Miller's Cyberinfrastructure Laboratory (MCIL)

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NSF, NIH, DOE, NIMA, NYS, HP

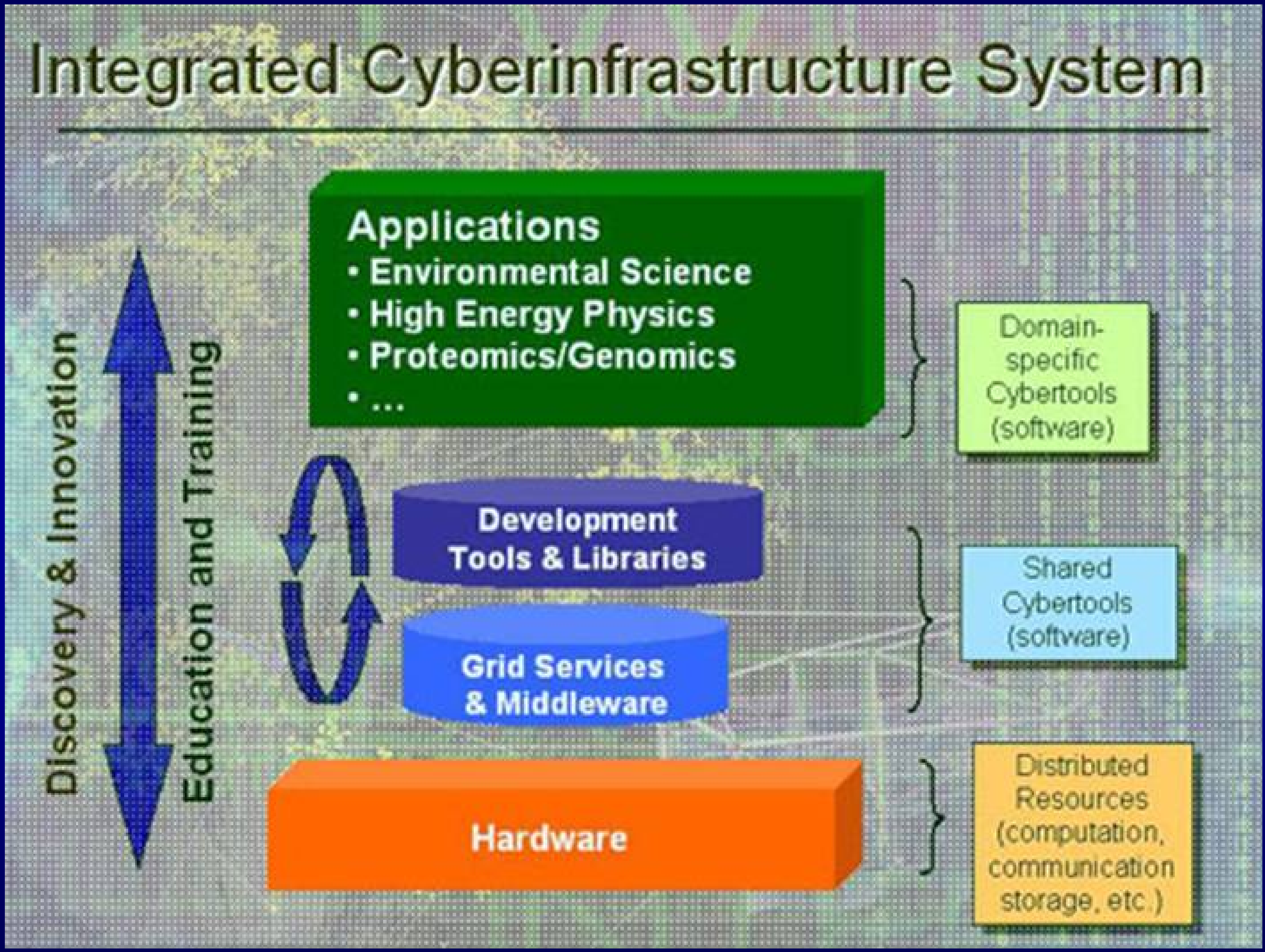
www.cse.buffalo.edu/faculty/miller/CI/

GRID
Advanced
Center for Computational Research
Data
Center

Cyberinfrastructure

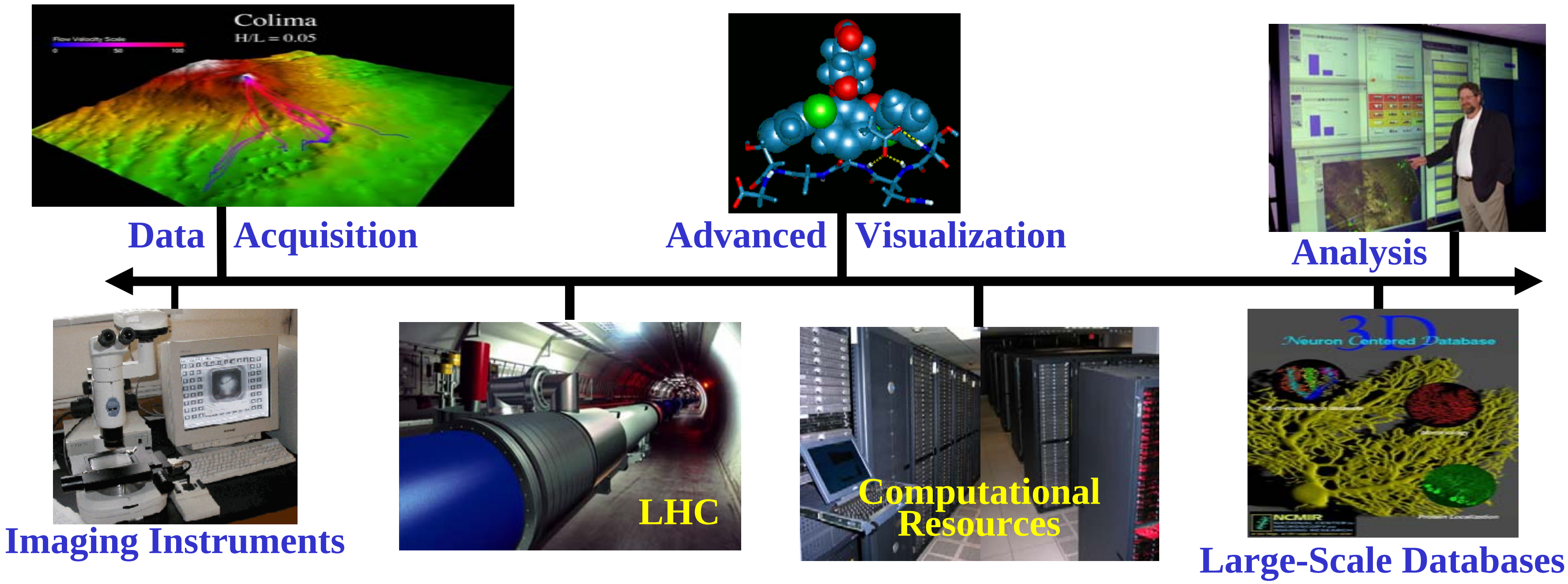
- **Foster & Kesselman: "a domain-independent computational infrastructure designed to support science."**
- **NSF: "comprehensive phenomenon that involves creation, dissemination, preservation, and application of knowledge"**
- **Generic: transparent and ubiquitous application of technologies central to contemporary engineering and science**
- **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."

Grid Computing Overview



- 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

Home Page - Netscape

File Edit View Go Bookmarks Tools Window Help

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

Mail Home Netscape

New Tab | Home Page

Cyberinfrastructure Laboratory

Ubiquitous High-End Computing, Data, Networking, & Visualization

Dr. Russ Miller

UB Distinguished Professor

- CI Lab
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Introduction

In the 21st century, leading academic institutions will embrace our digital data-driven society and empower students to compete in this knowledge-based economy. In order to support research, scholarship, education, and community outreach, the Cyberinfrastructure Laboratory (CI Lab) is dedicated to the integration of research in disciplinary domains, including science, engineering, and biomedicine, with research in enabling technologies and interfaces. The goal is to allow students and scientists to transparently collect, manage, organize, analyze, and visualize data without having to worry about details such as where the data is stored, where the data is processed, where the data is rendered, and so forth. This ease of use and high availability of data and information processing tools will allow for revolutionary advances in all areas of science, engineering, and beyond.

Cyberinfrastructure sits at the core of modern simulation and modeling, which allows for entirely new methods of investigation that allow scholars to address previously unsolvable problems. Specifically, the development of necessary software, algorithms, portals, and interfaces that will enable research and scholarship by freeing end-users from dealing with the complexity of various computing environments is critical to extending the reach of high-end computing, storage, networking, and visualization to the general user community.

Projects in the CI Lab are currently supported by an NSF ITR grant, an NSF CRI grant, and the Center for Computational

Miller's Cyberinfrastructure Lab

- **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

- **Experimental Equipment (1.25 TF; 140 Cores; 22TB)**
  - **Clusters**
    - **Head Nodes: Dell 1950 (Intel)**
    - **Workers: Intel 8×2 ×4 & AMD 8×2×2**
  - **Virtual Memory Machines (2 × Intel 4×4)**
  - **Dell GigE Managed Switches**
  - **InfiniBand**
  - **22 TB Dell Storage (2)**
  - **Condor Flock (35 Intel/AMD)**
  - ***In process*: 40-50TF system**
- **Production Equipment**
  - **Dell Workstations; Dell 15 TB Storage**
  - **Access to CCR equipment (13TF Dell/Intel clusters)**

Evolution of CI Lab Projects

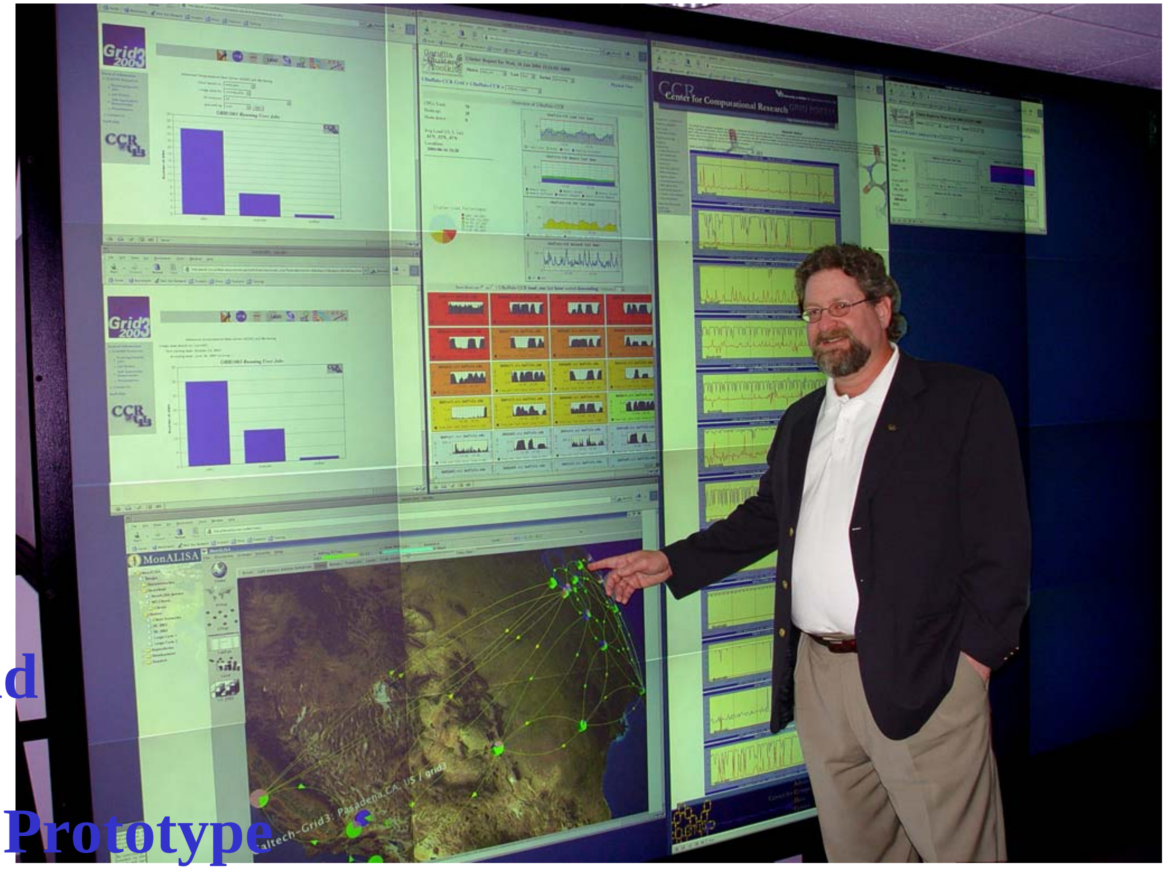
- **Buffalo-Based Grid**
  - **Experimental Grid: Globus & Condor**
  - **Integrate Data & Compute, Monitor, Portal, Node Swapping, Predictive Scheduling/Resource Management**
  - **GRASE VO: Structural Biology, Groundwater Modeling, Earthquake Eng, Comp Chemistry, GIS/BioHazards**
  - **Buffalo, Buffalo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

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

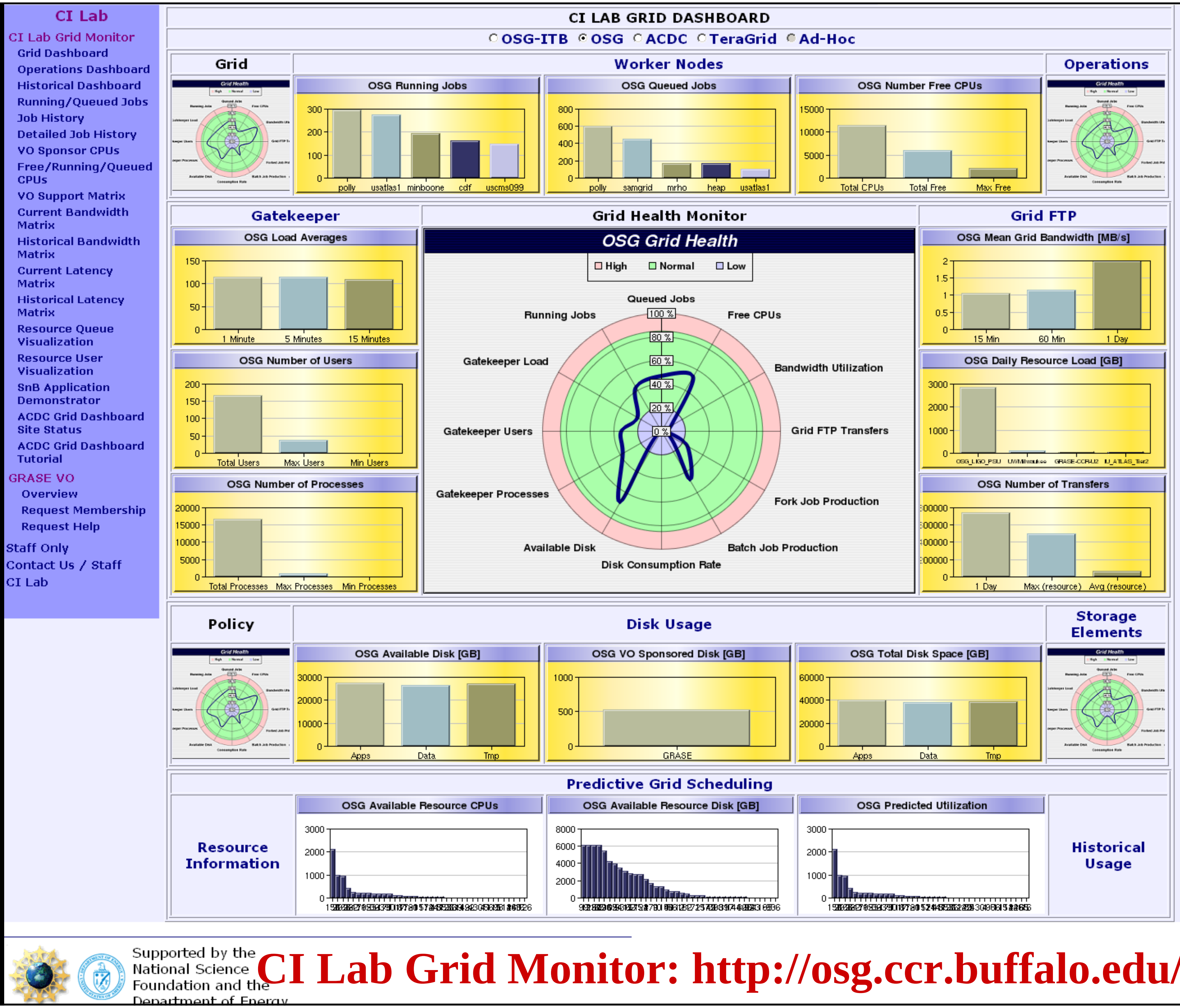
CI Lab Collaborations

- 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

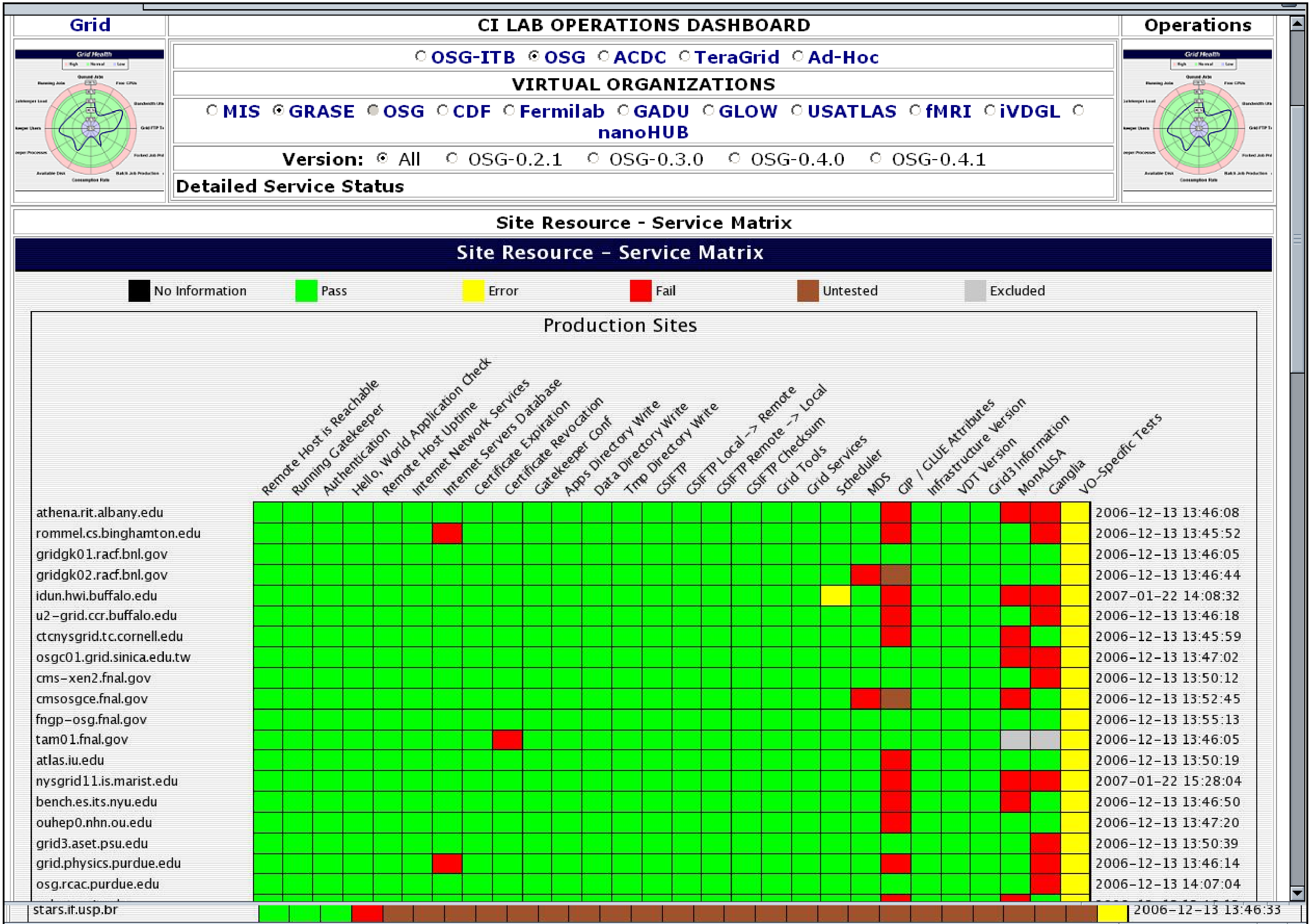


CI Lab Projects

- 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/

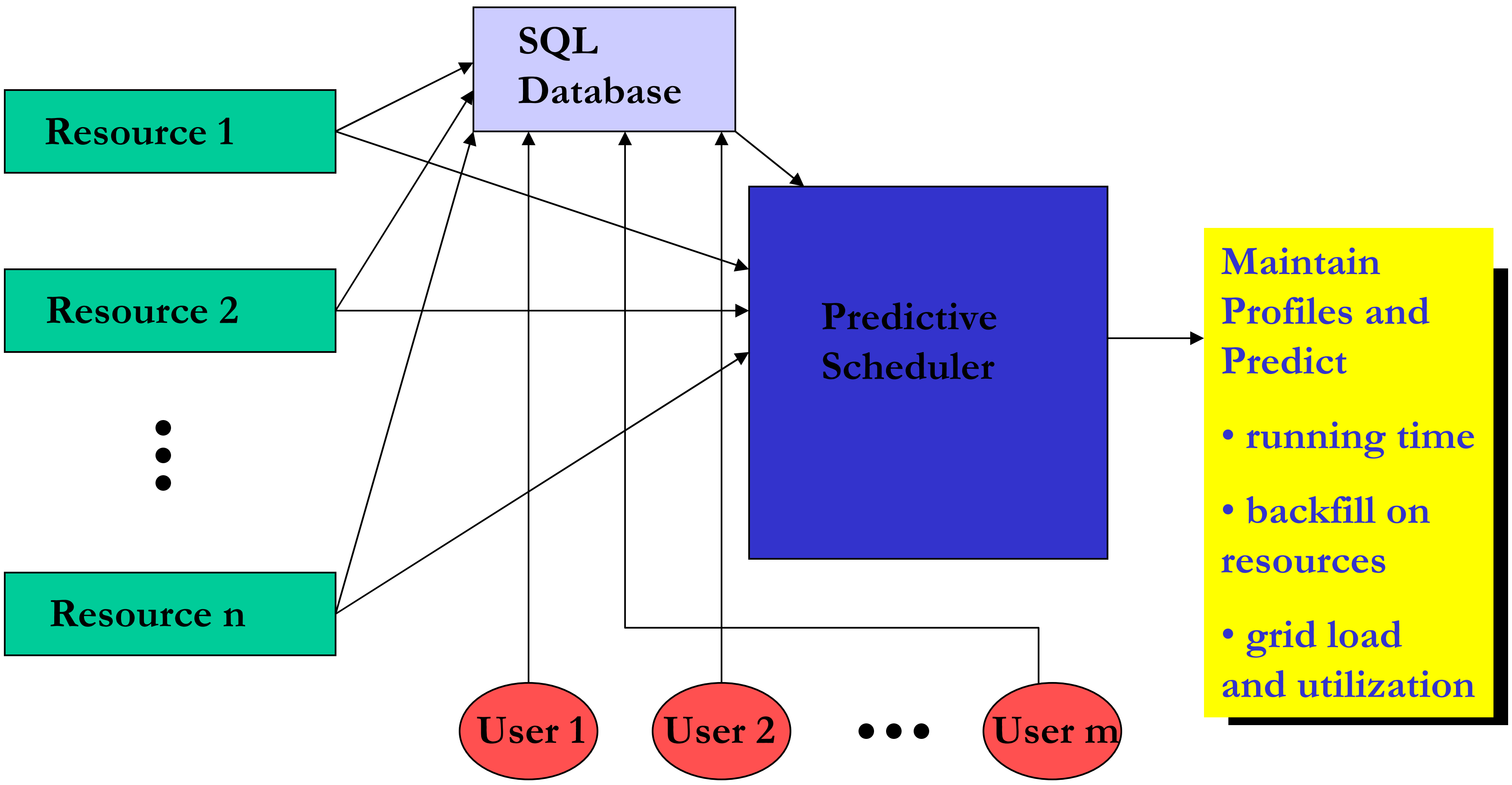


CI Lab Operations Dashboard

Predictive Scheduler

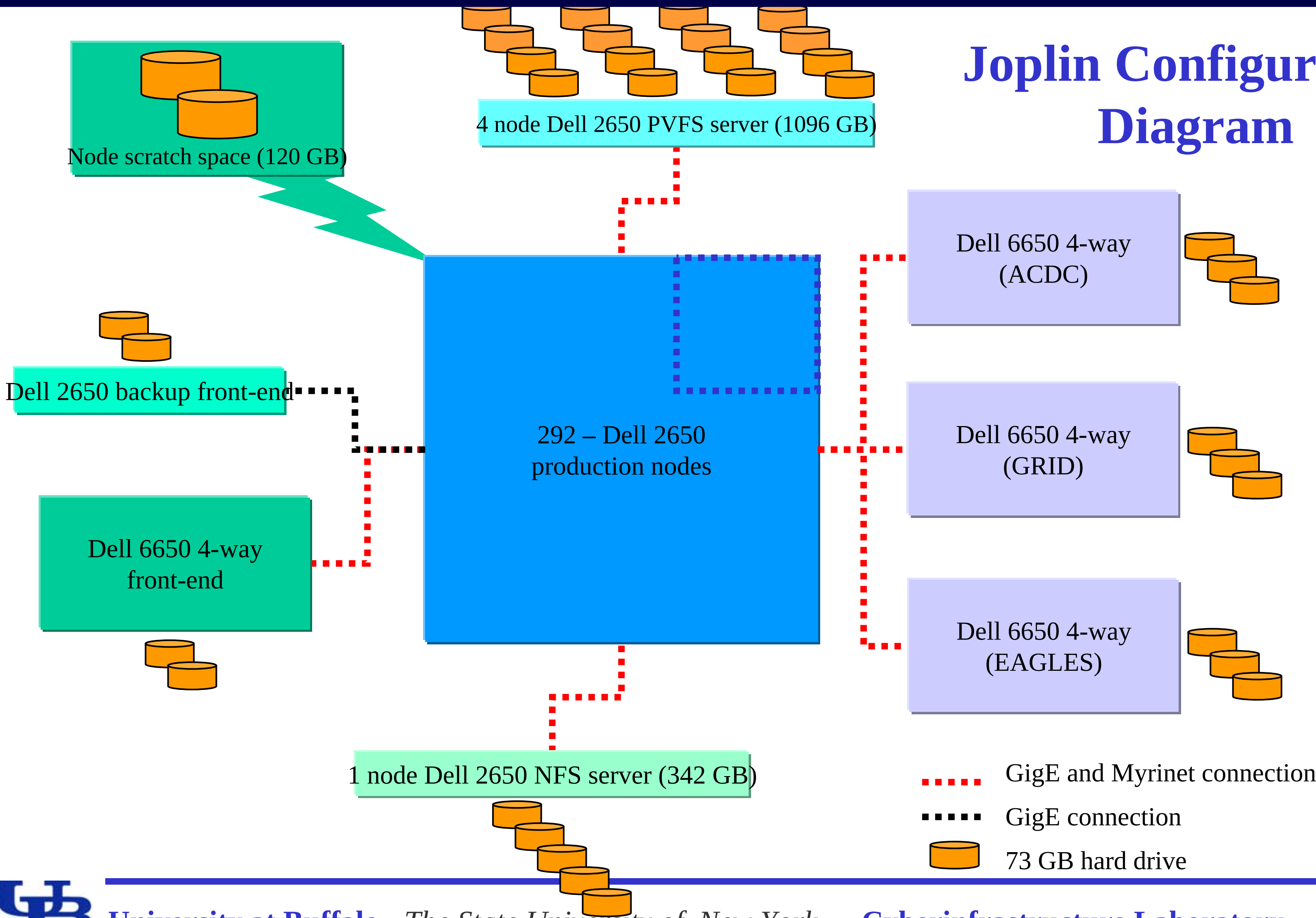
- Build profiles based on statistical analysis of logs of past jobs
  - Per User/Group
  - Per Resource
- Use these profiles to predict runtimes of new jobs
- Make use of these predictions to determine
  - Resources to be utilized
  - Availability of Backfill

System Diagram

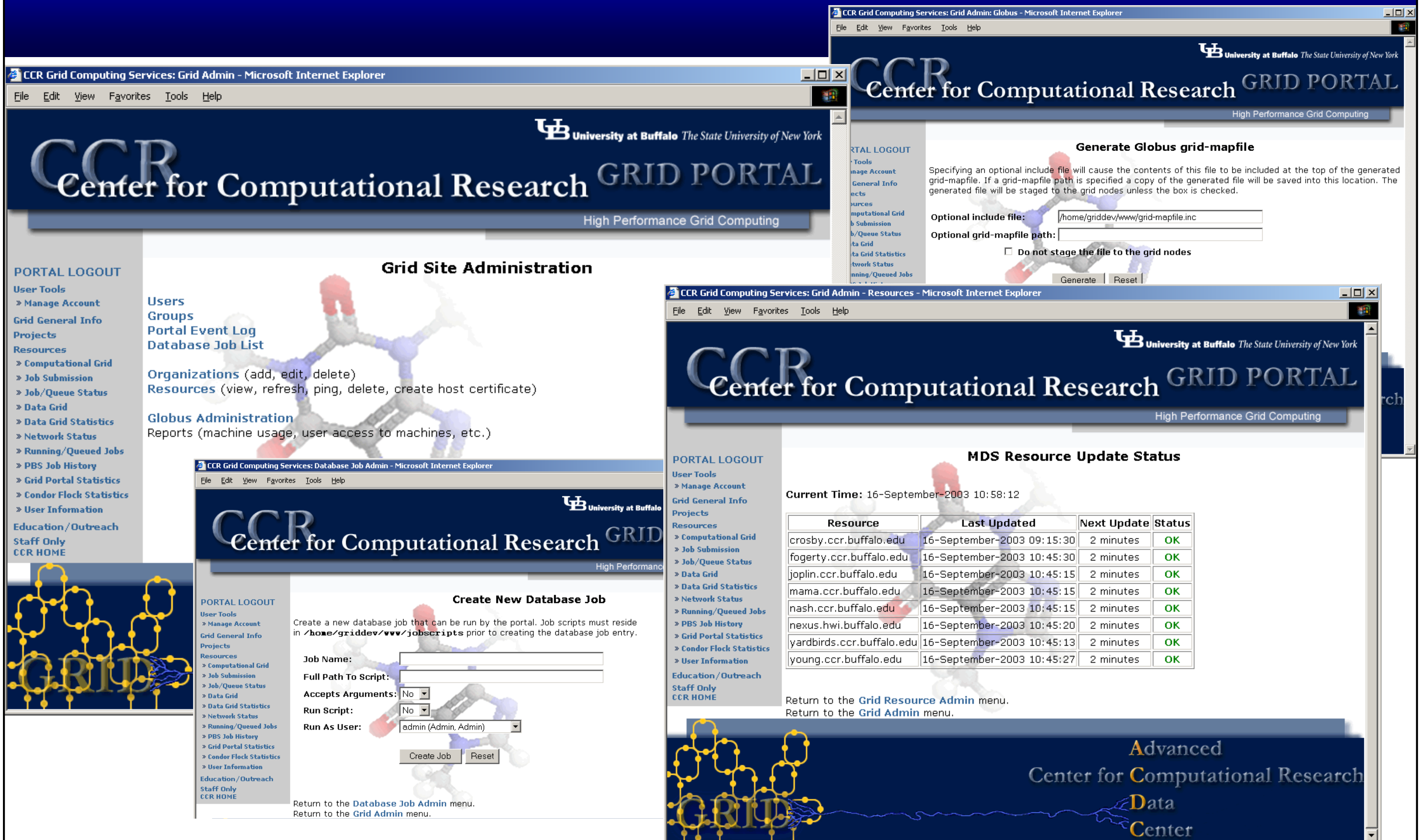


ACDC-Grid Dynamic Resource Allocation

Joplin Configuration Diagram



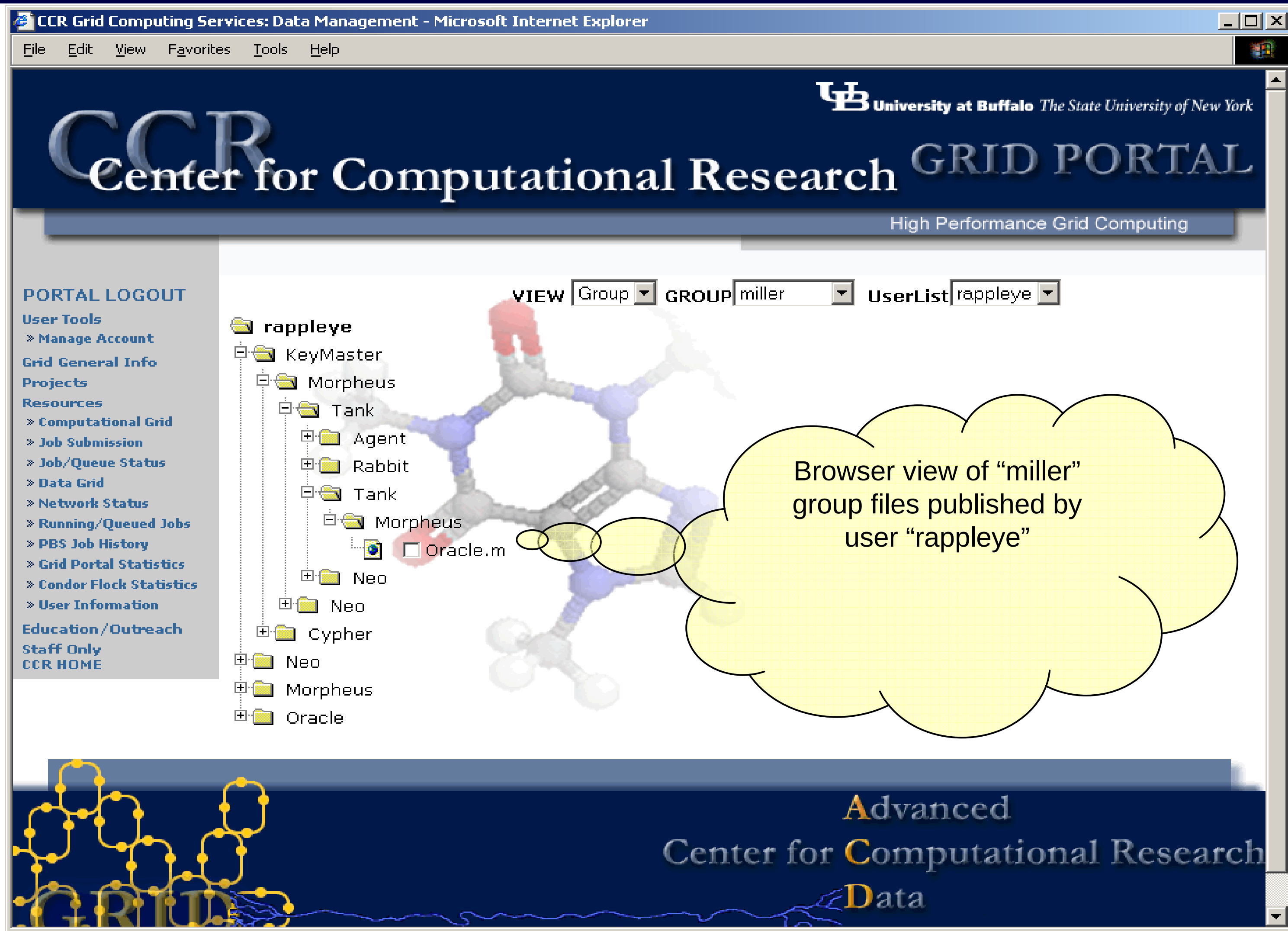
Grid Administration



Data Grid

- **Motivation:**
  - **Large data collections are emerging as important community resources.**
  - **Data Grids complement Computational Grids.**
- **Definition:** ***A data grid is a network of distributed storage resources, including archival systems, caches, and databases, which are linked logically to create a sense of global persistence.***
- **Goal: Design and implement transparent management of data distributed across heterogeneous resources.**

ACDC-Grid Data Grid



ACDC-Grid Data Grid Functionality

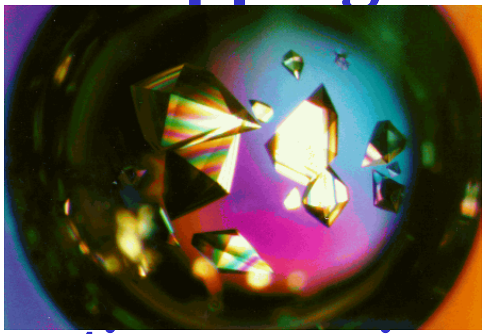
- Basic file management functions are accessible via a platform-independent web interface.
- User-friendly menus/interface.
- File Upload/Download to/from the Data Grid Portal.
- Simple Web-based file editor.
- Efficient search utility.
- Logical display of files (user/ group/ public).
- Ability to logically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

Grid-Enabling Application Templates (GATs)

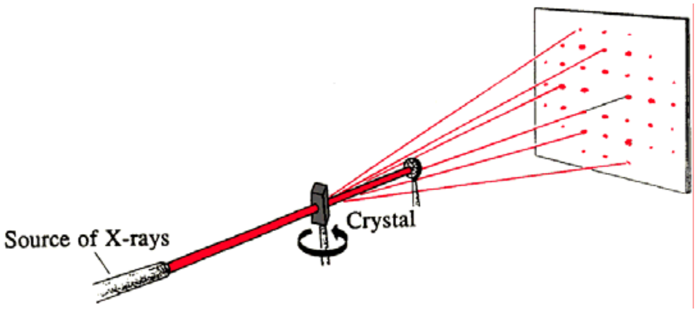
- Structural Biology
  - *SnB* and *BnP* for Molecular Structure Determination/Phasing
- Groundwater Modeling
  - *Ostrich*: Optimization and Parameter Estimation Tool
  - *POMGL*: Princeton Ocean Model Great Lakes for Hydrodynamic Circulation
  - *Split*: Modeling Groundwater Flow with Analytic Element 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

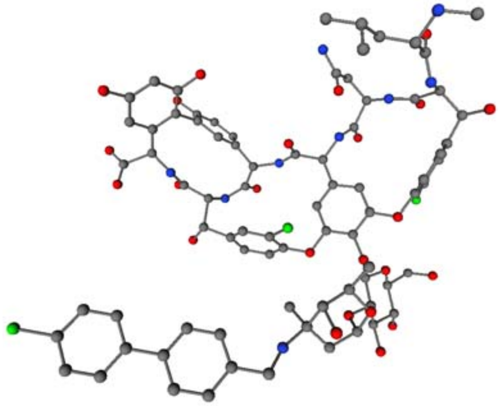
X-Ray Crystallography

- **Objective: Provide a 3-D mapping of the atoms in a crystal.**
- **Procedure:**



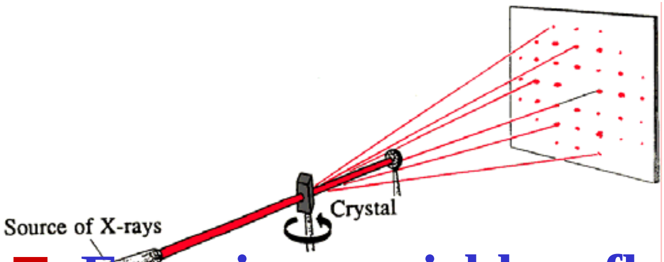
1. **Isolate a single crystal.**
2. **Perform the X-Ray diffraction experiment.**



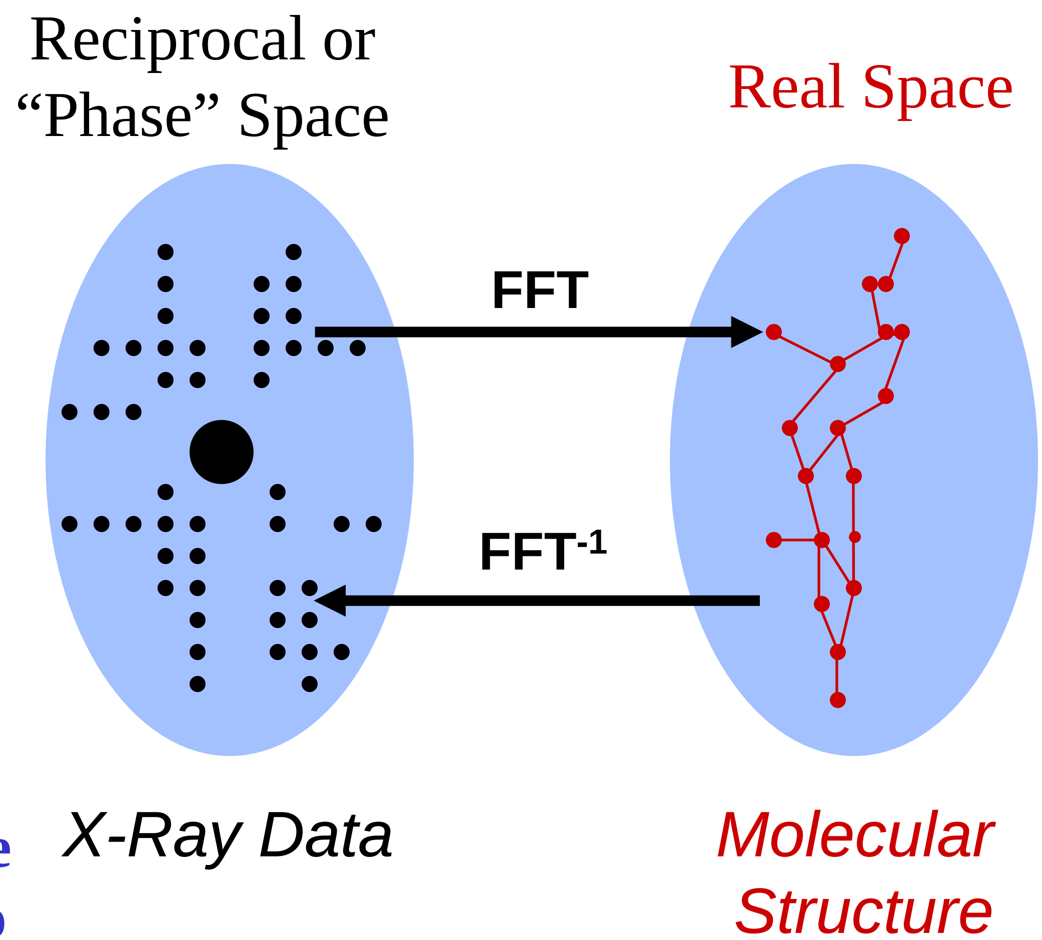


3. **Determine molecular structure that agrees with diffration data.**

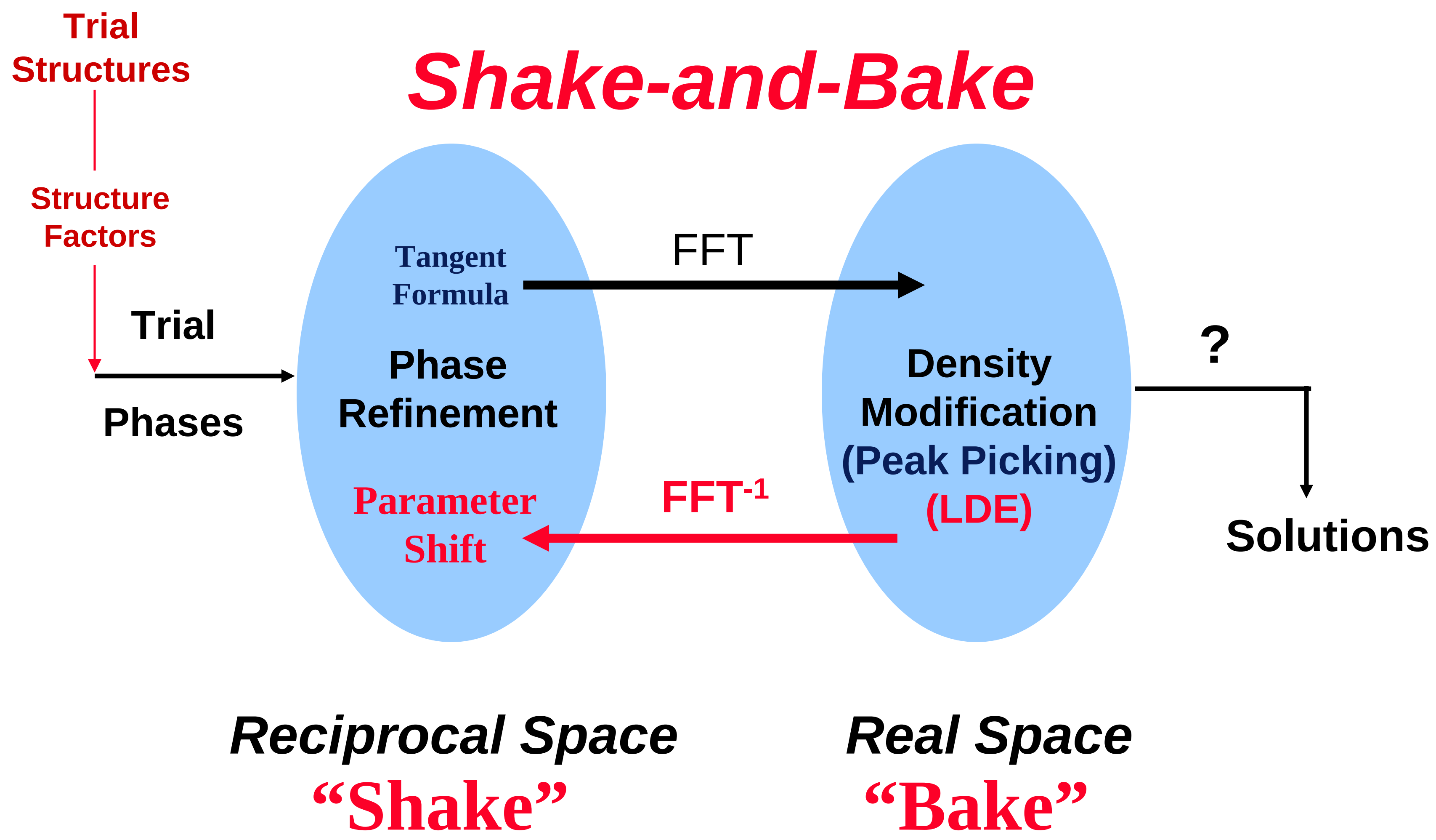
X-Ray Data & Corresponding Molecular Structure



- 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.



Shake-and-Bake Method: Dual-Space Refinement



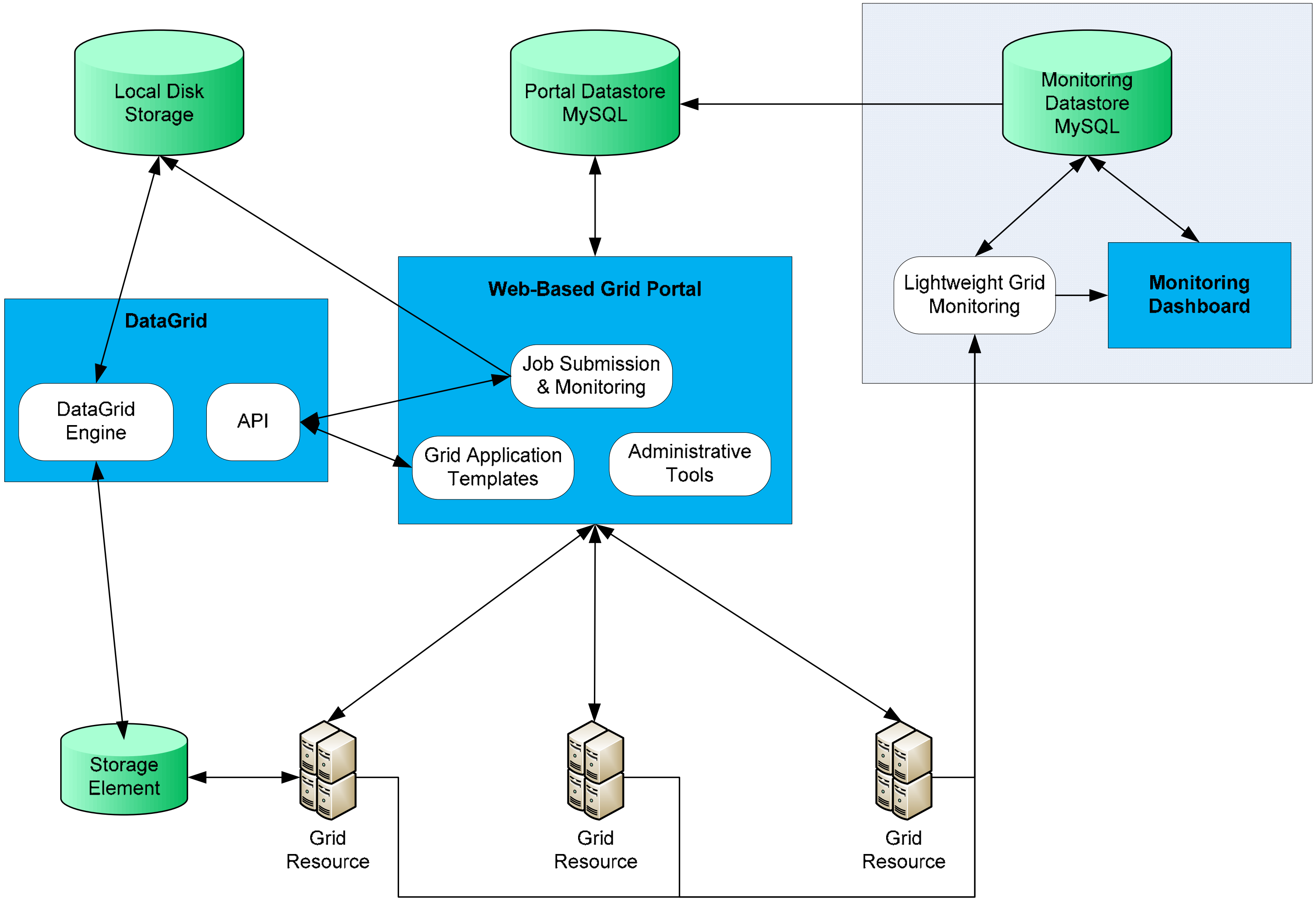
Grid Enabled *SnB*

- **Problem Statement**
  - Use all available resources for determining a single structure
- **Grid Enabling Criteria**
  - Run on heterogeneous set of resources
  - Store results in *SnB* database
  - Mine database (and automagically deploy new jobs) to improve parameter settings
- **Runtime Parameters Transparent to User**
  - Assembling Necessary Files
  - Number of Processors
  - Trials per Processor
  - Appropriate Queue and Running Times

Grid Enabled *SnB* Execution

- User
  - defines Grid-enabled *SnB* job using Grid Portal or *SnB*
  - supplies location of data files from Data Grid
  - supplies *SnB* mode of operation
- Grid Portal
  - assembles required *SnB* data and supporting files, execution scripts, database tables.
  - determines available ACDC-Grid resources.
- ACDC-Grid job management includes:
  - automatic determination of appropriate execution times, number of trials, and number/location of processors,
  - logging/status of concurrently executing resource jobs, &
  - automatic incorporation of *SnB* trial results into the molecular structure database.

NYS Grid Portal



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

Mail Home 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.

BnP

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

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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 applciations. 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.

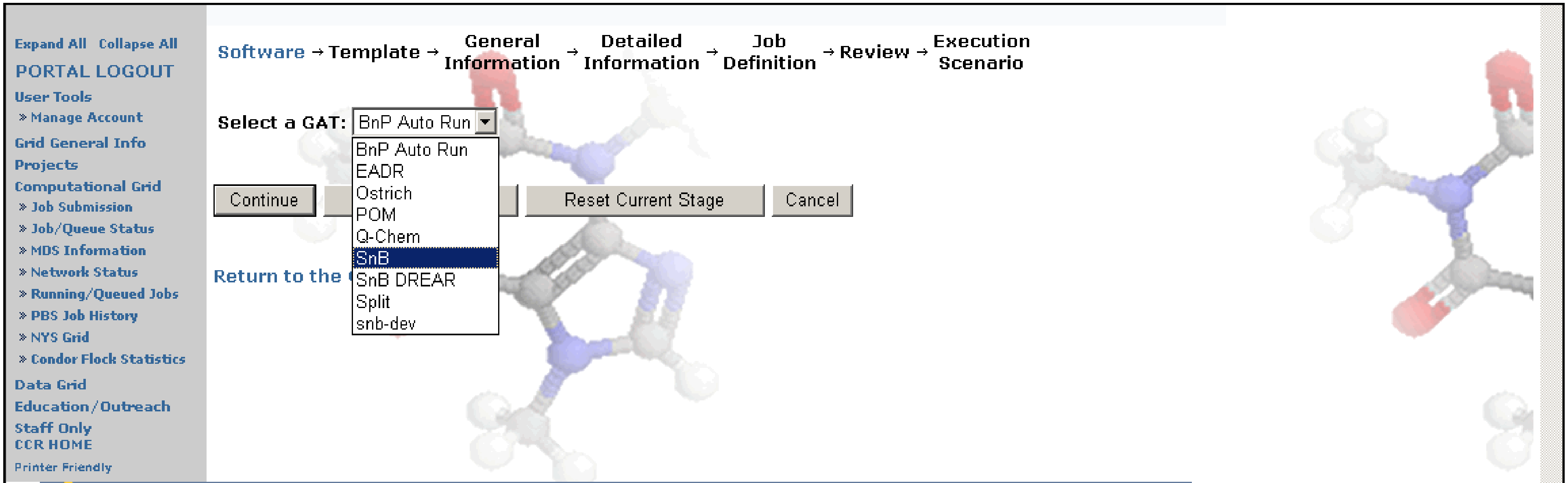
The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are require for execution in the ACDC-Grid environment. We have identified that sequentially defining milestones for the grid user to complete intuitively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

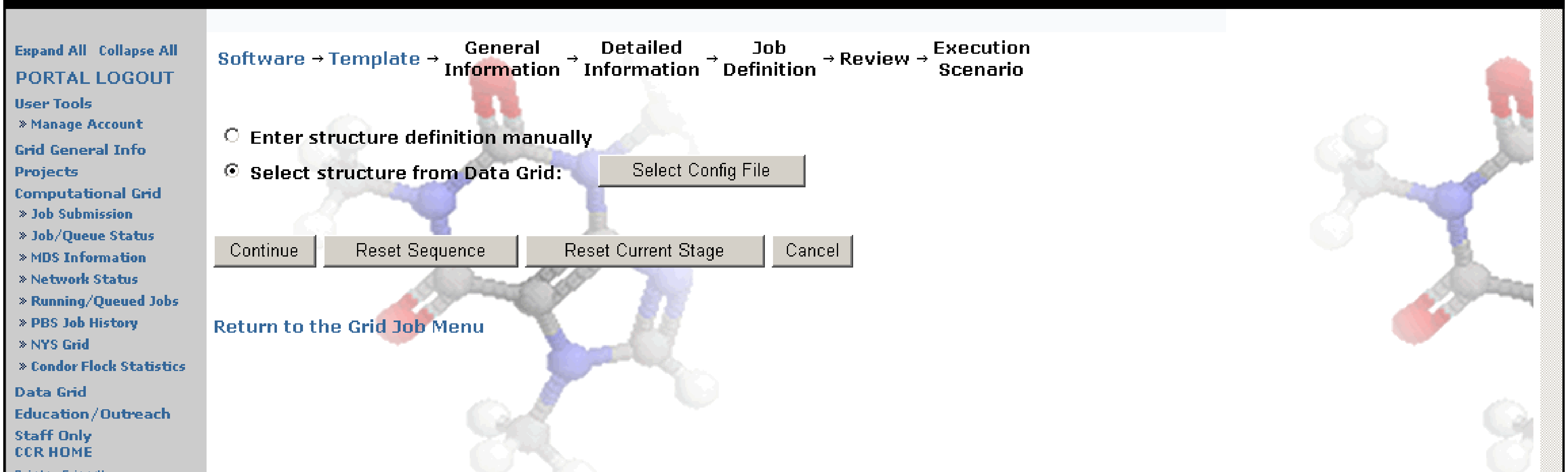
Each item of the job definition workflow is then stored in the ACDC-Grid Web Portal database so the grid user may use/modify any previously created workflow in creating new job definitions. The job definitions can also be accessed via batch script files for executing hundreds of similar workflows in 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



Software Package Selection



Full Structure / Substructure Template Selection

User Tools
» Manage Account
Grid General Info
Projects
Computational Grid
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» Job/Queue Status
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» Network Status
» Running/Queued Jobs
» PBS Job History
» NYS Grid
» Condor Flock Statistics
Data Grid
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General Information

Structure Information

Title: lled

Structure ID : iled

Space Group : 19 [Select]

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):

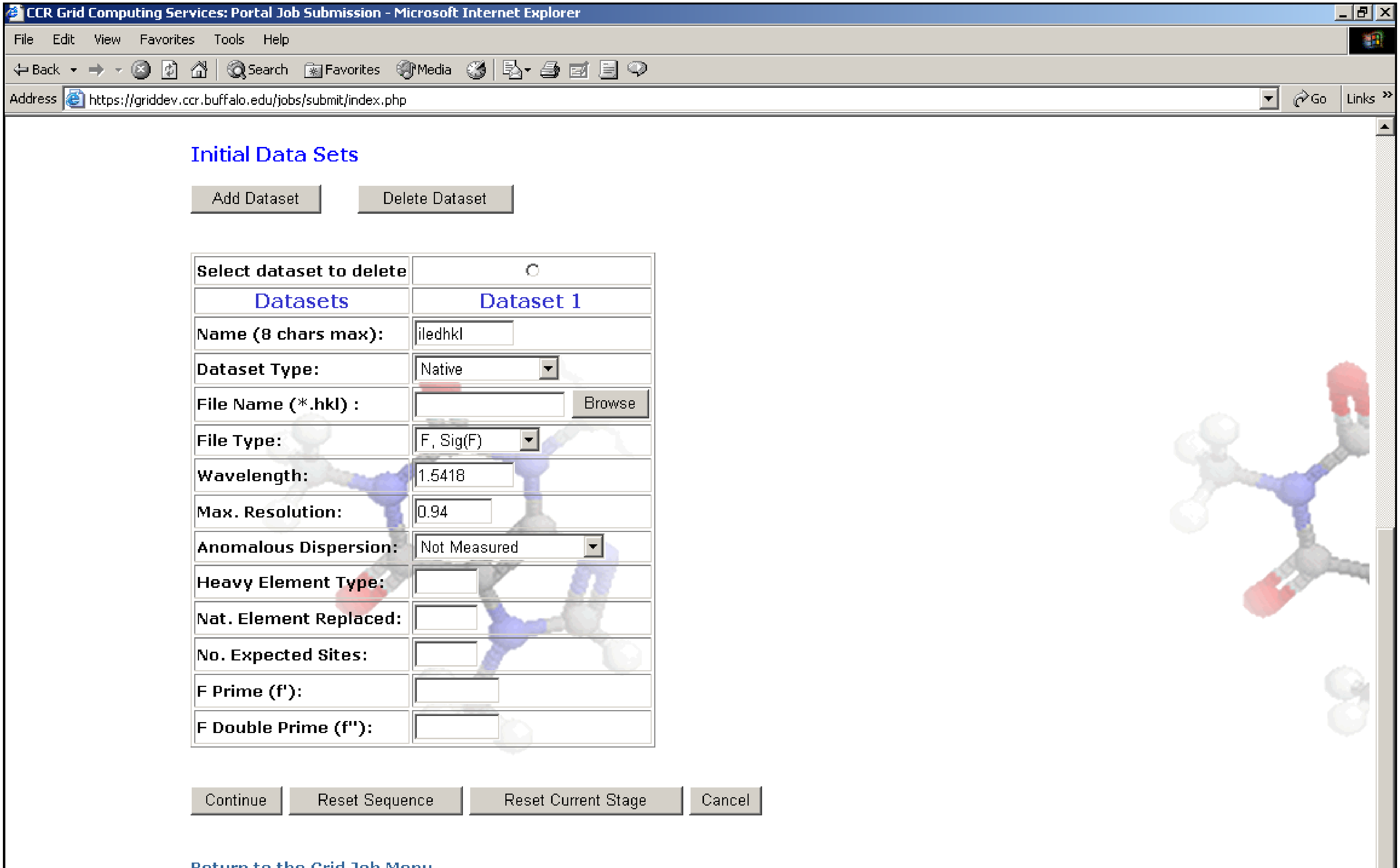
ASU Contents : C60H102N6O18 (examples: C6H12O6 OR C6 H12 O6)

Initial Data Sets

[Add Dataset] [Delete Dataset]

Select dataset to delete	○
Datasets	Dataset 1
Name (8 chars max):	iledhkl

Default Parameters Based on Template



Default Parameters (cont'd)

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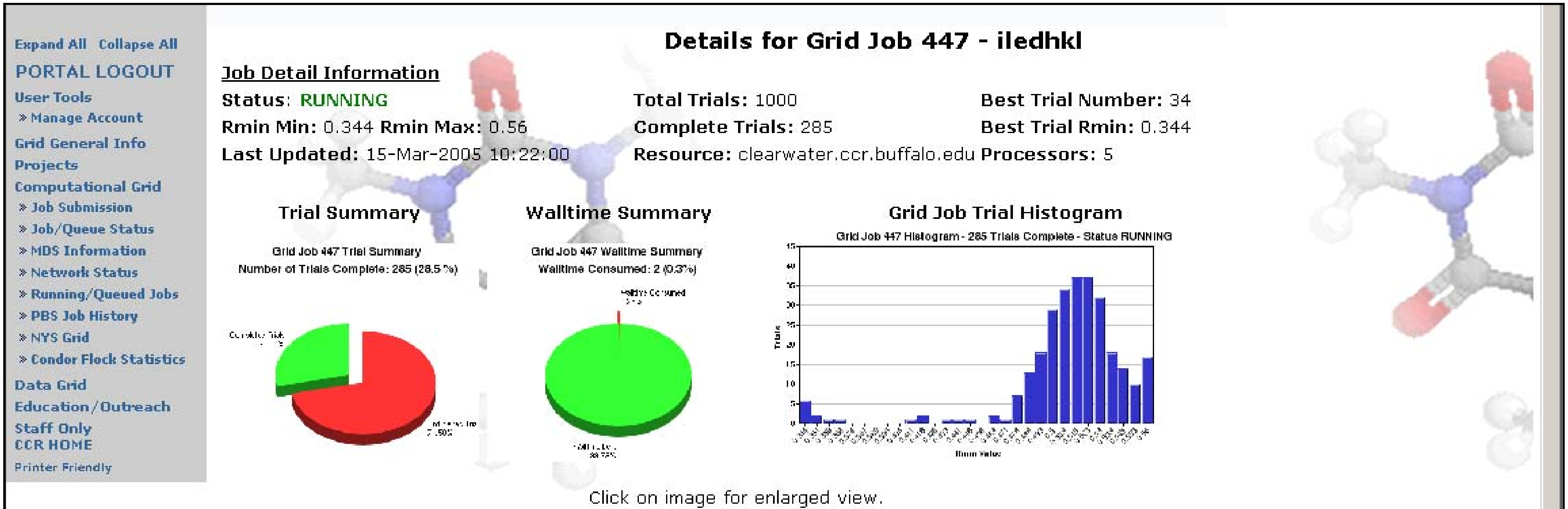
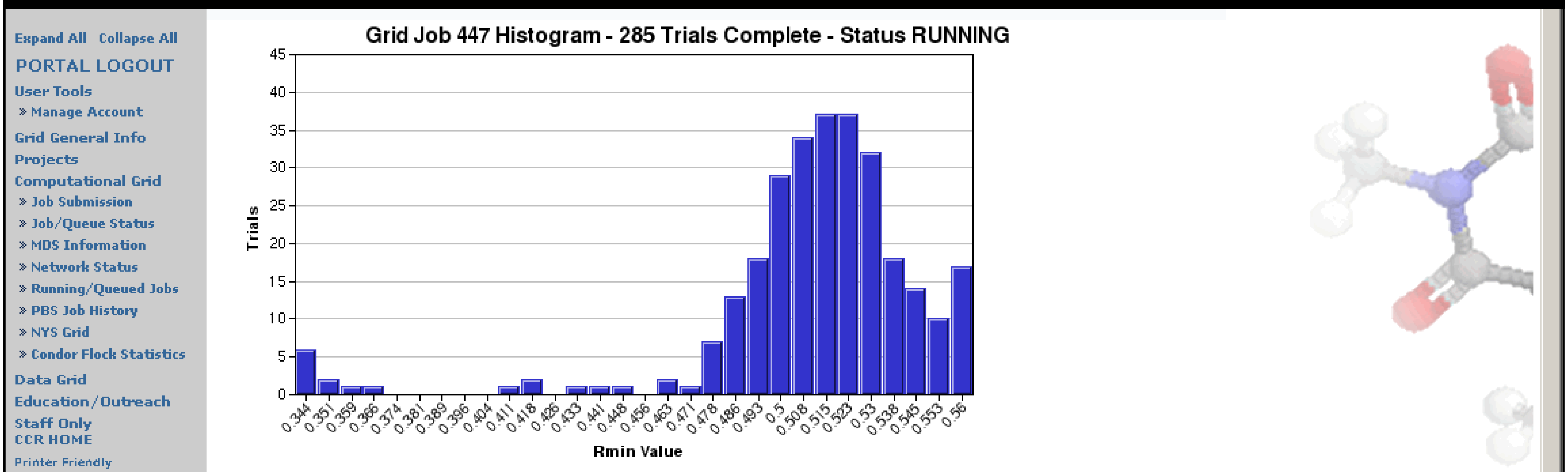
SnB Job Review

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

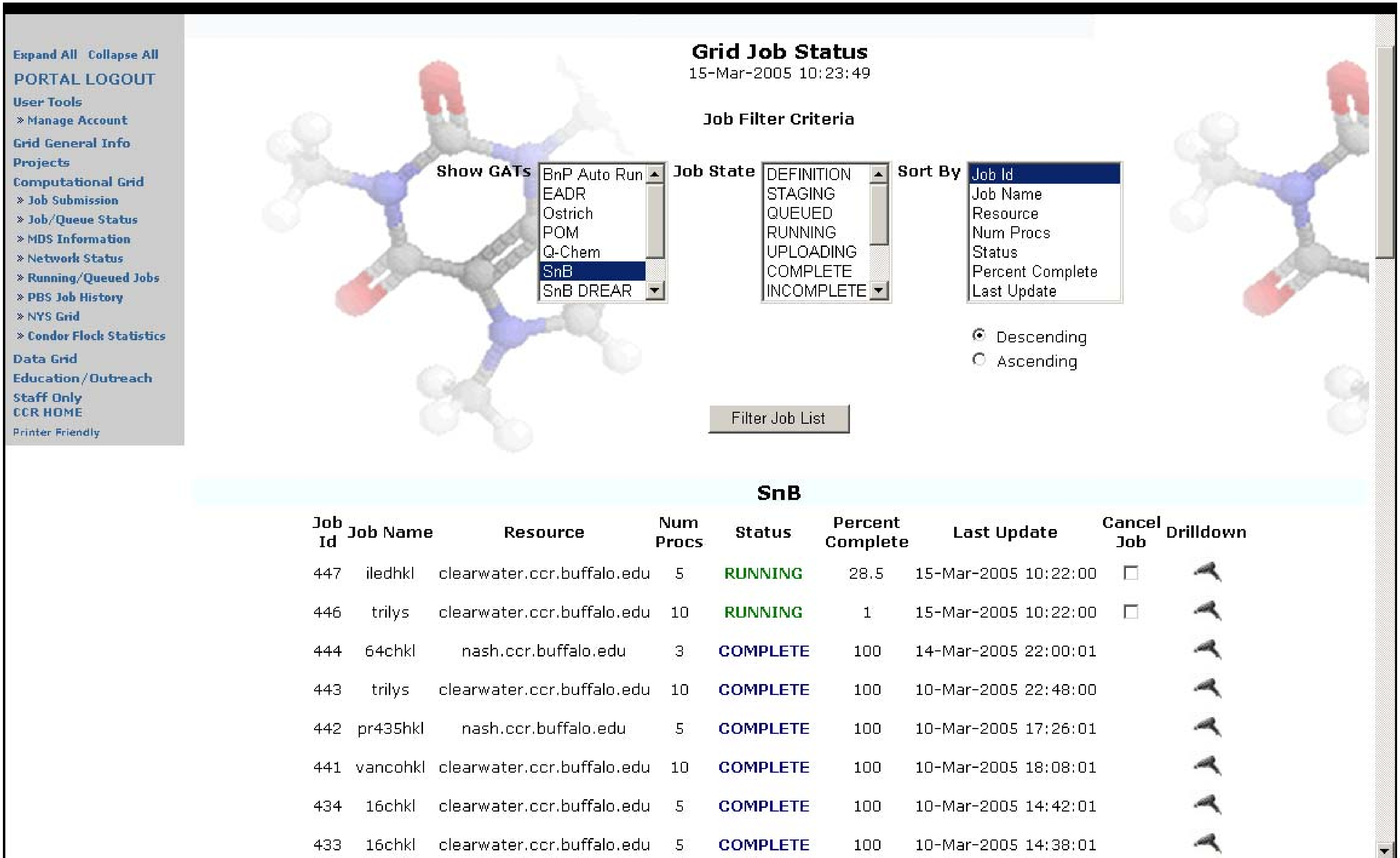
SnB Review (Grid job ID: 447)



Graphical Representation of Intermediate Job Status



Histogram of Completed Trial Structures



Expand All Collapse All
PORTAL LOGOUT
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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

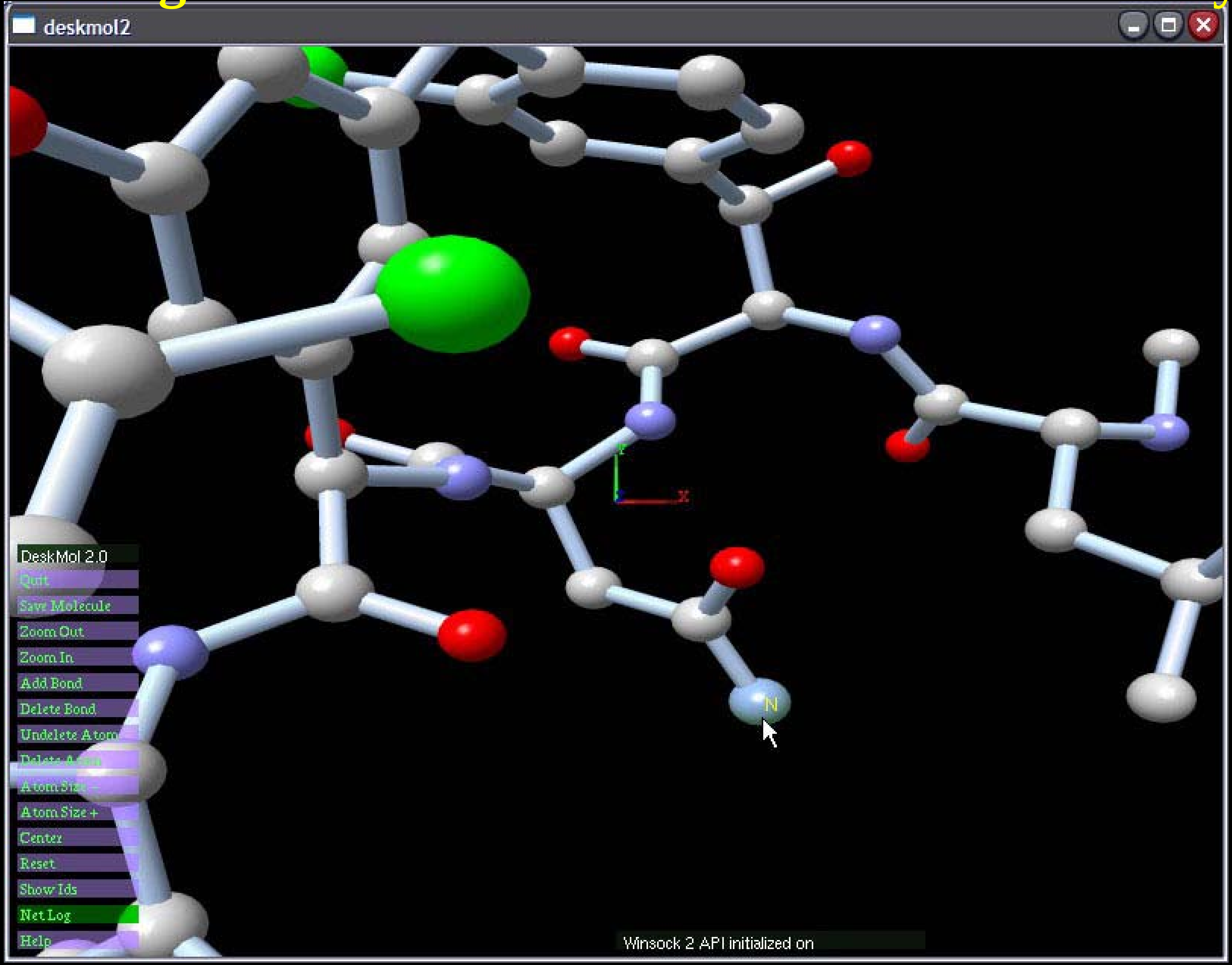
Filter Job List

SnB

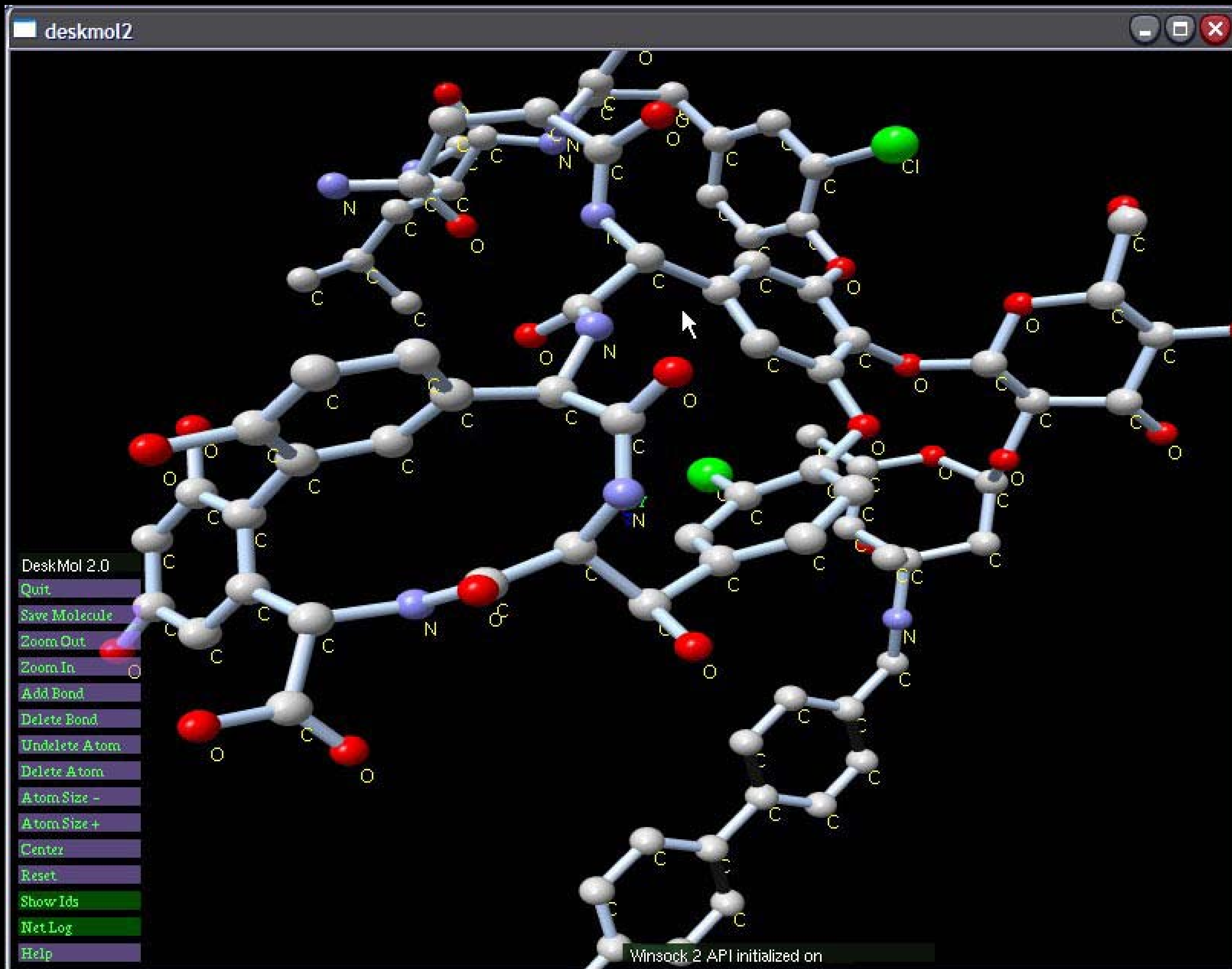
Job Id	Job Name	Resource	Num Procs	Status	Percent Complete	Last Update	Cancel Job	Drilldown
447	iledhkl	clearwater.ccr.buffalo.edu	5	RUNNING	28.5	15-Mar-2005 10:22:00	☐	
446	trilys	clearwater.ccr.buffalo.edu	10	RUNNING	1	15-Mar-2005 10:22:00	☐	
444	64chkl	nash.ccr.buffalo.edu	3	COMPLETE	100	14-Mar-2005 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.

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

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

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- NSF CRI
- NSF MRI
- NYS
- CCR


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