

Cyberinfrastructure & Grid Computing in New York State

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Hauptman-Woodward Med Res Inst



NSF, NIH, DOE, NIMA, NYS, HP

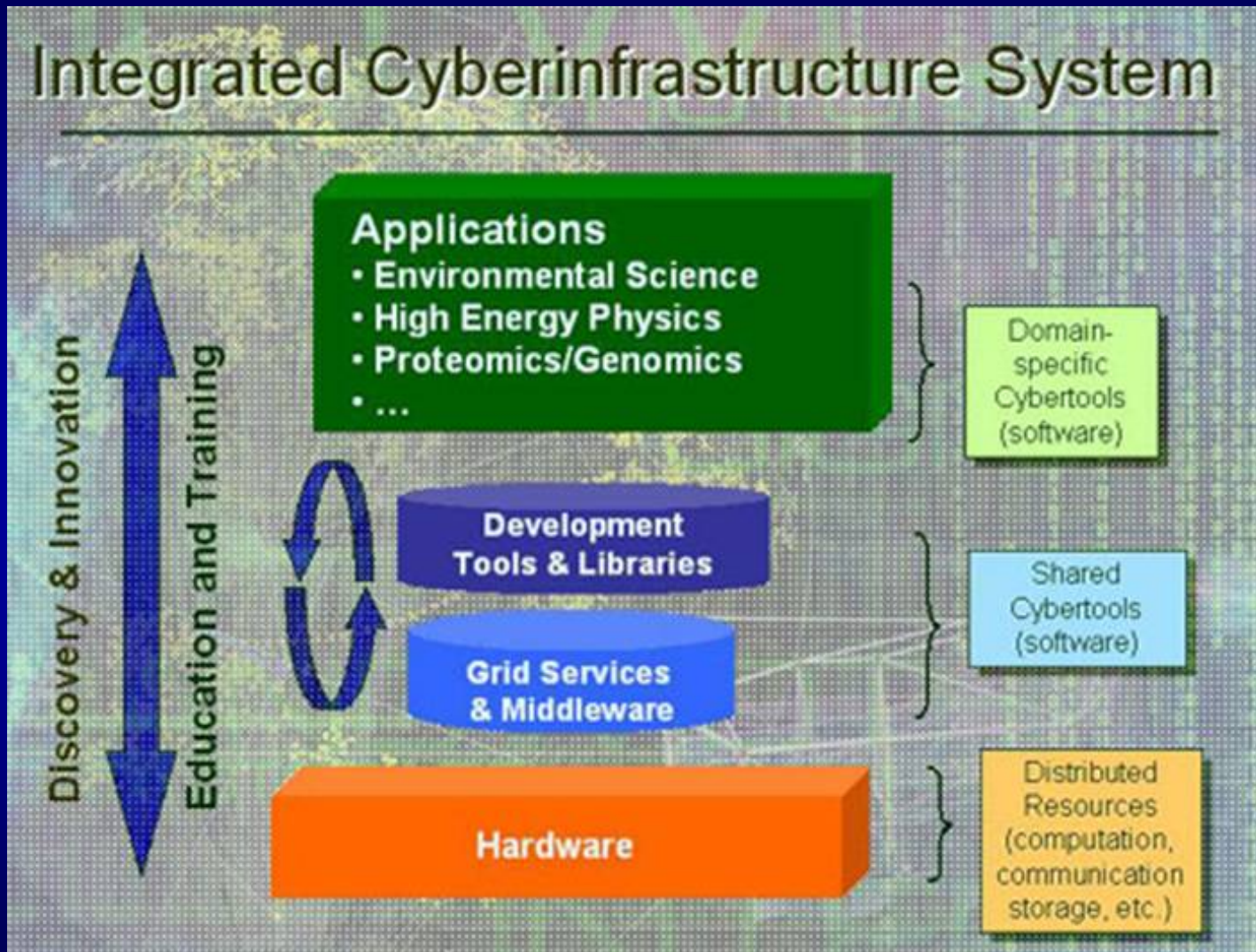
www.cse.buffalo.edu/faculty/miller/CI/

Cyberinfrastructure

- **Generic:** transparent and ubiquitous application of technologies central to contemporary engineering and science
- **NSF:** “comprehensive phenomenon that involves creation, dissemination, preservation, and application of knowledge”
- **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 Integrated Cyberinfrastructure



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."

Cyberinfrastructure in Academia

- **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**

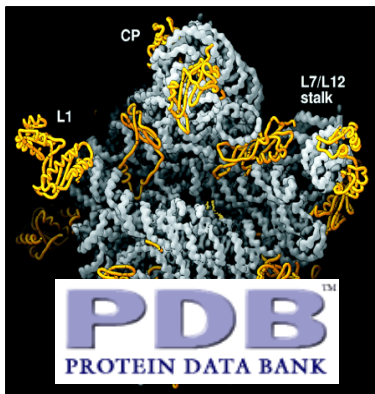
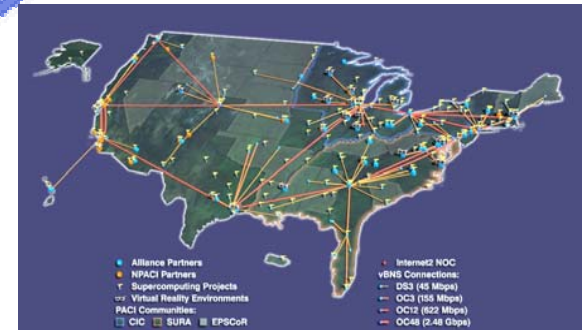
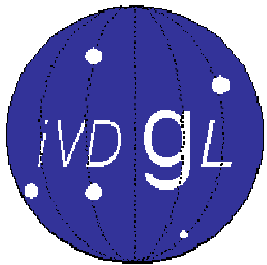


Critical Academic Initiatives

- **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)**
- **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**



Grid Computing



Asia-Pacific Advanced Network

Advanced
Center for Computational Research
Data
Center

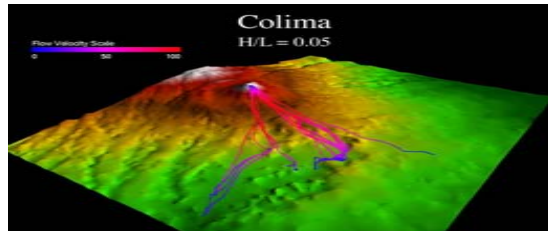


University at Buffalo The State University of New York

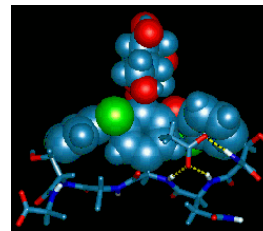
Cyberinfrastructure Laboratory

CI Lab

Grid Computing Overview



Data Acquisition



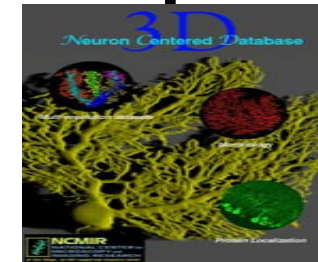
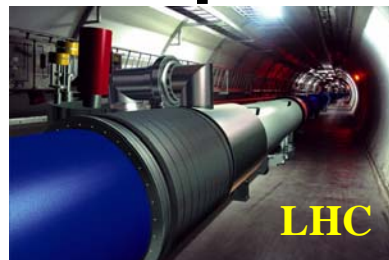
Advanced Visualization



Analysis



Imaging Instruments



Large-Scale Databases

- 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
 - ❑ 9 Sites; 250TF & 30PB
 - ❑ 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-ScienceE (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!

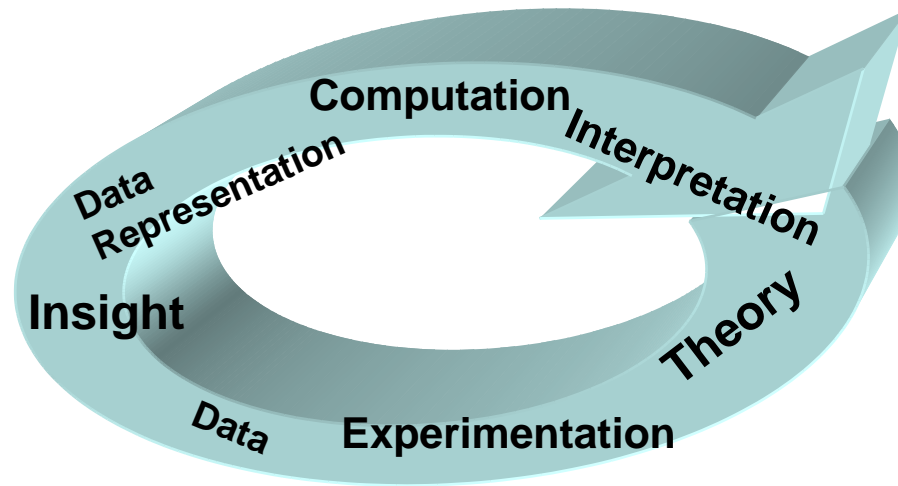


A Depiction of Cyber-enabled Discover (NSF)

*How will **CDI** (**C**yber-Enabled **D**iscover and **I**nnovation) change the way we will think about and practice science?*

“The Old Way: Classical Science”

Where, for the most part, classical science is practiced in a constrained domain.

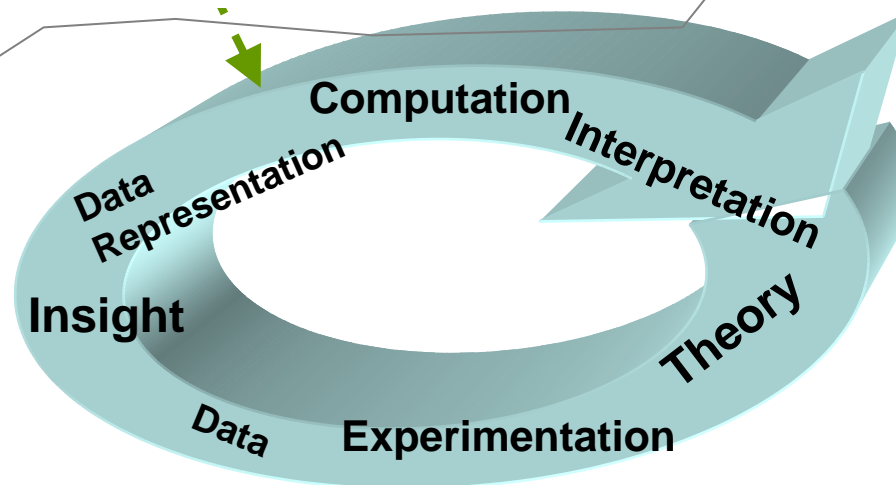


A Depiction of Cyber-enabled Discover (NSF)

Example:
Discovering causality of a phenomenon, such as a disease or weather pattern, by mining massive Data stores.

“The New Way: Cyber-Enabled Science”

For biologists, meteorologists, computational scientists, and others, a “cyber-layer” between their problem space and the way they traditionally engaged in science and may provide new sources of data, new ways of visualizing the data, new tools for extracting meaning from the data, new ways to collaborate with other scientists, and other enabling mechanisms and computational tools for discovery in new areas of science.

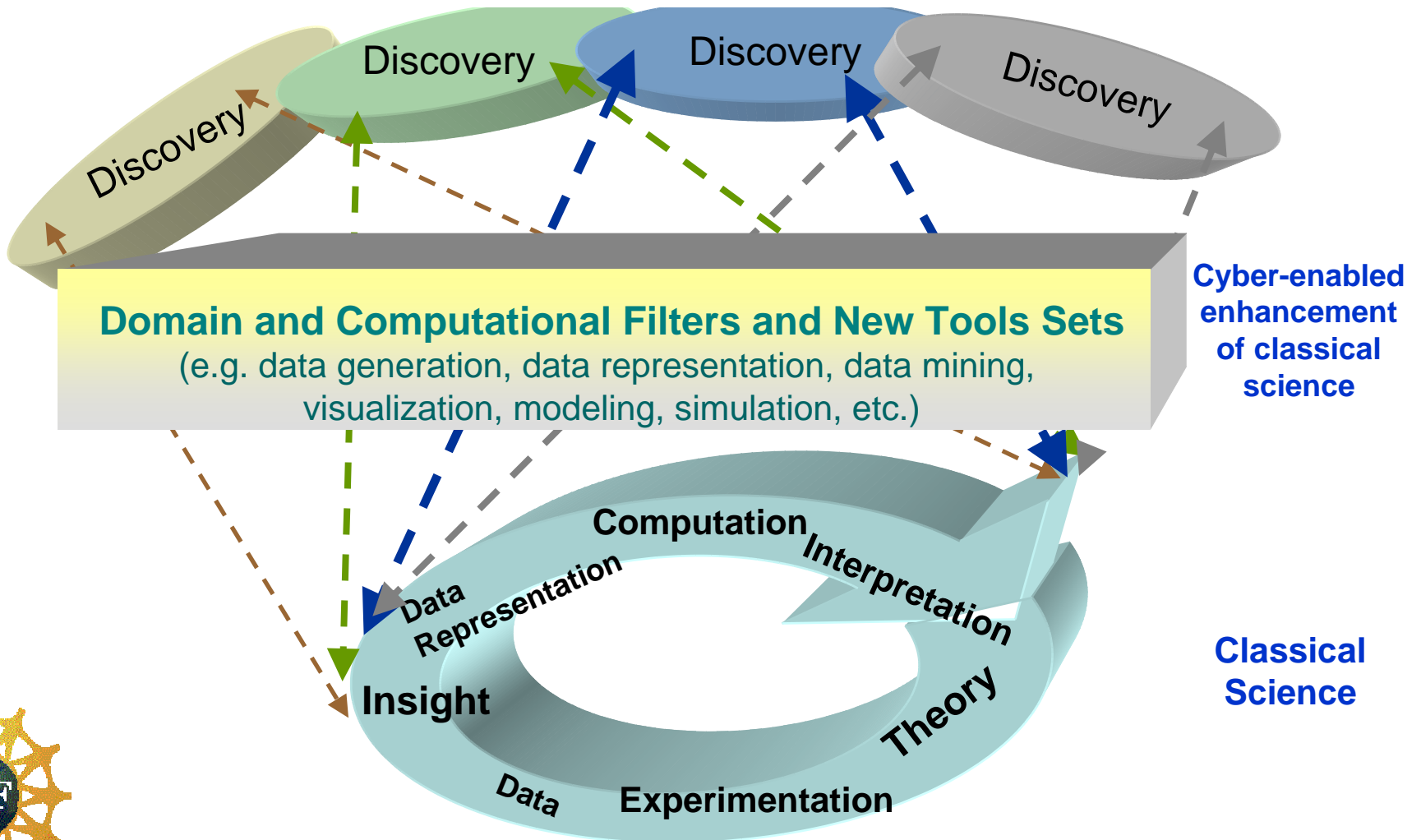


Classical Science



A Depiction of Cyber-enabled Discover (NSF)

Ubiquitous, cyber-enabled discovery across many fields.



Miller's Cyberinfrastructure Lab

- **CI sits at core of modern simulation & modeling**
- **CI allows for new methods of investigation to address previously unsolvable problems**
- **Focus on development of**
 - Algorithms
 - Portals
 - Interfaces
 - Middleware
- **Free end-users to do disciplinary work**
- **Funding (2001-pres): NSF ITR, NSF CRI, NSF MRI, NYS, Fed**



CI Lab Collaborations

- **High-Performance Networking Infrastructure**

- **Grid3+ Collaboration**

- **iVDGL Member**

- Only External Member

- **Open Science Grid**

- GRASE VO

- **NYSGrid.org**

- NYS CI Initiative

- Fndg Executive Director

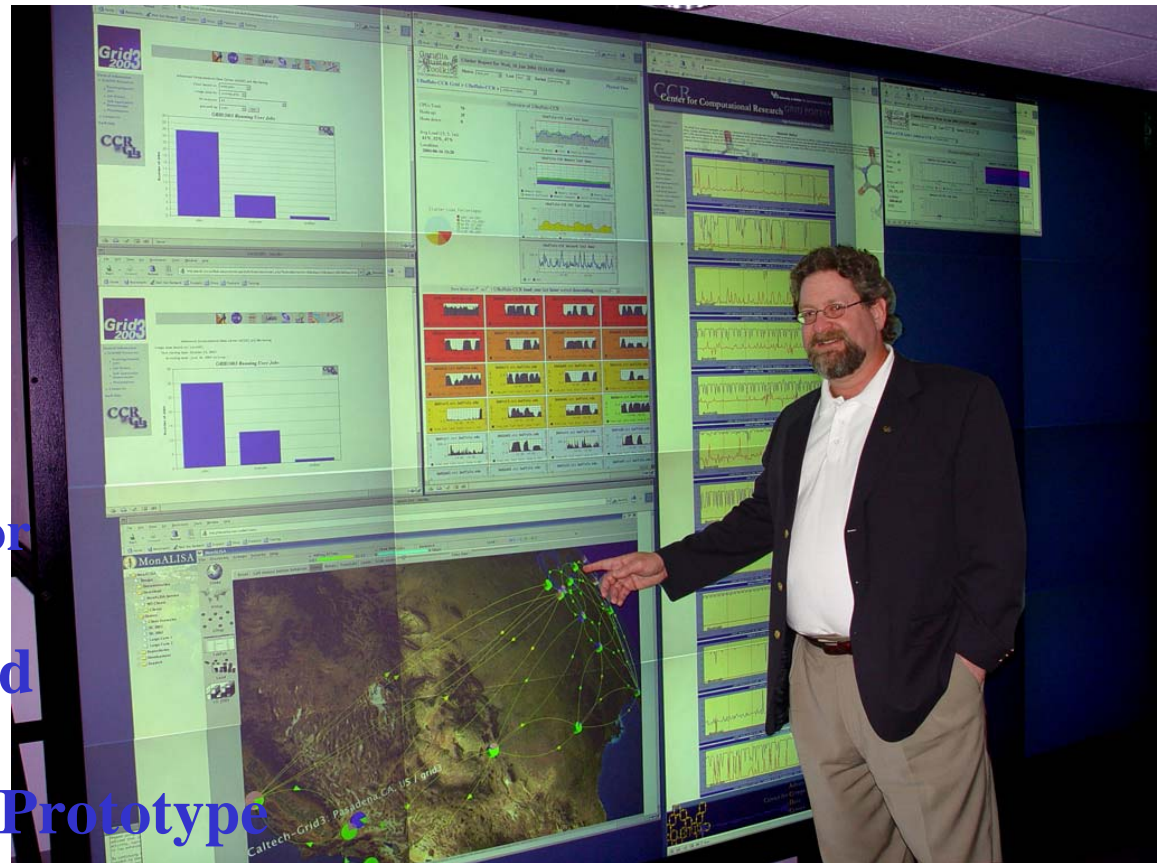
- Various WGs

- **Grid-Lite: Campus Grid**

- HP Labs Collaboration

- **Innovative Laboratory Prototype**

- Dell Collaboration



Evolution of CI Lab Projects

■ ACDC-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

■ WNY Grid

- ❑ Heterogeneous System: Hardware, Networking, Utilization
- ❑ Buffalo, Geneseo, Hauptman-Woodward, Niagara

■ NYS 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}
- ❑ VOs: Engage, GADU, GRASE, Nanohub, SDSS, USATLAS, USCMS



NYS Grid Resources

- **Albany: 8 Dual-Processor Xeon Nodes**
- **Binghamton: 15 Dual-Processor Xeon Nodes**
- **Buffalo: 1050 Dual-Processor Xeon Nodes**
- **Cornell: 30 Dual-Processor Xeon Nodes**
- **Geneseo State: Sun/AMD with 128 Compute Cores**
- **Hauptman-Woodward Institute: 50 Dual-Core G5 Nodes**
- **Marist: 9 P4 Nodes**
- **Niagara University: 64 Dual-Processor Xeon Nodes**
- **NYU: 58 Dual-Processor PowerPC Nodes**
- **RIT: 4 Dual-Processor Xeon Nodes**
- **Syracuse: 8 Dual-Processor Xeon Nodes**

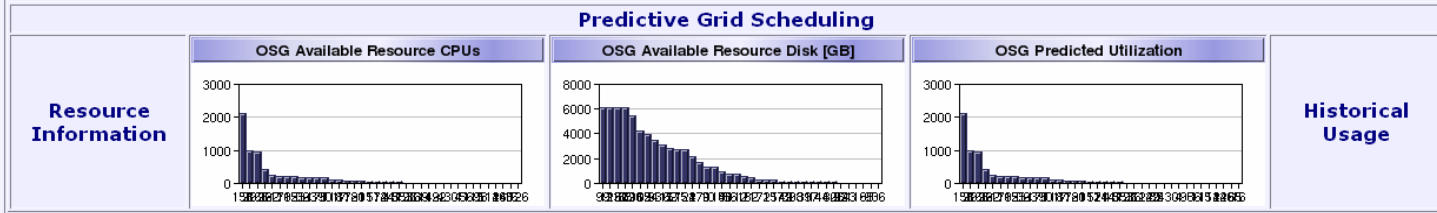
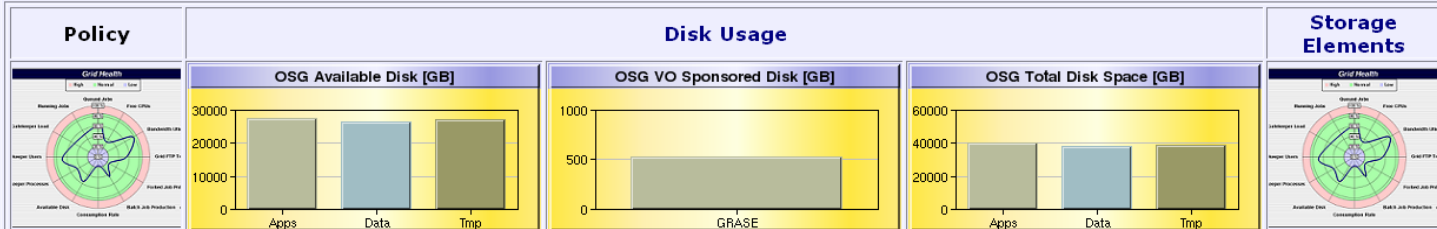
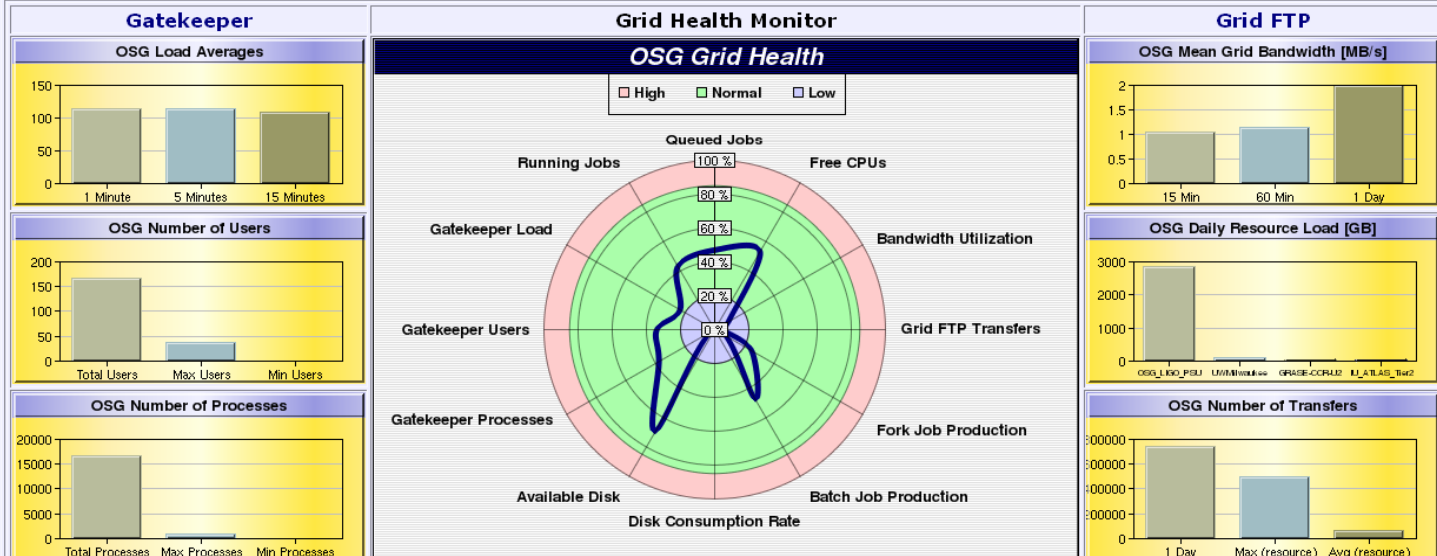
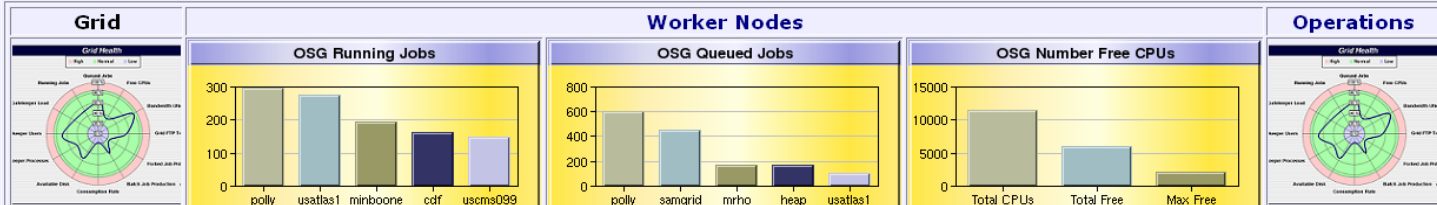


CI Lab

- CI Lab Grid Monitor
- Grid Dashboard
- Operations Dashboard
- Historical Dashboard
- Running/Queued Jobs
- Job History
- Detailed Job History
- VO Sponsor CPUs
- Free/Running/Queued CPUs
- VO Support Matrix
- Current Bandwidth Matrix
- Historical Bandwidth Matrix
- Current Latency Matrix
- Historical Latency Matrix
- Resource Queue Visualization
- Resource User Visualization
- SnB Application Demonstrator
- ACDC Grid Dashboard Site Status
- ACDC Grid Dashboard Tutorial
- GRASE VO
- Overview
- Request Membership
- Request Help
- Staff Only
- Contact Us / Staff
- CI Lab

CI LAB GRID DASHBOARD

OSG-ITB OSG ACDC TeraGrid Ad-Hoc



Supported by the National Science Foundation and the Department of Energy

CI Lab Grid Monitor: <http://osg.ccr.buffalo.edu/>

Predictive Scheduler

- **Build profiles based on statistical analysis of logs of past jobs**
 - Per User/Group
 - Per Resource
- **Use these profiles to predict runtimes of new jobs**
- **Make use of these predictions to determine**
 - Resources to be utilized
 - Availability of Backfill



ACDC-Grid Dynamic Resource Allocation at SC03 with Grid3

- **Small number (40) of CPUs were dedicated at night**
- **An additional 400 CPUs were dynamically allocated during the day**
- **No human intervention was required**
- **Grid applications were able to utilize the resources and surpassed the Grid3 goals**



ACDC-Grid Data Grid Functionality

- **Basic file management functions are accessible via a platform-independent web interface.**
- **User-friendly menus/interface.**
- **File Upload/Download to/from the Data Grid Portal.**
- **Simple Web-based file editor.**
- **Efficient search utility.**
- **Logical display of files (user/ group/ public).**
- **Ability to logically display files based on metadata (file name, size, modification date, etc.)**



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**
 - *Titan*: Computational Modeling of Hazardous Geophysical Mass Flows



Grid Enabled *Shake-and-Bake* (Molecular Structure Determination)

■ Required Layered Grid Services

□ Grid-enabled Application Layer

- *Shake-and-Bake* application
- Apache web server
- MySQL database

□ High-level Service Layer

- Globus, NWS, PHP, Fortran, and C

□ Core Service Layer

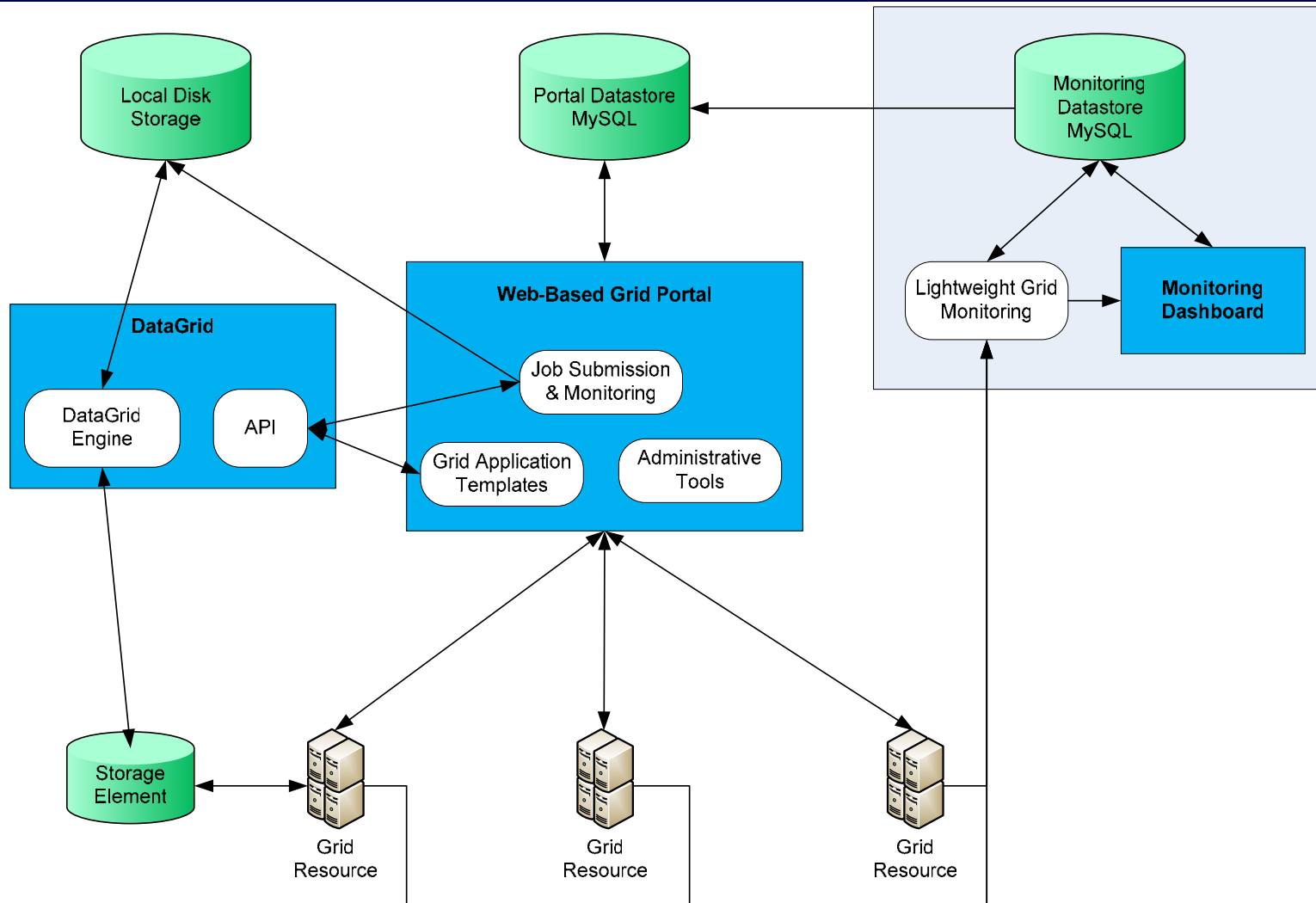
- Metacomputing Directory Service, Globus Security Interface, GRAM, GASS

□ Local Service Layer

- Condor, MPI, PBS, Maui, WINNT, IRIX, Solaris, RedHat Linux




NYS Grid Portal



https://grid.ccr.buffalo.edu/

Mail Home My Netscape

New Tab CCR Grid Computing Services:



Cyberinfrastructure Laboratory

Grid Portal

Dr. Russ Miller
UB Distinguished Professor of Computer Science & Engineering

CI Lab

- Grid Portal Info
 - Overview
 - Portal Login
 - Grid Account Info
- Computational Grid
 - Job Submission
 - Job/Queue Status
 - MDS Information
 - Network Status
 - Running/Queued Jobs
 - PBS Job History
 - Condor Flock Statistics
 - GAT/Resource Matrix
- Data Grid
 - Data Grid Tree
 - Data Grid Upload
 - Data Grid Download
 - Data Grid File Manager
 - Data Grid Replica Manager
 - Data Grid Simulator
 - Data Grid Admin Tools
 - Data Grid Admin File Tools
- Contact Us / Staff
 - CI Lab
 - Staff Only

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.



Software : BnP
Field : Protein crystal structure determination

Startup Screen for CI Lab Grid Job Submission

Expand All Collapse All

PORTAL LOGOUT

User Tools

» Manage Account

Grid General Info

Projects

Computational Grid

» Job Submission

» Job/Queue Status

» MDS Information

» Network Status

» Running/Queued Jobs

» PBS Job History

» NYS Grid

» Condor Flock Statistics

Data Grid

Education/Outreach

Staff Only

CCR HOME

Printer Friendly

Software → Template → **General Information** → Detailed Information → Job Definition → Review → Execution Scenario

Advanced Computational Data Center Grid Job Submission Instructions

The grid-enabling application templates used on the ACDC-Grid are created from the application developers grid user profiles that contain the users standard information uid, name, organization, address, etc., and more specific information such as group id and access level information for each of grid-enabled applications. 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. and statistics on application historical ACDC-Grid jobs for predictive runtime estimates. MySQL provides the speed and reliability required for this task and it is currently being used as the ACDC-Grid Web Portal database provider.

The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are require 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, BLOCKED, 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.

Continue

Reset Sequence

Reset Current Stage

Cancel

Instructions and Description for Running a Job on ACDC-Grid

Expand All Collapse All
PORTAL LOGOUT
User Tools
» Manage Account
Grid General Info
Projects
Computational Grid
» Job Submission
» Job/Queue Status
» MDS Information
» Network Status
» Running/Queued Jobs
» PBS Job History
» NYS Grid
» Conдор Flock Statistics
Data Grid
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Software → Template → General Information → Detailed Information → Job Definition → Review → Execution Scenario

Select a GAT: BnP Auto Run
BnP Auto Run
EADR
Ostrich
POM
Q-Chem
SnB
SnB DREAR
Split
snb-dev

Continue Reset Current Stage Cancel

Return to the

Software Package Selection

Expand All Collapse All
PORTAL LOGOUT
User Tools
» Manage Account
Grid General Info
Projects
Computational Grid
» Job Submission
» Job/Queue Status
» MDS Information
» Network Status
» Running/Queued Jobs
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» Conдор Flock Statistics
Data Grid
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CCR HOME
Printer Friendly

Software → Template → General Information → Detailed Information → Job Definition → Review → Execution Scenario

Enter structure definition manually
 Select structure from Data Grid: Select Config File

Continue Reset Sequence Reset Current Stage Cancel

Return to the Grid Job Menu

Full Structure / Substructure Template Selection

USER TOOLS

- » Manage Account
- Grid General Info**
- Projects
- Computational Grid
- » Job Submission
- » Job/Queue Status
- » MDS Information
- » Network Status
- » Running/Queued Jobs
- » PBS Job History
- » NYS Grid
- » Condor Flock Statistics
- Data Grid
- Education/Outreach
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- Printer Friendly

General Information

Structure Information

Title:

Structure ID :

Space Group :

Cell Constants and Cell Errors (Cell Errors optional)

A: +/-

B: +/-

C: +/-

Alpha: +/-

Beta: +/-

Gamma: +/-

Native Asymmetric Unit Contents

No Residues (Optional):

ASU Contents : (examples: C6H12O6 OR C6 H12 O6)

Initial Data Sets

| | |
|---------------------------------|--------------------------------------|
| Select dataset to delete | ○ |
| Datasets | Dataset 1 |
| Name (8 chars max): | <input type="text" value="iledhkl"/> |

Default Parameters Based on Template

User Tools
 » Manage Account
 Grid General Info
 Projects
 Computational Grid
 » Job Submission
 » Job/Queue Status
 » MDS Information
 » Network Status
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 » Condor Flock Statistics
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SnB Job Review

| | |
|--|----------------------------|
| Grid Job ID: | 447 |
| Selected resource: | clearwater.ccr.buffalo.edu |
| Number of processors: | 5 |
| Wallclock time requested: | 720 |
| Number of triplet invariant to use: | 8400 |
| Start Phases From: | Random Atoms |
| Random seed (prime): | 11909 |
| Number of trials: | 1000 |
| Starting Trial: | 1 |
| Input Phase File: | Unused |
| Input Atom File: | Unused |
| Keep complete (every trial) peak file? : | Yes |
| Number of Shake-and-bake cycles: | 20 |
| Keep complete (every cycle) trace file? : | No |
| Terminate trials failing the R-Ratio test? : | No |
| R-Ratio cutoff: | Unused |
| Phase Refinement Method: | Parameter Shift(Fast) |
| Number of passes through phase set: | 3 |
| Phase shift: | 90.0 |
| Number of shifts: | 2 |
| Number of peaks to select: | 84 |
| Minimum interpeak distance: | 3 |
| Minimum distance between symmetry-related peaks: | 3.0 |
| Number of special position peaks to keep: | 0 |
| Fourier grid size: | 0.31 |
| Perform extra cycles with more peaks? : | No |
| Number of extra cycles: | Unused |
| Number of peaks: | Unused |
| Trials for E-Fourier filtering (fourier refinement)? : | None |
| Number of cycles: | Unused |
| Number of peaks: | Unused |
| Minimum E : | Unused |

SnB Review (Grid job ID: 447)

Details for Grid Job 447 - iledhkl

Job Detail Information

Status: **RUNNING**

Rmin Min: 0.344 Rmin Max: 0.56

Last Updated: 15-Mar-2005 10:22:00

Total Trials: 1000

Complete Trials: 285

Resource: clearwater.ccr.buffalo.edu Processors: 5

Best Trial Number: 34

Best Trial Rmin: 0.344

Trial Summary

Grid Job 447 Trial Summary

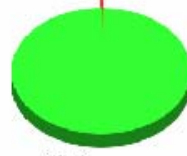
Number of Trials Complete: 285 (28.5%)



Walltime Summary

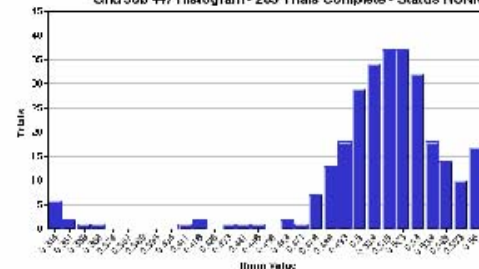
Grid Job 447 Walltime Summary

Walltime Consumed: 2 (0.3%)



Grid Job Trial Histogram

Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING



Click on image for enlarged view.

Graphical Representation of Intermediate Job Status

Expand All Collapse All

PORTAL LOGOUT

User Tools

» Manage Account

Grid General Info

Projects

Computational Grid

» Job Submission

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» Network Status

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» Condor Flock Statistics

Data Grid

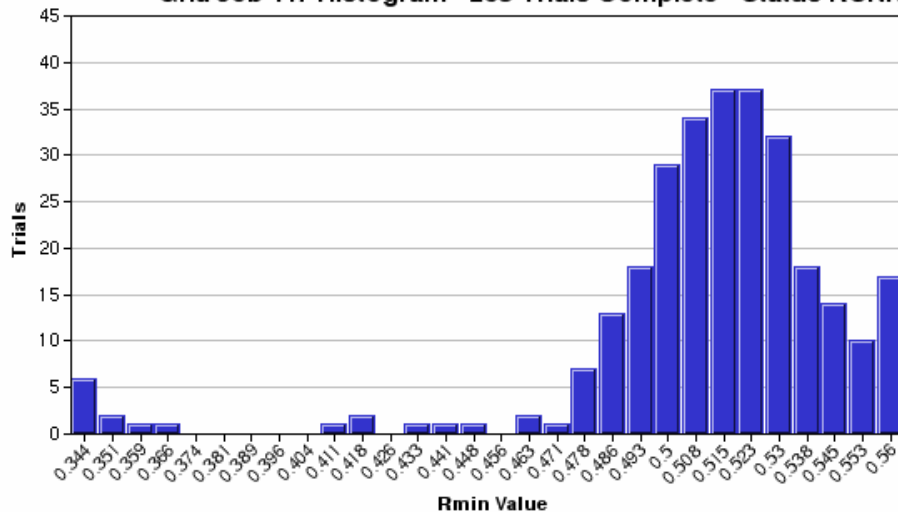
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Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING



Histogram of Completed Trial Structures

Expand All Collapse All

PORTAL LOGOUT

User Tools

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Data Grid

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Grid Job Status

15-Mar-2005 10:23:49

Job Filter Criteria

Show GATs

BnP Auto Run
EADR
Ostrich
POM
Q-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

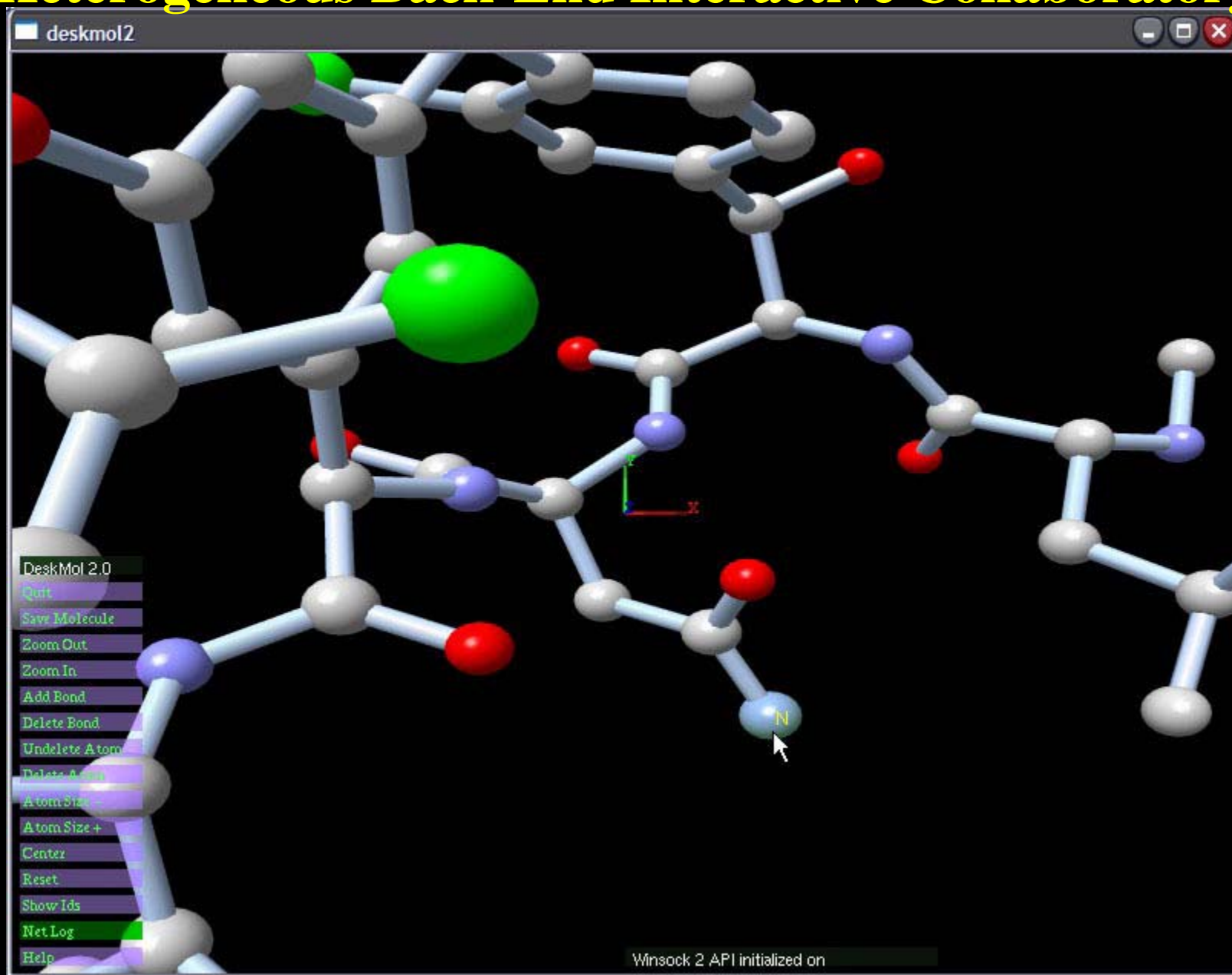
Filter Job List

SnB

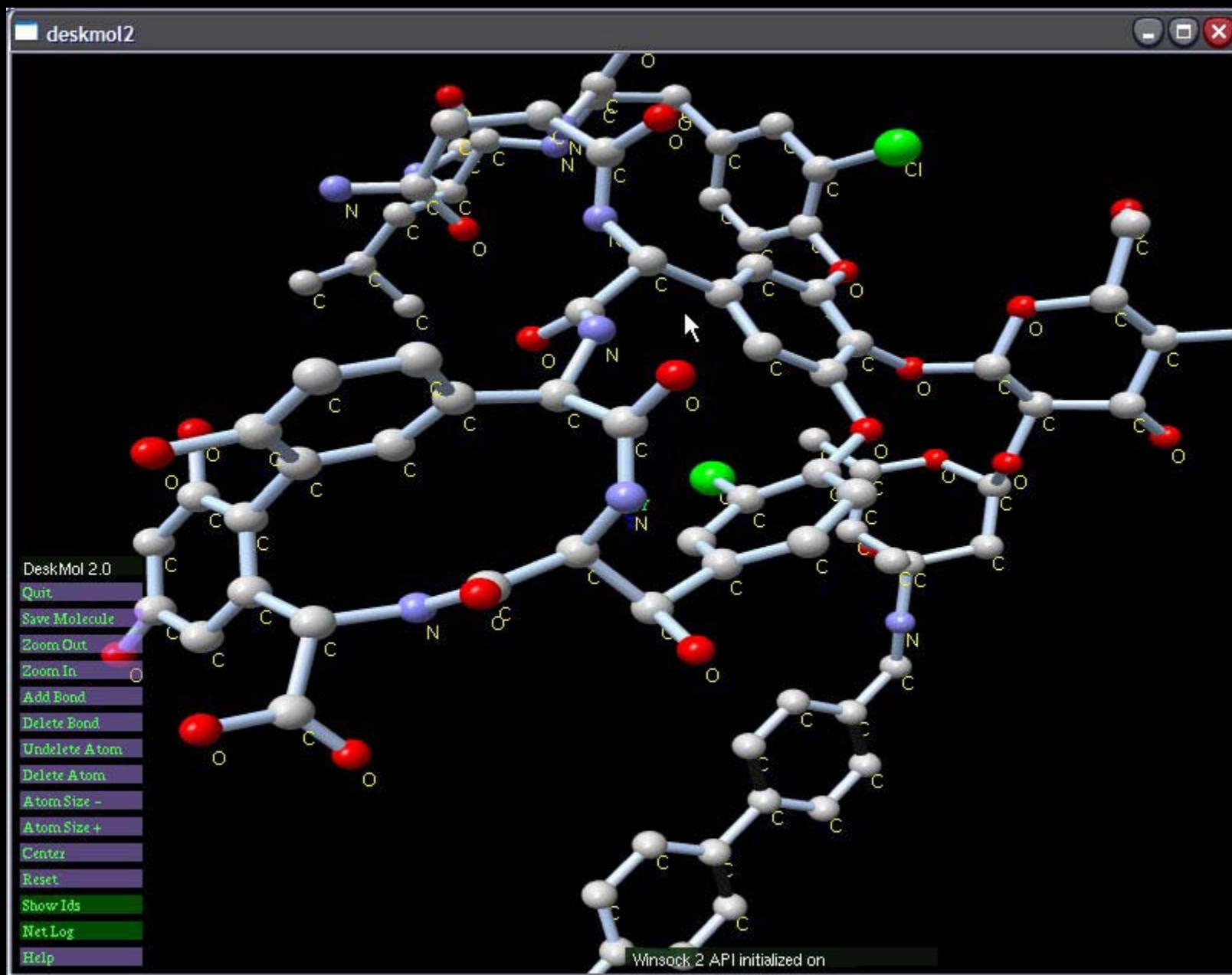
| Job Id | Job Name | Resource | Num Procs | Status | Percent Complete | Last Update | Cancel Job | Drilldown |
|--------|----------|----------------------------|-----------|----------|------------------|----------------------|--------------------------|---|
| 447 | iledhkl | clearwater.ccr.buffalo.edu | 5 | RUNNING | 28.5 | 15-Mar-2005 10:22:00 | <input type="checkbox"/> |  |
| 446 | trilys | clearwater.ccr.buffalo.edu | 10 | RUNNING | 1 | 15-Mar-2005 10:22:00 | <input type="checkbox"/> |  |
| 444 | 64chkl | nash.ccr.buffalo.edu | 3 | COMPLETE | 100 | 14-Mar-2005 22:00:01 | |  |
| 443 | trilys | clearwater.ccr.buffalo.edu | 10 | COMPLETE | 100 | 10-Mar-2005 22:48:00 | |  |
| 442 | pr435hkl | nash.ccr.buffalo.edu | 5 | COMPLETE | 100 | 10-Mar-2005 17:26:01 | |  |
| 441 | vancohkl | clearwater.ccr.buffalo.edu | 10 | COMPLETE | 100 | 10-Mar-2005 18:08:01 | |  |
| 434 | 16chkl | clearwater.ccr.buffalo.edu | 5 | COMPLETE | 100 | 10-Mar-2005 14:42:01 | |  |
| 433 | 16chkl | clearwater.ccr.buffalo.edu | 5 | COMPLETE | 100 | 10-Mar-2005 14:38:01 | |  |

Status of Jobs

Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Binghamton University

- **Grid Computing Research Laboratory**
- **Drs. Kenneth Chiu, Madhu Govindaraju, and Michael Lewis.**
- **Techniques for Web and grid service performance optimization**
- **Component frameworks for grids**
- **Instruments and sensors for grid environments**
- **Adaptive information dissemination protocols across grid overlays**
- **Emulation framework for grid computation on multi-core processors**
- **Secure grid data transfer**
- **www.grid.cs.binghamton.edu/**



NYSGrid.org

- **Grass-Roots Cyberinfrastructure Initiative in NYS.**
- **Open to academic and research institutions.**
- **Mission Stmt: 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.**
- **To date, no utilization on any Grid through their VO.**
- **www.nysgrid.org**
- **Recently made part of NYSERNet.**



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www.cse.buffalo.edu/faculty/miller