Discovery & Innovation via High-End Computational Resources

Russ Miller
Cyberinfrastructure Lab, SUNY-Buffalo Hauptman-Woodward Med Res Inst

NSF, NIH, DOE, NIMA, NYS, Dell

www.cse.buffalo.edu/faculty/miller/CI/
Academia in the 21st Century

- Empower students to compete in knowledge-based economy
- Embrace digital data-driven society
- Accelerate discovery and comprehension
- Enhance virtual organizations
- Provide increased education, outreach, and training
- Enhance and expand relationships between academia and the corporate world
Academia in the 21st Century: Implementation

- Support HPC infrastructure, research, and applications
- Deliver high-end cyberinfrastructure to enable efficient
  - Collection of data
  - Management/Organization of data
  - Distribution of data
  - Analysis of data
  - Visualization of data
- Create links between enabling technologists and disciplinary users
- Improve efficiency of knowledge-driven applications in myriad disciplines
  - New Techniques
  - New Algorithms
  - New Interactions (people & systems)
Cyberinfrastructure

- NSF: “comprehensive phenomenon that involves creation, dissemination, preservation, and application of knowledge”
- Generic: transparent and ubiquitous application of technologies central to contemporary engineering and science
- Foster & Kesselman: “a domain-independent computational infrastructure designed to support science.”
- NSF Cyberinfrastructure (OCI)
  - HPC Hardware and Software
  - Data Collections
  - Science Gateways/Virtual Organizations
  - Support of Next Generation Observing Systems
NSF Director Arden L. Bement: “leadership in cyberinfrastructure may determine America's continued ability to innovate – and thus our ability to compete successfully in the global arena.”
Academic HPC Initiative

- Must be Pervasive Across the Entire University
- Must Remove Barriers
- Groups Must Interact
  - Research Groups
  - Support Staff
  - Students
  - Departments
  - Colleges

Issues
- Tenure & Promotion
- University vs Colleges vs Departments vs Faculty vs Centers/Institutes vs Degrees vs Courses

Details are University Dependent
Center for Computational Research (CCR): 1998-2006

- Founding Director
- Facts & Figures
  - Top Academic HPC Center in World
  - ~25 TF of HPC
  - ~600 TB of High-End Storage
  - Significant Visualization
  - Special-Purpose Systems
  - ~30 FTEs Staff
  - 140 Projects Annually
- EOT

ROI: $7M → ~$300M @ UB
ROI: ~$450M to WNY
2008: 13 TF; 25 TB
CCR Highlights (1998-2006)

- Provide HE-Comp
- Provide HE-Vis + AGN
- Special Purpose Systems
  - Bioinformatics
  - Data Warehouse / Mining
- Support Local/National Efforts – Industry + Acad
- Create jobs in WNY
- Certificate Program
- Workshops + Tours
  - Campus, Industry
  - High-School
- Urban Planning & Design
- MTV Videos
- Peace Bridge, Med Campus
- Olmsted Parks, Thruway
- NYS Agencies
- Elected Officials
- Magnet on Campus
- Significant Funds
- Numerous Awards
- Significant Publicity
CCR Research & Projects

- Archaeology
- Bioinformatics/Protein Folding
- Computational Chemistry
- Computational Fluid Dynamics
- Data Mining/Database
- Earthquake Engineering
- Environ Modeling & Simulation
- Grid Computing
- Molecular Structure Determination
- Physics

- Videos: MTV
- Urban Simulation and Viz
  - StreetScenes
  - I-90 Toll Barrier
  - Medical Campus
  - Peace Bridge
- Accident Reconstruction
- Scientific Viz
  - Dental
  - Surgery
  - MRI/CT Scan
  - Confocal Microscopy
  - Crystallization Wells
  - Collaboratories
CCR Funding (1998-2006)

- CCR-Enabled to SUNY-Buffalo
  - $170M External Funds
  - $140M In-Kind Contributions
- CCR-Enabled to WNY
  - $200M External Funds
- Federal Appropriations
- New York State Appropriations
- Local WNY Foundations
- In-Kind Contributions (Dell, SGI, Sun, etc.)
- Grants (NSF, NIH, DOE, etc.)
- Projects with Local Companies
- Government Projects
- SUNY-Buffalo: staff and space
Real-Time Visualization
StreetScenes: Real-Time 3D Traffic Simulation

- Accurate local landmarks: Bridges, Street Signs, Business, Homes
- Can be viewed from driver’s perspective
- Real-Time Navigation
- Works with
  - Corsim
  - Synchro
- Generate AVI & MOV
- Multiple Simultaneous
  - Traffic Loads
  - Simulation
  - Varying POV
Animation & Simulation

Rendered Scenes
Williamsville Toll Barrier Improvement Project

Initial Photo Match incorporating real and computer-generated components
Peace Bridge Visualization: Animation & Simulation

The Problem
- 75 year old bridge
- 3 lanes – poor capacity
- Existing US plaza: small and poor design

Proposed Options
- Relocate US plaza
- Build a 3-lane companion span & rehab existing bridge
- Build a six lane signature span
Song: I’m OK (I Promise)
Band: Chemical Romance
Gaming Environment: Death Jr.

MTV
IBC Digital & CCR
Virtual Reality
Networked art application for CAVE
- Users from around the world
- First performance 2001

Dance-floor environment
- Inhabited by life-size puppets
- Dance with each other
- Synchro

Recording Booth
- User enters booth
- User dances
- System records dance from tracking on head and hands
- Dance mapped to Avatar

J. Anstey
Interactive virtual factory
- Creates digital mock-up of factory
- Drag & place modular machines
- Mathematical algorithms for consistency checks
Collaborative Visualization Environments

- Enable distributed collaboration via software developed at CCR
- Enable visualization and interaction with data across a geographically disparate network topology
- Integrate multiple data sources:
  - Scientific
  - Multimedia
- Research Topics
  - Distributed databases
  - OpenGL 3D programming
  - 3D Modeling
  - Character animation
  - User interaction
  - Virtual Reality

A. Ghadersohi, R. Miller, M. Green
Western New York

Some Facts
Buffalo, New York

- The Queen City: 2nd Largest City in NYS
- City of Lights
  - First U.S. city to have electric street lights
  - Pan American Exposition (1901)
    - Pres. McKinley Shot
- Architecture
  - Frederick Law Olmsted
  - Frank Lloyd Wright
- Underground Railroad
  - Slaves escaped to freedom in Canada
- Four straight Super Bowl appearances
- Culinary Delights
  - Beef on Weck, Pizza, Fish Fries
  - (Buffalo) Wings: Anchor Bar, 1964
- Health Problems
  - Heart Disease/Stroke
  - Multiple Sclerosis
Recent Biomedical Advances
(Buffalo, NY)

- PSA Test (screen for Prostate Cancer)
- Avonex: Interferon Treatment for Multiple Sclerosis
- Artificial Blood
- Nicorette Gum
- Fetal Viability Test
- Edible Vaccine for Hepatitis C
- Timed-Release Insulin Therapy
- Anti-Arrhythmia Therapy
  - Tarantula venom

- Direct Methods Structure Determination
  - Listed on “Top Ten Algorithms of the 20th Century”
- Vancomycin
- Gramacidin A
- High Throughput Crystallization Method: Patented
- NIH National Genomics Center: Northeast Consortium
- Howard Hughes Medical Institute: Center for Genomics & Proteomics
Scientific Visualization
Collaboration with Buffalo Neuroimaging Analysis Center (BNAC)

- Developers of Avonex, drug of choice for treatment of MS

MS Project examines patients and compares scans to healthy volunteers
3D Medical Visualization

- Reads data output from a CT or MRI Scan
- Collaboration with Children’s Hospital
- Visualize multiple surfaces and volumes
- Export images, movies or CAD file
- Pre-surgical planning
- Runs on a PC

M. Innus
Positron emission tomography (PET), shows sites activated and deactivated as subjects decide whether a sound is a target or not.

Current density maps of brain surface (1–700 ms after target) show dynamic pattern of brain activity during decision-making process.

A. Lockwood
Science & Engineering

Small Subset of Projects
Groundwater Flow Modeling

- Regional scale modeling of groundwater flow and contaminant transport (Great Lakes)
- Ability to include all hydrogeologic features as independent objects
- Based on Analytic Element Method

Key features:
- Highly parallel
- Object-oriented programming
- Intelligent user interface

Utilized 42 years of CPU time on CCR computers in 1 calendar year

A. Rabideau, I. Jankovic, M. Becker

Environmental Engineering
Avalanches, Volcanic and Mud Flows

- Modeling of Volcanic Flows, Mud flows (flash flooding), and avalanches
- Integrate information from several sources
  - Simulation results
  - Remote sensing
  - GIS data
- Present information to decision makers using custom visualization tools local & remote
- GRID enabled for remote access
- Key Features
  - Parallel Adaptive Computation
  - Integrated with GIS System for flows on natural terrain

A. Patra, B. Pitman, M. Sheridan, M. Jones

Flow models of Colima volcano in Mexico – courtesy Rupp et. al.’06
Literacy & Disability in Canada

- Exploring the relationship between illiteracy & disability across the Canadian landscape.
- Social Systems GIS Lab in the Dept. of Anthropology is working with researchers from York University & the Canadian Abilities Foundation.
- Sponsored by The Adult Learning & Literacy Directorate of the Ministry of Human Resources & Social Development Canada.

E. Zubrow
Verberie Paleolithic Site in France

- Intrasite spatial analysis and 3D modeling of the a Late Upper Paleolithic archaeological site in the Paris Basin of France
- Social Systems GIS Lab in the Dept. of Anthropology is working with researchers from the CNRS in Paris
- Sponsored by the National Science Foundation

E. Zubrow

University at Buffalo  The State University of New York  Cyberinfrastructure Laboratory
Cosmological Parameter Estimation

- Wealth of new precision cosmological data
- WMAP Cosmic Microwave Background Measurement
- Sloan Digital Sky Survey: 3-D map of a million galaxies
- Interpret implications of data for models of the first trillionth of a second of the universe: inflation
- *Monte Carlo Markov Chain data analysis: stochastic exploration of many-dimensional parameter spaces*

W. Kinney
UB’s Structural Engineering and Earthquake Simulation Laboratory (SEESL)

NEESWood: Development of a Performance-Based Seismic Design for Woodframe Construction:

M. Bruneau, A. Reinhorn, G. Lee
Understanding Combustion

- Flame-wall interaction modeling for a non-premixed flame propelled by a vortex ring.
- In this figure different time instants are shown during the interaction. White line contours and color contours represent vortex ring and flame, respectively.
- Key Features:
  - Parallel algorithm using mpi
  - 85-90% Parallel efficiency for up to 64 processors
- FWI study is important to determine
  - Engine Design
  - Quenching Distances
  - Flame Structure
  - Unburned hydrocarbon
  - Maximum Wall heat fluxes

C. Madnia
Nanomedicine Program

World class Research Program Melding Nanotechnology with Biomedical Sciences

Building from the Bottom Up

State of the Art Molecular Imaging and Nanocharacterization Facilities
- Multiphoton Laser Scanning System
- Confocal Imaging including FRET, FLIM & FRAP analysis
- Coherent Anti-Stokes Raman Imaging
- Optical Trapping/Dissection
- Advanced Laser Systems

P. Prasad

www.biophotonics.buffalo.edu

"Leading the Way to Technology through Innovation"
Miller’s Cyberinfrastructure Laboratory (MCIL)
MCIL Overview

- **Working Philosophy**
  - CI sits at core of modern simulation & modeling
  - CI allows for new methods of investigation to address previously unsolvable problems

- **Focus of MCIL** is on development of *algorithms, portals, interfaces, middleware*

- **Goal of MCIL** is to free end-users to do disciplinary work

- **Funding (2001-pres)**
  - NSF: ITR, CRI, MRI
  - NYS appropriations
  - Federal appropriations
MCIL Equipment (50+ TF)

- **Experimental Equipment (57.5 TF; 22TB; 156 Traditional Cores; 15 nVidia Tesla GPGPUs)**
  - Clusters
    - Head Nodes: Dell 1950 (Intel)
    - Workers: Intel 8×2×4, Intel 8×1×2, & AMD 8×2×2
    - 13 nVidia S1070s & 2 nVidia S870s
  - Virtual Memory Machines (2 × Intel 4×4)
  - Dell GigE Managed Switches
  - InfiniBand
  - 22 TB Dell Storage (2)
  - Condor Flock (35 Intel/AMD)

- **Production Equipment**
  - Dell Workstations; Dell 15 TB Storage
  - Access to CCR equipment (13TF Dell/Intel clusters)
Coordinate Computing Resources, People, Instruments in Dynamic Geographically-Distributed Multi-Institutional Environment

Treat Computing Resources like Commodities
- Compute cycles, data storage, instruments
- Human communication environments

No Central Control; No Trust
Major Grid Initiatives

- **TeraGrid (NSF)**
  - Integrates High-End Resources
  - High-Performance (Dedicated) Networks
  - 11 Sites; 1.2PF, 4PB Disk, 30PB Tape
  - 100+ Databases Available

- **OSG (DOE, NSF)**
  - High-Throughput Distributed Facility
  - Open & Heterogeneous
  - Biology, Computer Science, Astrophysics, LHC
  - 57 Compute Sites; 11 Storage Sites;
  - 10K CPUS; 6PB

- **EGEE: Enabling Grids for E-Science (European Commission)**
  - Initial Focus on CERN (5PB of Data/Year)
    - High-Energy Physics and Life Sciences
  - Expanded Focus Includes Virtually All Scientific Domains
  - 200 Institutions; 40 Countries
  - 20K+ CPUs; 5PB; 25,000 jobs per day!
Evolution of MCIL Lab Projects

- **Buffalo-Based Grid**
  - Experimental Grid: Globus & Condor
  - Integrate Data & Compute, Monitor, Portal, Node Swapping, Predictive Scheduling/Resource Management
  - GRASE VO: Structural Biology, Groundwater Modeling, Earthquake Eng, Comp Chemistry, GIS/BioHazards
  - Buffalo, Buffalo State, Canisius, Hauptman-Woodward

- **Western New York Grid**
  - Heterogeneous System: Hardware, Networking, Utilization
  - Buffalo, Geneseo, Hauptman-Woodward, Niagara

- **New York State Grid**
  - Extension to Hardened Production-Level System State-Wide
  - Albany, Binghamton, Buffalo, Geneseo, Canisius, Columbia, HWI, Niagara, [Cornell, NYU, RIT, Rochester, Syracuse, Marist], {Stony Brook, RPI, Iona}
MCIL Lab Collaborations

- High-Performance Networking Infrastructure
- Grid3+ Collaboration
- iVDGL Member
  - Only External Member
- Open Science Grid
  - GRASE VO
- NYS CI Initiative
  - Executive Director
  - Various WGs
- Grid-Lite: Campus Grid
  - HP Labs Collaboration
- Innovative Laboratory Prototype
  - Dell Collaboration
MCIL Lab Projects

- **Lightweight Grid Monitor (Dashboard)**
- **Predictive Scheduler**
  - Define quality of service estimates of job completion, by better estimating job runtimes by profiling users.
- **Dynamic Resource Allocation**
  - Develop automated procedures for dynamic computational resource allocation.
- **High-Performance Grid-Enabled Data Repositories**
  - Develop automated procedures for dynamic data repository creation and deletion.
- **Integrated Data Grid**
  - Automated Data File Migration based on profiling users.
- **Grid Portal**
CI Lab Grid Monitor: http://osg.ccr.buffalo.edu/
CI Lab Operations Dashboard

Grid: OSG-ITB, OSG, ACDC, TeraGrid, Ad-Hoc, MIS, GRASE, OSG, CDF, Fermilab, GADU, GLOW, USATLAS, fMRI, iVDGL, nanoHUB

Version: All, OSG-0.2.1, OSG-0.3.0, OSG-0.4.0, OSG-0.4.1

Site Resource - Service Matrix

Production Sites

- athena.nt.albany.edu
- rommel.cs.binghamton.edu
- gridgk01.rad.bnl.gov
- gridgk02.rad.bnl.gov
- icdun.hwi.buffalo.edu
- u2-grid.ccr.buffalo.edu
- ctcnysgrid.tc.cornell.edu
- osgc01.grid.smi.east.tw
- cms-xen2.fnal.gov
- cmsosgcf.fnal.gov
- fnop-osgf.fnal.gov
- tam01.fnal.gov
- atlas.iu.edu
- nysgrid1.lis.manist.edu
- benches.it.syu.edu
- ouhep0.rhnu.edu
- grid3.scat.psu.edu
- grid.physics.purdue.edu
- osgrcar.purdue.edu
- starsit.usp.br

- Version: 2006-12-13 13:46:33
Grid-Enabling Application Templates (GATs)

- Structural Biology
  - SnB and BnP for Molecular Structure Determination/Phasing

- Groundwater Modeling
  - Ostrich: Optimization and Parameter Estimation Tool
  - POMGL: Princeton Ocean Model Great Lakes for Hydrodynamic Circulation
  - Split: Modeling Groundwater Flow with Analytic Element Method

- Earthquake Engineering
  - EADR: Evolutionary Aseismic Design and Retrofit; Passive Energy Dissipation System for Designing Earthquake Resilient Structures

- Computational Chemistry
  - Q-Chem: Quantum Chemistry Package

- Geographic Information Systems & BioHazards
Experiment yields reflections and associated intensities.

Underlying atomic arrangement is related to the reflections by a 3-D Fourier transform.

Phase angles are lost in experiment.

Phase Problem: Determine the set of phases corresponding to the reflections.
Ph8755: SnB Histogram
Phasing and Structure Size

- **Se-Met with *Shake-and-Bake***
  - 567 kDa (160 Se)
- **Multiple Isomorphous Replacement**
- **Conventional Direct Methods**
  - **Vancomycin**

Number of Atoms in Structure

- 0
- 100
- 1,000
- 10,000
- 100,000
Shake-and-Bake Applications: Structure Size and Data Resolution

- **Basic Data (Full Structure)**
  - ~750 unique non-H atoms (equal)
  - ~2000 such atoms including 8 Fe’s
  - 1.1-1.2Å data (equal atom)
  - 1.3-1.4Å data (unequal atoms, sometimes)

- **SAS or SIR Difference Data (substructures)**
  - 160 Se (567 kDa / ASU)
  - 3-4Å data
  - 5Å truncated data have also worked
Vancomycin

- Interferes with formation of bacterial walls
- *Last line of defense* against deadly
  - streptococcal and staphylococcal bacteria strains
- Vancomycin resistance exists (Michigan)
- Can’t just synthesize variants and test
- Need structure-based approach to predict
- Solution with *SnB* (*Shake-and-Bake*)
  - Pat Loll
  - George Sheldrick
Grid Enabled \textit{SnB}

- **Required Layered Grid Services**
  - **Grid-enabled Application Layer**
    - \textit{Shake – and – Bake} application
    - Apache web server
    - MySQL database
  - **High-level Service Layer**
    - Globus, NWS, PHP, Fortran, and C
  - **Core Service Layer**
    - Metacomputing Directory Service, Globus Security Interface, GRAM, GASS
  - **Local Service Layer**
    - Condor, MPI, PBS, Maui, WINNT, IRIX, Solaris, RedHat Linux
Welcome to the Cyberinfrastructure Laboratory Grid Portal

The Cyberinfrastructure Laboratory, in conjunction with the Center for Computational Research, has created an Integrated Data and Computational Grid. This site is devoted to a Grid Portal that provides access to applications that can be run on a variety of grids. A related site contains a Grid Monitoring System designed by the Cyberinfrastructure Laboratory.

Applications may be run on the Cyberinfrastructure Laboratory’s ACDC Grid, Western New York Grid, and New York State Grid, which includes computational and data storage systems from dozens of institutions throughout the State of New York.

The applications available to the users cover a variety of disciplines, including Bioinformatics, Computational Chemistry, Crystallography and Medical Imaging, to name a few.

The grids developed by the CI Lab support teaching and research activities, as well as providing infrastructure that includes high-end data, computing, imaging, grid-enabled software, all of which relies on the New York State Research Network (NYSERNet).

This work is funded by the National Science Foundation (ITR, MRI, CRI), three program projects from The National Institutes of Health, and the Department of Energy.
Advanced Computational Data Center Grid Job Submission Instructions

The grid-enabling application templates used on the ACDC-Grid are created from the application developer's grid user profile, which contains the user's standard information such as name, organization, address, etc., and more specific information such as group ID and access level. This information is stored in a database for each of the grid-enabled applications and can be accessed through selected queries throughout the ACDC-Grid Web Portal.

Additionally, each grid-enabled scientific application profile contains information about specific execution parameters, required data files, optional data files, computational requirements, etc. This information is stored in a database for each of the grid-enabled applications and can be accessed through selected queries throughout the ACDC-Grid Web Portal.

The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are required for execution in the ACDC-Grid environment. We have identified that sequentially defining milestones for the grid user to complete intuitively guides them through the application workflow.

**Software Application:** Grid user chooses a grid-enabled software application.

**Template:** Grid user selects the required and/or optional data files from the ACDC Data Grid. User-defined computational requirements are input or a template-defined computational requirement runtime estimate is selected.

**Job Definition:** Grid user defines application specific runtime parameters or accepts default template parameter definitions.

**Review:** Grid user accepts the template complete job definition workflow or corrects any part of job definition.

**Execution Scenario:** The grid user has the ability to input an execution scenario or select a ACDC-Grid determined template defined execution scenario.

**Grid Job Status:** The grid user can view specific grid job completion status, grid job current state (COMPLETE, RUNNING, QUEUED, BLOKED, FAILED, etc.), detailed information on all running or queued grid jobs and grid-enabled application specific intermediate and post-processing grid job graphics, plots and tables.

Each item of the job definition workflow is then stored in the ACDC-Grid Web Portal database so the grid user may use/modify any previously created workflow in creating new job definitions. The job definitions can also be accessed via batch script files for executing hundreds of similar workflows in an automated fashion. For example, a grid user would first define/save a relatively generic job workflow template for the grid-enabled application and then use the batch script capabilities to change the job definition workflow data files or application parameters and execute a series of new grid jobs.
Structure Information

Title: Iled
Structure ID: Iled
Space Group: 19

Cell Constants and Cell Errors (Cell Errors optional)

A: 11.516 +/-
B: 15.705 +/-
C: 39.310 +/- 0.004
Alpha: 90.0 +/-
Beta: 90.0 +/-
Gamma: 90.0 +/-

Native Asymmetric Unit Contents

No Residues (Optional):
ASU Contents: C6H12O6 (examples: C6H12O6 OR C6 H12 O6)

Initial Data Sets

Add Dataset  Delete Dataset

Select dataset to delete: C

Datasets  Dataset 1
Name (8 chars max): ilcdhkl
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<tr>
<th>Grid Job ID:</th>
<th>447</th>
</tr>
</thead>
<tbody>
<tr>
<td>Selected resource:</td>
<td>clearwater.ccr.buffalo.edu</td>
</tr>
<tr>
<td>Number of processors:</td>
<td>5</td>
</tr>
<tr>
<td>Wallclock time requested:</td>
<td>720</td>
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<tr>
<td>Number of triplet invariant to use:</td>
<td>8400</td>
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<td>Start Phases From:</td>
<td>random atoms</td>
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<tr>
<td>Random seed (prime):</td>
<td>11909</td>
</tr>
<tr>
<td>Number of trials:</td>
<td>1000</td>
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<tr>
<td>Starting Trial:</td>
<td>1</td>
</tr>
<tr>
<td>Input Phase File:</td>
<td>unused</td>
</tr>
<tr>
<td>Input Atom File:</td>
<td>unused</td>
</tr>
<tr>
<td>Keep complete (every trial) peak file?</td>
<td>yes</td>
</tr>
<tr>
<td>Number of Shake-and-bake cycles:</td>
<td>20</td>
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<tr>
<td>Keep complete (every cycle) trace file?</td>
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<tr>
<td>Terminate trials failing the R-Ratio test?</td>
<td>no</td>
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<td>Phase Refinement Method:</td>
<td>Parameter Shift(Fast)</td>
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<td>Minimum distance between symmetry-related peaks:</td>
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<td>Number of peaks:</td>
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</tr>
<tr>
<td>Minimum</td>
<td></td>
</tr>
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</table>
Graphical Representation of Intermediate Job Status

Details for Grid Job 447 - iledhkl

Job Detail Information
Status: RUNNING
Rmin Min: 0.344 Rmin Max: 0.56
Last Updated: 15-Mar-2008 10:22:00

Total Trials: 1000
Complete Trials: 265
Best Trial Number: 34
Best Trial Rmin: 0.344
Resource: clearwater.ccr.buffalo.edu Processors: 5

Trial Summary
Completed Trials: 285 (28.5%)

Walltime Summary
Walltime Consumed: 2 (0.2%)

Grid Job Trial Histogram
- Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING

Histogram of Completed Trial Structures
## Status of Jobs

### Grid Job Status

### Job Filter Criteria

#### Show GATs
- BrP Auto Run
- EACR
- Ostrich
- POM
- C-Chem
- SnB
- SnB DREAR

#### Job State
- DEFINITION
- STAGING
- QUEUED
- RUNNING
- UPLOADING
- COMPLETE
- INCOMPLETE

#### Sort By
- Job Id
- Job Name
- Resource
- Num Procs
- Status
- Percent Complete
- Last Update

#### Descending
- Ascending

### SnB

<table>
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<th>Resource</th>
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<th>Status</th>
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Heterogeneous Back-End Interactive Collaboratory

User starts up – default image of structure.
Molecule scaled, rotated, and labeled.
New York State Grass Roots Cyberinfrastructure Initiative

- Miller’s NYS Grid used as fundamental infrastructure.
- Currently an initiative of NYSERNet.
- Open to academic and research institutions.
- Mission Statement: To create and advance collaborative technological infrastructure that supports and enhances the research and educational missions of institutions in NYS.
- Enable Research, Scholarship, and Economic Development in NYS.
- Currently, no significant utilization.
TRUN: Transborder Research University Network

- Ontario: York, Toronto, Western Ontario, McMaster, Queen’s, Waterloo, Guelph
- NYS: Buffalo, Rochester, Syracuse, Cornell, Albany, RIT
- Mission Statement: Expand and support cooperation among research universities in the border region of Province of Ontario and NYS:
  - Collaborative/consortial research
  - Joint applications for external funding
  - Cooperative academic programs
  - Faculty and student exchanges
  - Shared facilities
  - Joint conferences, symposia, workshops

www.trun.ca
TRUN: Transborder Research University Network

- **Current Focus**
  - Great Lakes Sustainable Energy
  - IT-Supported Disciplinary Research
  - High Performance Computing
  - Canada-U.S. Policy and Standardization of Binational Data

- **General Issues**
  - Public Policy Issues, Regional Governance
  - Border Security and Mobility
  - Economic and Workforce Development
  - University Partnerships with Government and Industry
  - Health Care and Policy
  - Basic Research and Technology Transfer

www.trun.ca
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- George DeTitta
- Herb Hauptman
- Charles Weeks
- Steve Potter
- Alan Rabideau
- Igor Janckovic
- Michael Sheridan
- Abani Patra
- Matt Jones
- NSF ITR
- NSF CRI
- NSF MRI
- NYS
- CCR