

The Cyberinfrastructure Laboratory: Middleware Overview

Russ Miller

Director, CI Laboratory

Dept of Comp Sci & Eng

Hauptman-Woodward Med Res Inst

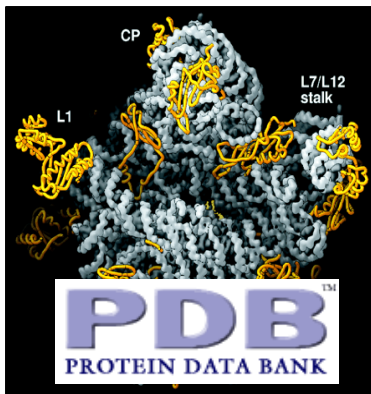
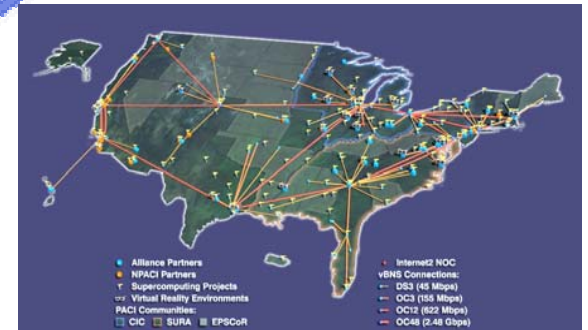
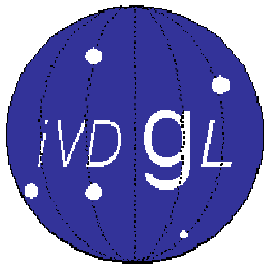
Executive Director, NYSGrid

NSF, NIH, DOE, NIMA, NYS, HP

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



Grid Computing



Asia-Pacific Advanced Network

Advanced
Center for Computational Research
Data
Center

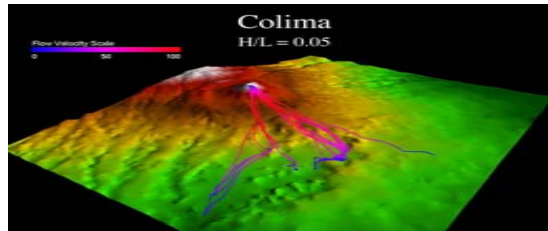


University at Buffalo The State University of New York

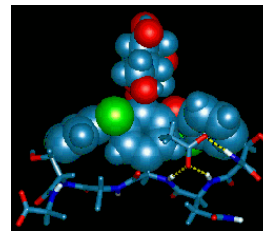
Cyberinfrastructure Laboratory

CI Lab

Grid Computing Overview



Data Acquisition



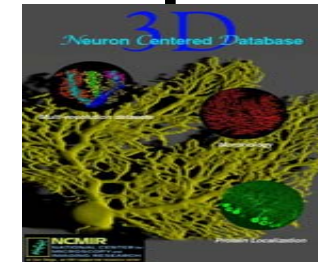
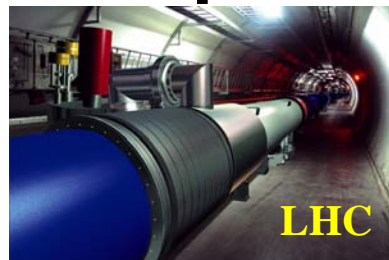
Advanced Visualization



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



ACDC-Grid Collaborations I

- **High-Performance Networking Infrastructure**
- **Grid3+ Collaboration**
- **iVDGL Member**
 - ❑ Only External Member
- **Open Science Grid**
 - ❑ Organizational Committee
 - ❑ Blueprint Committee
 - ❑ Security Working Group
 - ❑ Data Working Group
 - ❑ GRASE VO
- **Grid-Lite: Campus Grid**
 - ❑ HP Labs Collaboration
- **Innovative Laboratory Prototype**
 - ❑ Dell Collaboration



ACDC-Grid Collaborations II

■ Grass Roots NYS Grid (pre-NYSGrid.org)

- SUNY-Albany
- SUNY-Binghamton
- SUNY-Buffalo
- SUNY-Geneseo
- Canisius College
- Columbia
- Hauptman-Woodward Inst.
- Niagara University

■ GRASE VO: Grid Resources for Advanced Science and Engineering Virtual Organization

- (Non-Physics Research)
- Structural Biology
- Groundwater Modeling
- Earthquake Engineering
- Computational Chemistry
- GIS/BioHazards



"Middleware"

- **Intermediate Software Layer between Application Codes and Grid Resources**
- **Required for applications, users, and resource providers to operate effectively in a manner transparent to the user**
- **Security; Resource Management; Data Access; Policies; Accounting;**
- **Globus; Condor**
- **Checks availability of Resources**
 - CPUs; Storage; Networking; Render Farms; etc.
- **Scheduling / Workload Management System**
- **Resource Broker**
 - Evaluates Job and Breaks Up/Submits



NSF Middleware Initiative (NMI)

- **Develop, improve, and deploy a suite of reusable software components for use in national-scale “cyberinfrastructure”.**
- **APST, Condor, CPM, DataCutter, DataCutter STORM, Globus Toolkit, GPT, Gridconfig, GridPort, GridSolve, GSI OpenSSH, Inca, KX.509/KCA, Look, MPICH-G2, MyProxy, Network Weather Service, OpenSAML, PERMIS, PyGlobus, Shibboleth, SRB Client, UberFTP, and WebISO (Web Initial Sign-on).**



Grid Issues

- **High-Throughput Computing**
- **Transparent Integration of Data, Computing, Sensors/Devices, Networking**
- **Heterogeneous Resources**
- **Standards (Grid, Data)**
- **Major User Communities**
 - **High-Energy Physics and Astrophysics**
 - **Medicine and Biological Sciences**
 - **Earth Sciences**
- **Public Funding Still Critical**
- **Grids are in their Infancy**



Major Grid Initiatives

- **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!
- **OSG (DOE, NSF)**
 - ❑ High-Throughput Distributed Facility
 - ❑ Open & Heterogeneous
 - ❑ Biology, Computer Science, Astrophysics, LHC
 - ❑ 57 Compute Sites; 11 Storage Sites;
 - ❑ 10K CPUS; 6PB
- **TeraGrid (NSF)**
 - ❑ Integrates High-End Resources
 - ❑ High-Performance (Dedicated) Networks
 - ❑ 9 Sites; 100TF & 15PB
 - ❑ 100+ Databases Available

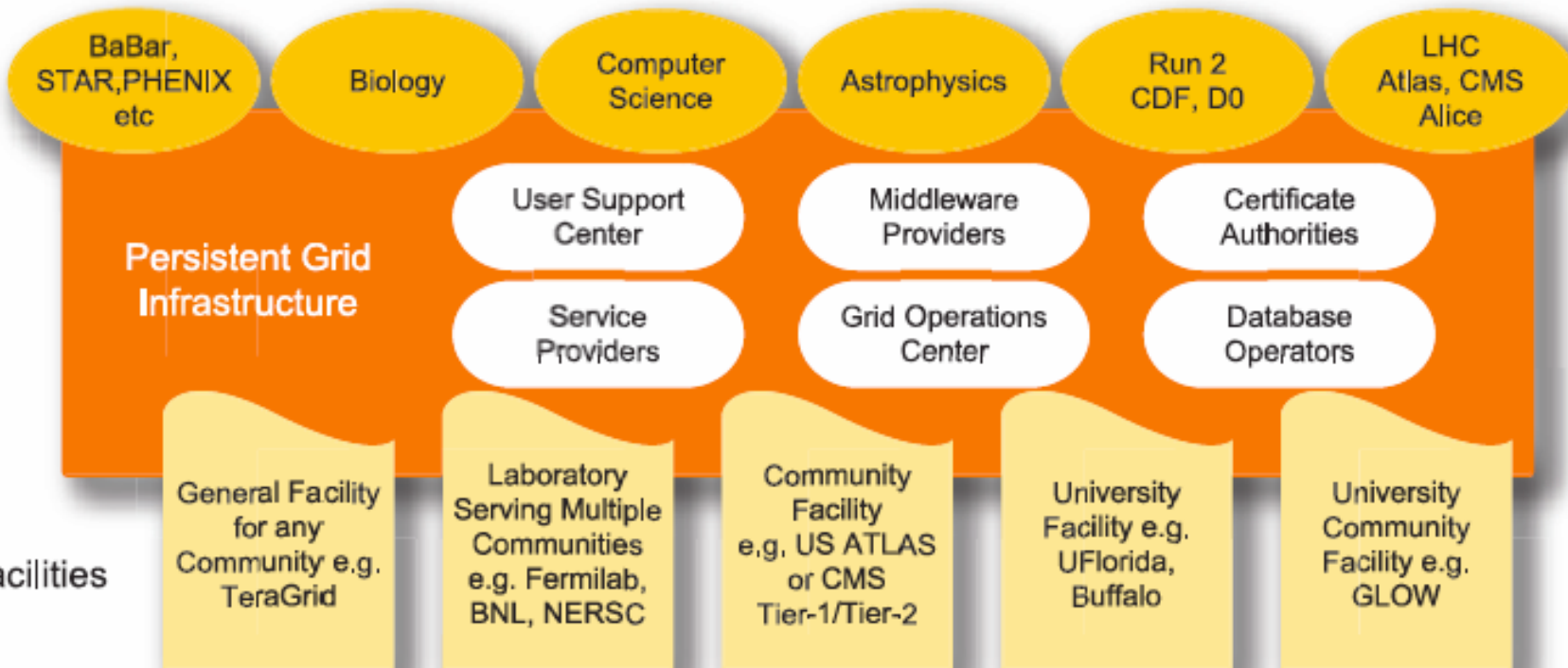


Open Science Grid

Courtesy of Paul Avery

Open Science Grid *Applications, Infrastructure, and Facilities*

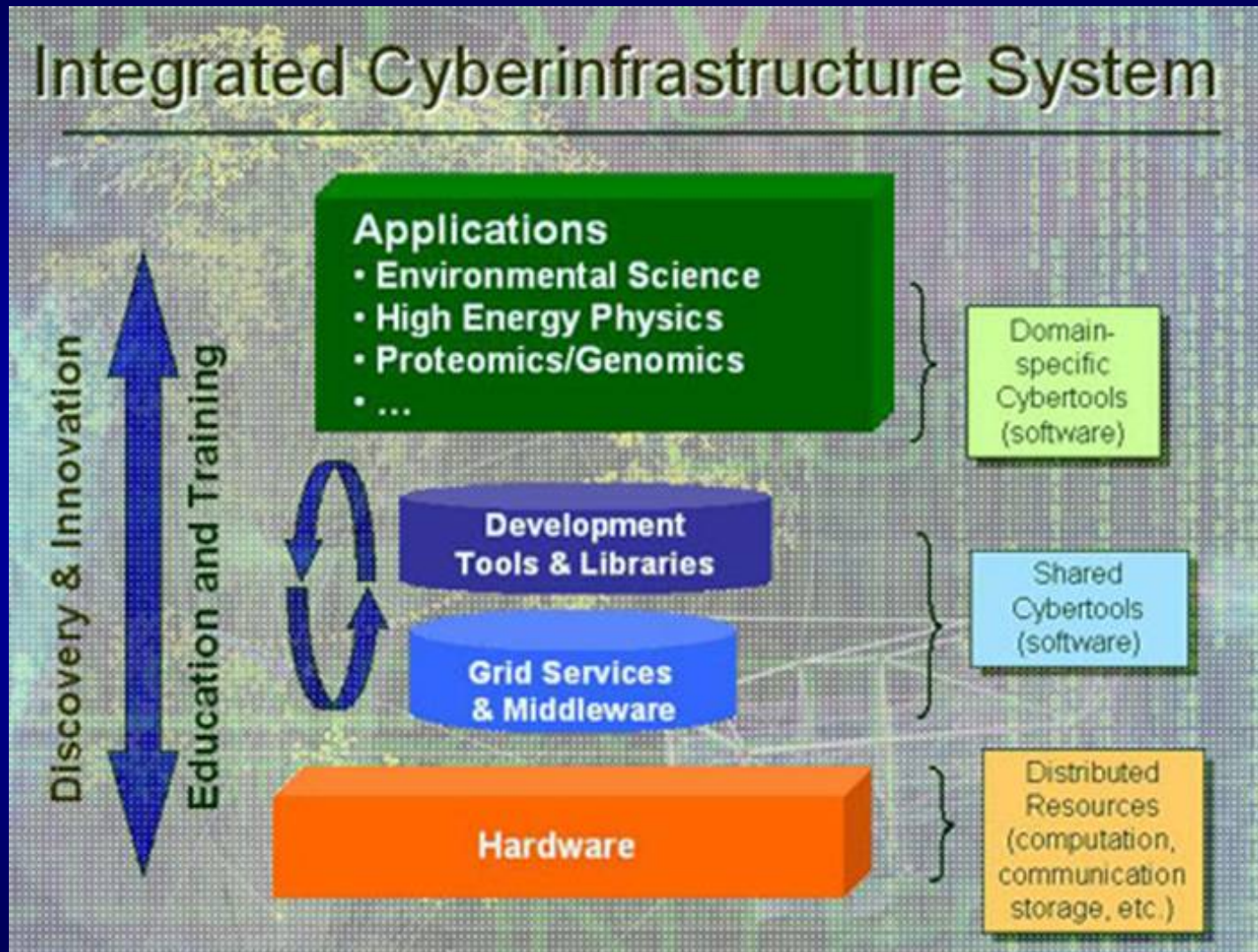
Applications



Facilities



NSF Integrated Cyberinfrastructure



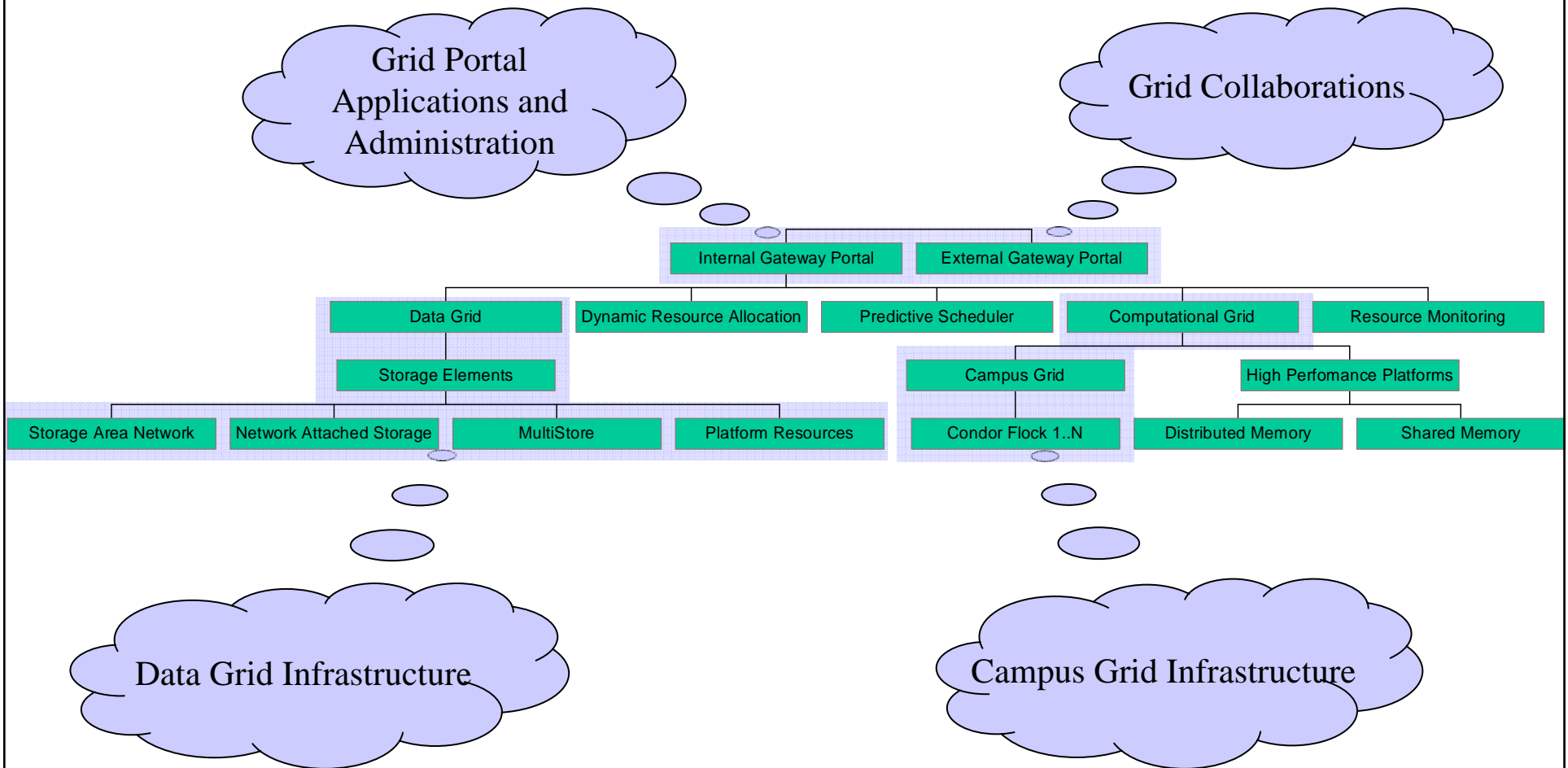
NSF Director Arden L. Bement: "leadership in cyberinfrastructure may determine America's continued ability to innovate – and thus our ability to compete successfully in the global arena."

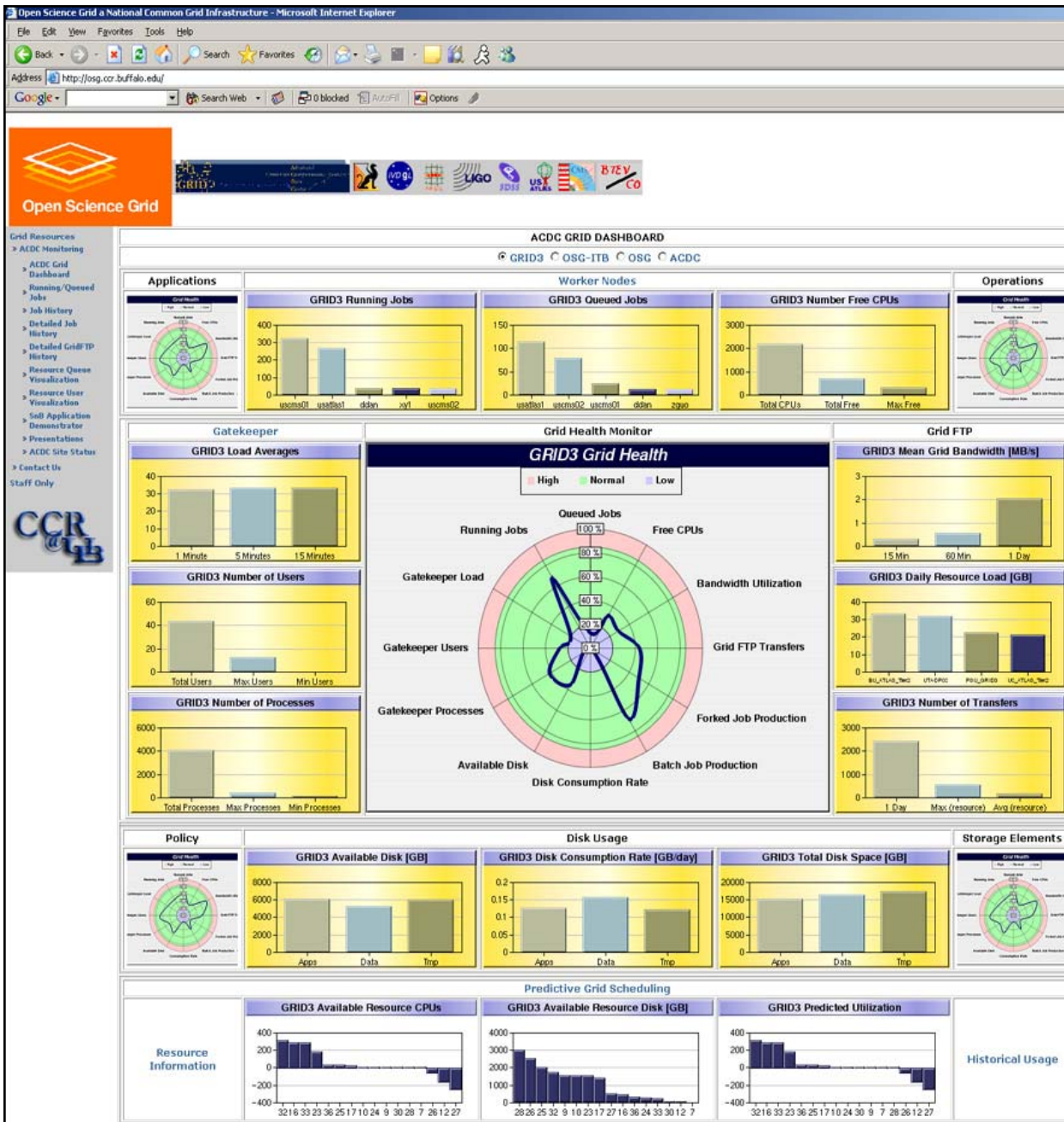
ACDC-Grid Cyberinfrastructure

- **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**



ACDC-Grid System Architecture

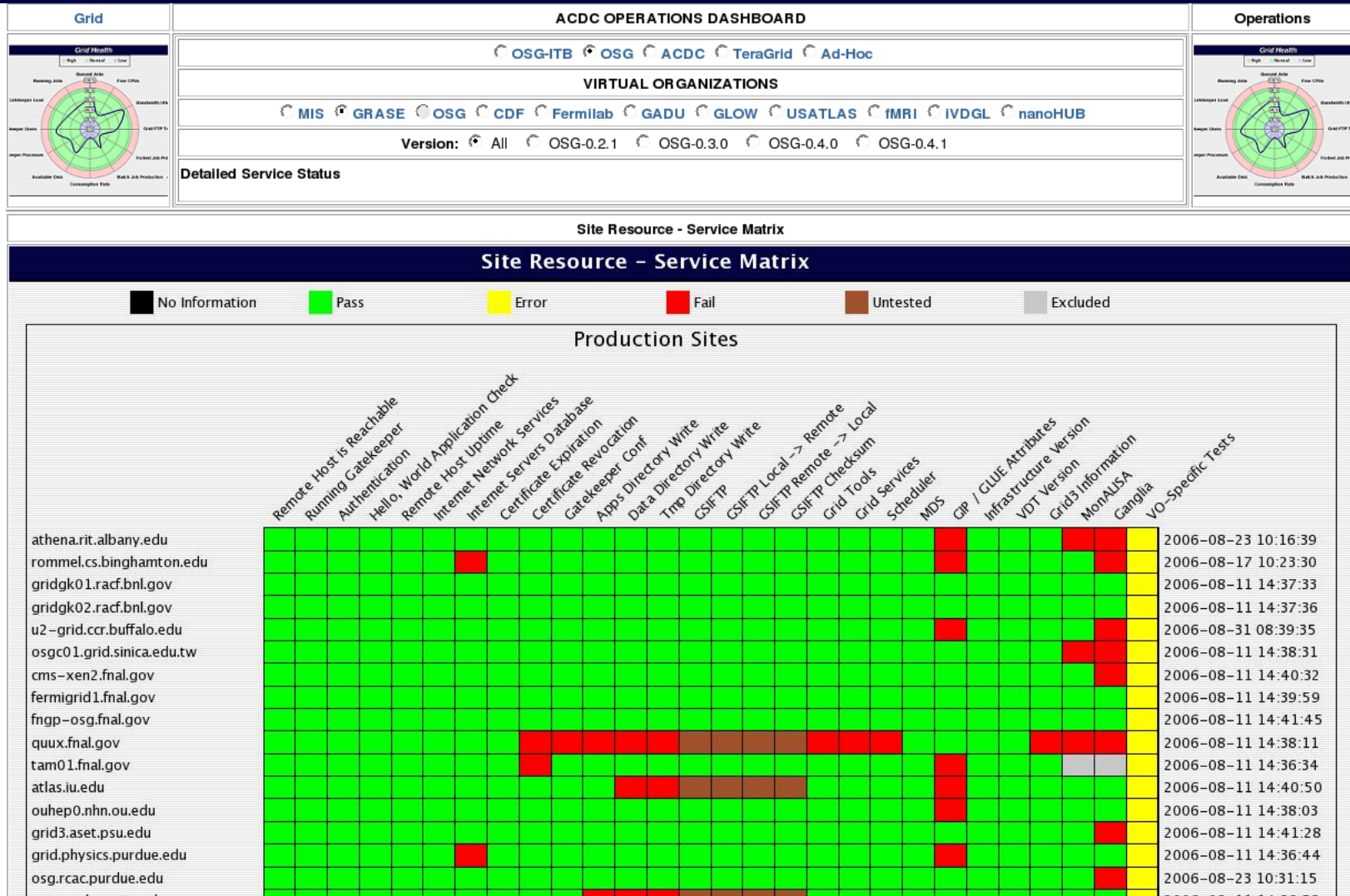




ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD

ACDC Monitor

<http://osg.ccr.buffalo.edu/operations-dashboard.php?grids=3&vos=10>



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

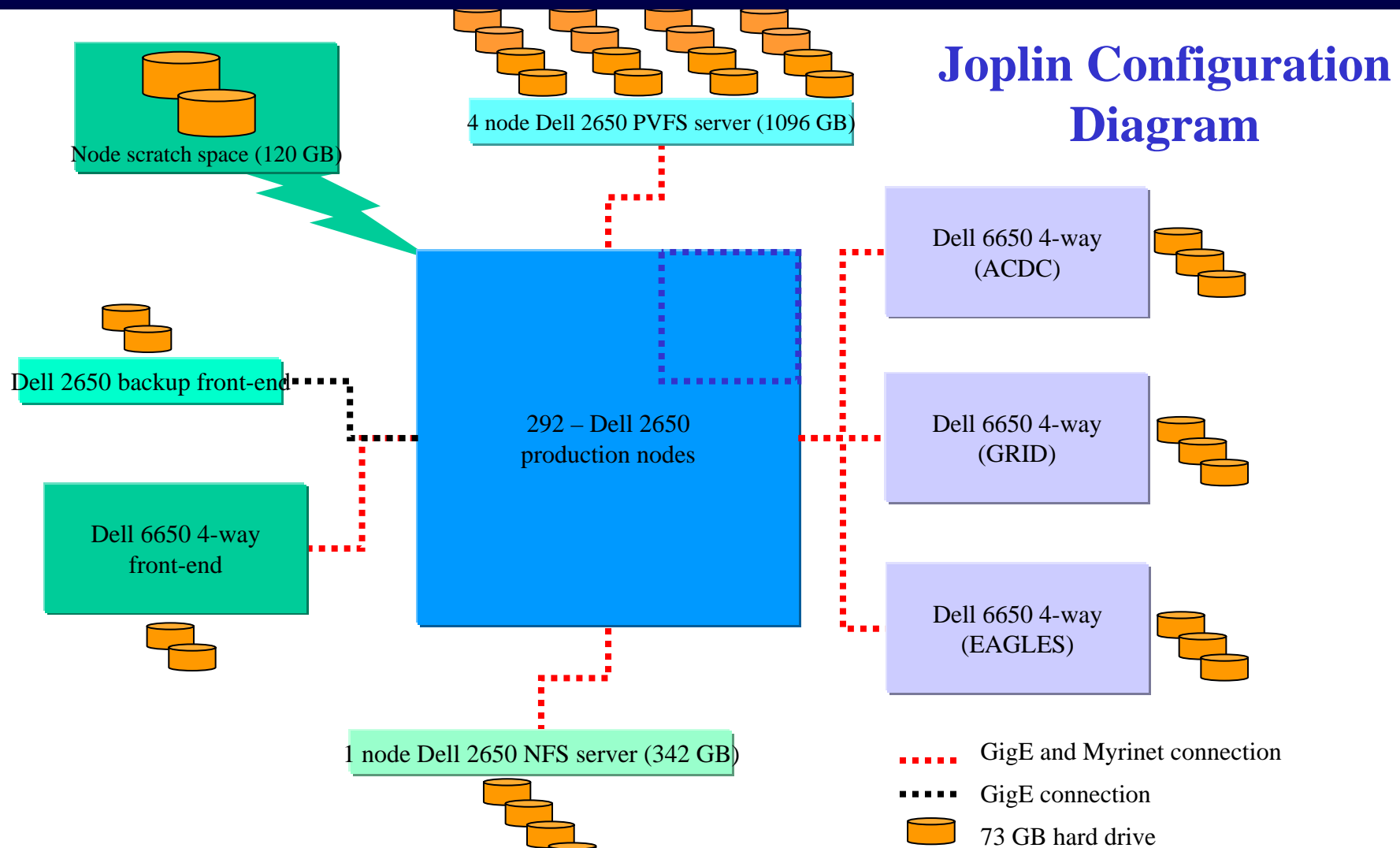


ACDC-Grid Dynamic Resource Allocation at SC03 with Grid3

- **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 Dynamic Resource Allocation



ACDC-Grid Administration

CCR Grid Computing Services: Grid Admin - Microsoft Internet Explorer

Center for Computational Research **GRID PORTAL**
High Performance Grid Computing

Grid Site Administration

Users
Groups
Portal Event Log
Database Job List

Organizations (add, edit, delete)
Resources (view, refresh, ping, delete, create host certificate)

Globus Administration
Reports (machine usage, user access to machines, etc.)

CCR Grid Computing Services: Grid Admin - Globus - Microsoft Internet Explorer

Center for Computational Research **GRID PORTAL**
High Performance Grid Computing

Generate Globus grid-mapfile

Specifying an optional include file will cause the contents of this file to be included at the top of the generated grid-mapfile. If a grid-mapfile path is specified a copy of the generated file will be saved into this location. The generated file will be staged to the grid nodes unless the box is checked.

Optional include file:

Optional grid-mapfile path:

Do not stage the file to the grid nodes

Generate Reset

CCR Grid Computing Services: Database Job Admin - Microsoft Internet Explorer

Center for Computational Research **GRID PORTAL**
High Performance Grid Computing

Create New Database Job

Create a new database job that can be run by the portal. Job scripts must reside in `/home/griddev/www/jobscripts` prior to creating the database job entry.

Job Name:

Full Path To Script:

Accepts Arguments:

Run Script:

Run As User:

Return to the Database Job Admin menu.
Return to the Grid Admin menu.

CCR Grid Computing Services: Grid Admin - Resources - Microsoft Internet Explorer

Center for Computational Research **GRID PORTAL**
High Performance Grid Computing

MDS Resource Update Status

Current Time: 16-September-2003 10:58:12

Resource	Last Updated	Next Update	Status
crosby.ccr.buffalo.edu	16-September-2003 09:15:30	2 minutes	OK
fogerty.ccr.buffalo.edu	16-September-2003 10:45:30	2 minutes	OK
joplin.ccr.buffalo.edu	16-September-2003 10:45:15	2 minutes	OK
mama.ccr.buffalo.edu	16-September-2003 10:45:15	2 minutes	OK
nash.ccr.buffalo.edu	16-September-2003 10:45:15	2 minutes	OK
nexus.hwi.buffalo.edu	16-September-2003 10:45:20	2 minutes	OK
yardbirds.ccr.buffalo.edu	16-September-2003 10:45:13	2 minutes	OK
young.ccr.buffalo.edu	16-September-2003 10:45:27	2 minutes	OK

Return to the Grid Resource Admin menu.
Return to the Grid Admin menu.

GRID
Advanced
Center for Computational Research
Data
Center



ACDC-Grid Data Grid

CCR Grid Computing Services: Data Management - Microsoft Internet Explorer

File Edit View Favorites Tools Help

UB University at Buffalo The State University of New York

CCR Center for Computational Research GRID PORTAL

High Performance Grid Computing

PORTAL LOGOUT

- User Tools
 - » Manage Account
- Grid General Info
- Projects
- Resources
 - » Computational Grid
 - » Job Submission
 - » Job/Queue Status
 - » Data Grid
 - » Network Status
 - » Running/Queued Jobs
 - » PBS Job History
 - » Grid Portal Statistics
 - » Conder Flock Statistics
 - » User Information
- Education/Outreach
- Staff Only
- CCR HOME

VIEW Group GROUP miller UserList rappleye

- rappleye
 - KeyMaster
 - Morpheus
 - Tank
 - Agent
 - Rabbit
 - Tank
 - Morpheus
 - Oracle.m
 - Neo
 - Neo
 - Cypher
 - Neo
 - Morpheus
 - Oracle

Advanced
Center for Computational Research
Data



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 Services and Applications

**ACDC-Grid
Computational
Resources**



Applications

Shake-and-Bake

Apache

MySQL

Oracle

High-level Services and Tools

Globus
Toolkit

NWS

MPI

MPI-IO

C, C++, Fortran, PHP

globusrun

Core Services

Metacomputing
Directory
Service

Globus
Security
Interface

GRAM

GASS

**ACDC-Grid
Data
Resources**



Local Services

Condor

Stork

MPI

RedHat Linux

WINNT

LSF

PBS

Maui Scheduler

TCP

UDP

Irix

Solaris

Adapted from Ian Foster and Carl Kesselman



University at Buffalo *The State University of New York*

Cyberinfrastructure Laboratory

CI Lab

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 *SnB*

■ 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



Required Grid Services

■ Application Layer

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

■ High-level Services

- ❑ Globus, PHP, Fortran, C

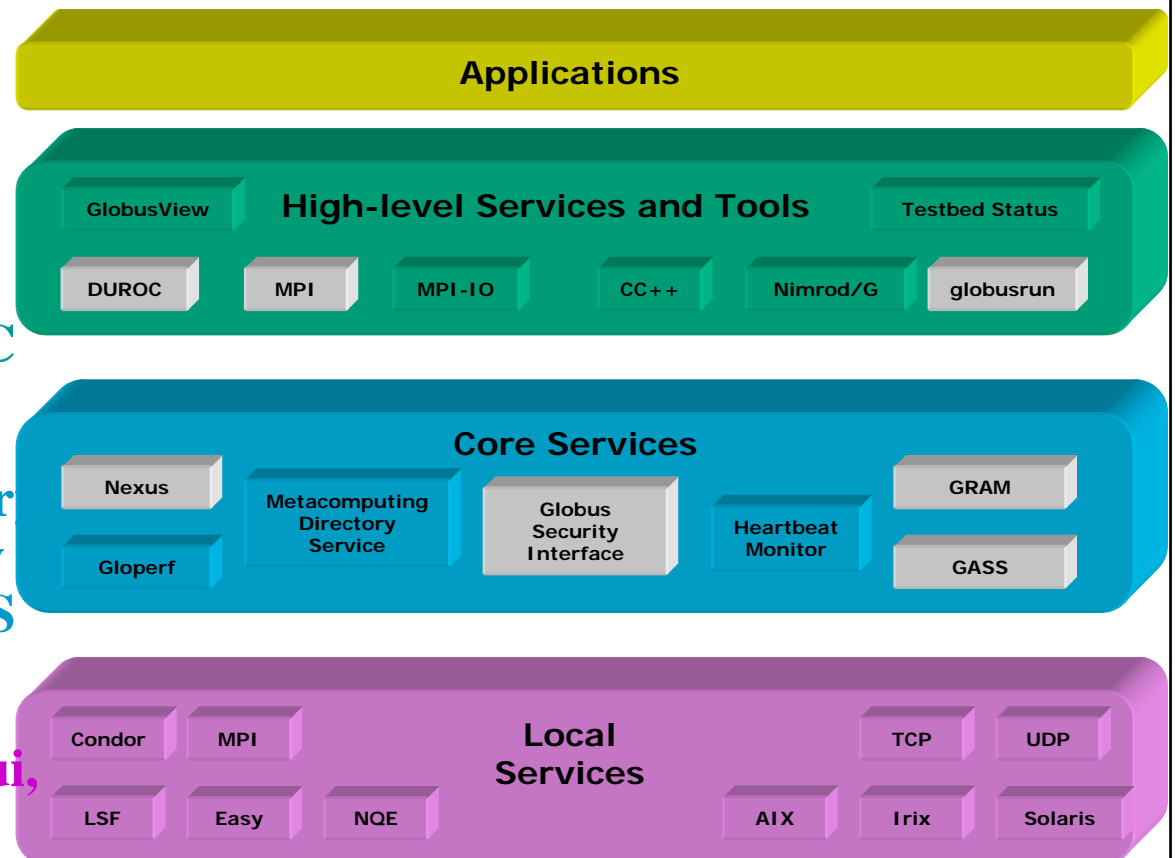
■ Core Services

- ❑ Metacomputing Director Service, Globus Security Interface, GRAM, GASS

■ Local Services

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

Grid Implementation as a Layered Set of Services



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.



CCR Grid Computing Services: Advanced Computational Data Center Grid Jobs - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/>


University at Buffalo *The State University of New York*
CCR **Center for Computational Research** **GRID PORTAL**
 High Performance Grid Computing

Advanced Computational Data Center Grid Jobs

Grid Job Submission: This section contains forms for the selection of a grid-enabled application, modification of an application template, grid job definition review and grid job submission.

Grid Job Status: This section contains grid user based 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.

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
 » Conder Flock Statistics
Data Grid
Education/Outreach
Staff Only
CCR HOME
 Printer Friendly

Advanced
Center for Computational Research
Data
Center

Startup Screen for ACDC-Grid Job Submission ** Development Portal **

Done Internet

Start | Gmail - Inbox (1) - Micros... | Center for Computational... | CCR Grid Computing S... | SnB | Screenshots-Grid job sub... | 10:04 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

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.

Instructions and Description for Running a Job on ACDC-Grid

Done

Start | Gmail - Inbox (1) - Micros... | Center for Computational... | CCR Grid Computing S... | SnB | Screenshots-Grid job sub... | 10:04 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

University at Buffalo The State University of New York

CCR Center for Computational Research GRID PORTAL

High Performance Grid Computing

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
Education/Outreach
Staff Only
CCR HOME
Printer Friendly

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

Advanced
Center for Computational Research
Data
Center

**** Development Portal ****
Software Package Selection

Done Internet

Start Gmail - Inbox (1) - Micros... Center for Computational... CCR Grid Computing S... SnB Screenshots-Grid job sub... 10:05 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

University at Buffalo The State University of New York

CCR Center for Computational Research GRID PORTAL

High Performance Grid Computing

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
Education/Outreach
Staff Only
CCR HOME
Printer Friendly

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

Enter structure definition manually

Select structure from Data Grid:

[Return to the Grid Job Menu](#)

Advanced
Center for Computational Research
Data
Center

Full Structure / Substructure Template Selection

Done

Start | Gmail - Inbox (1) - Micros... | Center for Computational... | CCR Grid Computing S... | SnB | Screenshots-Grid job sub... | Internet | 10:05 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

Address: <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

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)	

Default Parameters Based on Template

Done

Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:16 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

Initial Data Sets

[Add Dataset](#) [Delete Dataset](#)

Select dataset to delete	<input type="radio"/>
Datasets	Dataset 1
Name (8 chars max):	<input type="text" value="iledhkl"/>
Dataset Type:	<input type="text" value="Native"/>
File Name (*.hkl) :	<input type="text"/> Browse
File Type:	<input type="text" value="F, Sig(F)"/>
Wavelength:	<input type="text" value="1.5418"/>
Max. Resolution:	<input type="text" value="0.94"/>
Anomalous Dispersion:	<input type="text" value="Not Measured"/>
Heavy Element Type:	<input type="text"/>
Nat. Element Replaced:	<input type="text"/>
No. Expected Sites:	<input type="text"/>
F Prime (f'):	<input type="text"/>
F Double Prime (f''):	<input type="text"/>

[Continue](#) [Reset Sequence](#) [Reset Current Stage](#) [Cancel](#)

[Return to the Grid Job Menu](#)

Default Parameters (cont'd)

Advanced
Center for Computational Research

Done

Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:16 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

Address: <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

Reflections and Invariants

Drear Table

Data Set	Job Type	Native Data	Derivative Data	Norm Method	Select
iledhkl	BASIC	iledhkl	NULL	Wilson (Anisotropic)	

Normalization Data

Data resolution cutoffs (in Angstroms)? Low: High:

Use Bayesian estimates for weak reflections?

Min |F| / sig(|F|) for local scaling:

SIR and SAS cutoffs: TMax : ZMax :
 XMIN : YMIN :

Generate Invariants

Data resolution cutoffs ? Low: High:

Minimum allowed |E| / sig(|E|): Maximum |E| :

Minimum allowed invariants / reflection ratio:

Initial values for adjustable parameters

Minimum |E| / sig(|E|) = ZMin:

Number of reflections to use:

Number of invariants to save:

Generating Reflections (Drear)

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

Address: <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

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
 - » Conder Flock Statistics
- Data Grid
- Education/Outreach
- Staff Only
- CCR HOME
- Printer Friendly

Reflections and Invariants

Declar Table

Data Set	Job Type	Native Data	Derivative Data	Norm Method	Select
iledhkl	BASIC	iledhkl	NULL	Wilson (Anisotropic)	<input type="radio"/>

Normalization Data

Data resolution cutoffs (in Angstroms)? Low: High:

Use Bayesian estimates for weak reflections?

Min |F| / sig(|F|) for local scaling:

SIR and SAS cutoffs:

TMax : ZMax :

XMIN : YMIN :

Generate Invariants

Data resolution cutoffs ? Low: High:

Minimum allowed |E| / sig(|E|): Maximum |E| :

Minimum allowed invariants / reflection ratio:

Initial values for adjustable parameters

Minimum |E| / sig(|E|) = ZMin:

Number of reflections to use:

Number of invariants to save:

Invariant Generation

Done

Start | Internet | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | 10:17 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

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
- » Conder Flock Statistics

Data Grid

Education/Outreach

Staff Only

CCR HOME

Printer Friendly

SnB Setup

Grid Parameters

Preferred resource name:

Number of processors:

Wallclock time requested: (mins)

Job Prefix for results:

Queue:

SnB Run Parameters

- *Invariants*

Number of triplet invariants to use:

- *Trials To Process*

Starting phases from:

Random seed (prime):

Number of Trials:

Starting Trial:

Input Phase File:

Input Atom File:

Keep complete (every trial) peak file? :

- *Cycles Information*

Number of Shake-and-Bake cycles:

Keep complete (every cycle) trace file? :

Terminate trials failing the R-Ratio test? :

R-Ratio cutoff:

- *Phase Refinement Method*

SnB Setup

Done

Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:17 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

- *Phase Refinement Method*
Phase Refinement Method :
Number of passes through phase set:
Phase shift:
Number of shifts:
- *Real-Space Constraints*
Number of peaks to select:
Minimum interpeak distance:
Minimum distance between symmetry-related peaks:
Number of special position peaks to keep:
Fourier grid size:
Perform extra cycles with more peaks? :
Number of extra cycles :
Number of peaks :
- *Twice Baking*
Trials for E-Fourier filtering (fourier refinement)? :
Number of cycles :
Number of peaks :
Minimum |E| :
- *Automatic solution identification criteria*
Rmin Improvement (%):
Rcryst Improvement (%):

SnB Setup (cont'd)

Done

Start | Internet

Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | 10:18 AM

CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer

Address: <https://griddev.ccr.buffalo.edu/jobs/submit/index.php>

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

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)

Done

Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:18 AM

CCR Grid Computing Services: Grid Job Status Detail - Microsoft Internet Explorer

Address: https://griddev.ccr.buffalo.edu/jobs/job_detail.php?id=447&gat=snb

CCR Center for Computational Research **GRID PORTAL**
 High Performance Grid Computing

University at Buffalo The State University of New York

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

Best Trial Number: 34
 Best Trial Rmin: 0.344
 Processors: 5

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

Return to the Grid Job Menu

Advanced Center for Computational Research Data

Address: https://griddev.ccr.buffalo.edu/jobs/submit/snb/display_chart.php?id=447&gat=snb&chart=rmin_histogram

Start | G-mail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:21 AM

CCR Grid Computing Services: Grid Job Status Detail - Microsoft Internet Explorer

Address: https://griddev.ccr.buffalo.edu/jobs/submit/snb/display_chart.php?id=447&gat=snb&chart=rmin_histogram

CCR University at Buffalo The State University of New York
Center for Computational Research **GRID PORTAL**
 High Performance Grid Computing

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

Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING

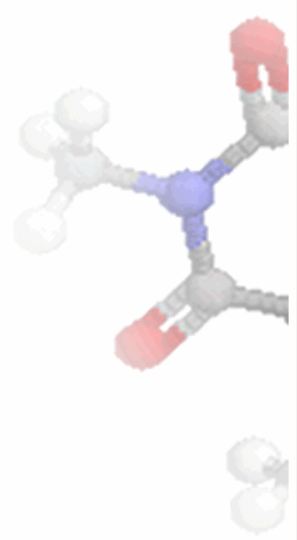
Rmin Value	Trials
0.344	6
0.351	2
0.359	1
0.366	1
0.374	1
0.381	0
0.389	0
0.396	0
0.404	0
0.411	1
0.418	2
0.426	0
0.433	1
0.441	1
0.448	1
0.456	0
0.463	2
0.471	1
0.478	7
0.486	13
0.493	18
0.5	29
0.508	34
0.515	37
0.523	37
0.53	32
0.538	18
0.545	14
0.553	10
0.56	17

Return to Job Details
 Return to the Grid Job Status List
 Return to the Grid Job Menu

Advanced
 Center for Computational Research

Done
 Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:22 AM

Histogram of Completed Trial Structures



CCR Grid Computing Services: Grid Job Status - Microsoft Internet Explorer

Address: https://griddev.ccr.buffalo.edu/jobs/job_status_list.php

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

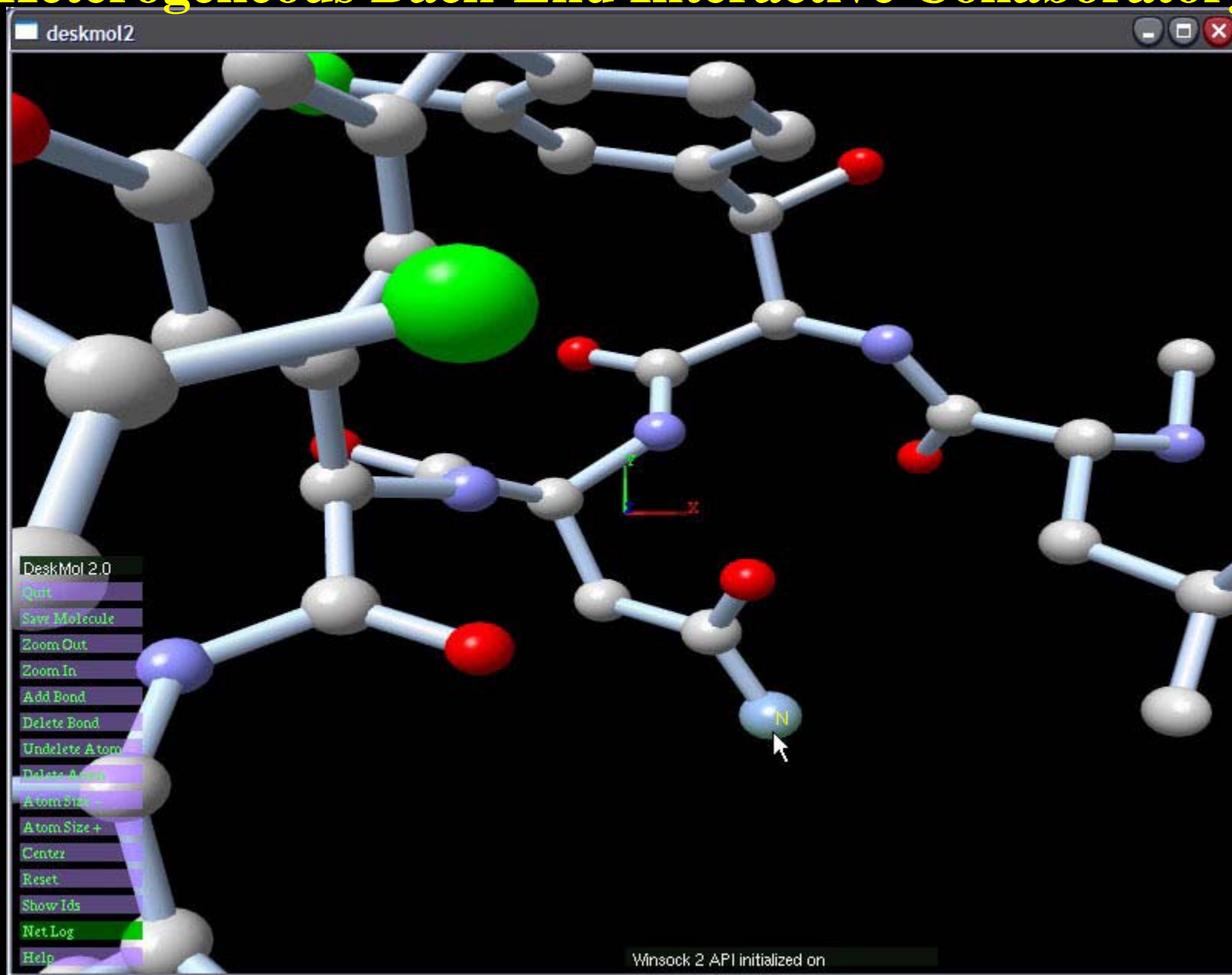
SnB									
Job Id	Job Name	Resource	Num Procs	Status	Percent Complete	Last Update	Cancel Job	Drilldown	
447	iledhkl	clearwater.ccr.buffalo.edu	5	RUNNING	28.5	15-Mar-2005 10:22:00	<input type="checkbox"/>		
446	trilys	clearwater.ccr.buffalo.edu	10	RUNNING	1	15-Mar-2005 10:22:00	<input type="checkbox"/>		
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	3	COMPLETE	100	10-Mar-2005 14:38:01			

Status of Jobs

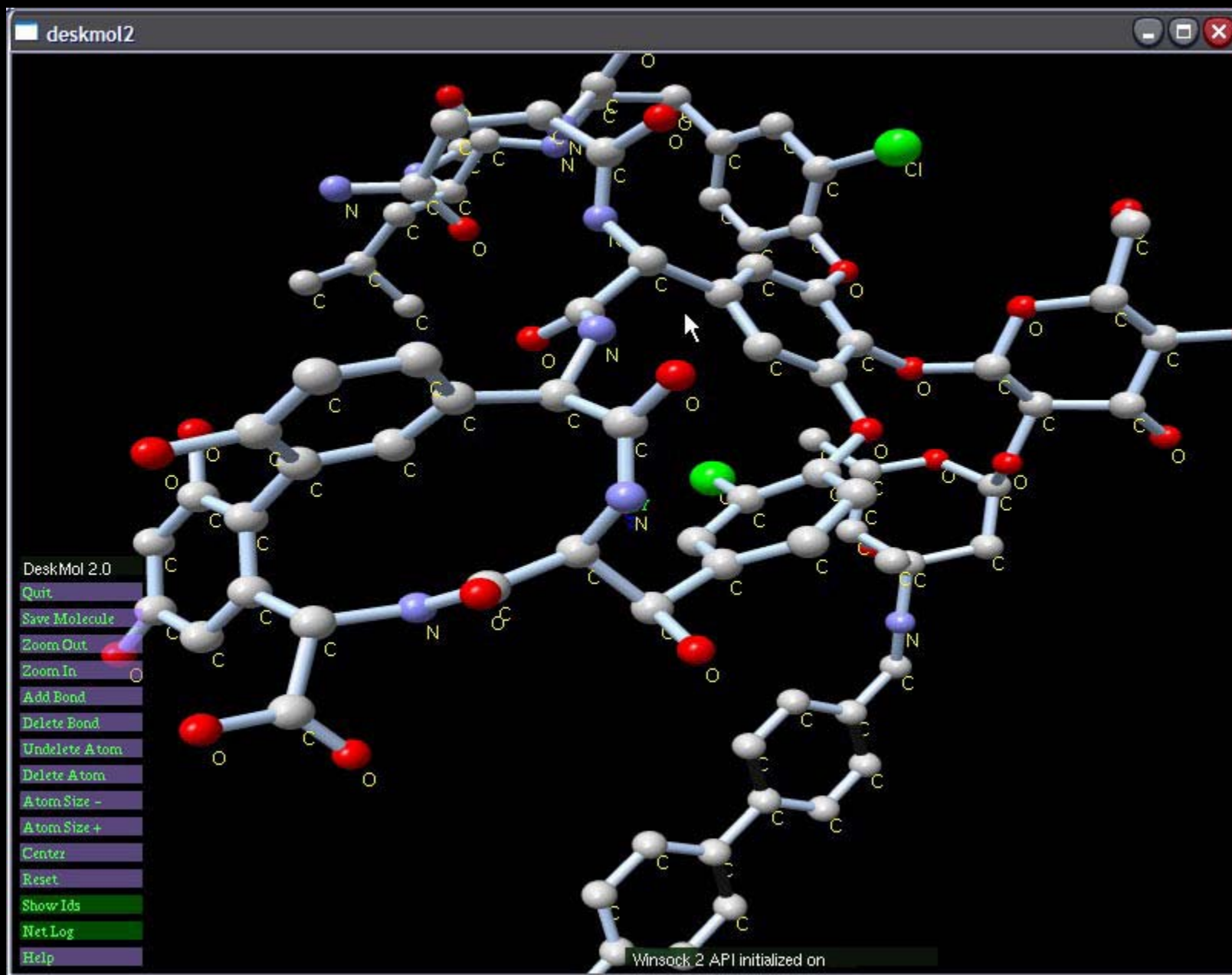
Done

Start | Gmail - Inbox - Mi... | Center for Comp... | CCR Grid Comp... | SnB | Screenshots-Grid ... | clearwater.ccr.bu... | Internet | 10:24 AM

Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Acknowledgments

- Mark Green
 - Cathy Ruby
 - Amin Ghadersohi
 - Naimesh Shah
 - Steve Gallo
 - Jason Rappleye
 - Jon Bednasz
 - Sam Guercio
 - Martins Innus
 - Cynthia Cornelius

 - 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





www.cse.buffalo.edu/faculty/miller