Turbine Separated Flow and its Control

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

Principal Investigator: Michael Hanson
Institution: Wesleyan Univ
Proposal Number: SES030003
Proposal Type: New
Proposal Title: The "Price Puzzle" Reconsidered

Resources(SUs): **Approved**
NCSA SGI Origin2000 7,000

Principal Investigator: Steve Heister
Institution: Purdue Univ
Proposal Number: ASC030023
Proposal Type: New
Proposal Title: 3-D Modelings for Hydrodynamic Flow Instabilities of Co-axial Injector in a Recessed Region

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

Principal Investigator: Bruce Hietbrink
Institution: California State Univ, Northridge
Proposal Number: CHE030021
Proposal Type: New
Proposal Title: Organic and Organometallic Reaction Mechanism

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

Principal Investigator: Predrag Hrnjak
Institution: Univ of Illinois, Urbana
Proposal Number: CTS020011
Proposal Type: Renewal
Proposal Title: An Experimental and Computational Study of Disperse Two-Phase Flow in Headers

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

Principal Investigator: Joonkyung Jang
Institution: Northwestern Univ
Proposal Number: CHE030019
Proposal Type: New
Proposal Title: Capillary force on a nanoscale AFM tip

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

Principal Investigator: Kalju Kahn
Institution: Univ of California, Santa Barbara
Proposal Number: DMR030028
Proposal Type: New
Proposal Title: Electronic and Optical Properties of Paracyclophanes

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

Principal Investigator: Abdelkader Kara
Institution: Kansas State Univ
Proposal Number: DMR030027
Proposal Type: New
Proposal Title: Electronic Structure of Metal Vicinal Surfaces With Adsorbates

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

Principal Investigator: Diego Klabjan
Institution: Univ of Illinois, Urbana
Proposal Number: DDM020001
Proposal Type: Renewal
Proposal Title: Next Generation Linear Optimization

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

Principal Investigator: Gregory Kobidze
Institution: Michigan State Univ
Proposal Number: ECS010007
Proposal Type: Renewal
Proposal Title: Electromagnetic Scattering Analysis for Electrically Large Conducting Bodies

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

Principal Investigator: John B. Kogut
Institution: Univ of Illinois, Urbana
Proposal Number: PHY030006
Proposal Type: New
Proposal Title: Scaling of a Lattice Gauge Theory Code on The NCSA Origin

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

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

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

Principal Investigator: Frederick V Lawrence
Institution: Univ of Illinois, Urbana
Proposal Number: MSS030005
Proposal Type: New
Proposal Title: Reliability of Improved Thermite Welds

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

Principal Investigator: Alex Li
Institution: Washington State Univ
Proposal Number: CHE030038
Proposal Type: New
Proposal Title: Folding versus Assembling of Perylene Dimer

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

Principal Investigator: Steve Liebling
Institution: Long Island University
Proposal Number: PHY030010
Proposal Type: New
Proposal Title: Using Distributed Adaptive Mesh Refinement for Threshold Behavior

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

Principal Investigator: Lorie Liebrock
Institution: New Mexico Inst of Mining and Tech
Proposal Number: ASC030016
Proposal Type: New
Proposal Title: Automatic Data Distribution for Galaxy Quest

Resources(SUs): **Approved**
NCSA IA32 Linux Supercluster 4,800
NCSA IA64 Linux Supercluster 4,800

Principal Investigator: Yong Liu
Institution: Univ of Illinois, Urbana
Proposal Number: ASC030024
Proposal Type: New
Proposal Title: Grid-aware High Performance and High Throughput MPI Blast

Resources(SUs): **Approved**
NCSA IA32 Linux Supercluster 10,000
NCSA IA64 Linux Supercluster 10,000

Principal Investigator: Qiang Lu
Institution: Univ of California, Irvine
Proposal Number: MCB030023
Proposal Type: New
Proposal Title: The Molecular Dynamics Study of Cancer Guardian Protein:p53

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

Principal Investigator: Mark Mascal
Institution: Univ of California, Los Angeles
Proposal Number: CHE030039
Proposal Type: New
Proposal Title: A Computational Study of Novel Modes of Cation and Anion Binding in Cyclophanes

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 Bullseye Effect and the Large-Scale Structure of the Universe

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

Principal Investigator: Zach Miller
Institution: Univ of Wisconsin, Madison
Proposal Number: BIO030003
Proposal Type: New
Proposal Title: BLAST on the Grid

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

Principal Investigator: Jay Mittenthal
Institution: Univ of Illinois, Urbana
Proposal Number: MCB030025
Proposal Type: New
Proposal Title: An Evolutionary Computation Model of Intracellular Signaling Networks

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

Principal Investigator: Alireza Namazifard
Institution: Univ of Illinois, Urbana
Proposal Number: ASC030025
Proposal Type: New
Proposal Title: Benchmarks of Integrated Solid Propellant Rocket Simulations.

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

Principal Investigator: Harvey B. Newman
Institution: California Institute of Technology
Proposal Number: PHY030009
Proposal Type: New
Proposal Title: Proposal to use NCSA Resources for Higgs Boson Background Studies on CMS (LHC)

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

Principal Investigator: Mark R. Nimlos
Institution: Colorado School of Mines
Proposal Number: CHE010026
Proposal Type: Renewal
Proposal Title: Electronic Structure Calculations of Transient Molecules

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

Principal Investigator: Dimitrios Papavassiliou
Institution: Univ of Oklahoma
Proposal Number: CTS010024
Proposal Type: Renewal
Proposal Title: COMPLEX TRANSPORT PROCESSES

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

Principal Investigator: Ranjit Pati
Institution: Rensselaer Polytechnic Institute
Proposal Number: DMR020005
Proposal Type: Renewal
Proposal Title: Quantum Conductivity Calculation in Nanotube for Nanoelectronic Application

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

Principal Investigator: Charles S. Peskin
Institution: New York Univ
Proposal Number: DMS030007
Proposal Type: New
Proposal Title: Monte Carlo Simulation of Gene Networks with Spatial Diffusion

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

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

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

Principal Investigator: Elizabeth Praton
Institution: Franklin and Marshall College
Proposal Number: AST030014
Proposal Type: New
Proposal Title: Quantifying the Bull's-Eye Effect in Maps of the Large-Scale Structure of the Universe

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

Principal Investigator: Robert Preece
Institution: Univ of Alabama, Huntsville
Proposal Number: AST030017
Proposal Type: New
Proposal Title: Relativistic Plasma Simulations

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

Principal Investigator: Robert Quandt
Institution: Illinois State Univ
Proposal Number: CHE030013
Proposal Type: New
Proposal Title: An ab Initio Study of the Two-Photon Photodissociation of CXBr3 and CBr4 (X=H, CH3 or CH3CH2) Halocarbons.

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

Principal Investigator: Anisur Rahman
Institution: Drexel Univ
Proposal Number: MSS030008
Proposal Type: New
Proposal Title: Fracture Parameters for Damage Tolerance Evaluation of Aircraft Fuselages

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

Principal Investigator: Sumathy Raman
Institution: Massachusetts Institute of Technology
Proposal Number: CHE030014
Proposal Type: New
Proposal Title: Minimization of Soot Formation During Combustion - a Thermodynamic Approach

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

Principal Investigator: Antonis Rokas
Institution: Univ of Wisconsin, Madison
Proposal Number: DEB030003
Proposal Type: New
Proposal Title: Yeast Phylogenomics

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

Principal Investigator: Vivek Shenoy
Institution: Brown Univ
Proposal Number: MSS030006
Proposal Type: New
Proposal Title: Density-Functional Studies of Stepped Titanium Nitride Surfaces

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

Principal Investigator: Michael Silver
Institution: Hope College
Proposal Number: DMR030018
Proposal Type: New
Proposal Title: Development of Molecular Dynamics Parameters for Analysis of the Structure and Reactivity of Novel Silicone Polymers

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

Principal Investigator: Garrison Sposito
Institution: Univ of California, Berkeley
Proposal Number: EAR030001
Proposal Type: New
Proposal Title: Molecular Simulations of Smectite-Organic Matter Complexes

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 Carbon and Sulphur Chemisorption on Vicinal Pd Surfaces

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

Principal Investigator: Yuri Strukov
Institution: Univ of Illinois, Urbana
Proposal Number: MCB030019
Proposal Type: New
Proposal Title: Condensation of Mitotic Chromosomes: Fixed Folding Pathways vs. Random Folding

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

Principal Investigator: Andrei Tokmakoff
Institution: Massachusetts Institute of Technology
Proposal Number: CHE030020
Proposal Type: New
Proposal Title: QM/MM Studies of Solvation of N-Methylacetamide

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

Principal Investigator: Blair Tuttle
Institution: Pennsylvania State Univ
Proposal Number: DMR030020
Proposal Type: New
Proposal Title: Electronic Structure of Semiconductor Materials

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

Principal Investigator: John Scott Walker
Institution: Univ of Illinois, Urbana
Proposal Number: DMS030009
Proposal Type: New
Proposal Title: Magnetic Damping of Float-zone Crystal Growth Instabilities

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

Principal Investigator: Benjamin Wandelt
Institution: Univ of Illinois, Urbana
Proposal Number: AST020005
Proposal Type: Renewal
Proposal Title: Power Spectrum Analysis of BEAST Data

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

Principal Investigator: Junmei Wang
Institution: Univ of California, San Francisco
Proposal Number: MCB000017
Proposal Type: Renewal
Proposal Title: Development of a general AMBER force field (GAFF)

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

Principal Investigator: Tao Ye
Institution: Univ of Michigan
Proposal Number: ASC030021
Proposal Type: New
Proposal Title: Direct Numerical Simulation of Bubble-Wall Interaction in Medicine

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

Principal Investigator: Tao Ye
Institution: Univ of Michigan
Proposal Number: BIO030007
Proposal Type: New
Proposal Title: Direct Numerical Simulation of Bubble, Non-Newtonian Fluid and Elastic Wall Interaction in Capillary

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

Principal Investigator: A. Peter Young
Institution: Univ of California, Santa Cruz
Proposal Number: DMR030023
Proposal Type: New
Proposal Title: Simulation of Vector Spin Glasses

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

Principal Investigator: Jon Zubieta
Institution: Syracuse Univ
Proposal Number: CHE030016
Proposal Type: New
Proposal Title: Theory and Experiment of Metal Carbonyl Complexes

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

Principal Investigator: Jon Zubieta
Institution: Syracuse Univ
Proposal Number: CHE030017
Proposal Type: New
Proposal Title: Computation of Zeolitic Structures and Inorganic Cluster Energetics

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