

High-Performance Computing & High-End Visualization in Buffalo

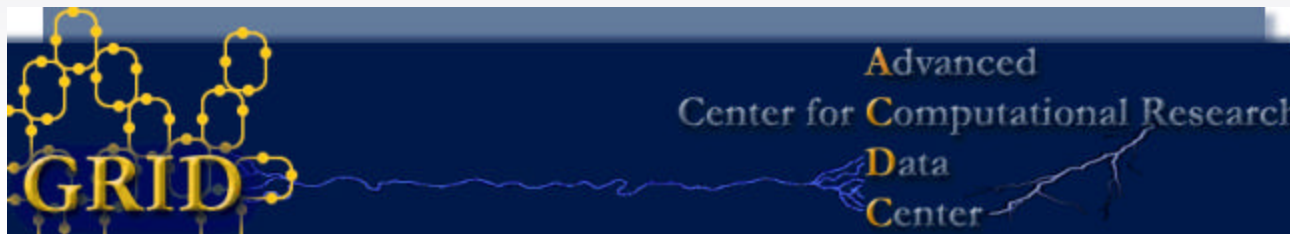
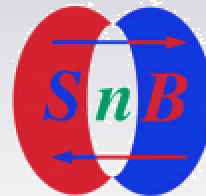
Russ Miller

Center for Computational Research
Computer Science & Engineering
SUNY-Buffalo

Hauptman-Woodward Medical Inst



NSF, NIH, DOE
NIMA, NYS, HP



University at Buffalo
The State University of New York

Center for Computational Research 1998-2005 Overview

■ High-End Computing, Storage, Networking, and Visualization

□ ~140 Research Groups in 37 Depts

○ Physical Sciences

○ Life Sciences

○ Engineering

○ Scientific Visualization, Medical Imaging, Virtual Reality

□ 13 Local Companies

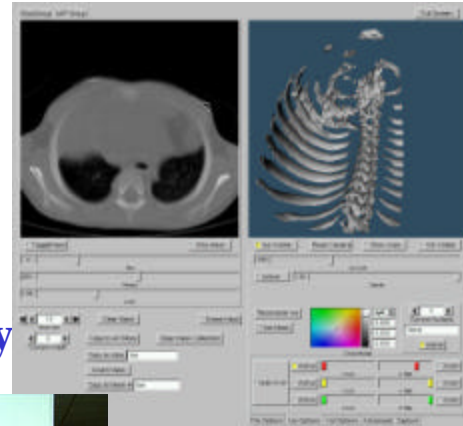
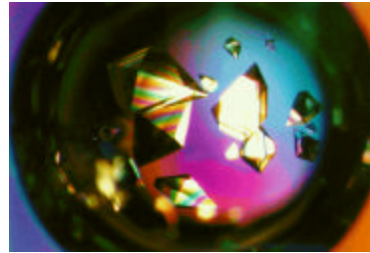
□ 10 Local Institutions

■ External Funding: \$300M+

■ Total Leveraged WNY: \$500M+

■ 1100+ Publications

■ EOT, Economic Development, Software, Media, Algorithms, Consulting, Training, CPU Cycles...



Major Compute/Storage Resources

- **Dell Linux Cluster (10TF peak)**
 - ❑ 1600 Xeon EM64T Processors (3.2 GHz)
 - ❑ 2 TB RAM; 65 TB Disk
 - ❑ Myrinet / Force10
 - ❑ 30 TB EMC SAN
- **Dell Linux Cluster (2.9TF peak)**
 - ❑ 600 P4 Processors (2.4 GHz)
 - ❑ 600 GB RAM; 40 TB Disk; Myrinet
- **Dell Linux Cluster (6TF peak)**
 - ❑ 4036 Processors (PIII 1.2 GHz)
 - ❑ 2TB RAM; 160TB Disk; 16TB SAN
- **IBM BladeCenter Cluster (3TF peak)**
 - ❑ 532 P4 Processors (2.8 GHz)
 - ❑ 5TB SAN
- **SGI Altix3700 (0.4TF peak)**
 - ❑ 64 Processors (1.3GHz ITF2)
 - ❑ 256 GB RAM
 - ❑ 2.5 TB Disk
- **CCR Bioinformatics System**
 - ❑ Sun V880 (3), Sun 6800
 - ❑ Sun 280R (2)
 - ❑ Intel PIIIs
 - ❑ Sun 3960: 7 TB Disk Storage
- **HP/Compaq SAN**
 - ❑ 75 TB Disk; 190 TB Tape
 - ❑ 64 Alpha Processors (400 MHz)
 - ❑ 32 GB RAM; 400 GB Disk

CCR Visualization Resources

- **Fakespace ImmersaDesk R2**
 - ❑ Portable 3D Device
 - ❑ Onyx2: 6 R10000 @ 250MHz
 - ❑ 2 IR2 Pipes; 3 64MB texture memory mgrs
- **Tiled-Display Wall**
 - ❑ 20 NEC projectors: 15.7M pixels
 - ❑ Screen is 11' x 7'
 - ❑ Dell PCs with Myrinet2000
- **Access Grid Nodes (2)**
 - ❑ Group-to-Group Communication
 - ❑ Commodity components
- **SGI Reality Center 3300W**
 - ❑ Dual Barco's on 8' x 4' screen
 - ❑ Onyx300: 10 R14000 @ 500MHz
 - ❑ 2 IR4 Pipes; 1 GB texture mem per pipe



CCR Research & Projects

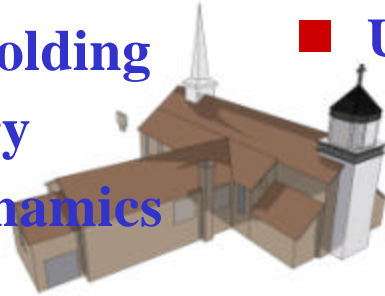
- Archaeology
- Bioinformatics/Protein Folding
- Computational Chemistry
- Computational Fluid Dynamics
- Data Mining/Database
- Earthquake Engineering
- Environ Modeling & Simulation
- Grid Computing
- Molecular Structure Determination

- Videos: MTV
- Urban Simulation and Viz

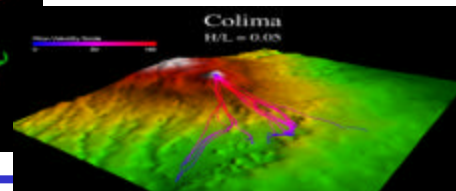
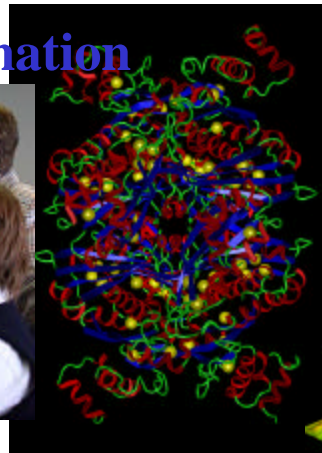
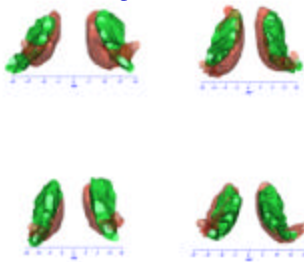
- StreetScenes
- I-90 Toll Barrier
- Medical Campus
- Peace Bridge

- Accident Reconstruction
- Scientific Viz

- Dental
- Surgery
- MRI/CT Scan
- Confocal Microscopy
- Crystallization Wells
- Collaboratories



Physics



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

■ Proposed Options

- ❑ Relocate US plaza
- ❑ Build a 3-lane companion span & rehab existing bridge

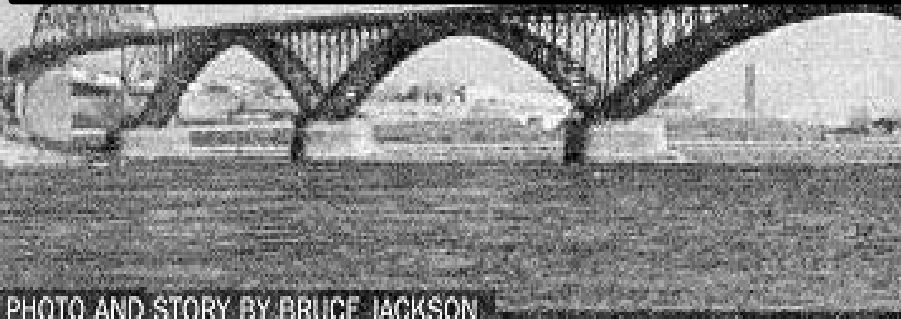


PHOTO AND STORY BY BRUCE JACKSON

MTV

IBC Digital & CCR

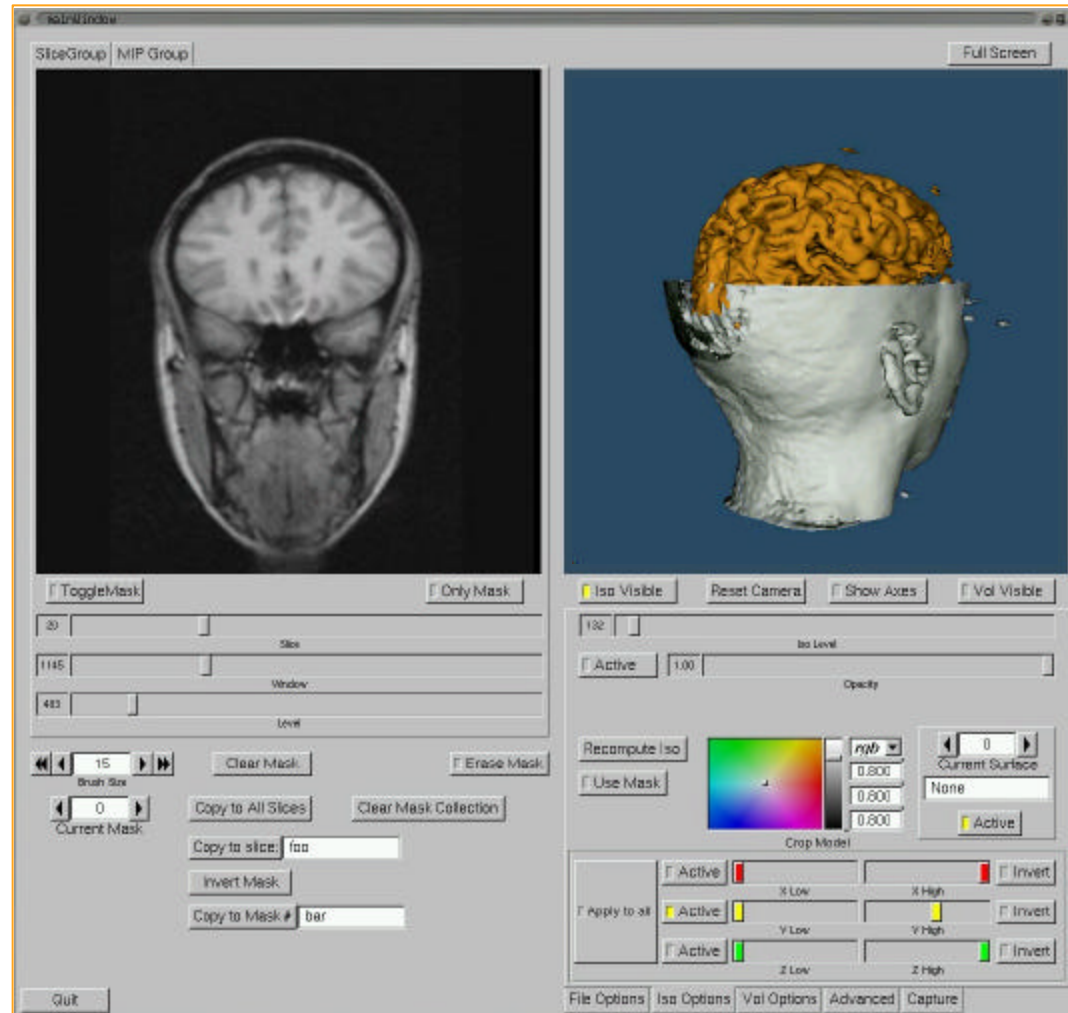
Song: I'm OK (I Promise)
Band: Chemical Romance
Gaming Environment: Death Jr.



Scientific Visualization

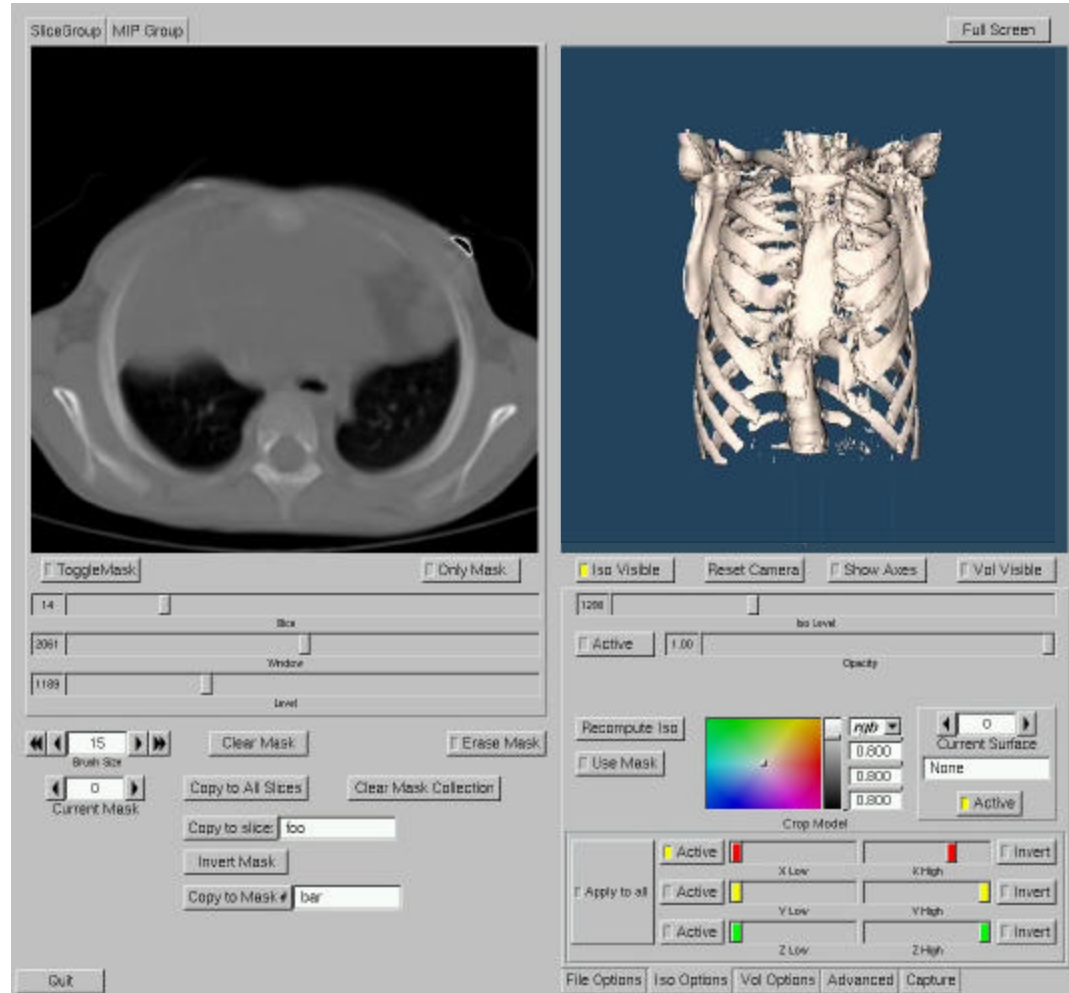
Multiple Sclerosis Project

- 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 App

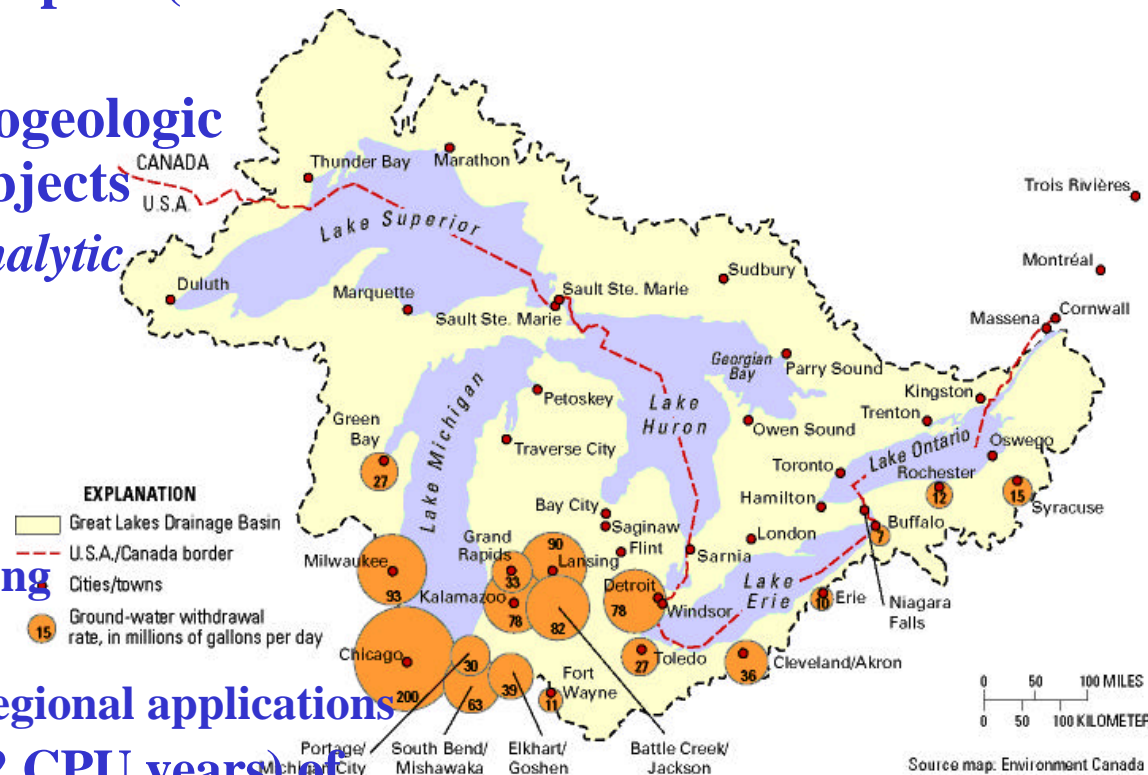
- Collaboration with Children's Hospital
 - Leading miniature access surgery center
- Application reads data output from a CT Scan
- Visualize multiple surfaces and volumes
- Export images, movies or CAD representation of model



Science & Engineering

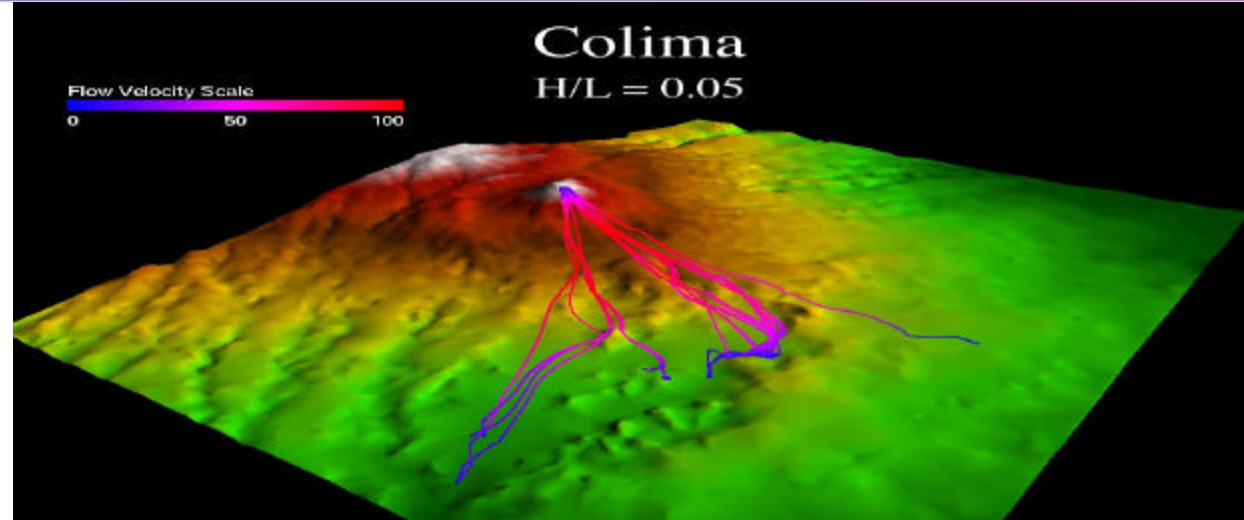
Groundwater Flow Modeling

- Regional-scale modeling of groundwater flow and contaminant transport (Great Lakes Region)
- Ability to include all hydrogeologic features as independent objects
- Current work is based on *Analytic Element Method*
- Key features:
 - High precision
 - Highly parallel
 - Object-oriented programming
 - Intelligent user interface
 - GIS facilitates large-scale regional applications
- Utilized 10,661 CPU days (32 CPU years) of computing in past year on CCR's commodity clusters



Geophysical Mass Flow Modeling

- Modeling of Volcanic Flows, Mud flows (flash flooding), and Avalanches
- Integrate information from several sources
 - Simulation results
 - Remote sensing
 - GIS data
- Develop realistic 3D models of mass flows
- Present information at appropriate level



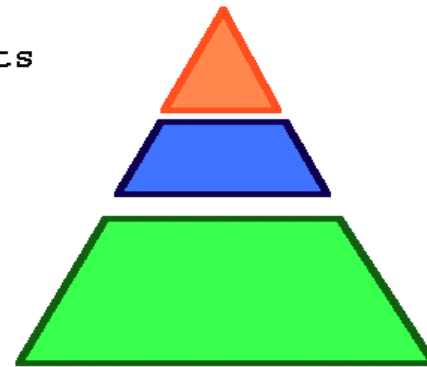
S
C
A
L
A
B
L
E

I
T

Scientists

Hazard
Managers

Public



High End Simulation
and Visualization

Remote Real time
visualization server

Web Servers

Web based
visualization

Shake-and-Bake

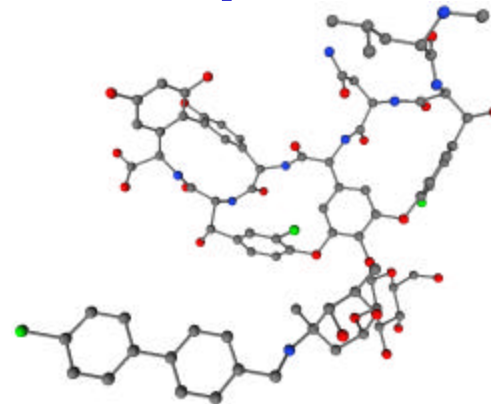
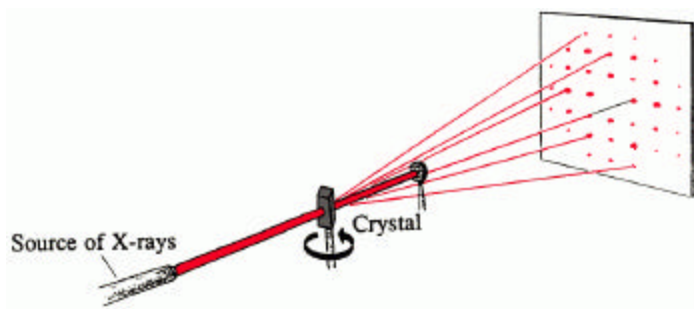
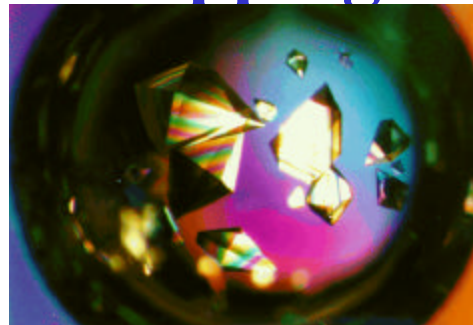
**Molecular Structure Determination
from X-Ray Crystallographic Data**

X-Ray Crystallography

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

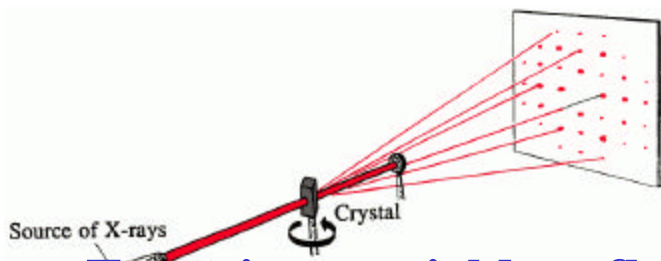
- **Procedure:**

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



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

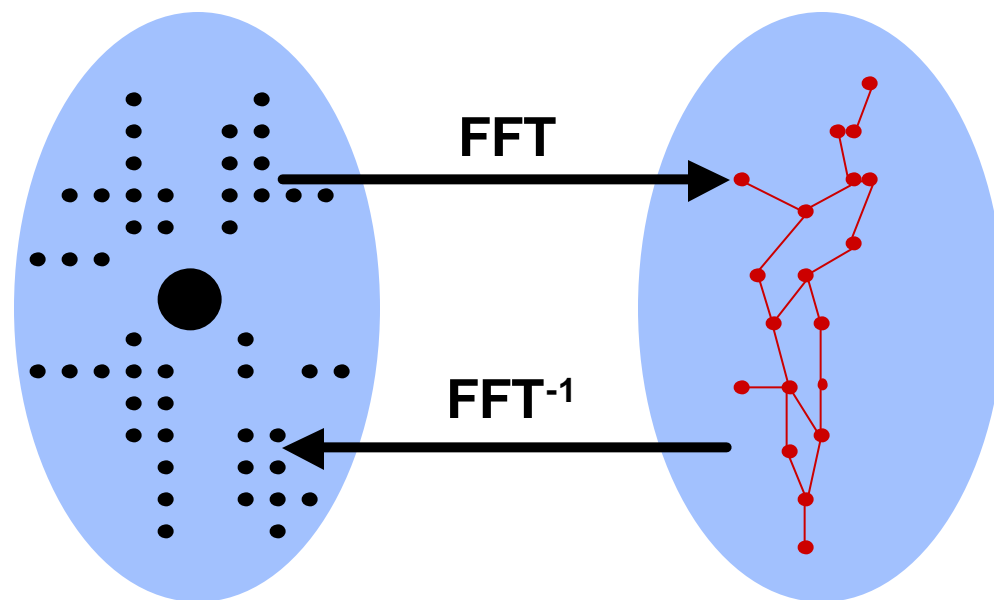
X-Ray Data & Corresponding Molecular Structure



- 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.*

Reciprocal or
“Phase” Space

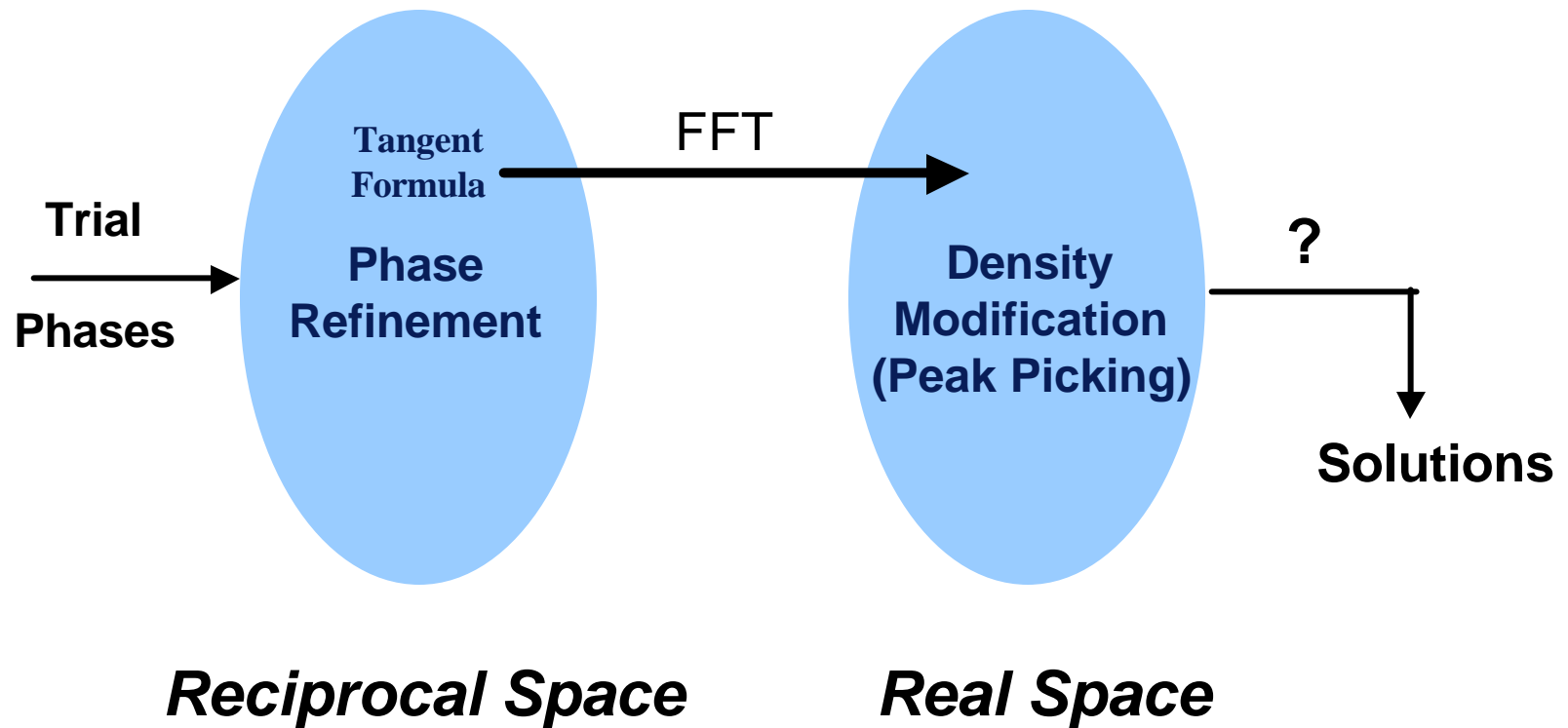
Real Space



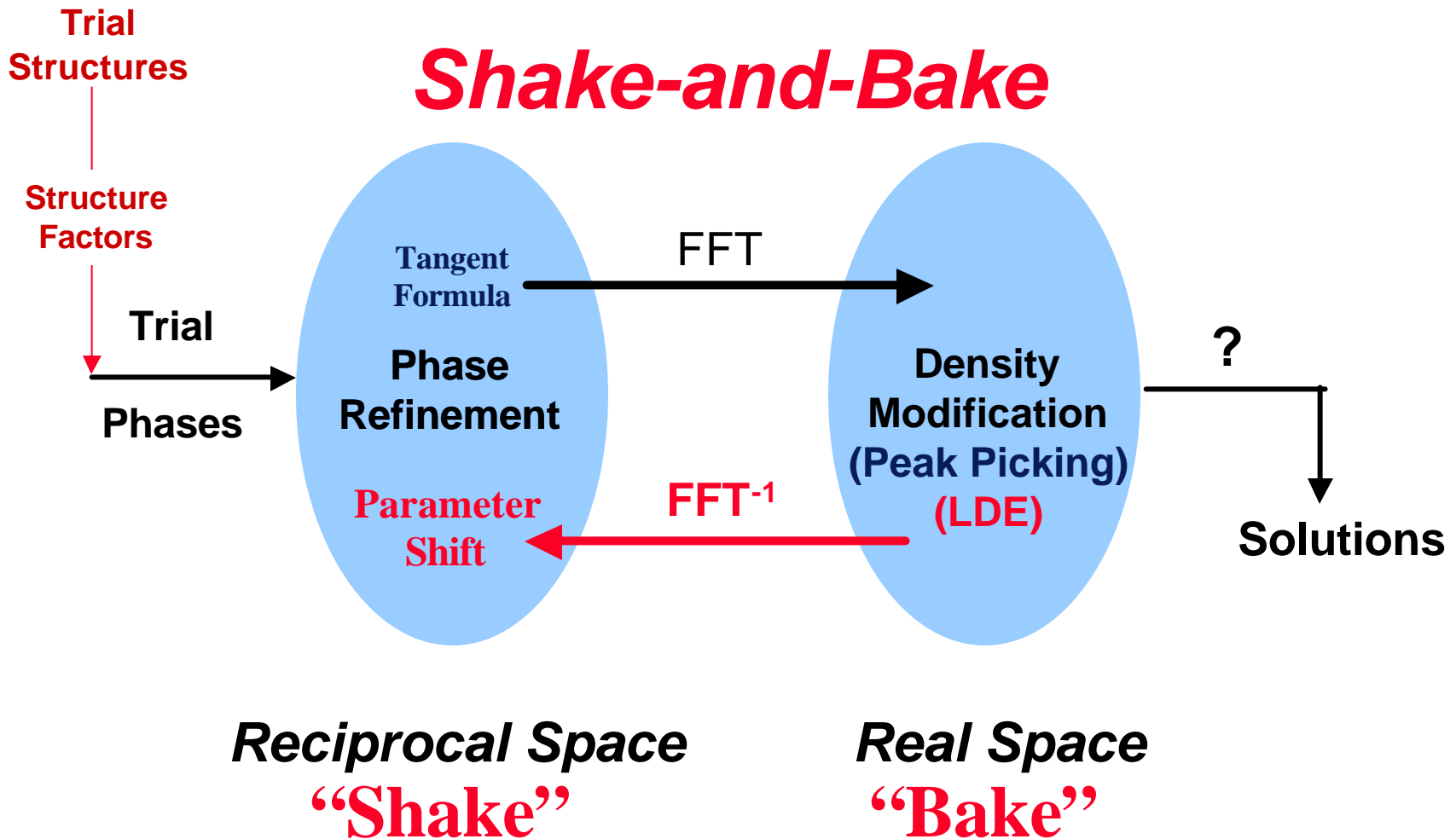
X-Ray Data

Molecular Structure

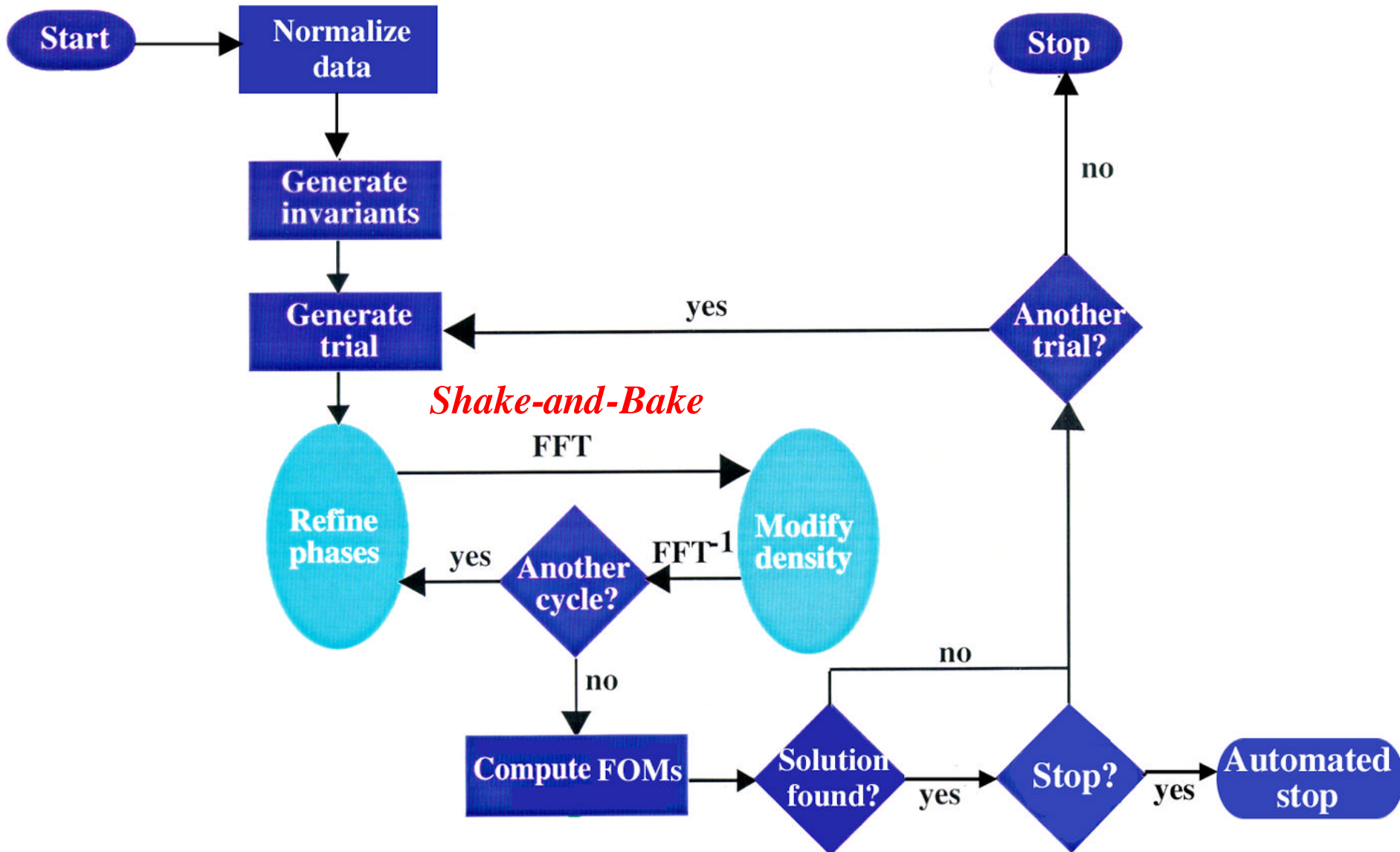
Conventional Direct Methods



Shake-and-Bake Method: Dual-Space Refinement



A Direct Methods Flowchart



Useful Relationships for Multiple Trial Phasing

Tangent
Formula

$$\tan \mathbf{f}_H = \frac{-\sum_K |E_K E_{-H-K}| \sin(\mathbf{f}_K + \mathbf{f}_{-H-K})}{\sum_K |E_K E_{-H-K}| \cos(\mathbf{f}_K + \mathbf{f}_{-H-K})}$$

Parameter Shift
Optimization

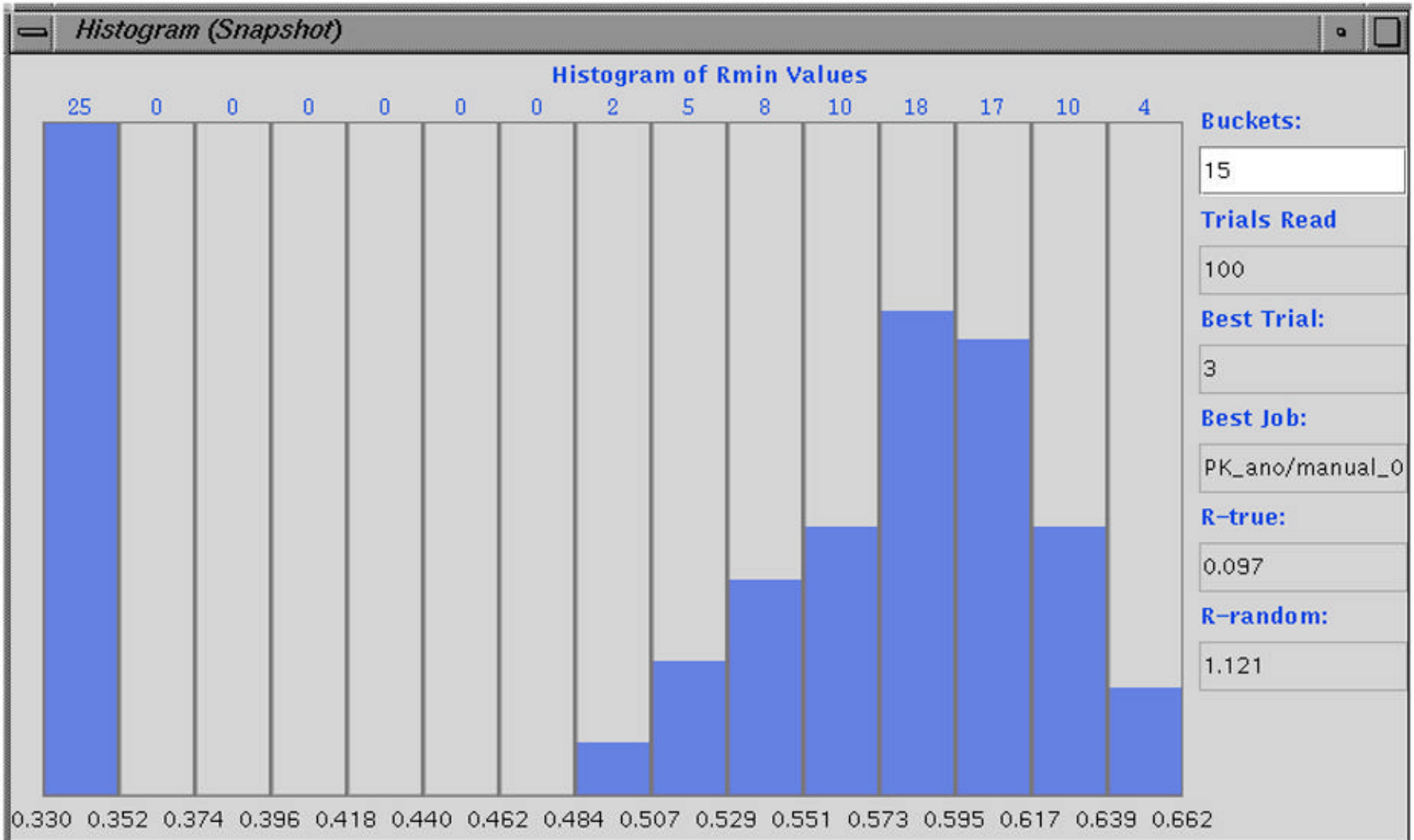
$$R(\mathbf{f}) = \frac{1}{\sum_{H,K} W_{HK}} \sum_{H,K} W_{HK} \left(\cos \Phi_{HK} - \frac{I_1(W_{HK})}{I_0(W_{HK})} \right)^2$$

where $|E_H| \propto |F_H|$ normalized in resolution shells

$$\text{Invariants : } \Phi_{HK} = \mathbf{f}_H + \mathbf{f}_K + \mathbf{f}_{-H-K} \approx 0$$

$$\text{Weights : } W_{HK} = A_{HK} = 2N^{-1/2} |E_H E_K E_{-H-K}|$$

Ph8755: SnB Histogram



Phasing and Structure Size

Se-Met with *Shake-and-Bake*?

Se-Met

567 kDa (160 Se)

Multiple Isomorphous Replacement?

Shake-and-Bake

Conventional Direct Methods

Vancomycin



Number of Atoms in Structure

Grid Computing

Grid Computing

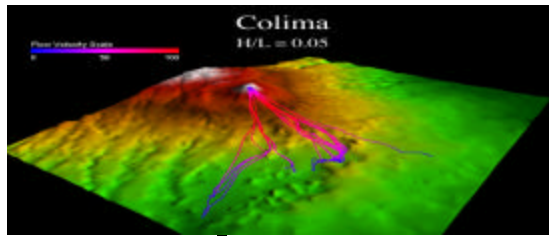


Asia-Pacific Advanced Network

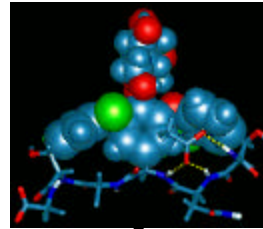


Advanced
Center for Computational Research
Data
Center

Grid Computing Overview



Data Acquisition



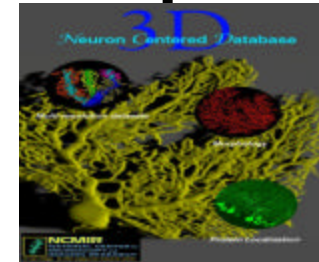
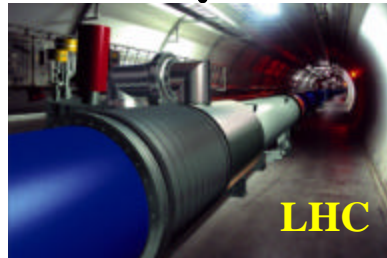
Advanced Visualization



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

- ❑ 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

ACDC-Grid Cyber-Infrastructure

■ Integrated Data Grid

- Automated Data File Migration based on profiling users.

■ 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.

ACDC-Grid Data Grid

The screenshot shows a web browser window titled "CCR Grid Computing Services: Data Management - Microsoft Internet Explorer". The page header includes the University at Buffalo logo and the text "Center for Computational Research GRID PORTAL High Performance Grid Computing".

On the left side, there is a "PORTAL LOGOUT" menu with the following items:

- 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
 - » Conдор Flock Statistics
 - » User Information
- Education/Outreach
- Staff Only
- CCR HOME

The main content area displays a file tree for the user "rappleye". At the top, there are controls: "VIEW Group", "GROUP miller", and "UserList rappleye". The file tree structure is as follows:

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

A yellow callout bubble points to the "Oracle.m" file in the tree, containing the text: "Browser view of 'miller' group files published by user 'rappleye'".

At the bottom of the page, there is a decorative graphic of a molecular structure and the text: "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.)**

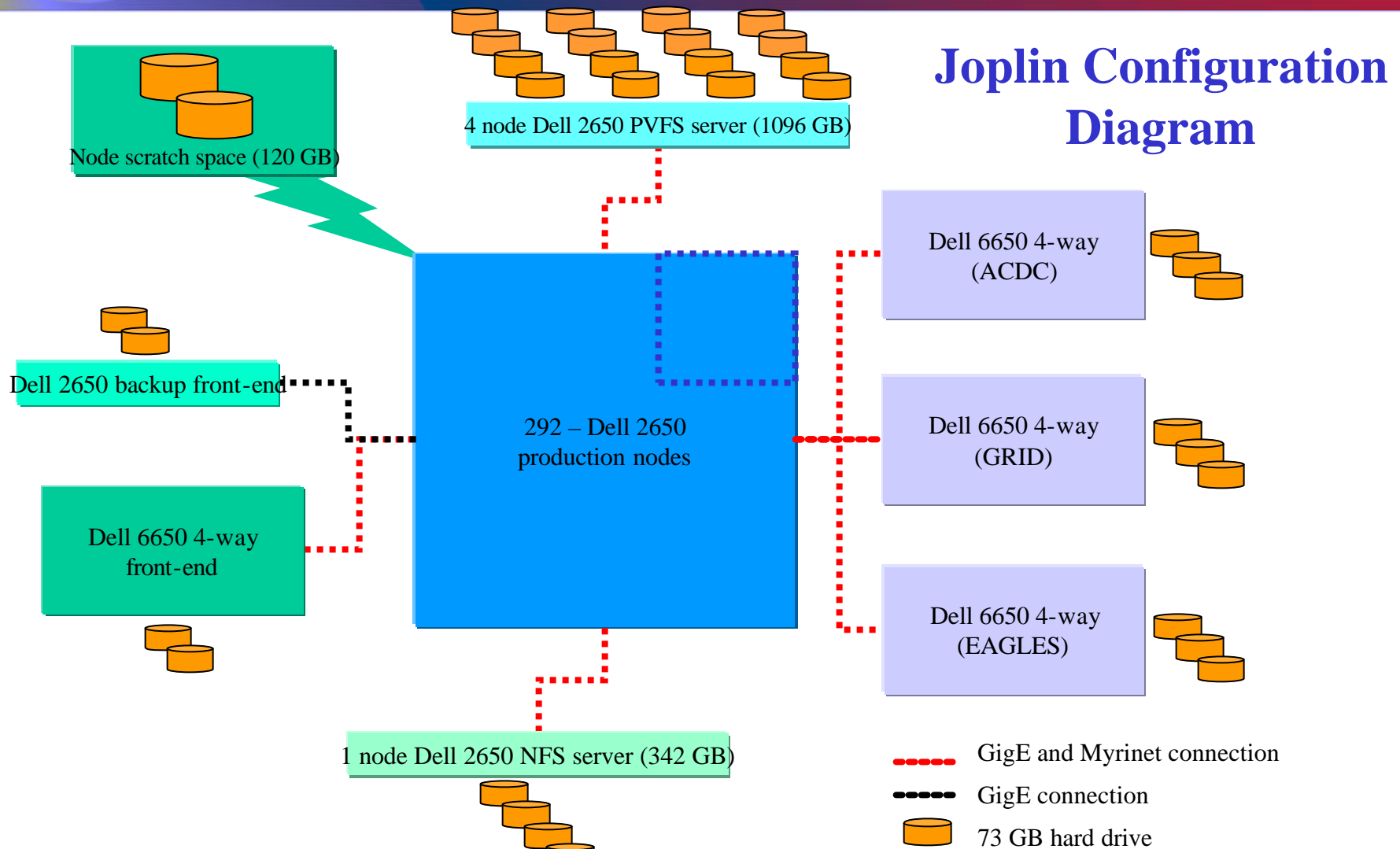
Predictive Scheduler

- **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**

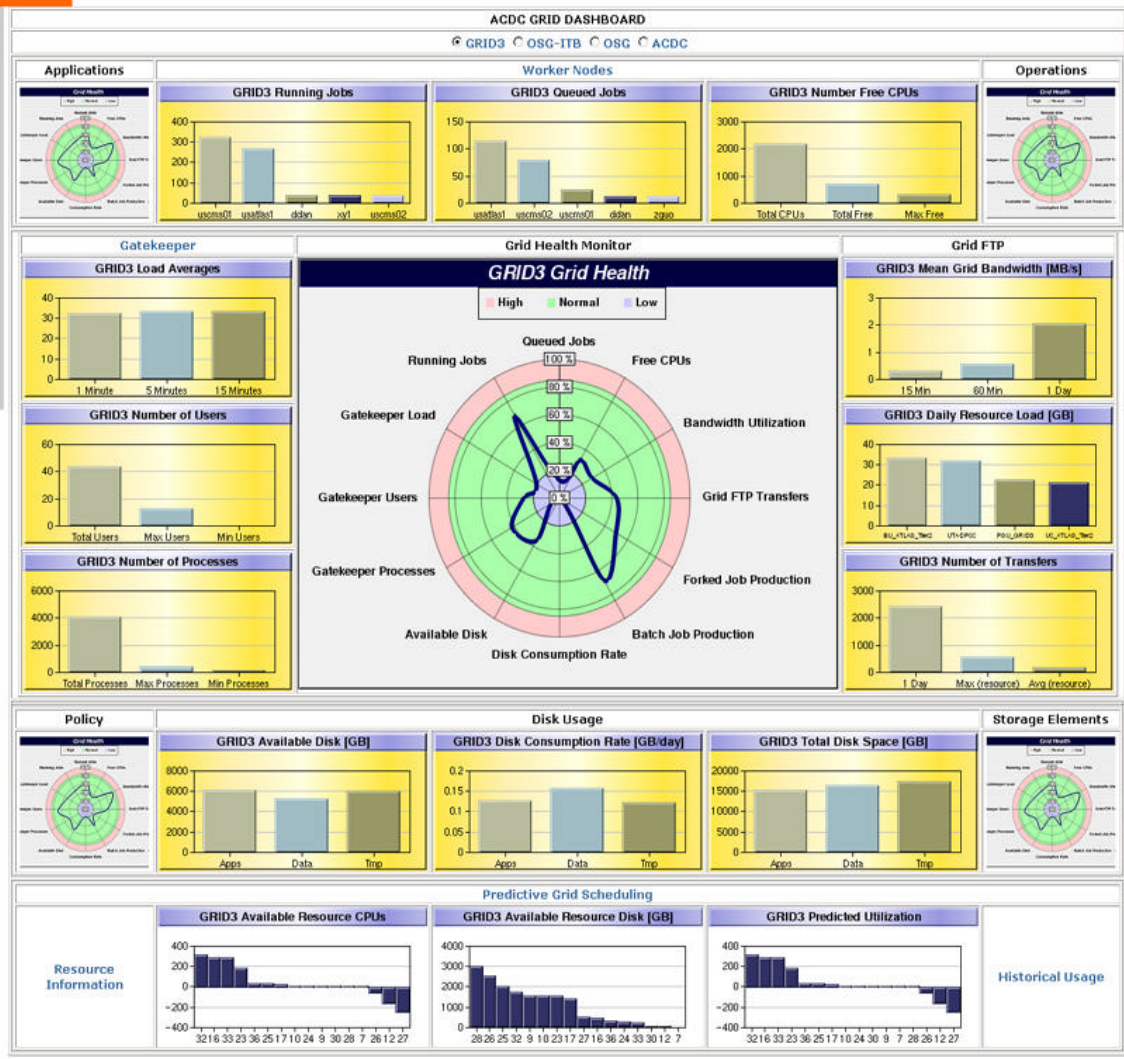
ACDC-Grid Dynamic Resource Allocation





ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD

- Grid Resources
- ACDC Monitoring
- ACDC Grid Dashboard
- Running/Queued Jobs
- Job History
- Detailed Job History
- Detailed GridFTP History
- Resource Queue Visualization
- Resource User Visualization
- Self Application Demonstrator
- Presentations
- ACDC Site Status
- Contact Us
- Staff Only



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

PORTAL LOGOUT
User Tools
Manage Account
Grid General Info
Projects
Resources
Computational Grid
Job Submission
Job/Queue Status
Data Grid
Data Grid Statistics
Network Status
Running/Queued Jobs
PBS Job History
Grid Portal Statistics
Center Fleck Statistics
User Information
Education/Outreach
Staff Only
CCR HOME

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.)

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 this file to the grid nodes

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 10:59:12

Resource	Last Updated	Next Update	Status
crasby.ccr.buffalo.edu	16-September-2003 09:15:30	2 minutes	OK
rogerty.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
newus.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.](#)

Advanced
Center for Computational Research
Data
Center



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

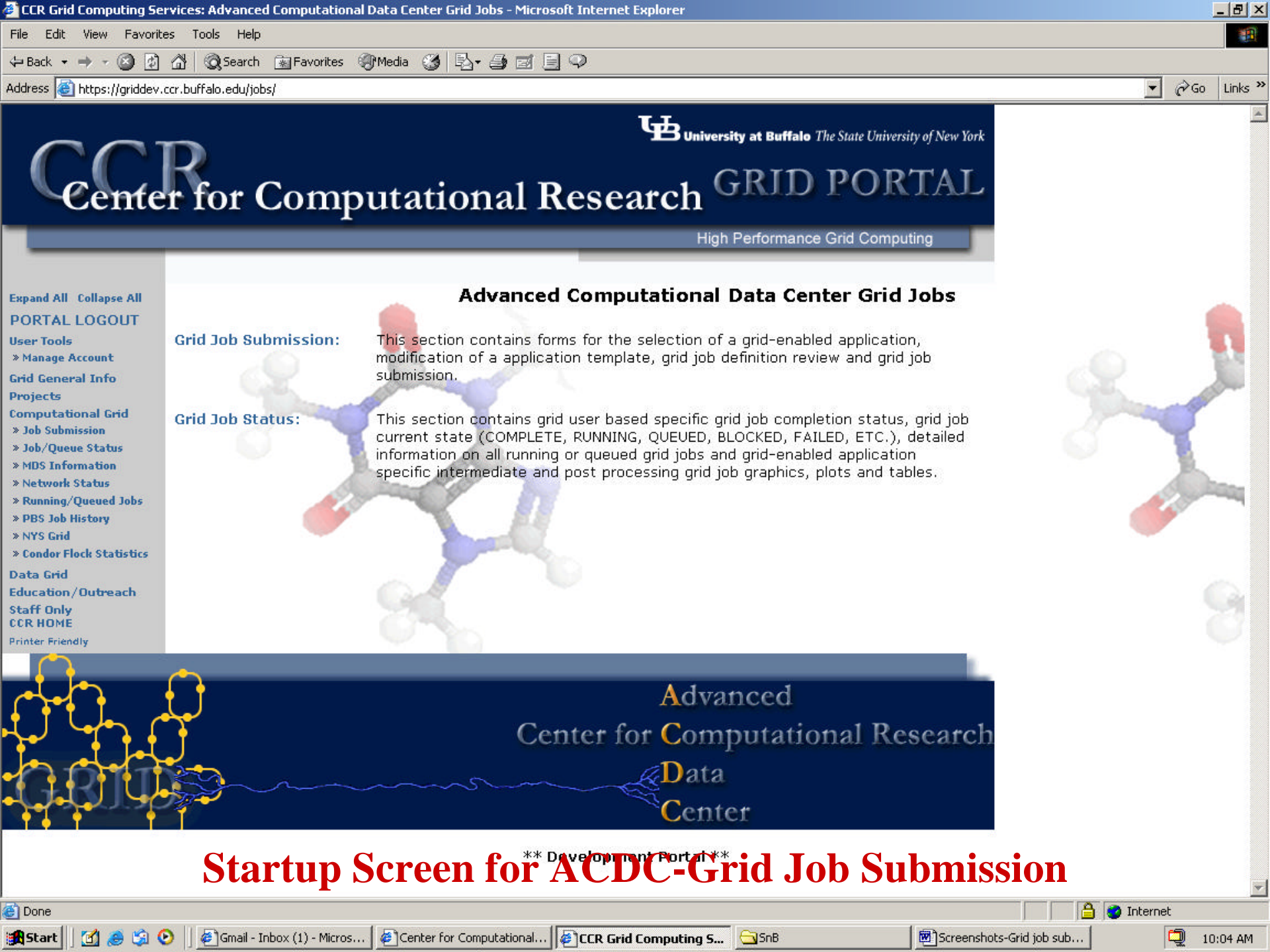
- ❑ *EADR*: Evolutionary Aseismic Design and Retrofit; Passive Energy Dissipation System for Designing Earthquake Resilient Structures

■ Computational Chemistry

- ❑ *Q-Chem*: Quantum Chemistry Package

■ Geographic Information Systems & BioHazards

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



CCR Center for Computational Research GRID PORTAL

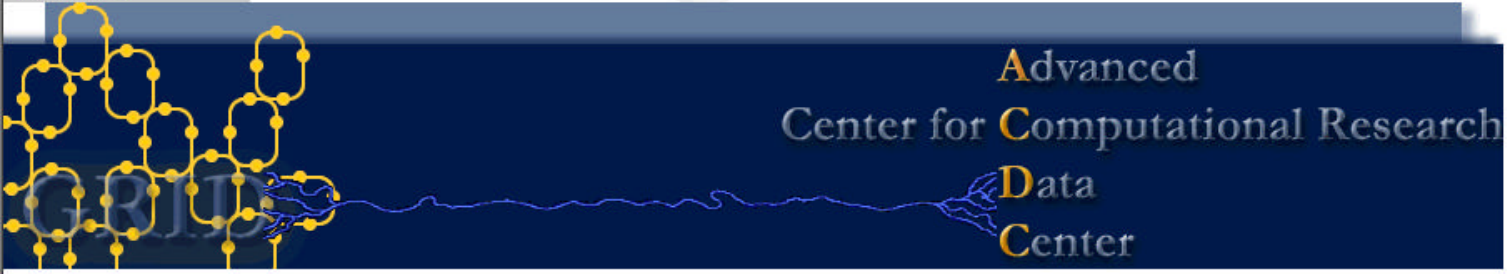
High Performance Grid Computing

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

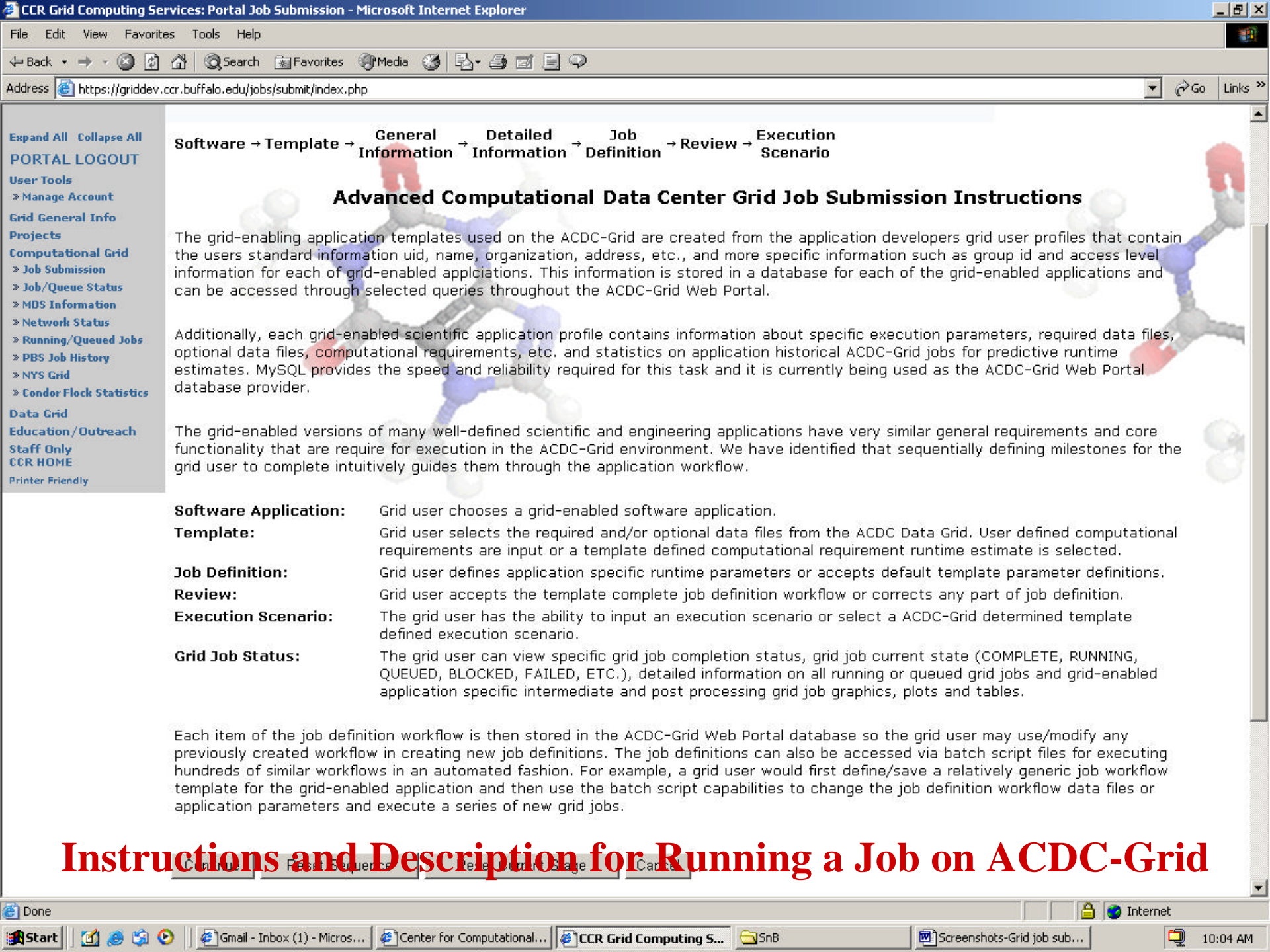
Advanced Computational Data Center Grid Jobs

Grid Job Submission: This section contains forms for the selection of a grid-enabled application, modification of a 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.



Startup Screen for ACDC-Grid Job Submission



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.

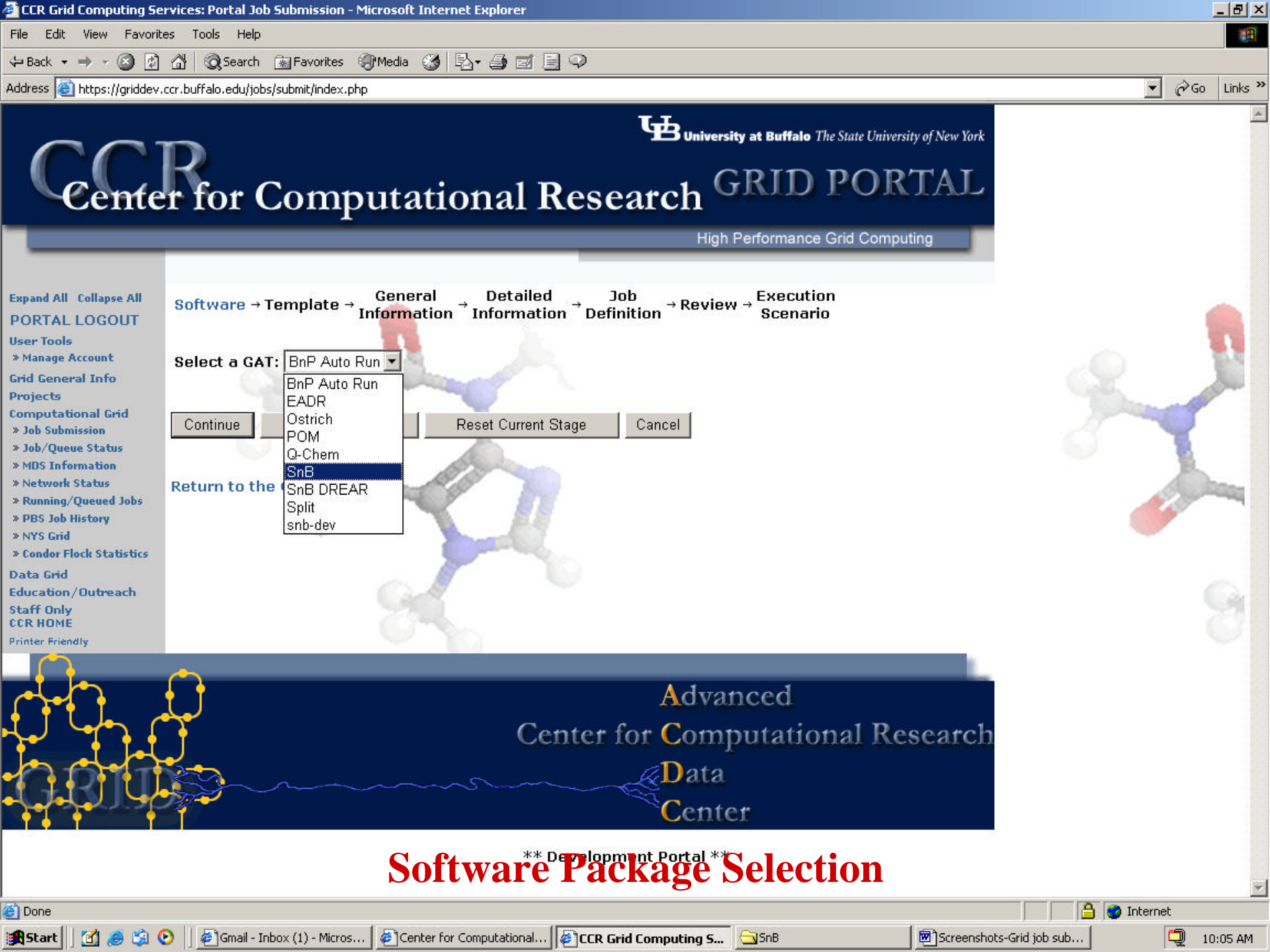
Additionally, each grid-enabled scientific application profile contains information about specific execution parameters, required data files, optional data files, computational requirements, etc. and statistics on application historical ACDC-Grid jobs for predictive runtime estimates. MySQL provides 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



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
 - » Condor 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

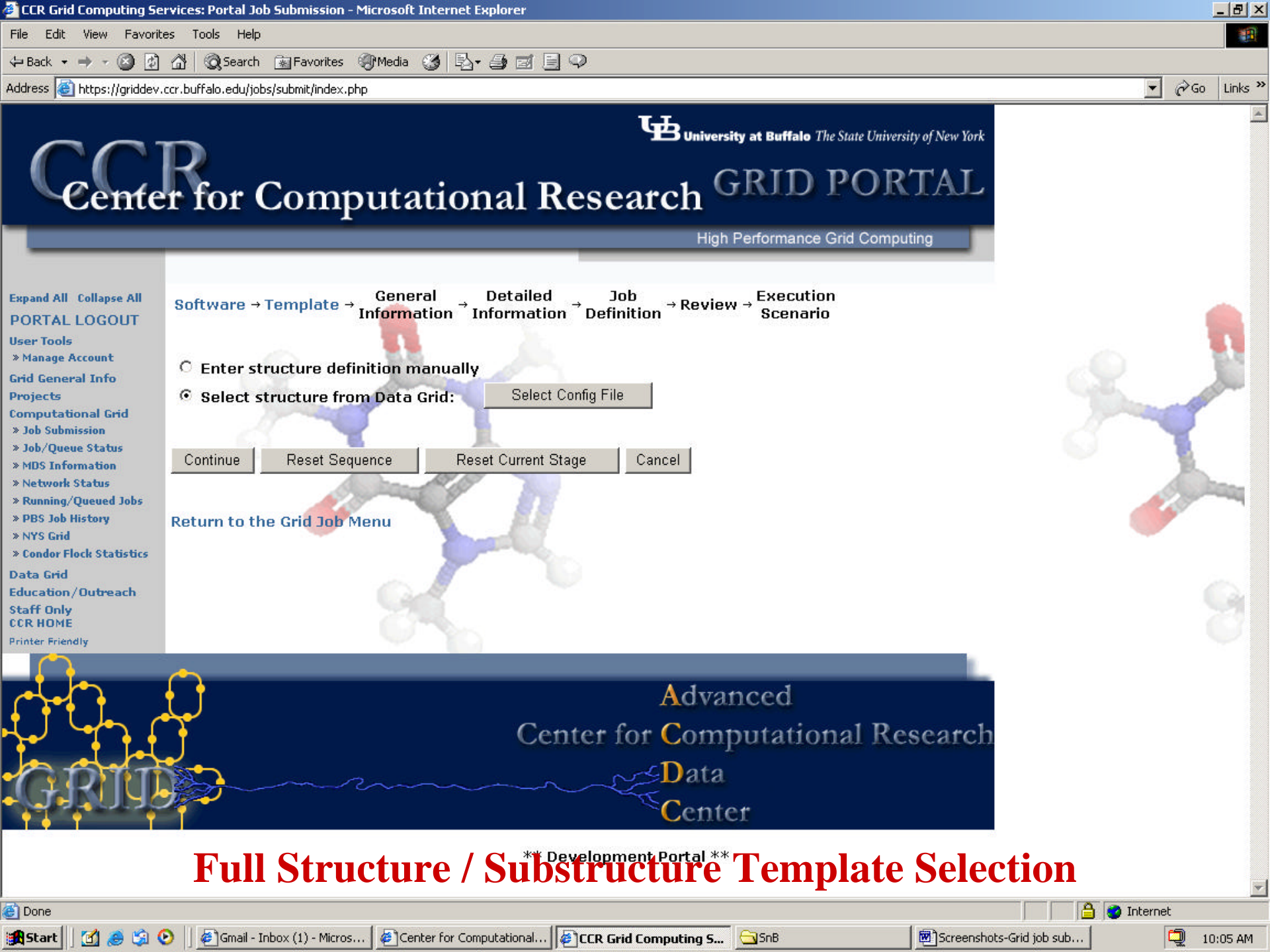
Reset Current Stage

Cancel

Return to the

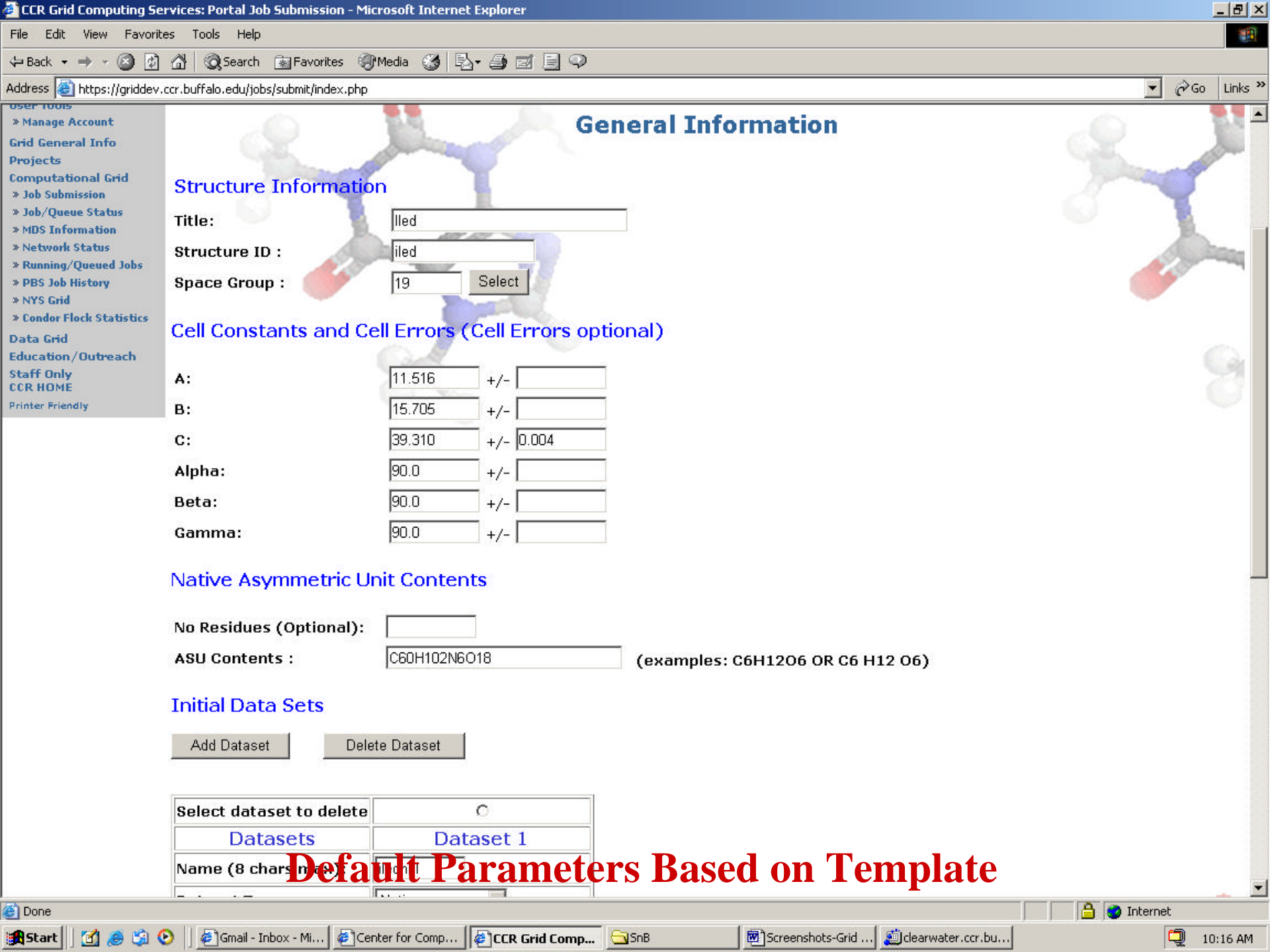


**** Development Portal ****
Software Package Selection



Full Structure / Substructure Template Selection

**** Development Portal ****



- 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

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

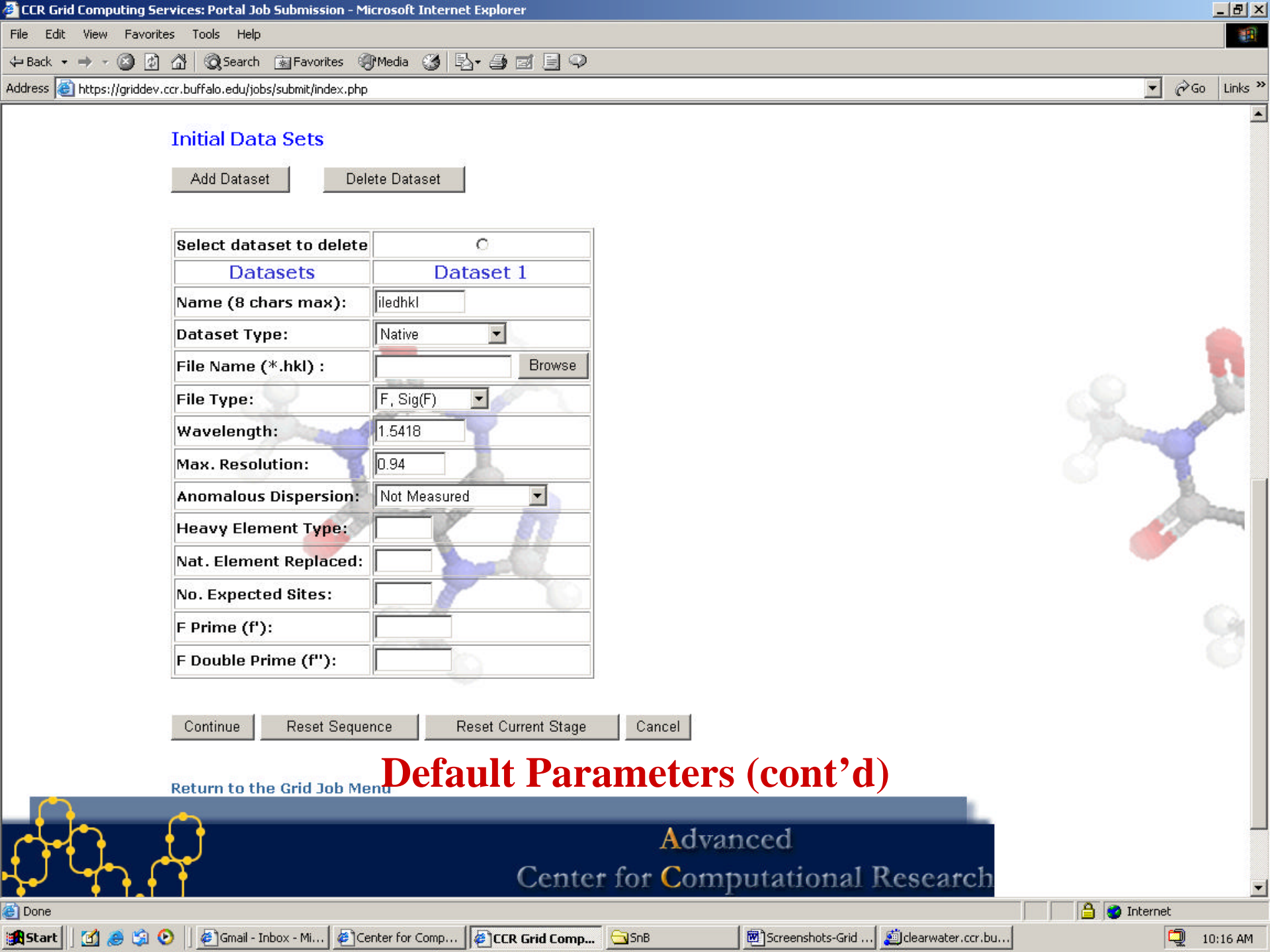
No Residues (Optional):

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

Initial Data Sets

Select dataset to delete	<input type="radio"/>
Datasets	<input type="radio"/>
Dataset 1	<input type="radio"/>
Name (8 chars max)	

Default Parameters Based on Template



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"/> <input type="button" value="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

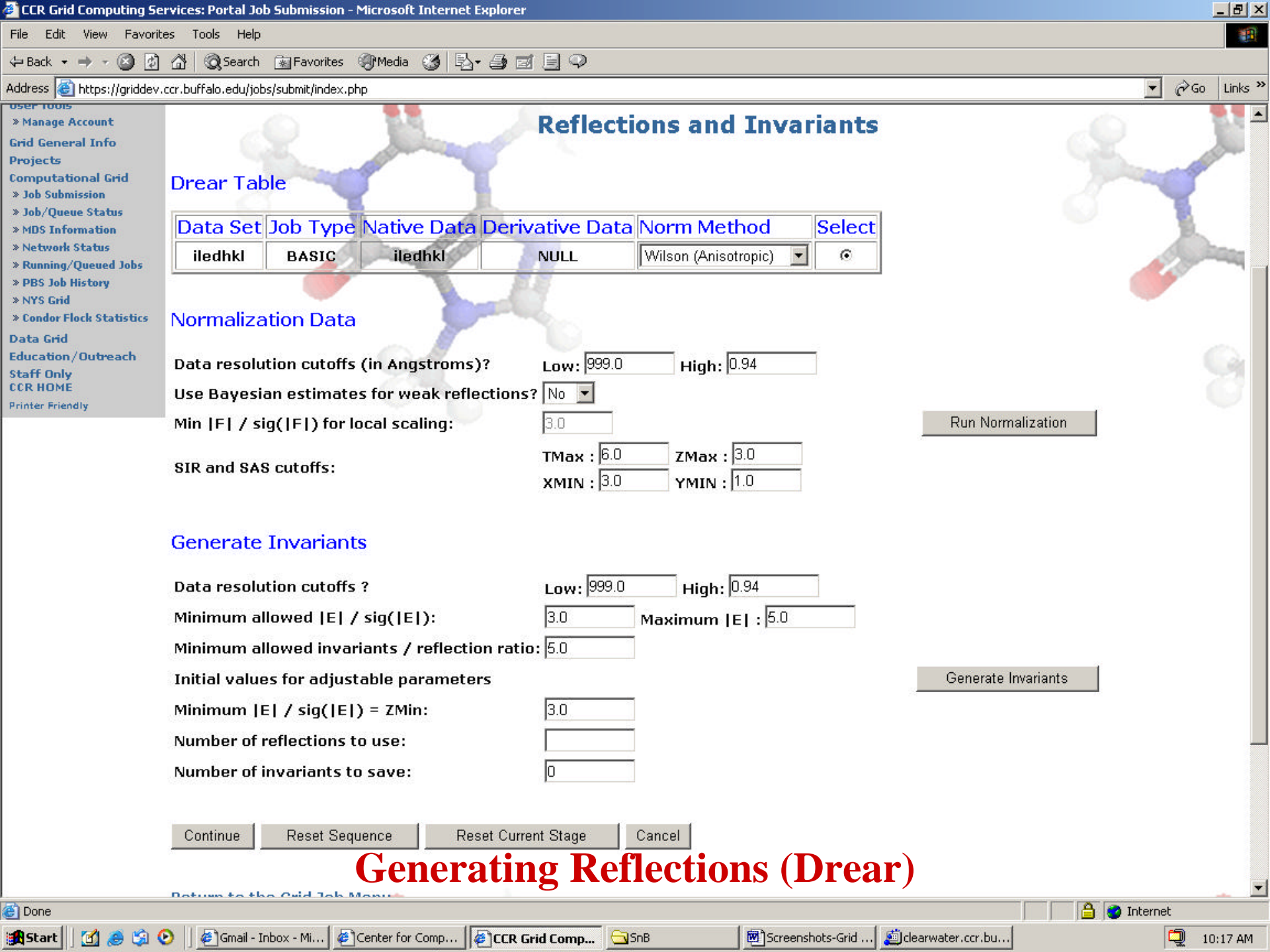
Reset Current Stage

Cancel

[Return to the Grid Job Menu](#)

Default Parameters (cont'd)

Advanced
Center for Computational Research



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 $|F| / \text{sig}(|F|)$ for local scaling:

SIR and SAS cutoffs:

TMax : ZMax :

XMIN : YMIN :

Run Normalization

Generate Invariants

Data resolution cutoffs ? Low: High:

Minimum allowed $|E| / \text{sig}(|E|)$: Maximum $|E|$:

Minimum allowed invariants / reflection ratio:

Initial values for adjustable parameters

Minimum $|E| / \text{sig}(|E|) = ZMin$:

Number of reflections to use:

Number of invariants to save:

Generate Invariants

Continue Reset Sequence Reset Current Stage Cancel

Generating Reflections (Drear)

- 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

Drear 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 :

Run Normalization

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:

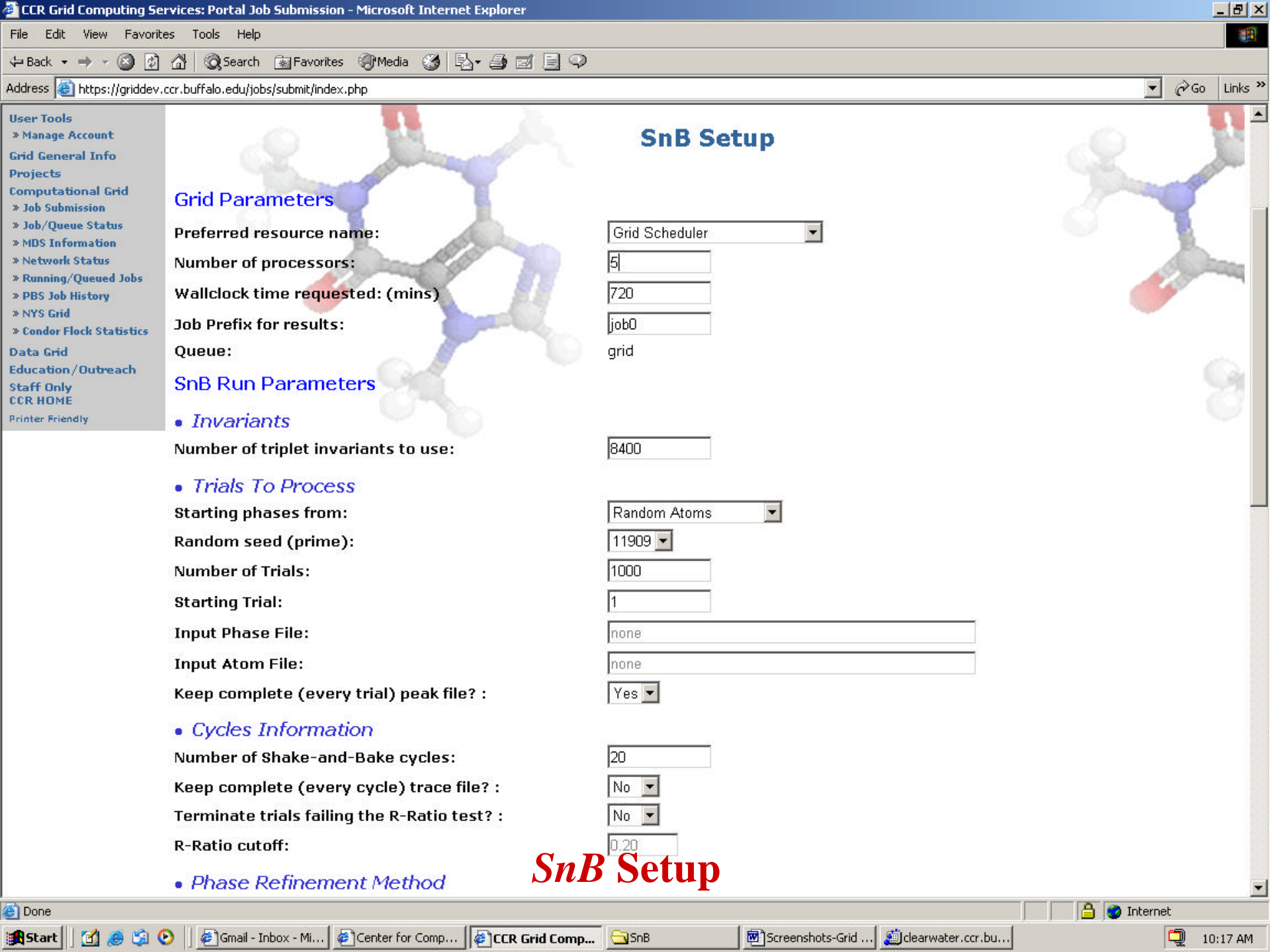
Number of reflections to use:

Number of invariants to save:

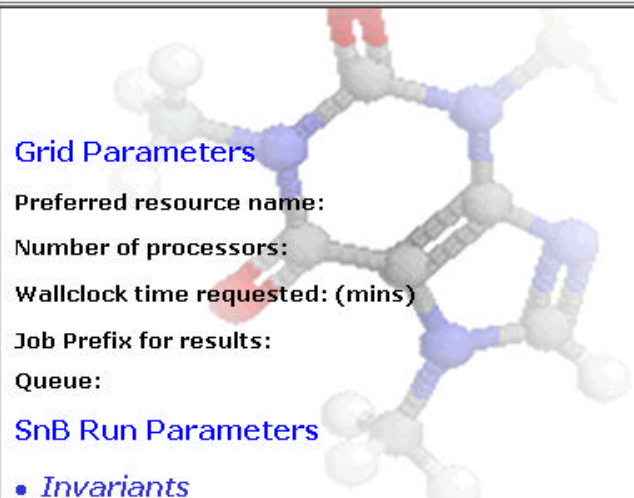
Generate Invariants

Continue Reset Sequence Reset Current Stage Cancel

Invariant Generation



- 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



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

CCR Grid Computing: Portal Job Submission - Microsoft Internet Explorer

File Edit View Favorites Tools Help

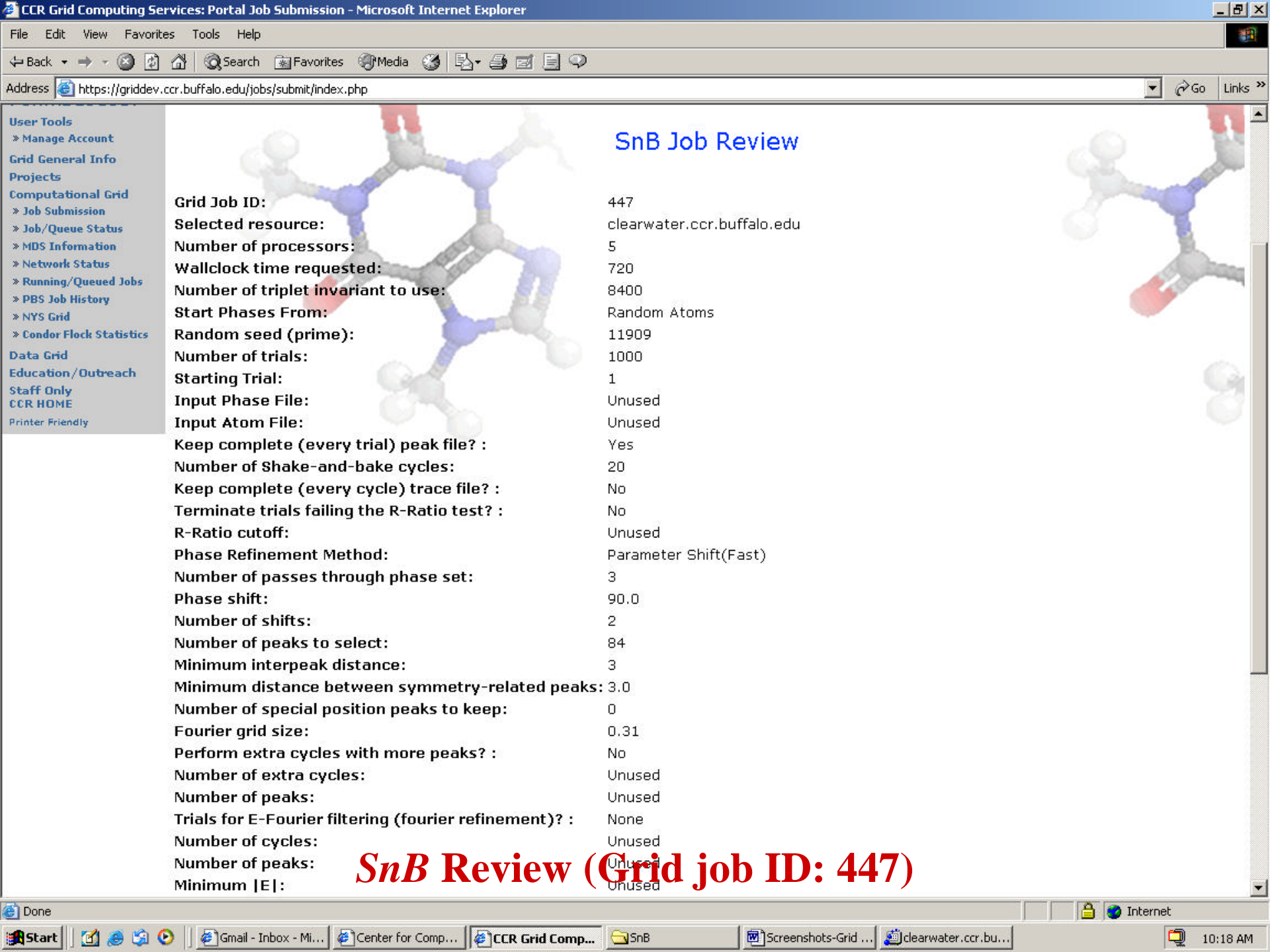
Address <https://griddev.ccr.buffalo.edu/jobs/submit/index.php> Go Links >>

- *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 Imporvement (%):

SnB Setup (cont'd)

Done Internet

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

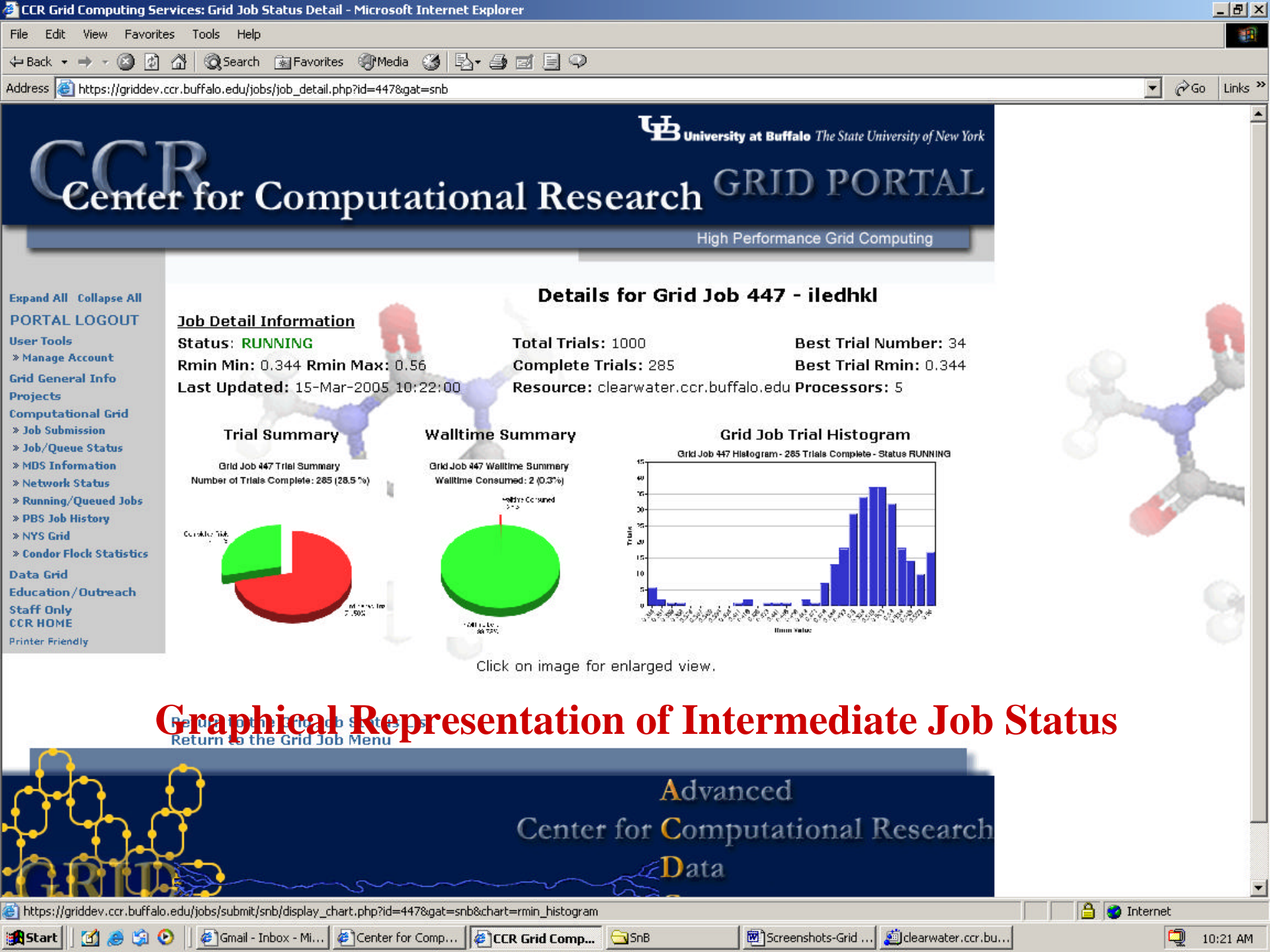


- User Tools
 - » Manage Account
- Grid General Info
- Projects
- Computational Grid
 - » Job Submission
 - » Job/Queue Status
 - » MDS Information
 - » Network Status
 - » Running/Queued Jobs
 - » PBS Job History
 - » NYS Grid
 - » Condor Flock Statistics
- Data Grid
- Education/Outreach
- Staff Only
- 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)



CCR Center for Computational Research

University at Buffalo The State University of New York

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

Details for Grid Job 447 - iledhkl

Job Detail Information

Status: **RUNNING** Total Trials: 1000 Best Trial Number: 34
 Rmin Min: 0.344 Rmin Max: 0.56 Complete Trials: 285 Best Trial Rmin: 0.344
 Last Updated: 15-Mar-2005 10:22:00 Resource: clearwater.ccr.buffalo.edu Processors: 5

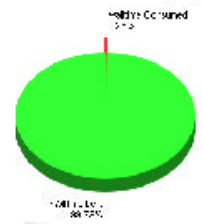
Trial Summary

Grid Job 447 Trial Summary
 Number of Trials Complete: 285 (28.5%)



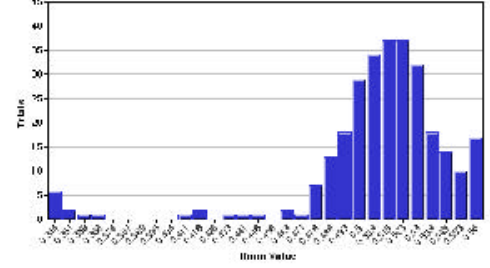
Walltime Summary

Grid Job 447 Walltime Summary
 Walltime Consumed: 2 (0.3%)



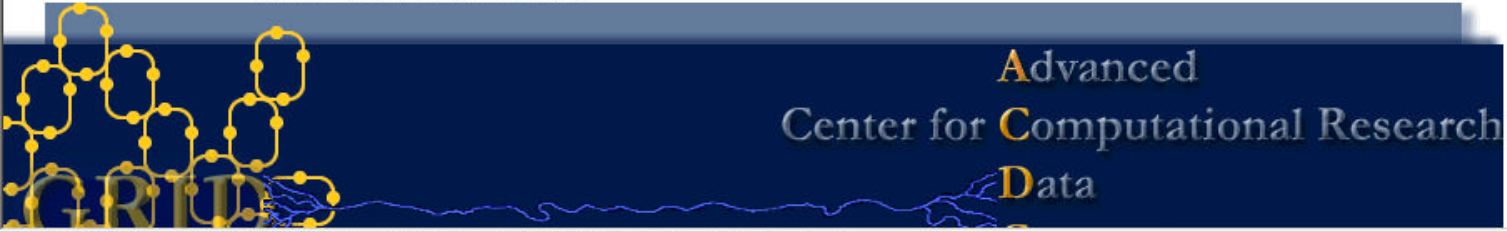
Grid Job Trial Histogram

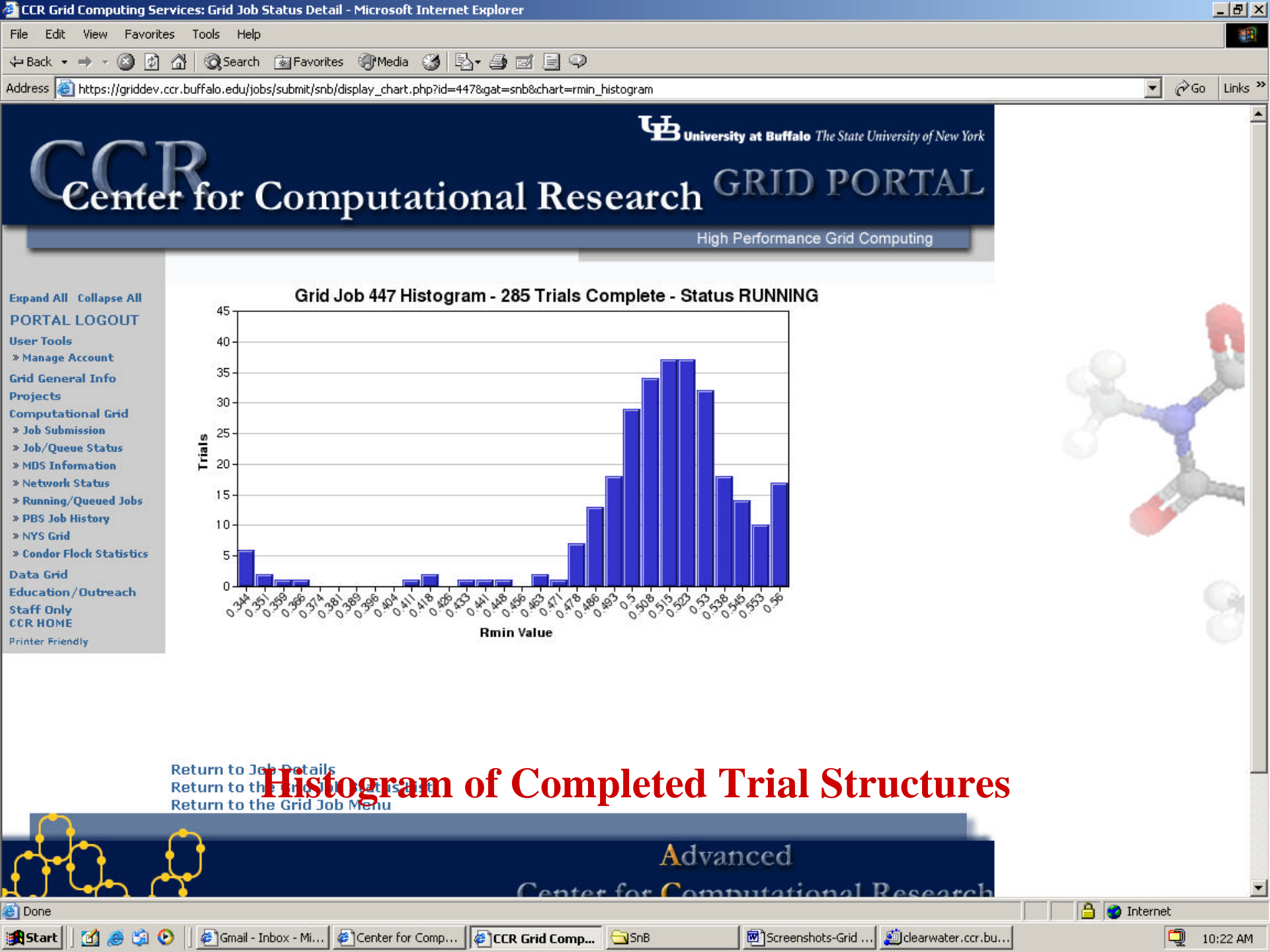
Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING



Click on image for enlarged view.

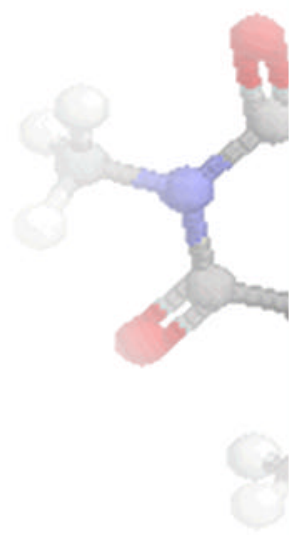
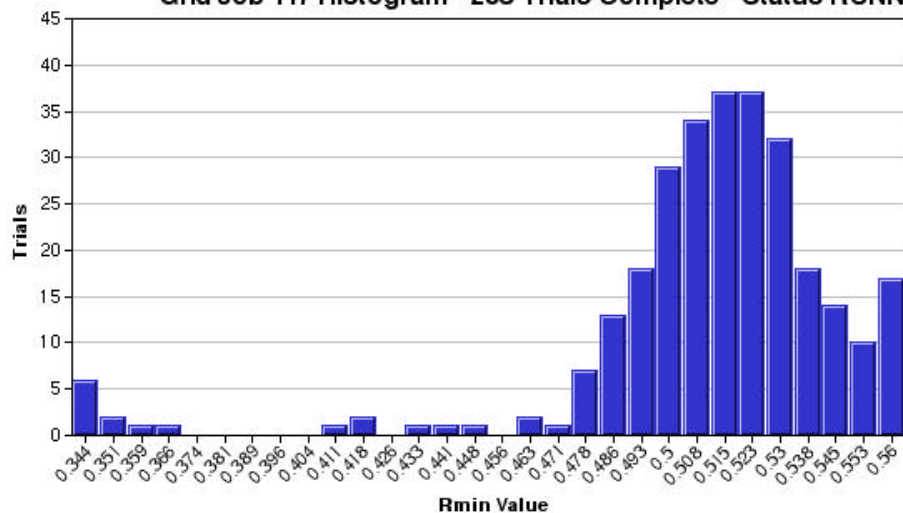
Graphical Representation of Intermediate Job Status





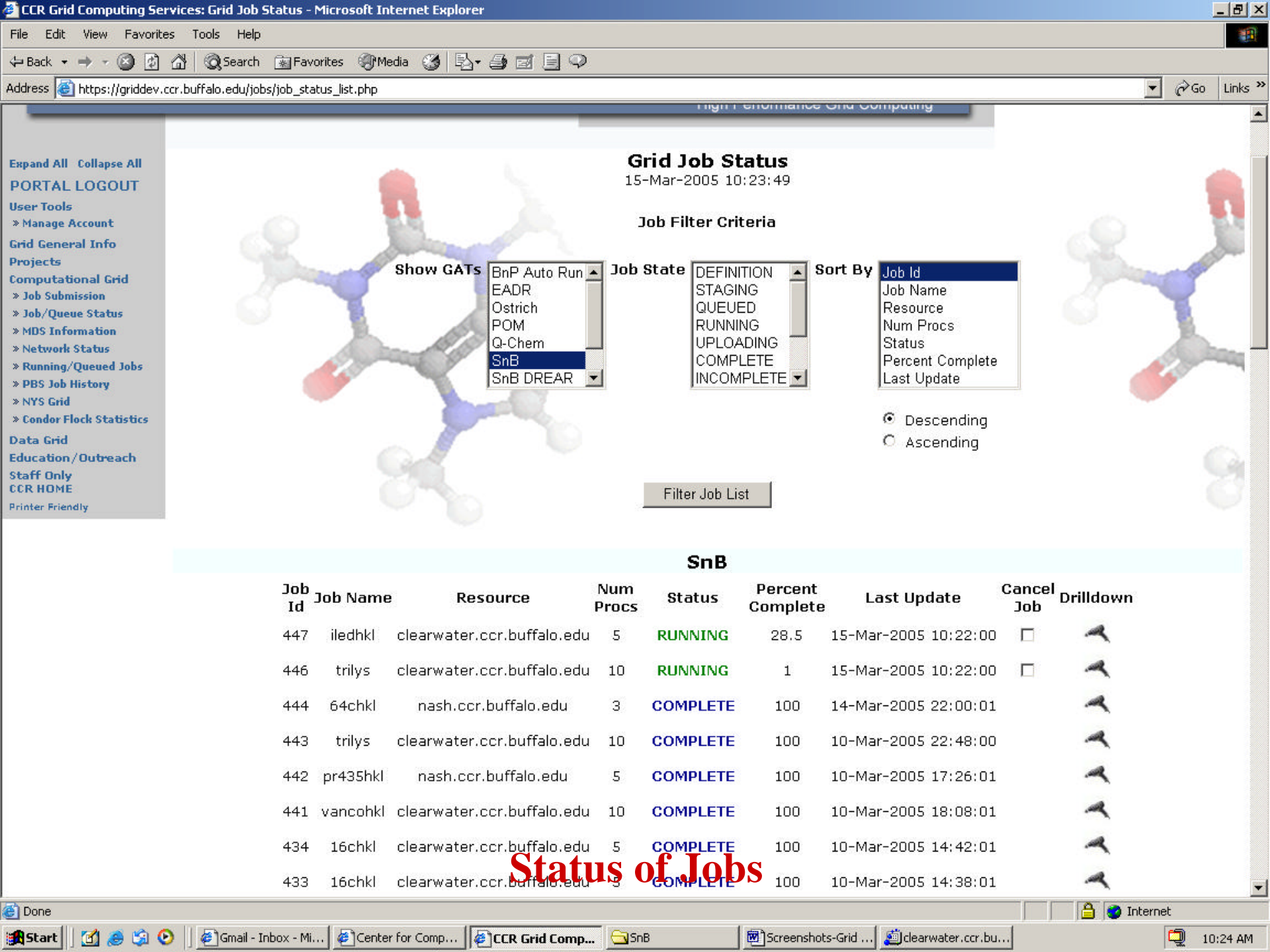
- Expand All Collapse All
- PORTAL LOGOUT
- User Tools
 - » Manage Account
- Grid General Info
- Projects
- Computational Grid
 - » Job Submission
 - » Job/Queue Status
 - » MDS Information
 - » Network Status
 - » Running/Queued Jobs
 - » PBS Job History
 - » NYS Grid
 - » Condor Flock Statistics
- Data Grid
- Education/Outreach
- Staff Only
- CCR HOME
- Printer Friendly

Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING



[Return to Job Details](#)
[Return to the Grid Job Status List](#)
[Return to the Grid Job Menu](#)

Histogram of Completed Trial Structures



- 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 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

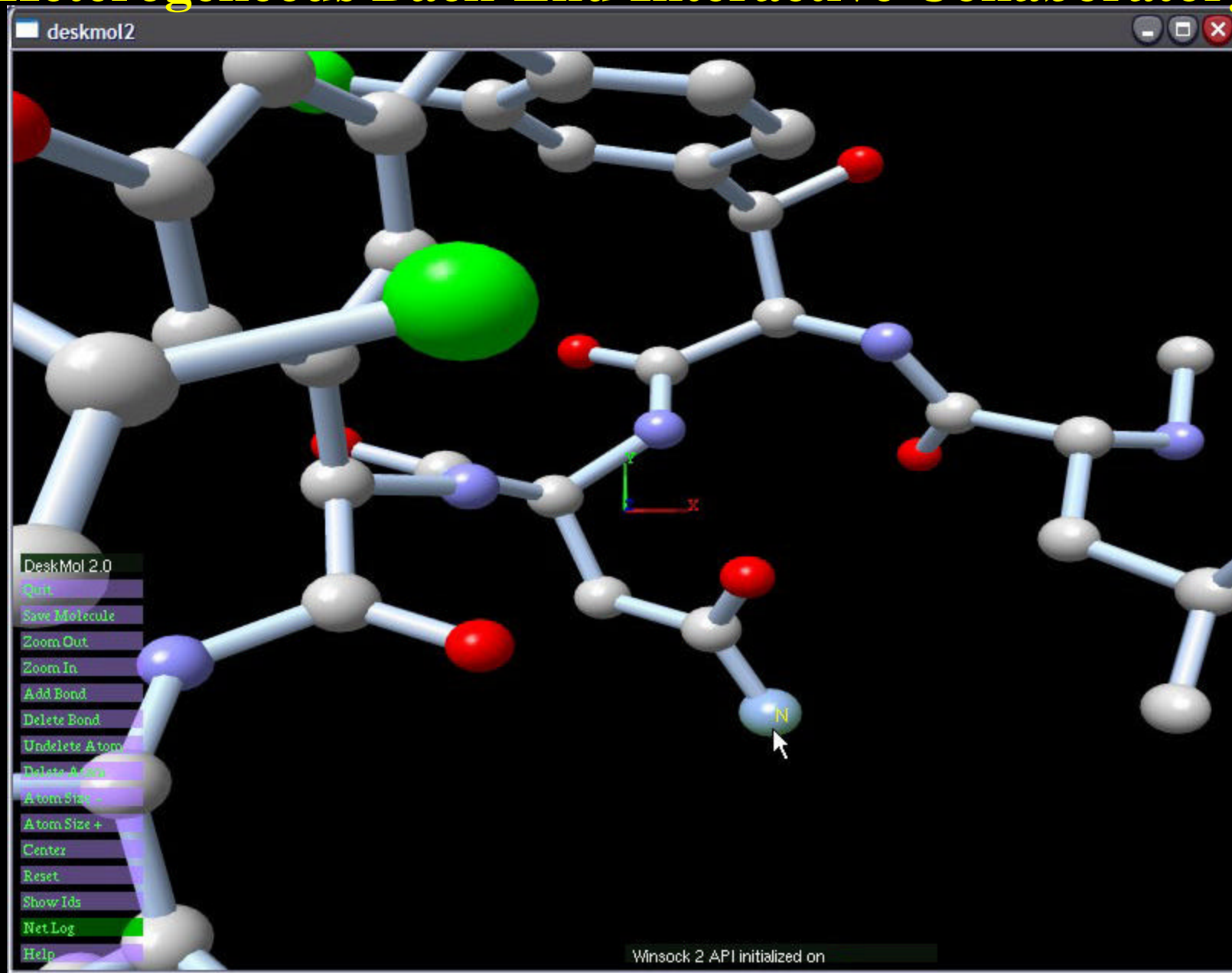
Filter Job List

SnB

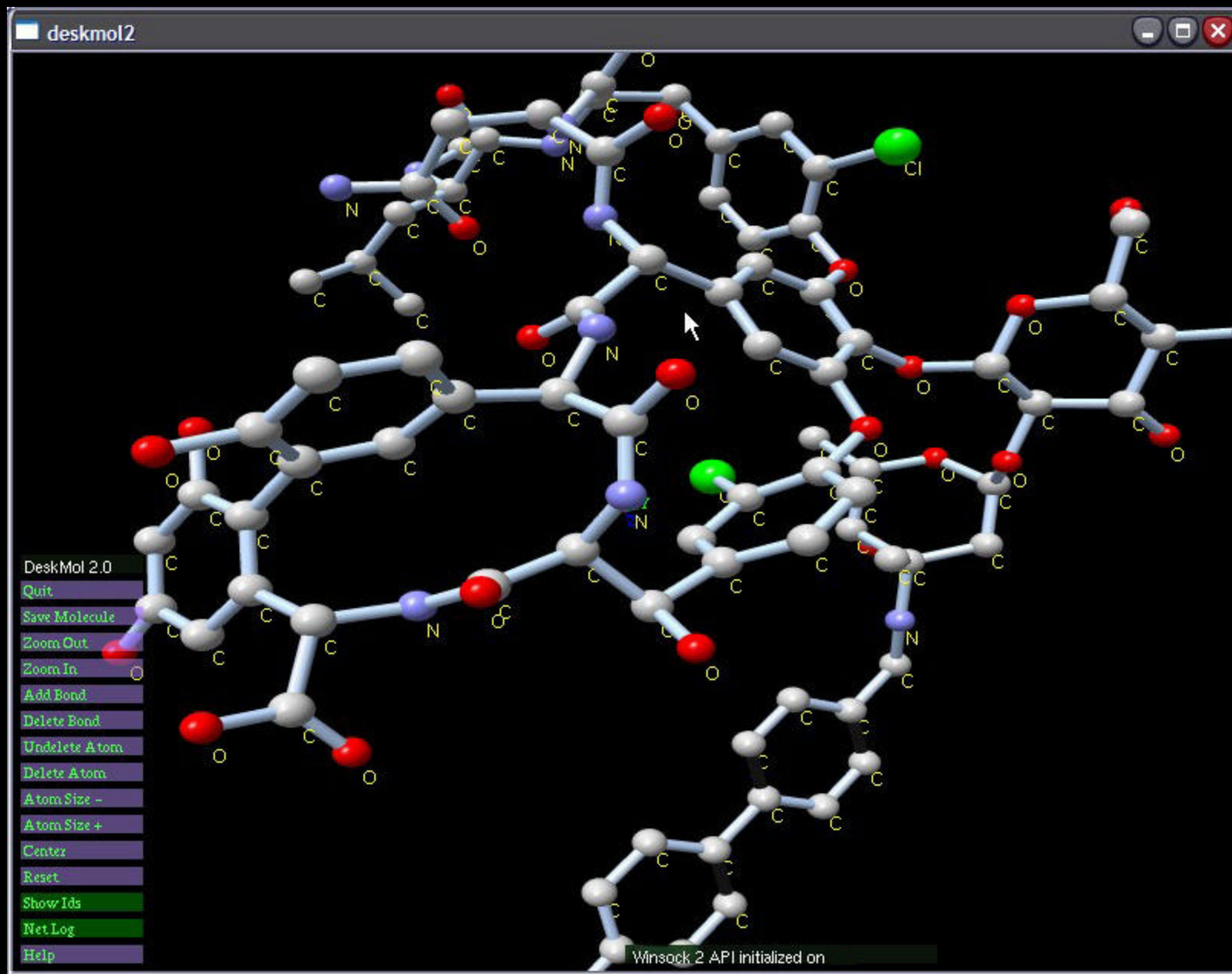
Job Id	Job Name	Resource	Num Procs	Status	Percent Complete	Last Update	Cancel Job	Drilldown
447	iledhkl	clearwater.ccr.buffalo.edu	5	RUNNING	28.5	15-Mar-2005 10:22:00	<input type="checkbox"/>	
446	trilys	clearwater.ccr.buffalo.edu	10	RUNNING	1	15-Mar-2005 10:22:00	<input type="checkbox"/>	
444	64chkl	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

Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Acknowledgments

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

- **George DeTitta**
- **Herb Hauptman**
- **Charles Weeks**
- **Steve Potter**

- **Phil Glick**
- **Rohit Bakshi**

- **Alan Rabideau**
- **Igor Janckovic**
- **Michael Sheridan**
- **Abani Patra**
- **Matt Jones**

- **IBC Digital**
- **TVGA**
- **Bergmann Associates**
- **Peace Bridge Authority**

- **Bruce Holm**
- **Janet Penksa**

- **NSF, NIH, NYS, NIMA, NTA, Oishei, Wendt, DOE**



University of Buffalo
College of Business

www.ccr.buffalo.edu

CCR

UB

