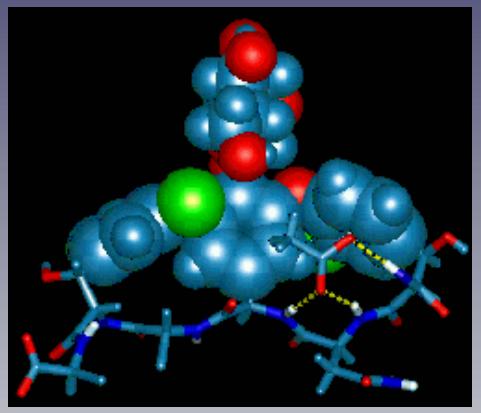
Cyberinfrastructure and Molecular Structure Determination



Russ Miller

State University of New York at Buffalo

Hauptman-Woodward Med Res Inst

NSF, NIH, DOE, NIMA, NYS, HP

GRID

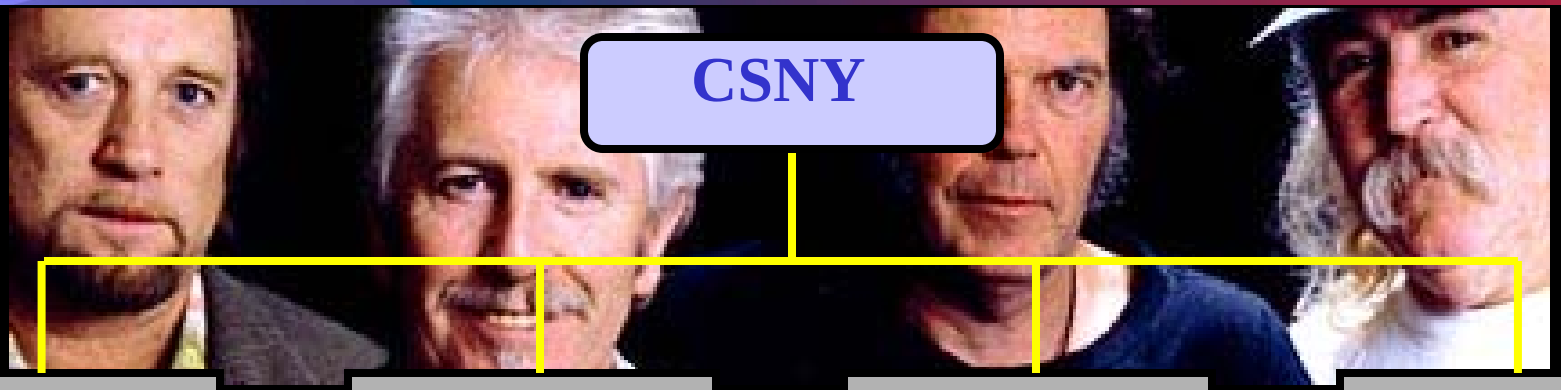
Advanced Center for Computational Research Data Center

SnB

Academia in the 21st Century

- Embrace digital data-driven society
- Empower students to compete in knowledge-based economy
- Support HPC infrastructure, research, and applications
- Support education, outreach, and training
- Deliver *high-end cyberinfrastructure* to enable efficient
  - Collection of data
  - Management/Organization of data
  - Distribution of data
  - Analysis of data
  - Visualization of data

Organization of CSNY
(Cyberinstitute of SUNY-Buffalo)



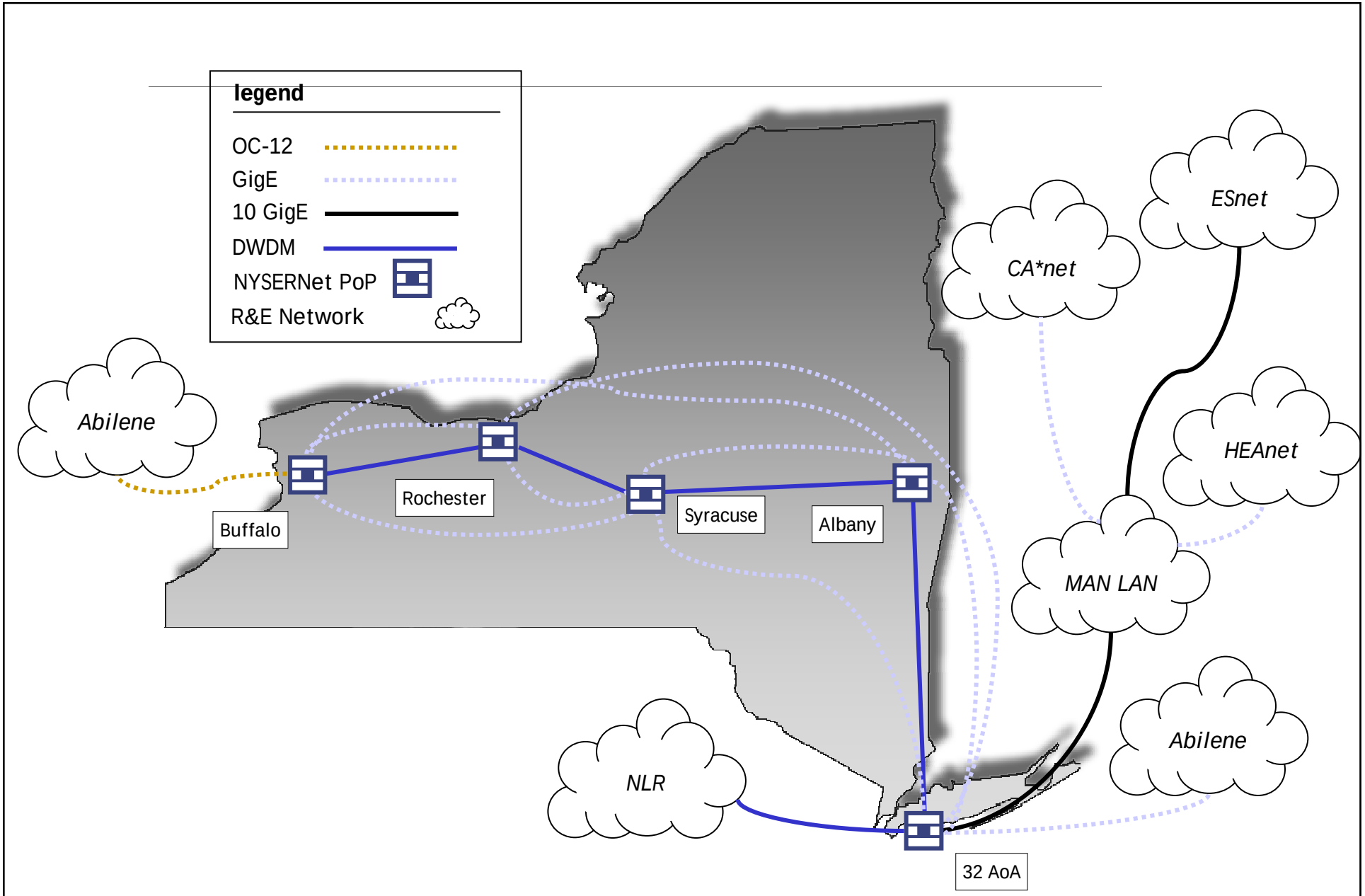
CSNY

HPC (CCR)
- Computing
- Data
- Visualization
- Networking

CSE
- MultiScale
- Sciences
- Engineering
- Life Sciences
- Media

CI
- Scheduling
- Monitoring
- Virtual Reality

Enabling
- Programmers
- GUI Design
- Integration



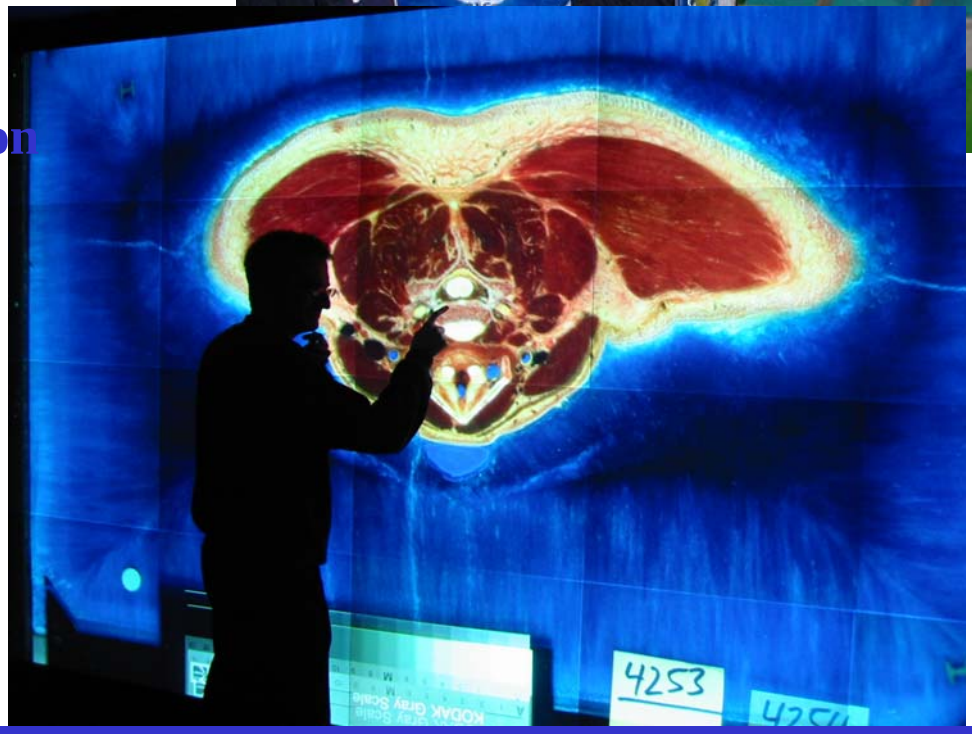
Courtesy of NYSER*Net*

Center for Computational Research

- 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 (3TF peak)
  - 600 P4 Processors (2.4 GHz)
  - 600 GB RAM; 40 TB Disk; Myrinet
- SGI Altix3700 (0.4TF peak)
  - 64 Processors (1.3GHz ITF2)
  - 256 GB RAM
  - 2.5 TB Disk
- BioACE: Bioinformatics System
  - Sun V880 (3), Sun 6800
  - Sun 280R (2), Intel PIIIs
  - Sun 3960: 7 TB Disk Storage
- EMC SAN
  - 35 TB Disk, 190 TB Tape
- Founding Director
  - 1998-2006
  - Peak of ~25 TF
  - Peak of ~600 TB Storage
  - Peak of 20/30 Staff
  - ROI: $7M → ~$300M @ UB
  - ROI: ~$500M to WNY

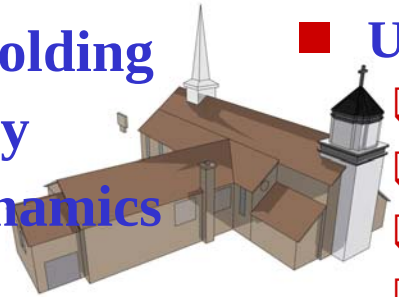
CCR Visualization Resources

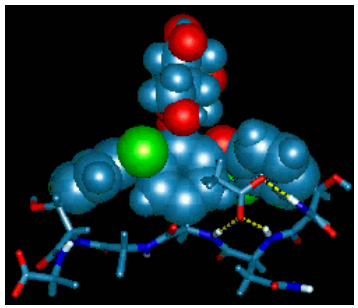
- **Tiled-Display Wall**
  - 20 NEC projectors: 15.7M pixels
  - Screen is 11'×7'
  - Dell PCs with Myrinet2000
- **Access Grid Nodes (2)**
  - Group-to-Group Communication
  - Commodity components
- **3D Passive Stereo Display**
  - VisDuo ceiling mounted system



CCR Research & Projects

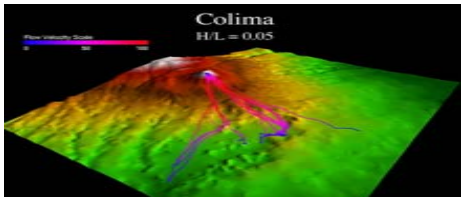
- Archaeology
- Bioinformatics/Protein Folding
- Computational Chemistry
- Computational Fluid Dynamics
- Data Mining/Database
- Earthquake Engineering
- Environ Modeling & Simulation
- Grid Computing
- Molecular Structure Determination
- Physics

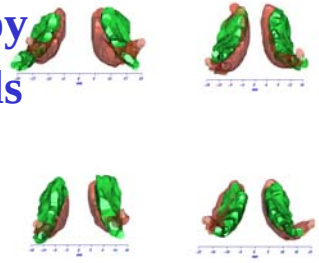




- Videos: MTV
- Urban Simulation and Viz
  - StreetScenes
  - I-90 Toll Barrier
  - Medical Campus
  - Peace Bridge

- Accident Reconstruction
- Scientific Viz
  - Dental
  - Surgery
  - MRI/CT Scan
  - Confocal Microscopy
  - Crystallization Wells
  - Collaboratories





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

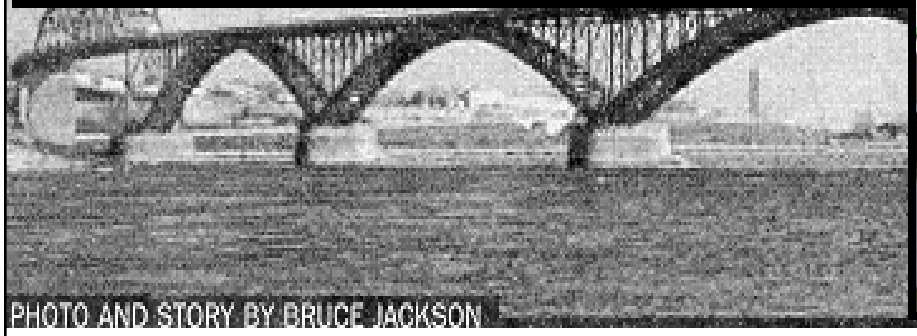
Animation & Simulation

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**

MTV

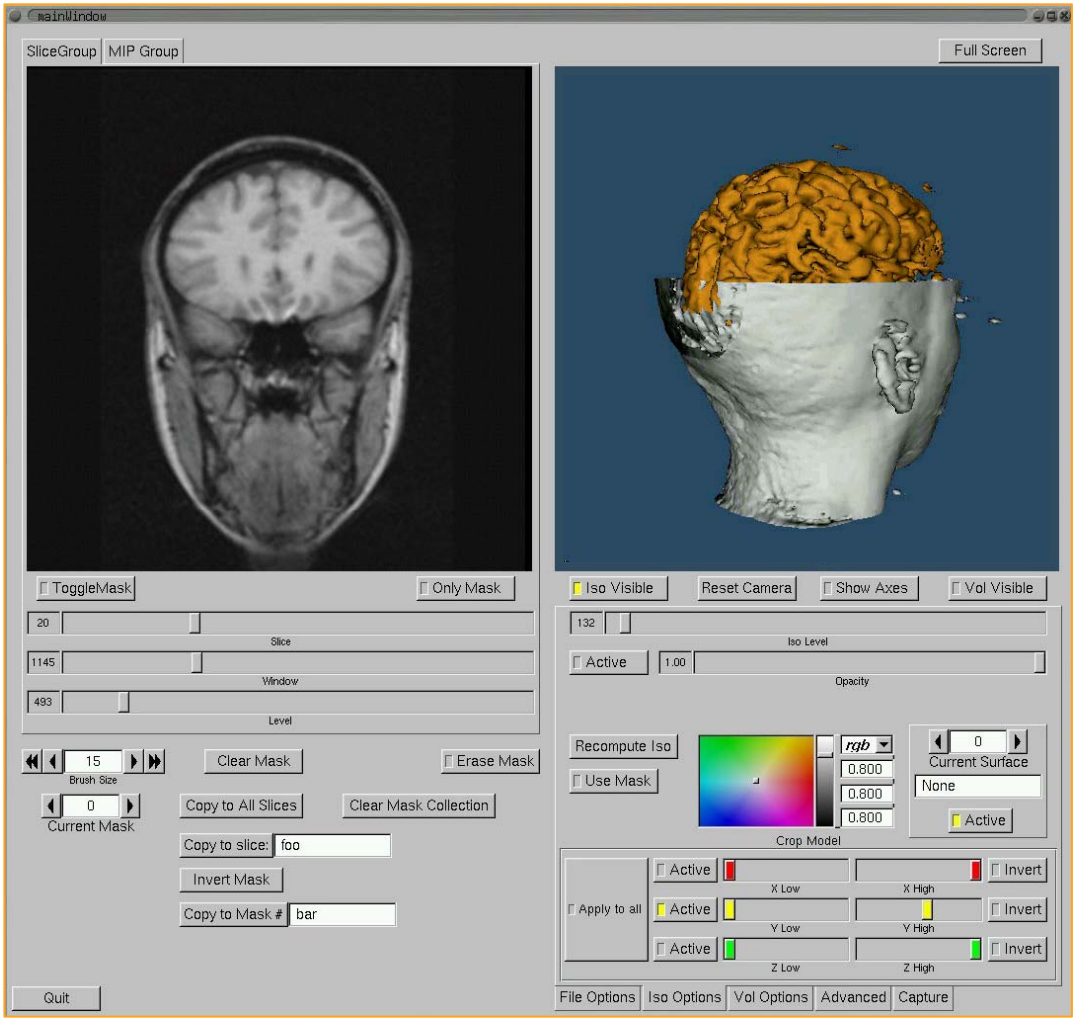
IBC Digital & CCR

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

Scientific Visualization

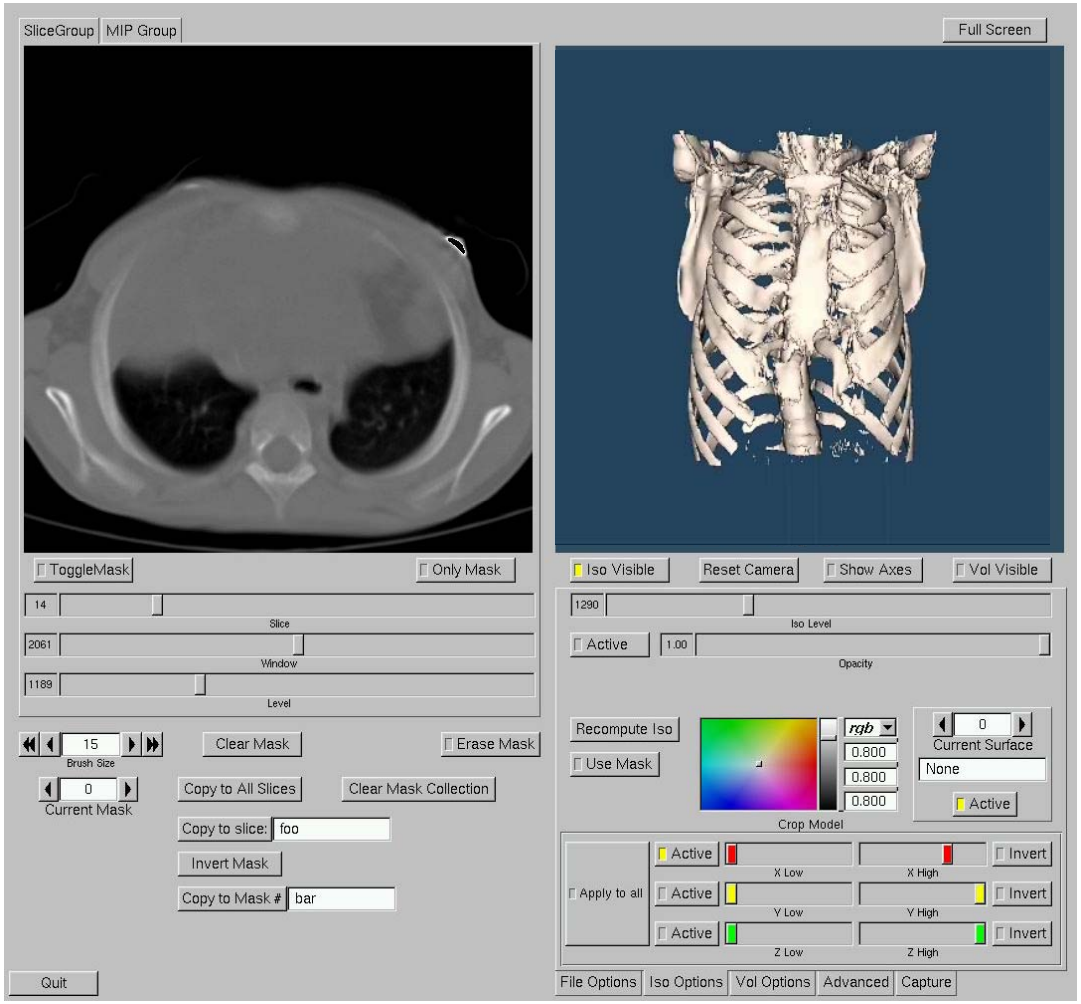
Multiple Sclerosis Project

- **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

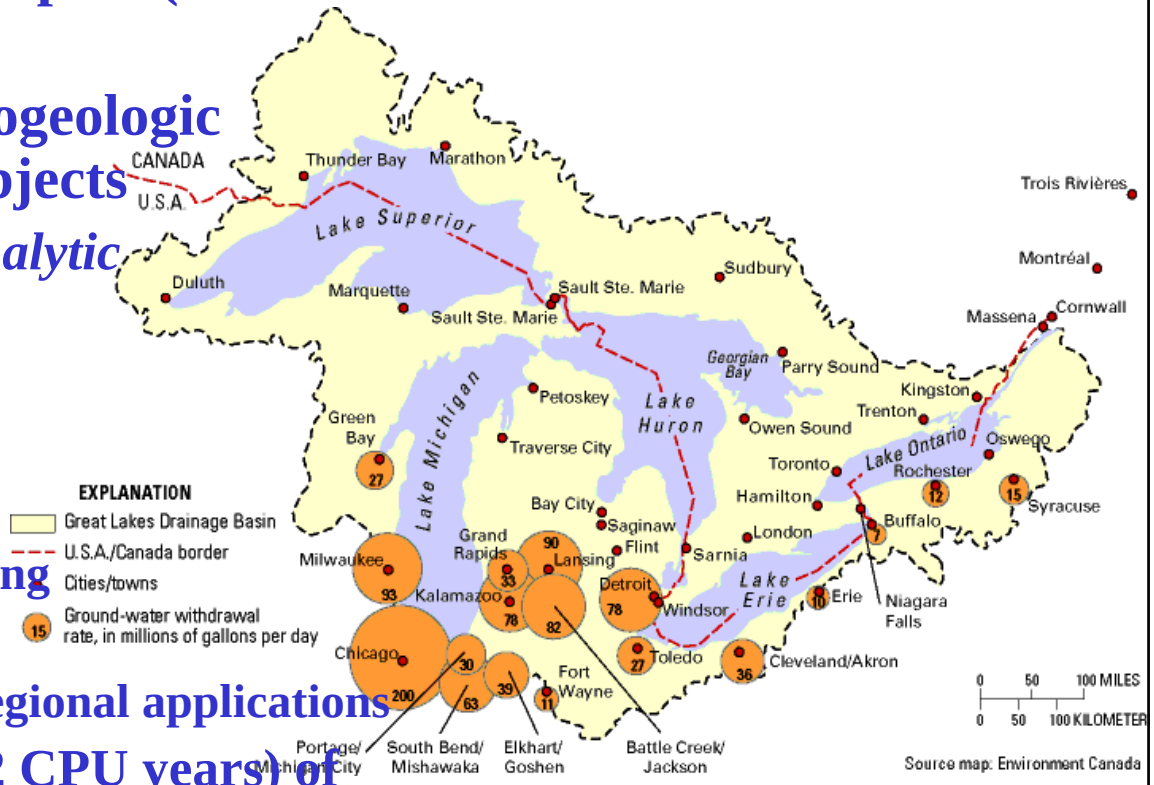
- Collaboration with Children's Hospital
  - Leading miniature access surgery center
- Application reads data output from a CT Scan
- Visualize multiple surfaces and volumes
- Export images, movies or CAD representation of model



Science & Engineering

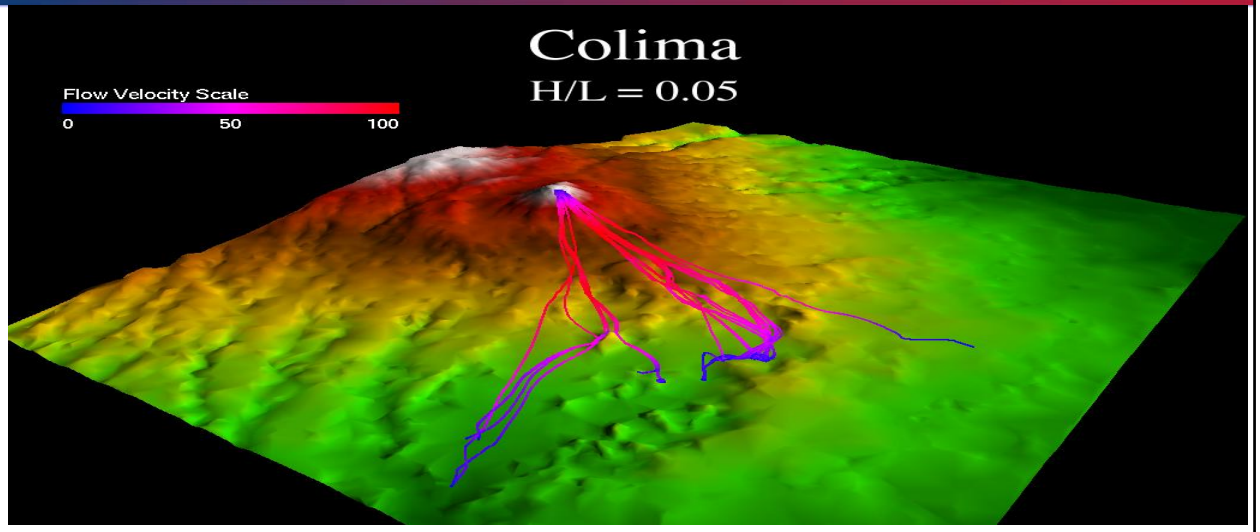
Groundwater Flow Modeling

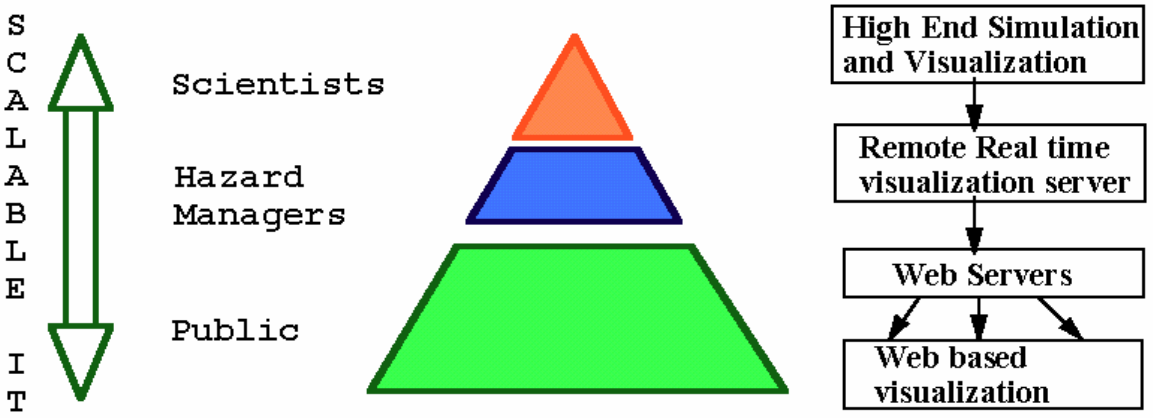
- **Regional-scale modeling of groundwater flow and contaminant transport (Great Lakes Region)**
- **Ability to include all hydrogeologic features as independent objects**
- **Current work is based on *Analytic Element Method***
- **Key features:**
  - **High precision**
  - **Highly parallel**
  - **Object-oriented 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



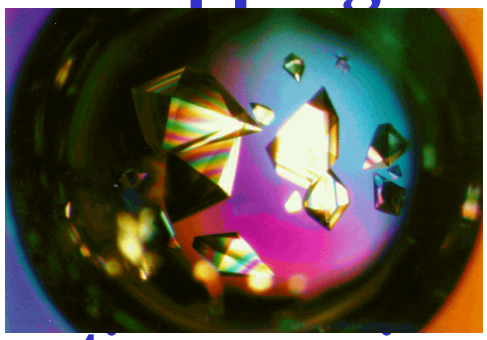


Shake-and-Bake

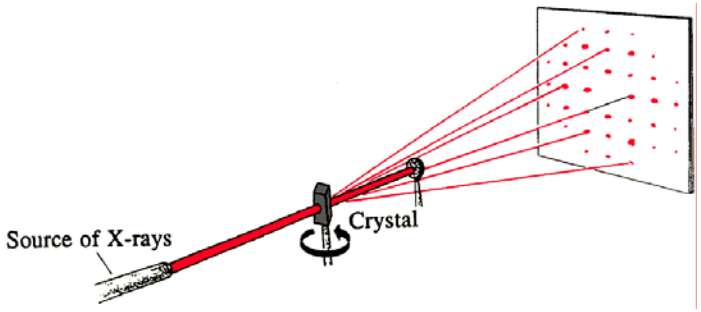
Molecular Structure Determination from X-Ray Crystallographic Data

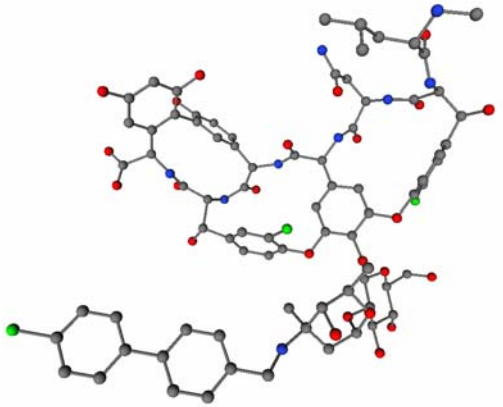
X-Ray Crystallography

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



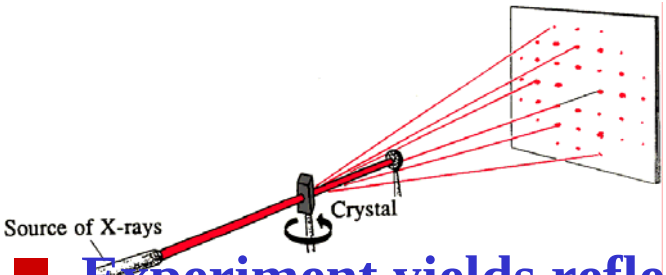
- **Procedure:**
  1. **Isolate a single crystal.**
  2. **Perform the X-Ray diffraction experiment.**



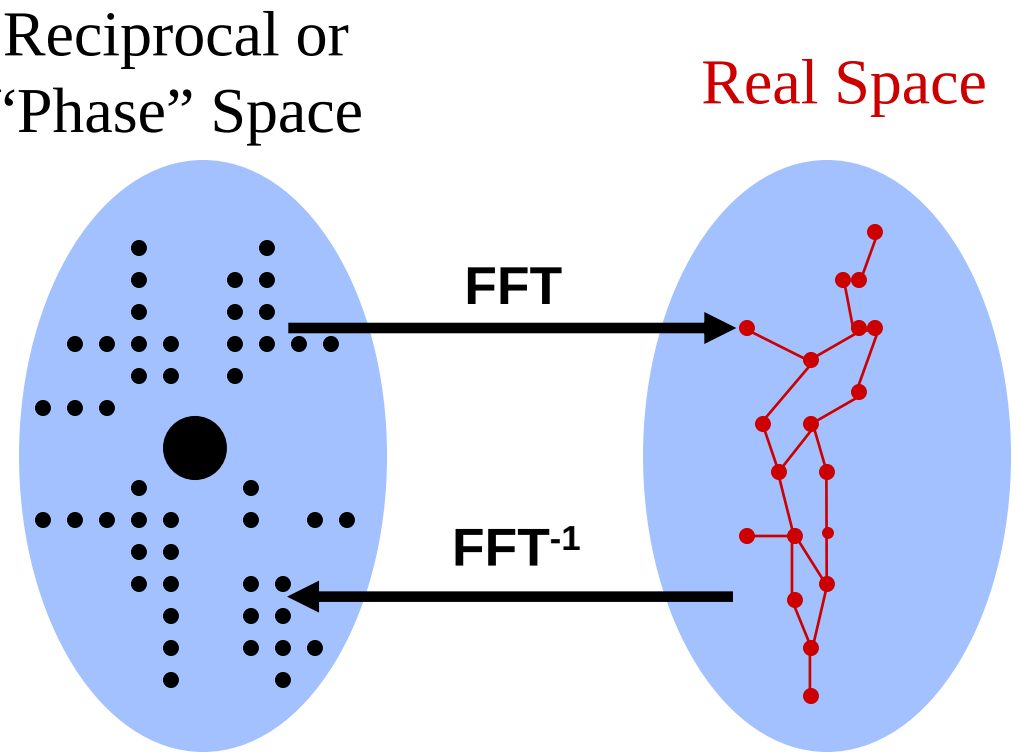


  3. **Determine molecular structure that agrees with diffration data.**

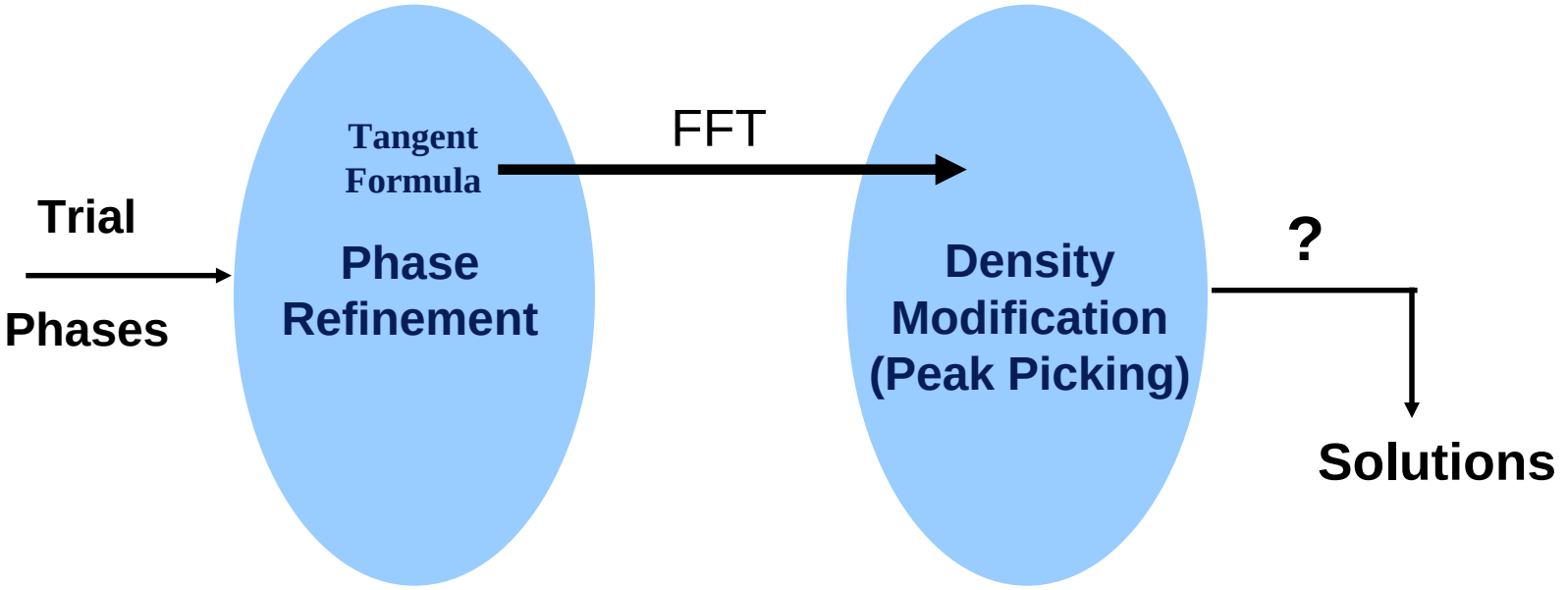
X-Ray Data & Corresponding Molecular Structure



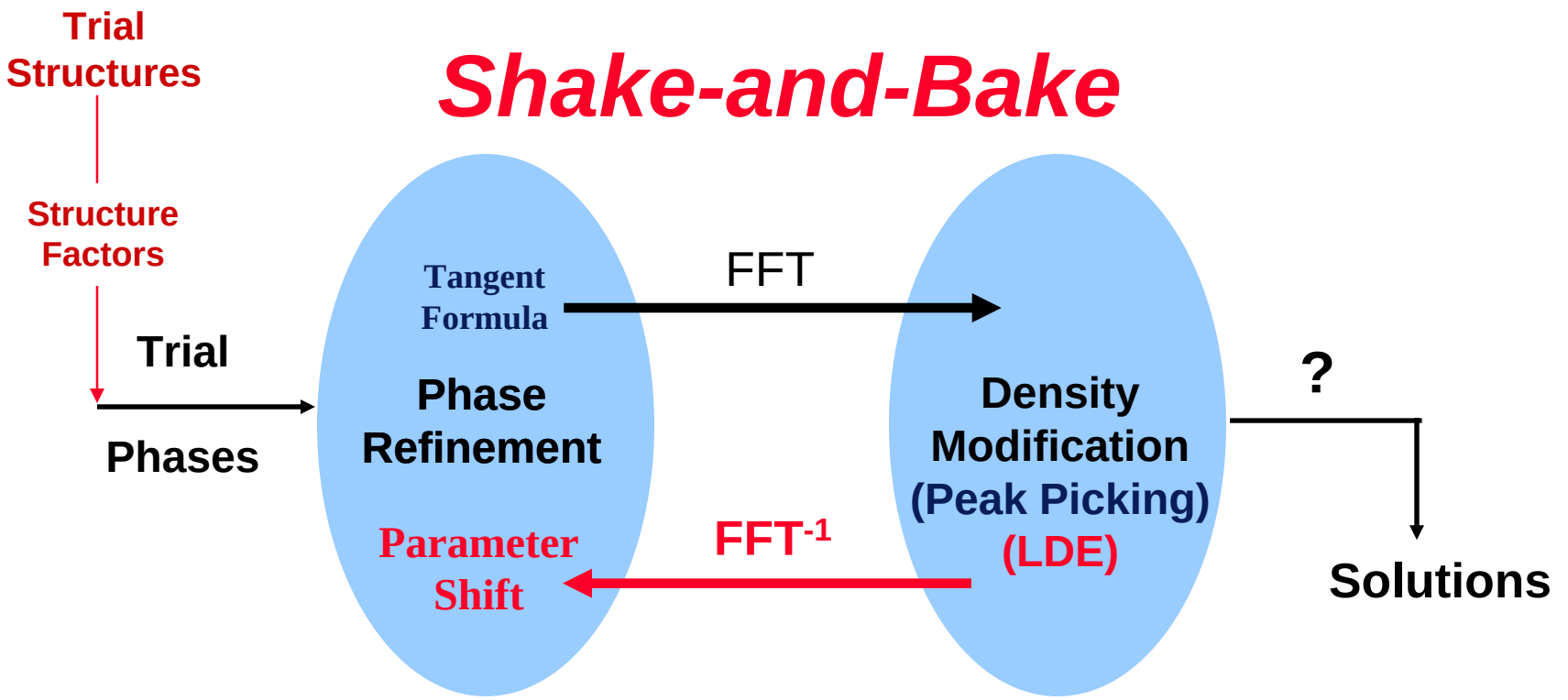
- **Experiment yields reflections and associated intensities.**
- **Underlying atomic arrangement is related to the reflections by a 3-D Fourier transform.**
- ***Phase angles are lost in experiment.***
- ***Phase Problem*: Determine the set of phases corresponding to the reflections.**



Conventional Direct Methods



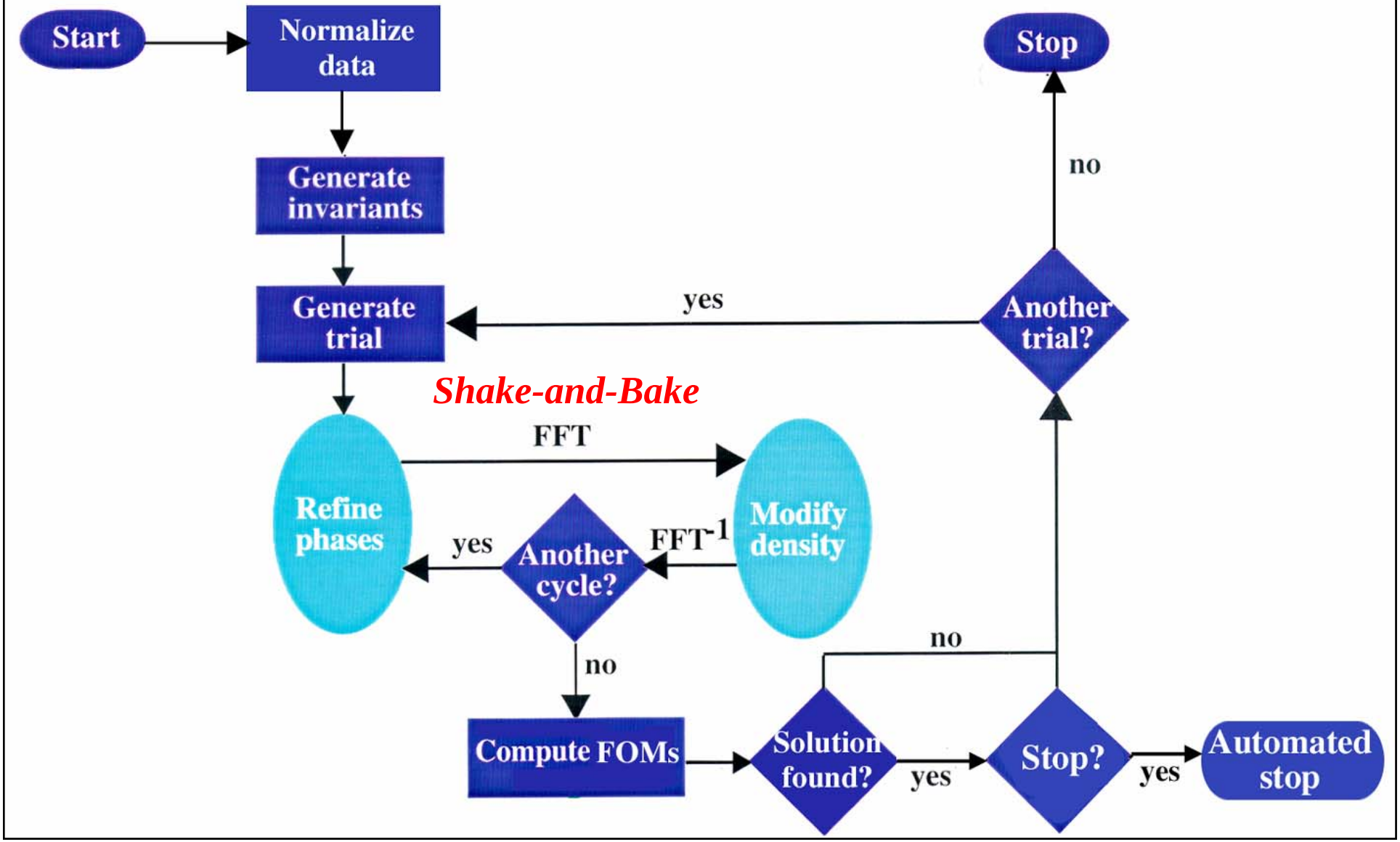
Shake-and-Bake Method: Dual-Space Refinement



Reciprocal Space
"Shake"

Real Space
"Bake"

A Direct Methods Flowchart



Useful Relationships for Multiple Trial Phasing

Tangent Formula

$$\tan\phi_H = \frac{-\sum_K |E_K E_{-H-K}| \sin(\phi_K + \phi_{-H-K})}{\sum_K |E_K E_{-H-K}| \cos(\phi_K + \phi_{-H-K})}$$

Parameter Shift Optimization

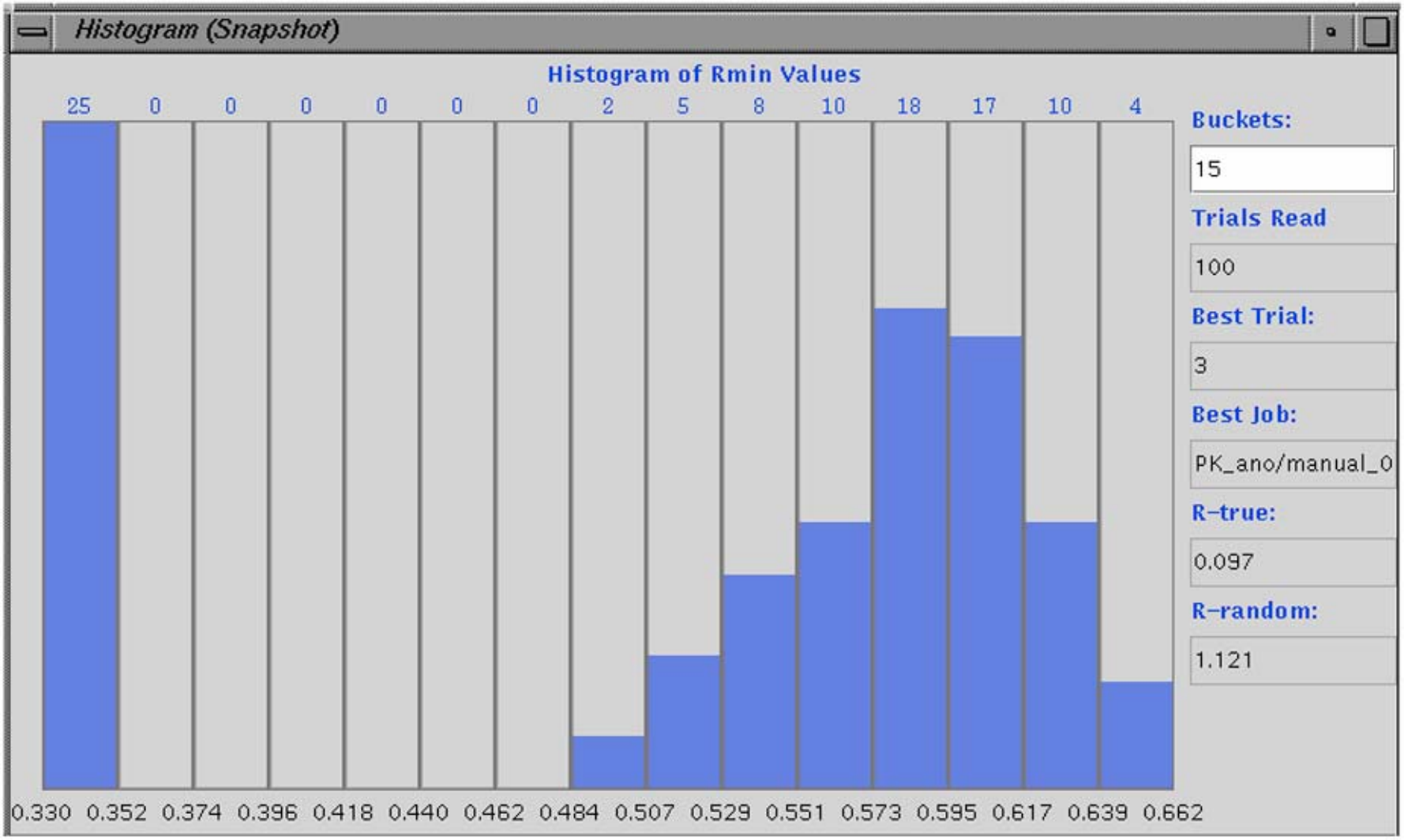
$$R(\phi) = \frac{1}{\sum_{H,K} W_{HK}} \sum_{H,K} W_{HK} \left(\cos\Phi_{HK} - \frac{I_1(W_{HK})}{I_0(W_{HK})} \right)^2$$

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

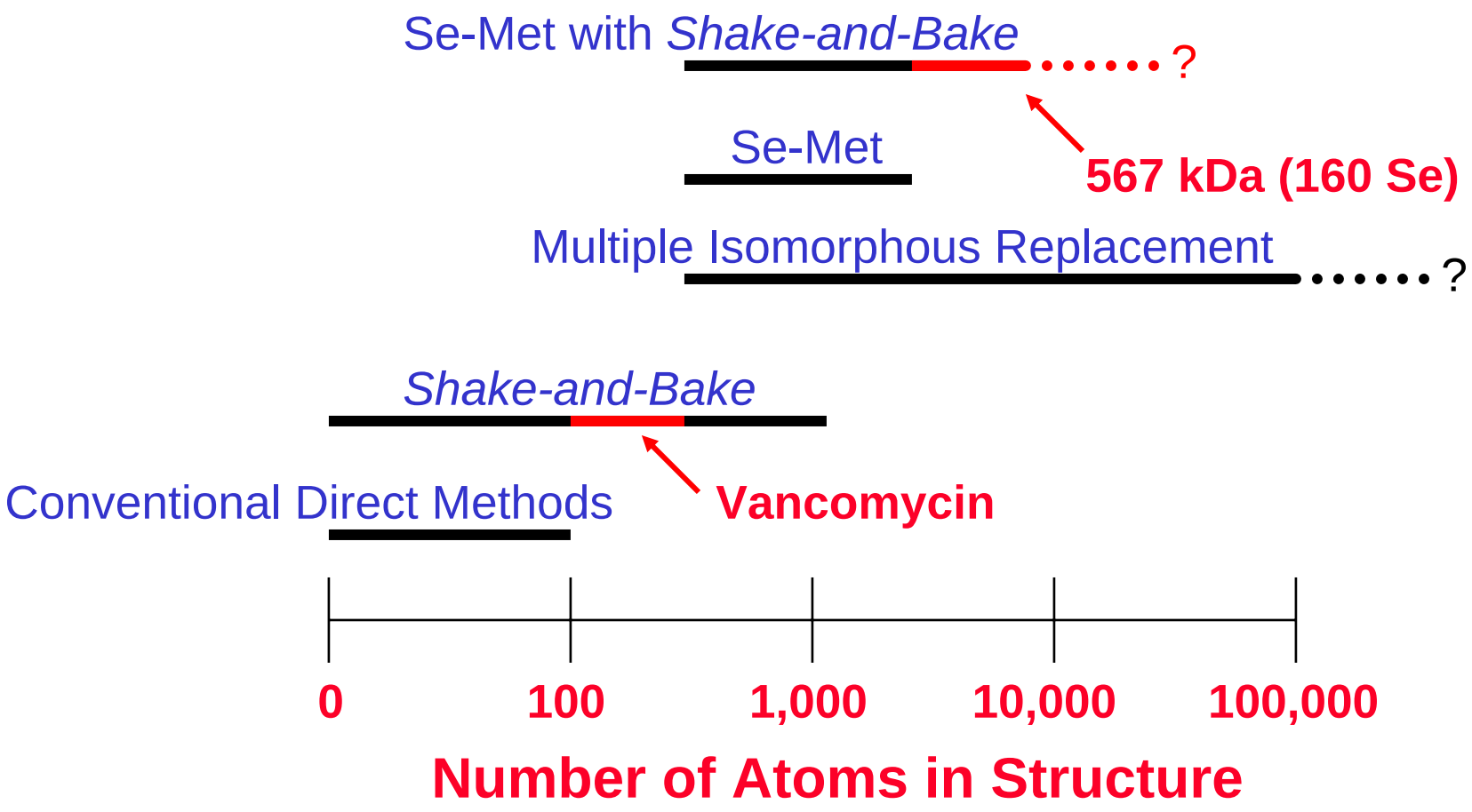
Invariants: $\Phi_{HK} = \phi_H + \phi_K + \phi_{-H-K} \approx 0$

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

Ph8755: *SnB* Histogram

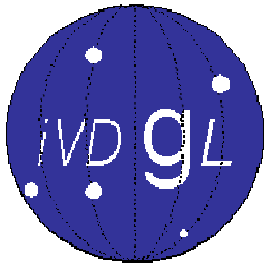


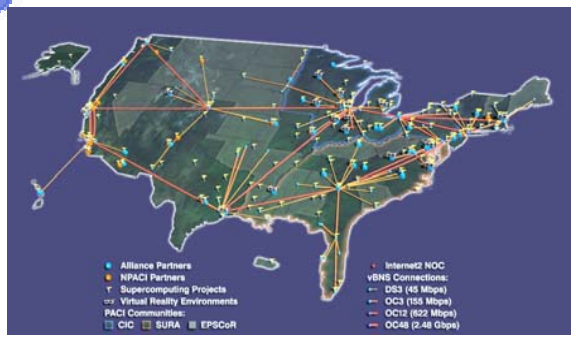
Phasing and Structure Size

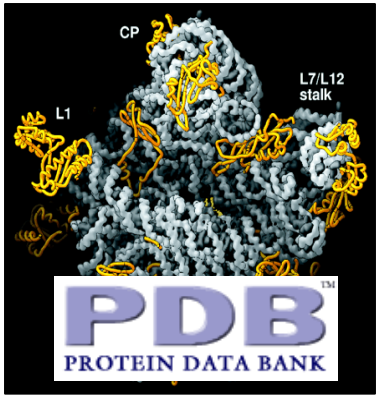


Grid Computing

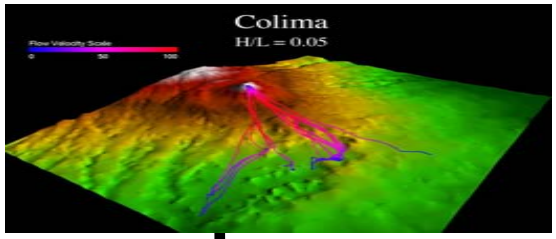
Grid Computing



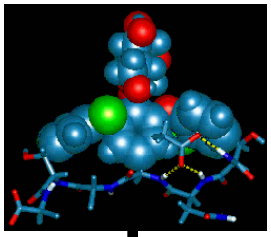




Grid Computing Overview



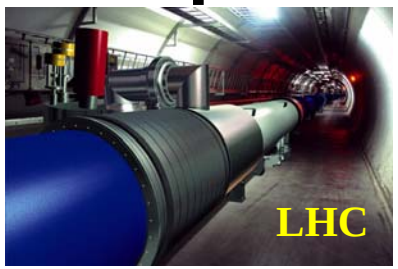
Data Acquisition



Advanced Visualization

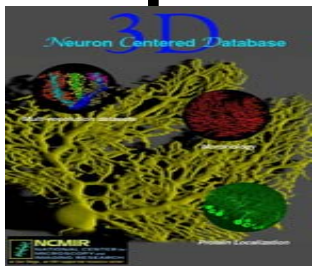
Analysis

Imaging Instruments



LHC

Computational Resources

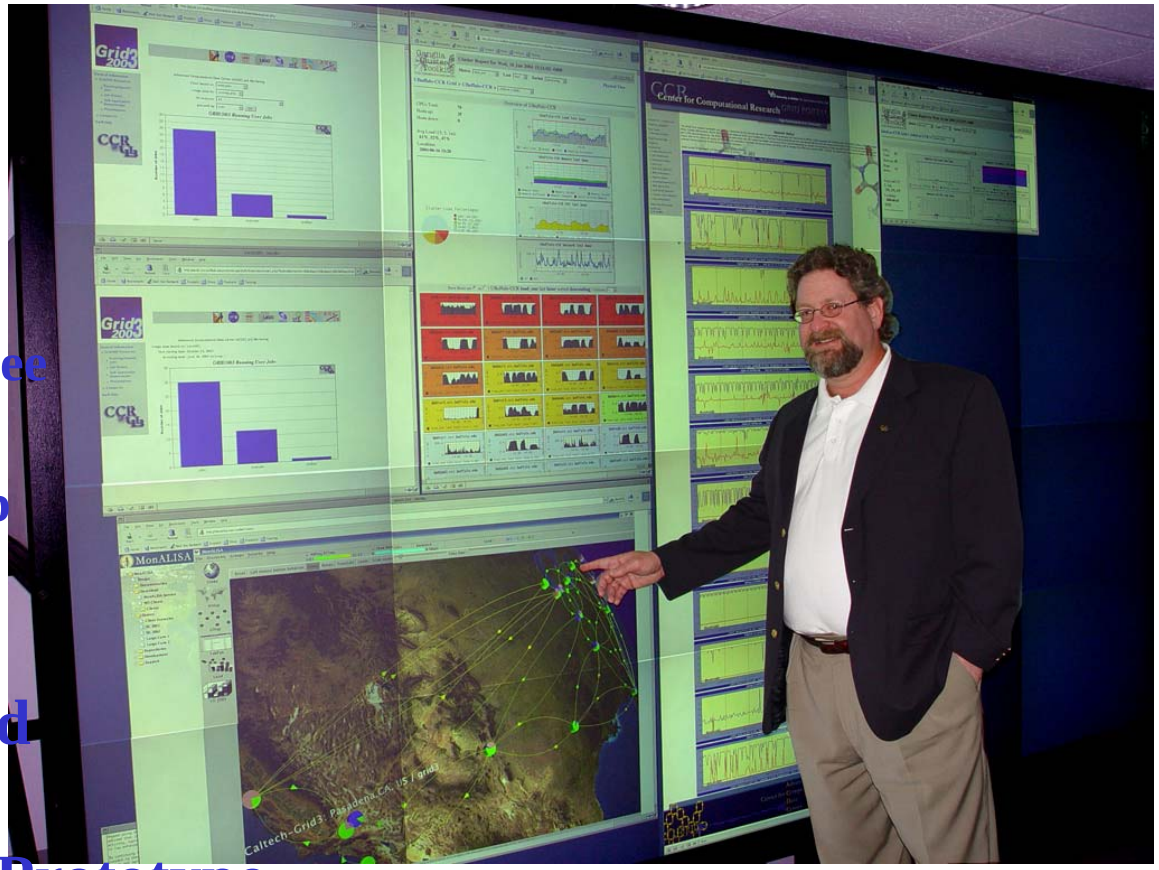


Large-Scale Databases

- 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



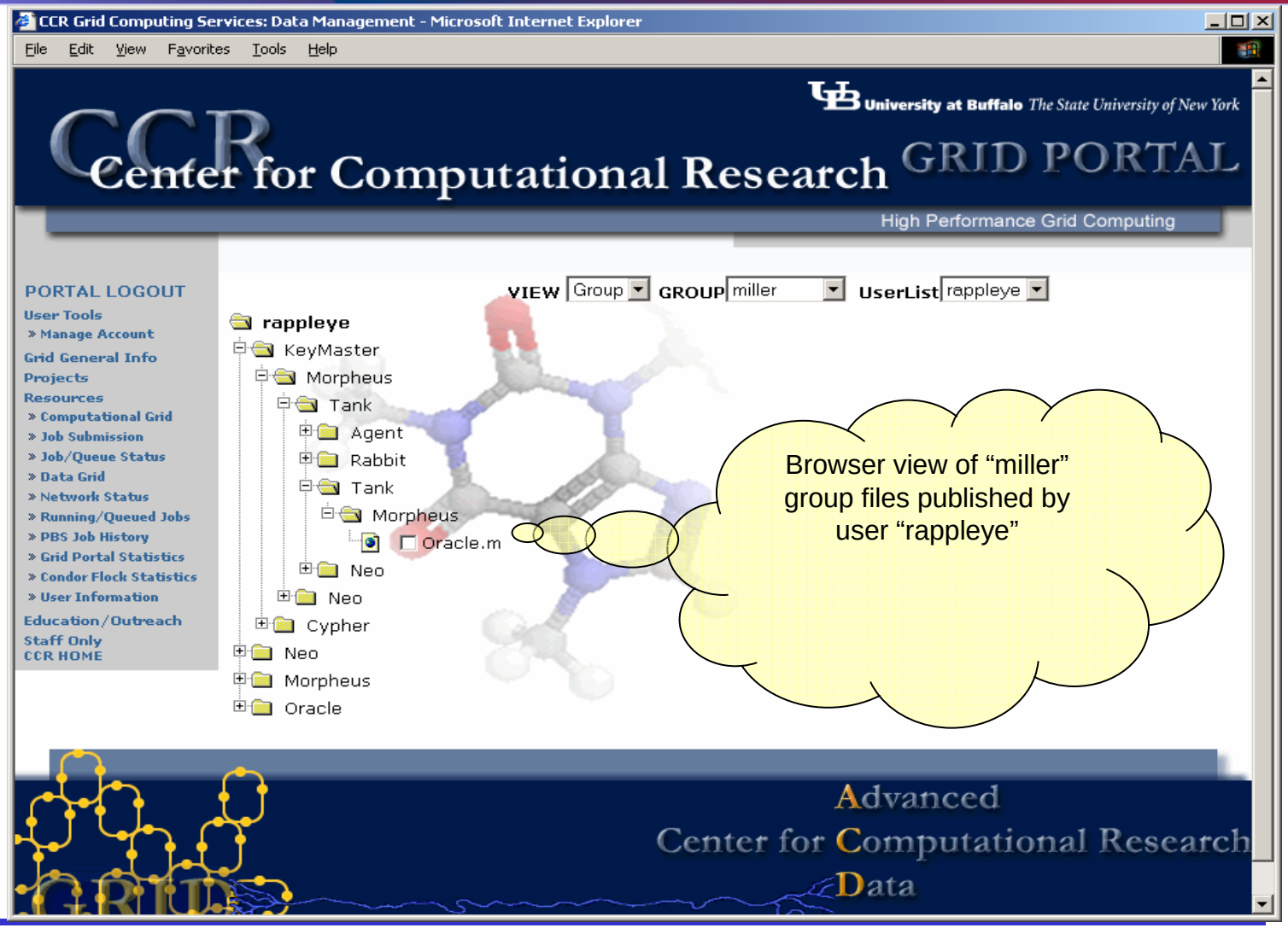
ACDC-Grid Collaborations II

- NYS Grid
  - Brookhaven
  - Canisius College
  - Columbia
  - Hauptman-Woodward Inst.
  - Niagara University
  - NYU
  - RIT
  - RPI
  - SUNY-Albany
  - SUNY-Binghamton
  - SUNY-Buffalo
  - SUNY-Geneseo
  - SUNY-Stony Brook
  - Syracuse
  - Univ of Rochester
- 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



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

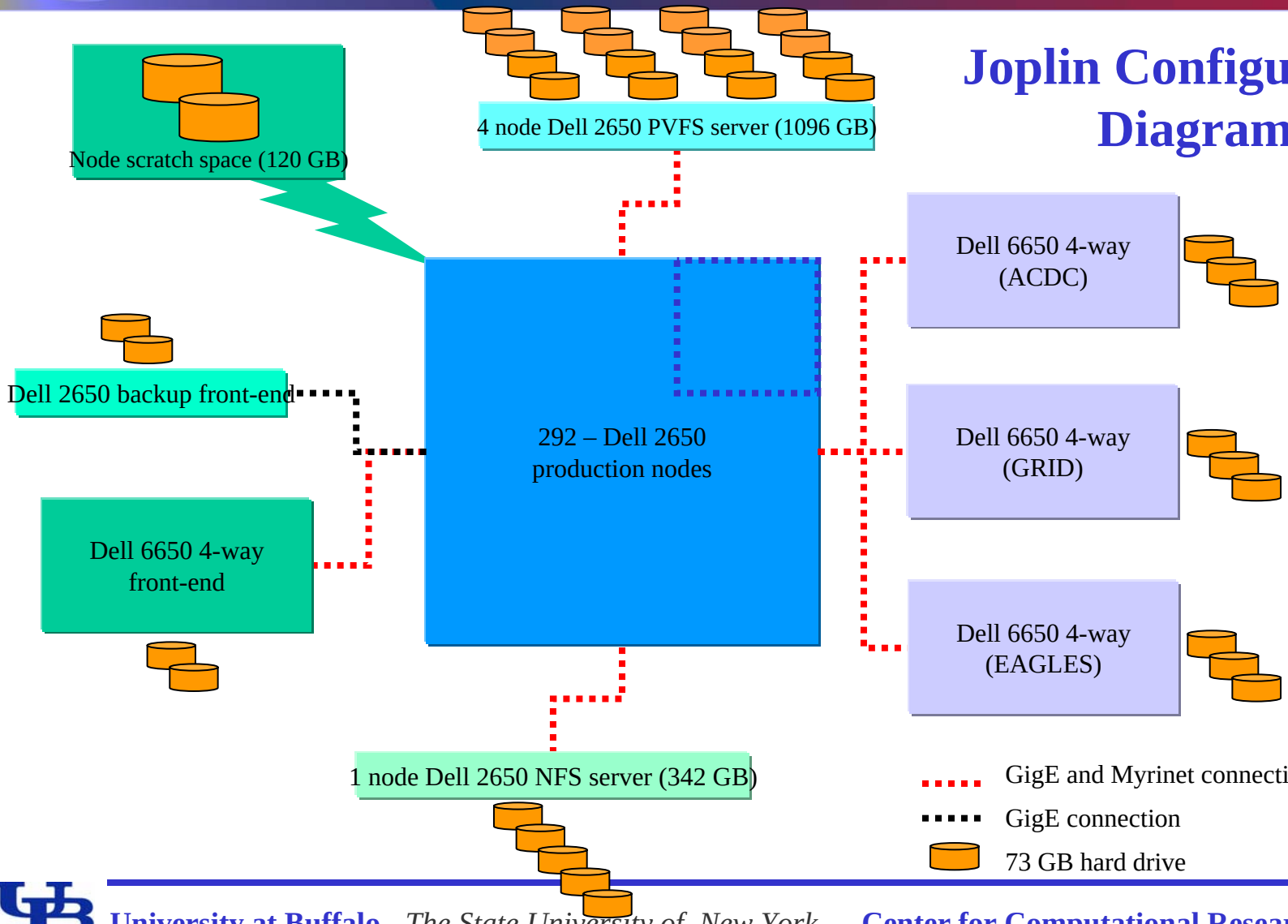
- **Build profiles based on statistical analysis of logs of past jobs**
  - **Per User/Group**
  - **Per Resource**
- **Use these profiles to predict runtimes of new jobs**
- **Make use of these predictions to determine**
  - **Resources to be utilized**
  - **Availability of Backfill**

ACDC-Grid Dynamic Resource Allocation at SC03 with Grid3

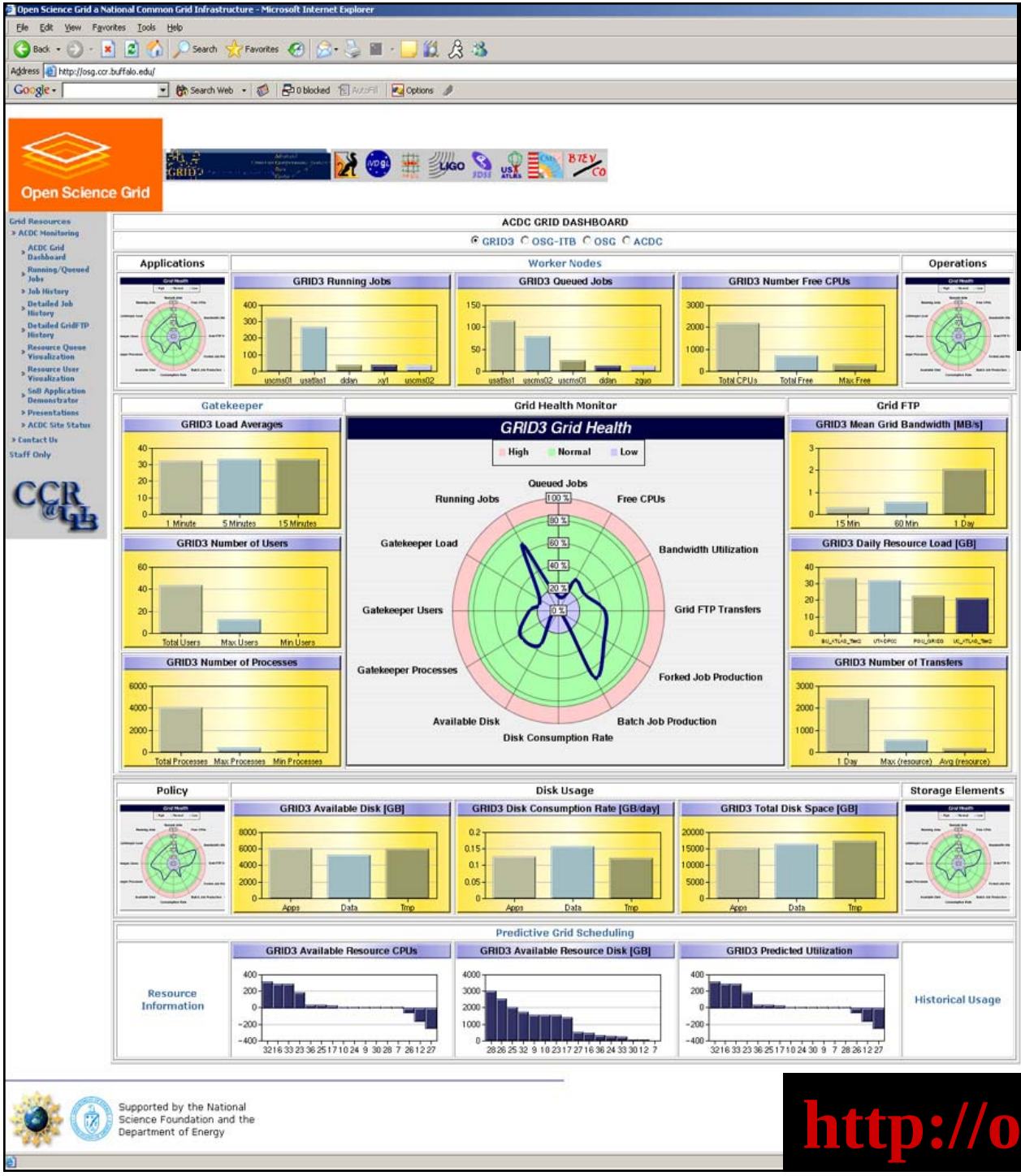
- **Small number (40) of CPUs were dedicated at night**
- **An additional 400 CPUs were dynamically allocated during the day**
- **No human intervention was required**
- **Grid applications were able to utilize the resources and surpassed the Grid3 goals**

ACDC-Grid Dynamic Resource Allocation

Joplin Configuration Diagram

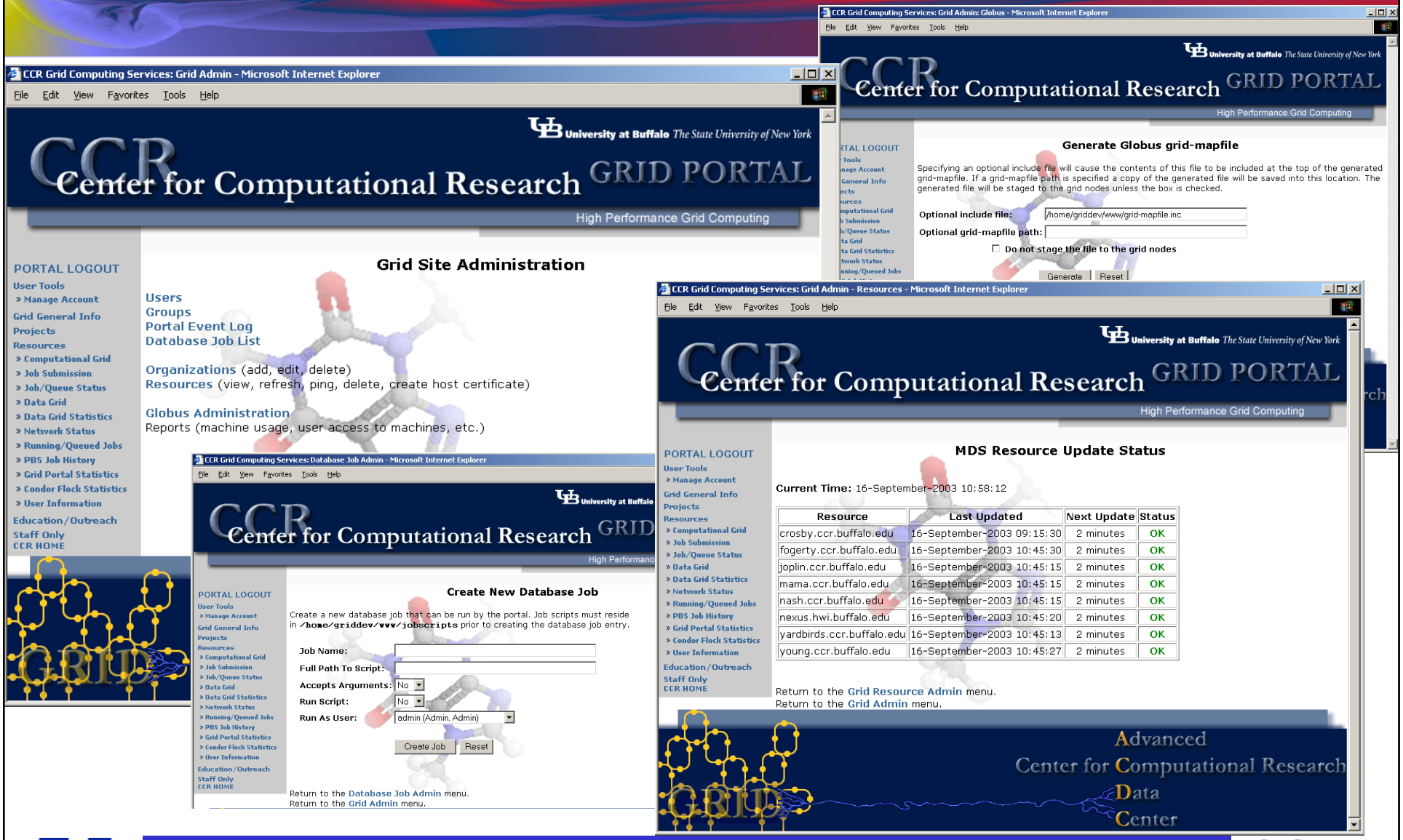


ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD



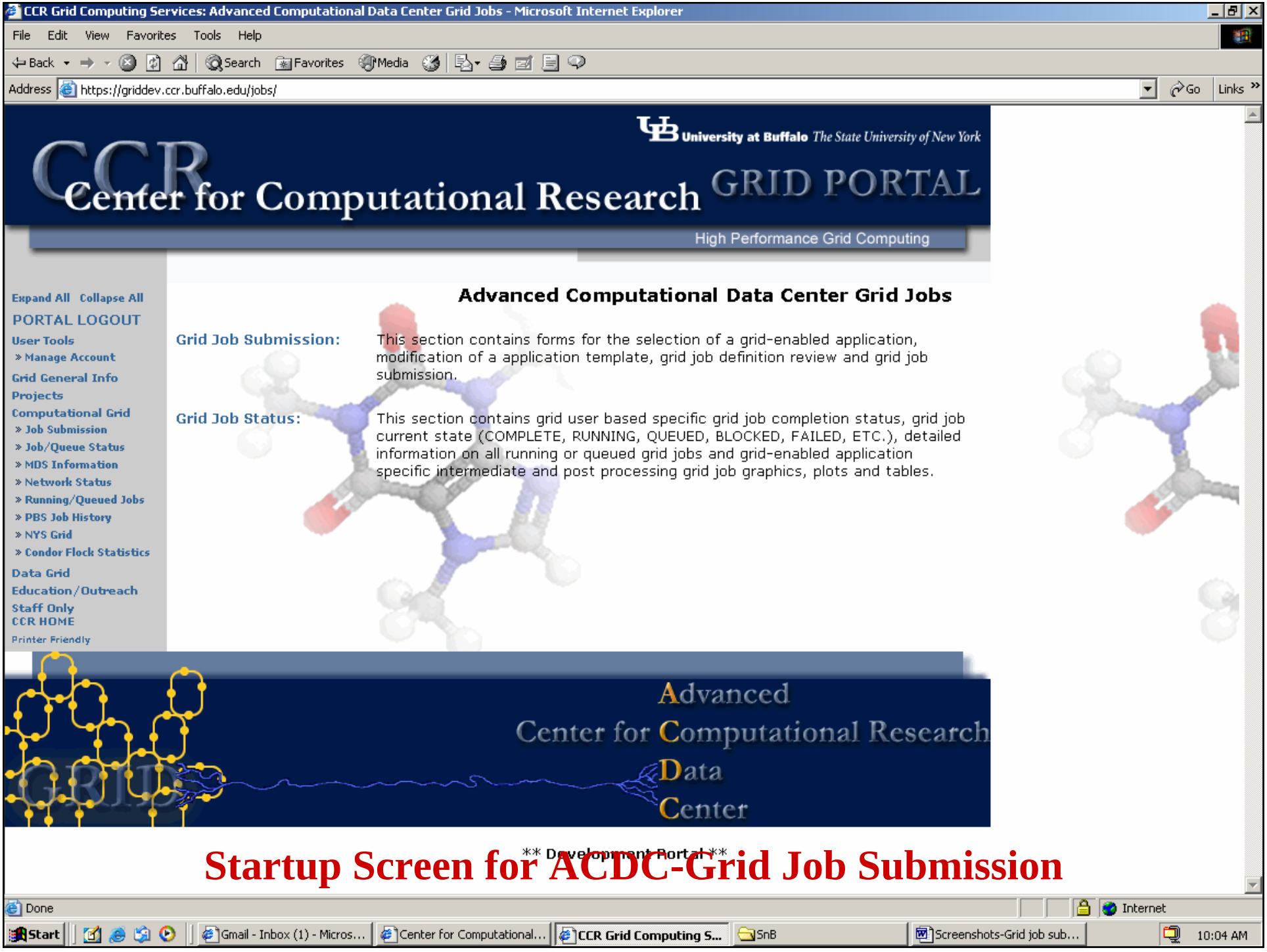
http://osg.ccr.buffalo.edu

ACDC-Grid Administration

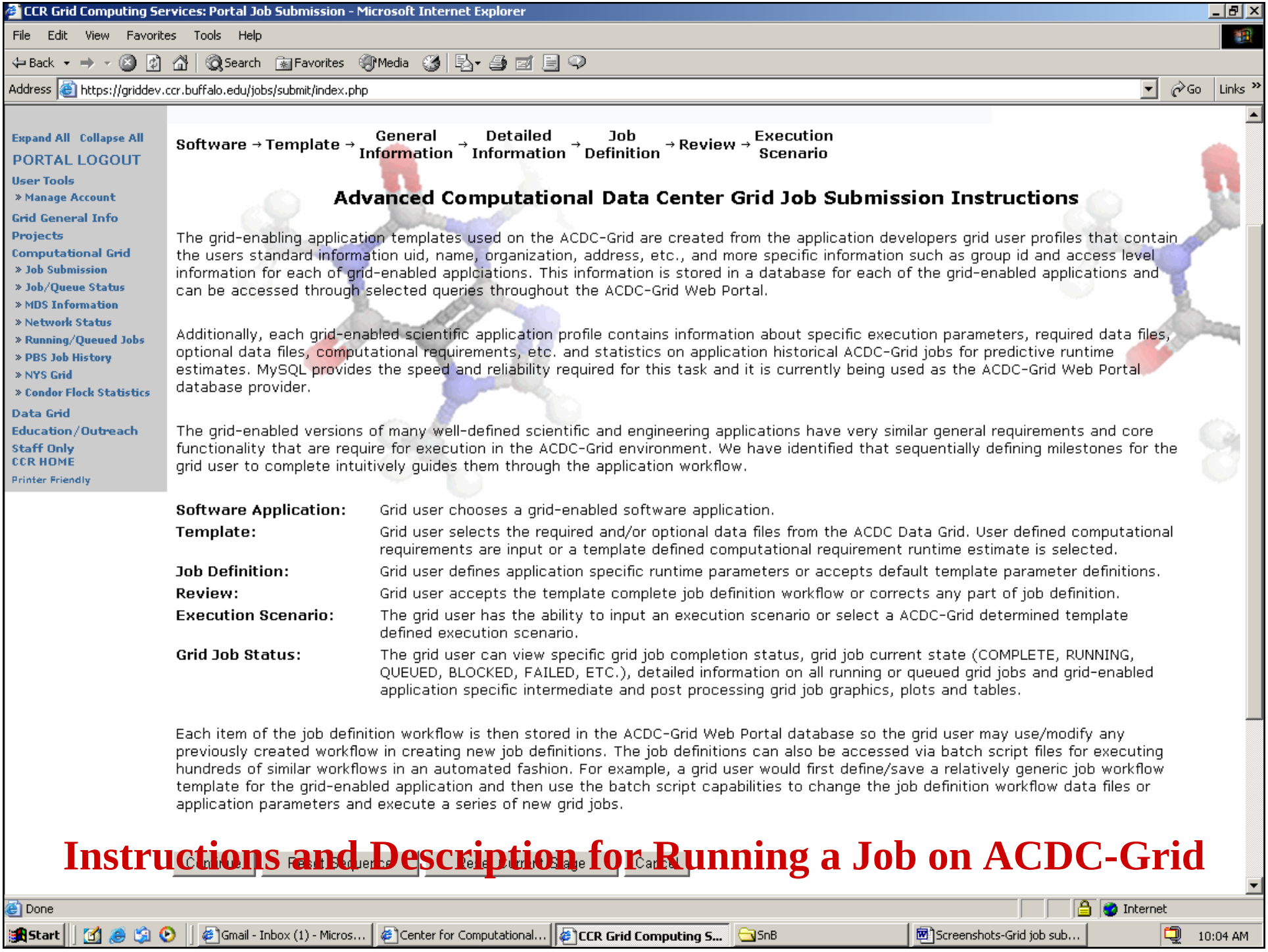


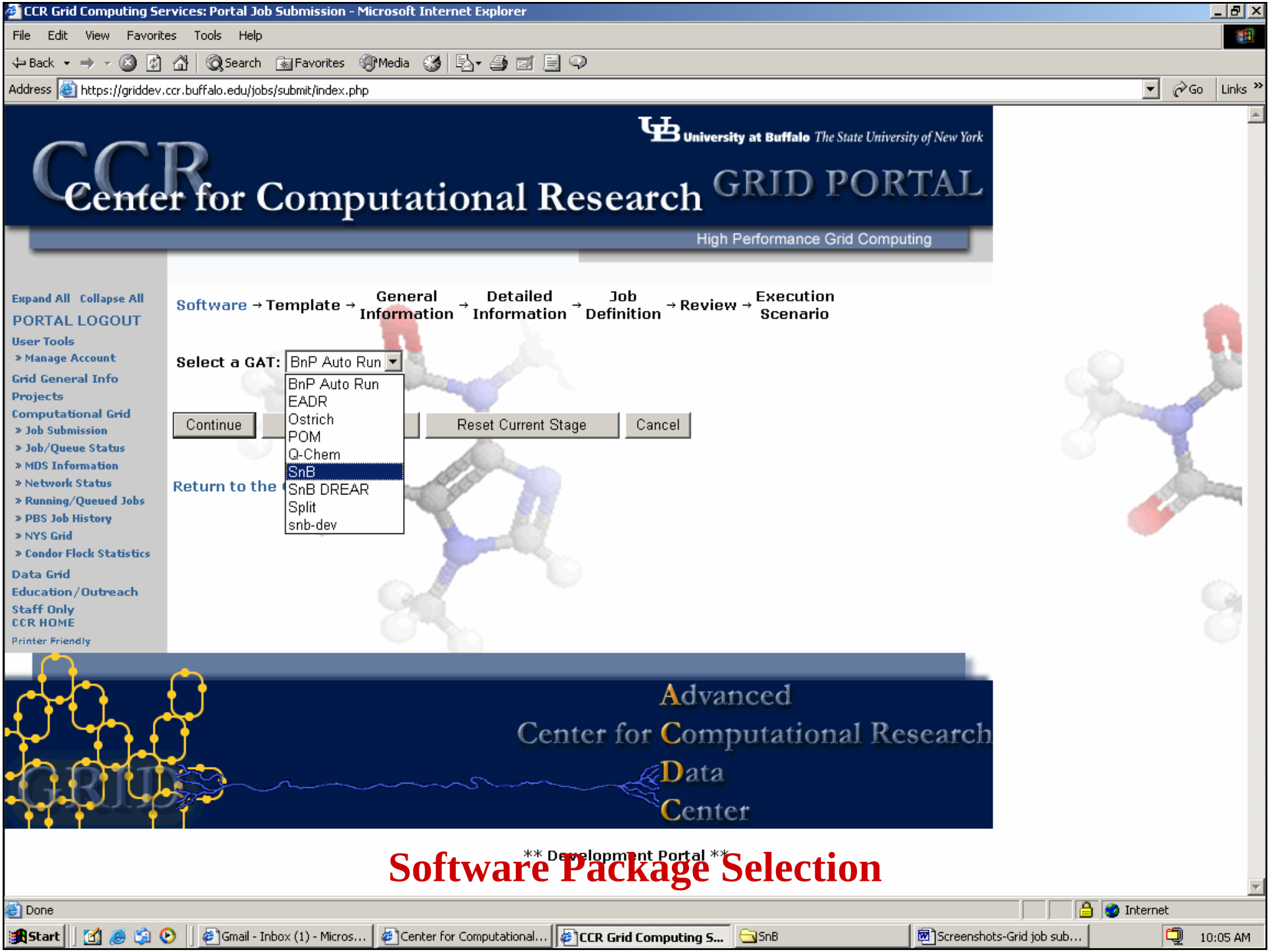
Grid-Enabling Application Templates (GATs)

- **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**



Startup Screen for ACDC-Grid Job Submission


CCR Grid Computing Services: Portal Job Submission - Microsoft Internet Explorer
File Edit View Favorites Tools Help
Back Search Favorites Media
Address https://griddev.ccr.buffalo.edu/jobs/submit/index.php
Go Links
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 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.
Instructions and Description for Running a Job on ACDC-Grid
Done
Internet
Start
Gmail - Inbox (1) - Micros...
Center for Computational...
CCR Grid Computing S...
SnB
Screenshots-Grid job sub...
10:04 AM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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
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Data
Center
** Development Portal **
Software Package Selection
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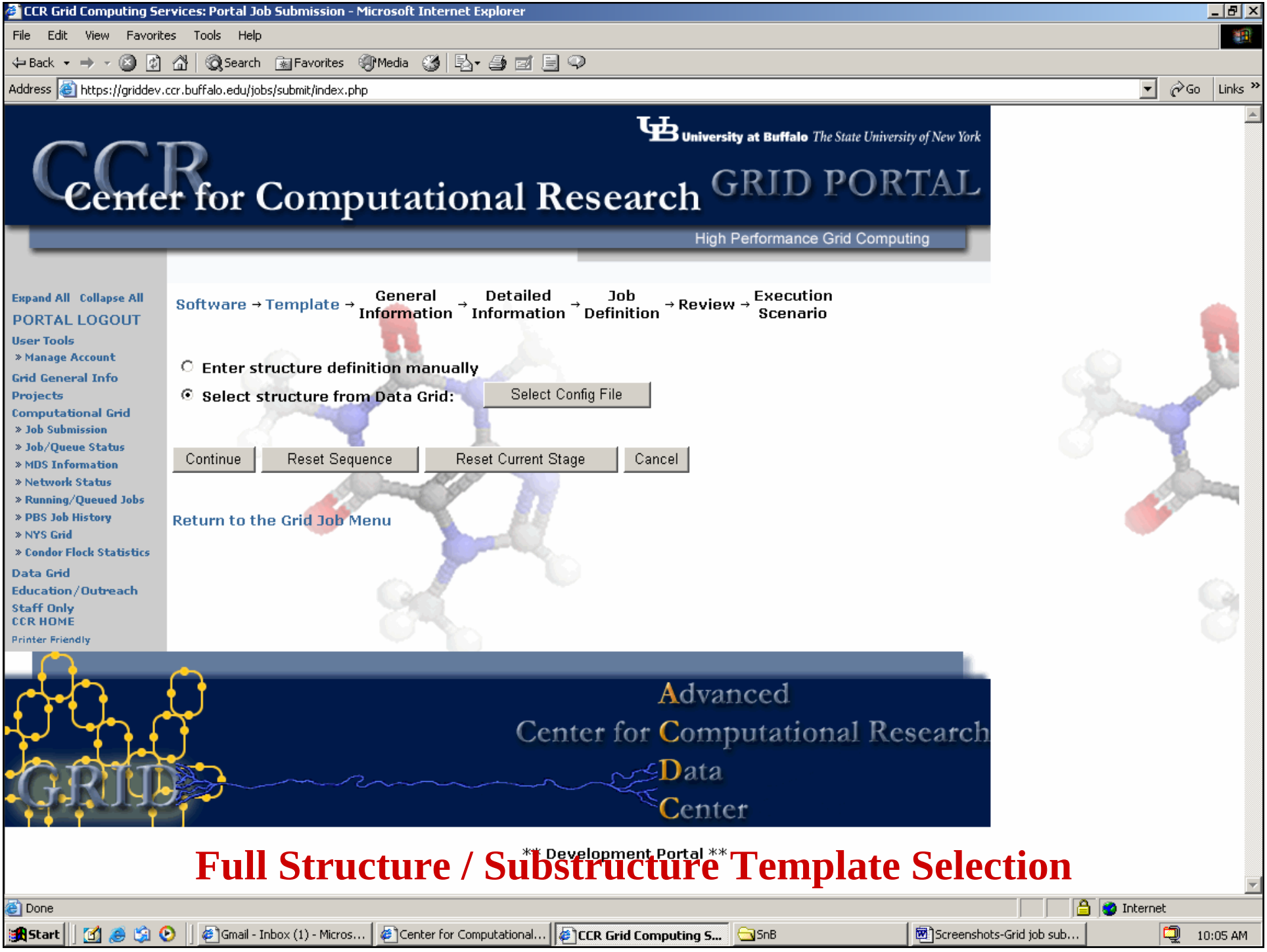
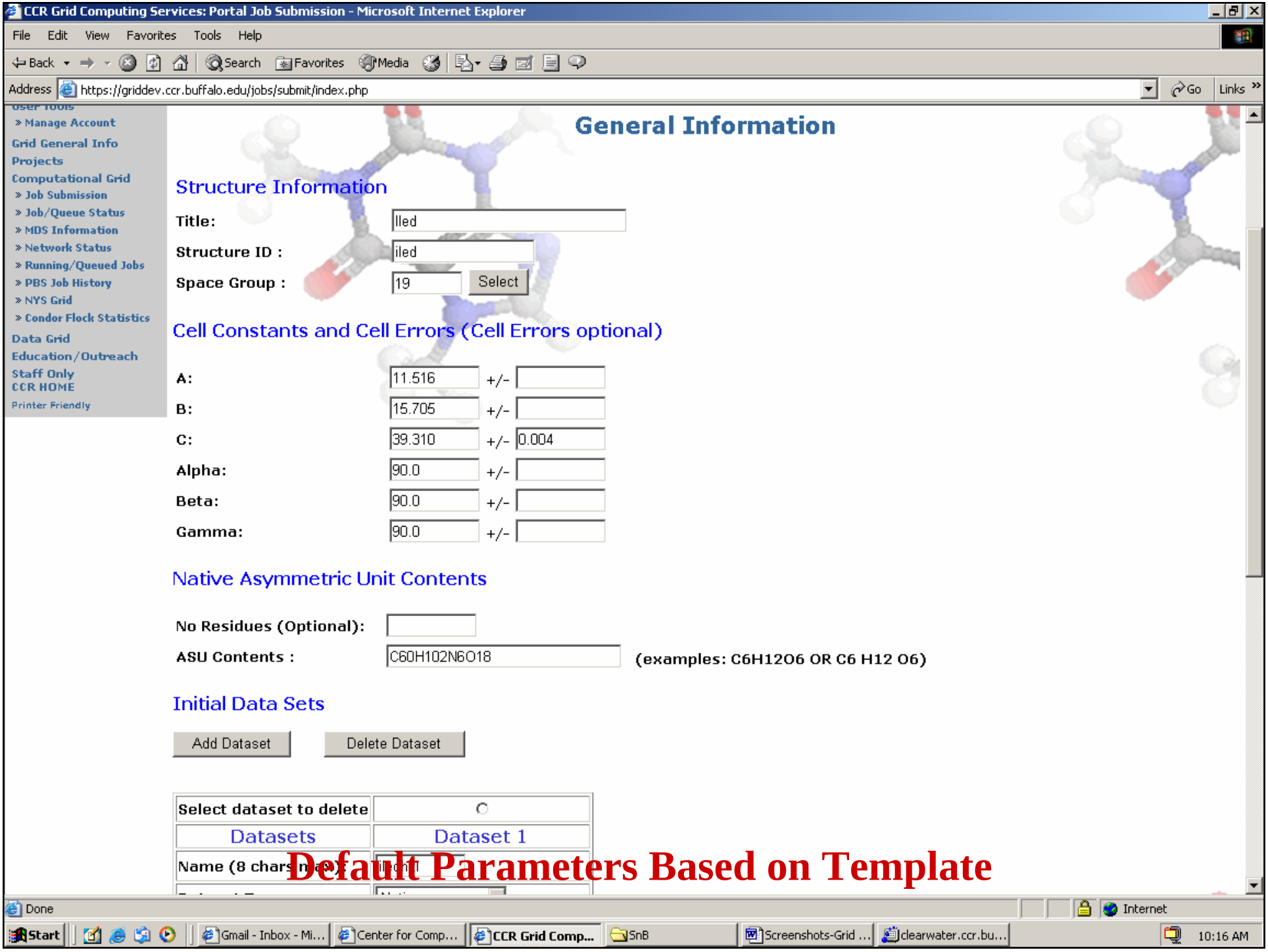


Full Structure / Substructure Template Selection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General Information
Structure Information
Title: lled
Structure ID : iled
Space Group : 19 Select
Cell Constants and Cell Errors (Cell Errors optional)
A: 11.516 +/-
B: 15.705 +/-
C: 39.310 +/- 0.004
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) Default
Default Parameters Based on Template
Done
Internet
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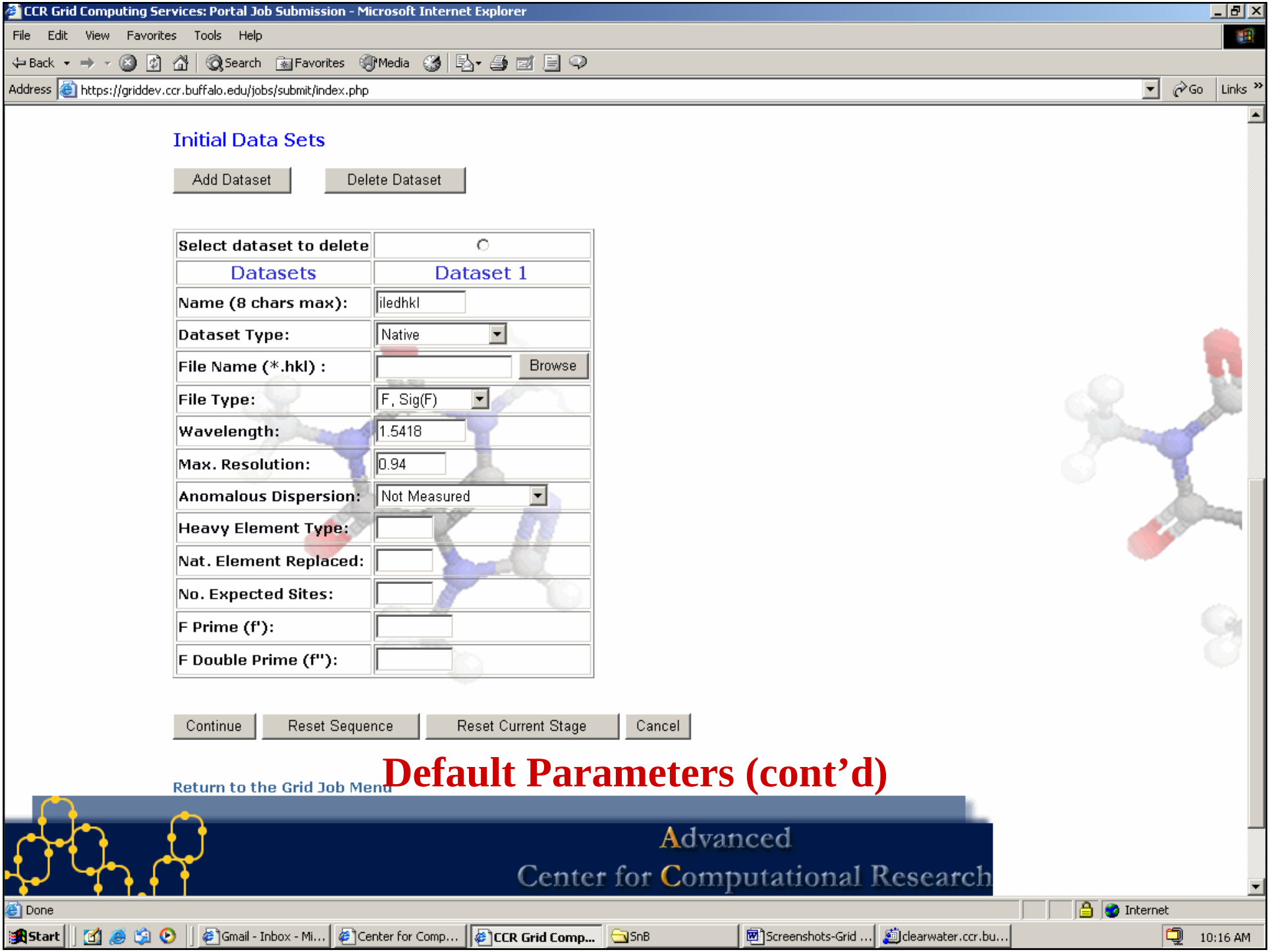
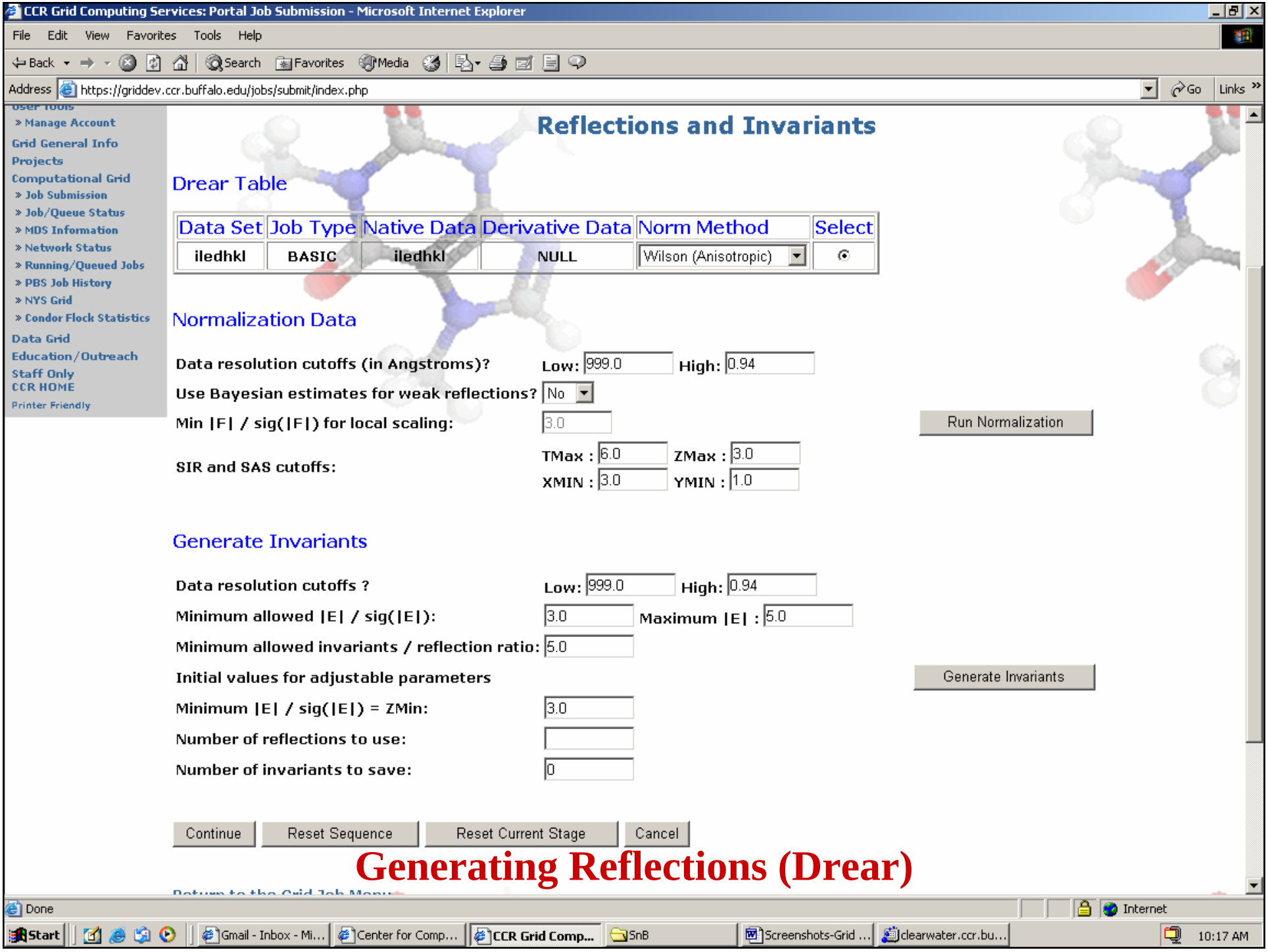
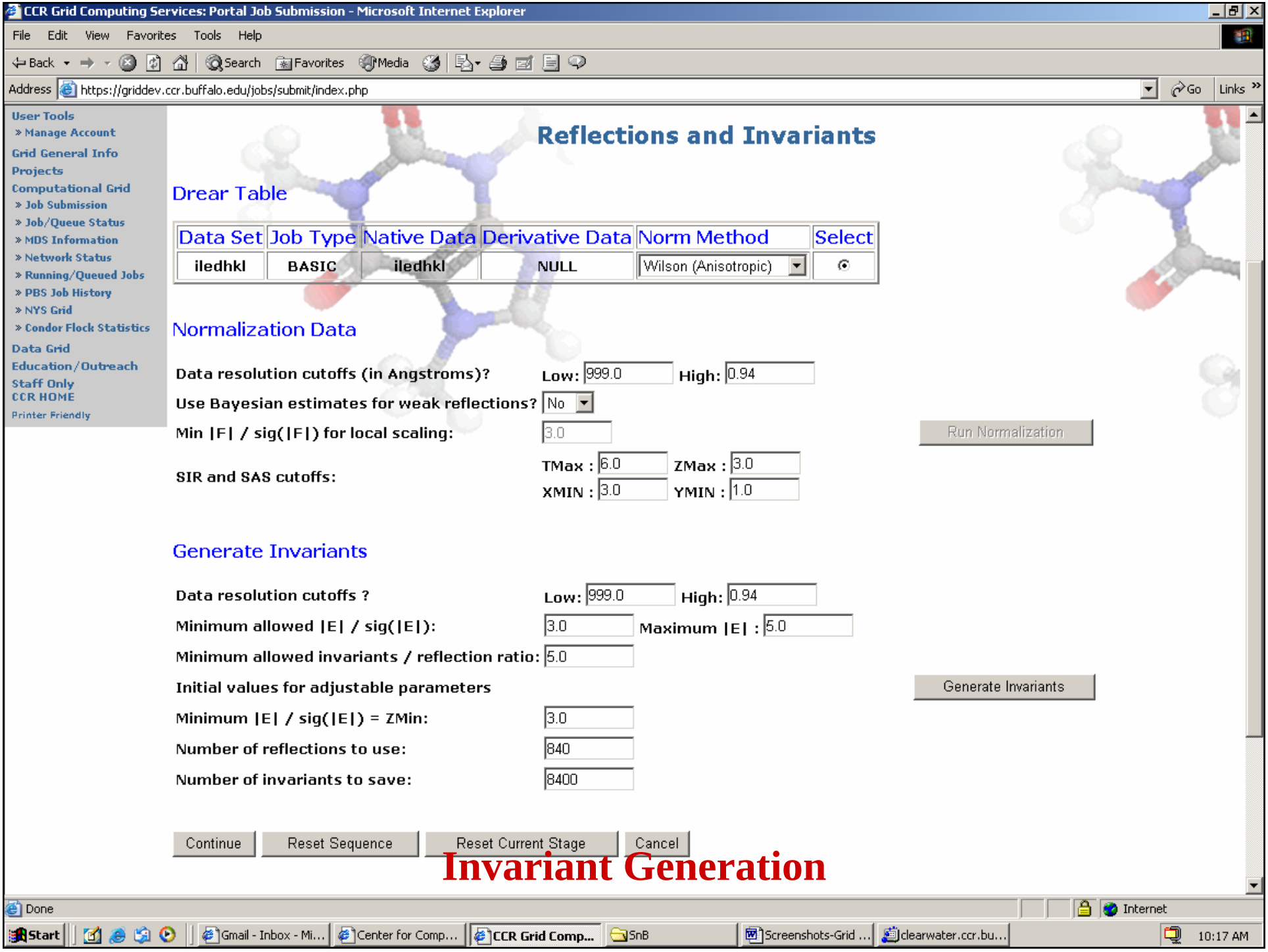


Default Parameters (cont'd)



Generating Reflections (Drear)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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: 999.0
High: 0.94
Use Bayesian estimates for weak reflections?
No
Min |F| / sig(|F|) for local scaling:
3.0
Run Normalization
SIR and SAS cutoffs:
TMax : 6.0
ZMax : 3.0
XMIN : 3.0
YMIN : 1.0
Generate Invariants
Data resolution cutoffs ?
Low: 999.0
High: 0.94
Minimum allowed |E| / sig(|E|):
3.0
Maximum |E| : 5.0
Minimum allowed invariants / reflection ratio:
5.0
Initial values for adjustable parameters
Generate Invariants
Minimum |E| / sig(|E|) = ZMin:
3.0
Number of reflections to use:
840
Number of invariants to save:
8400
Continue
Reset Sequence
Reset Current Stage
Cancel
Invariant Generation
Done
Internet
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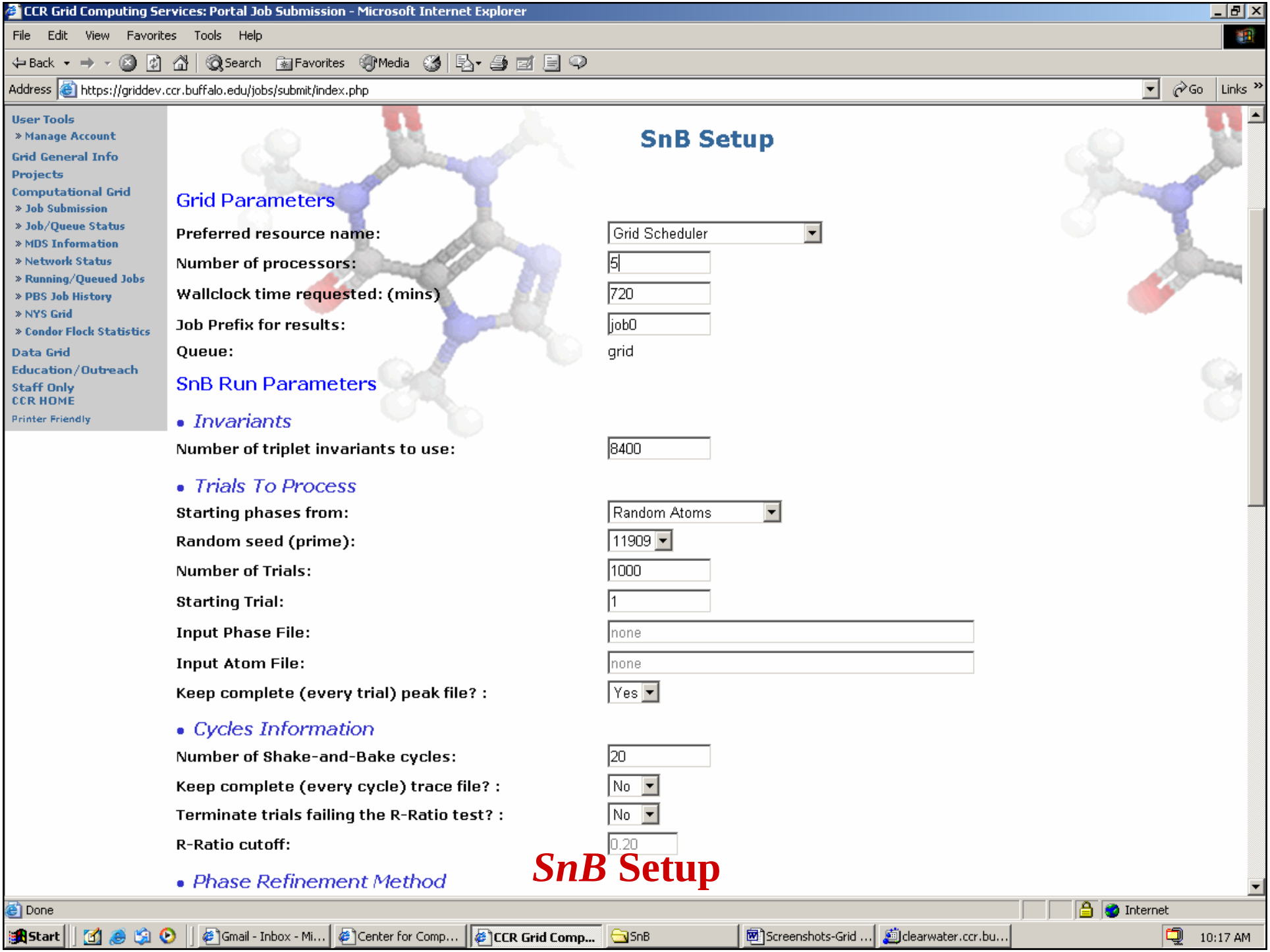
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SnB Setup
Grid Parameters
Preferred resource name: Grid Scheduler
Number of processors: 5
Wallclock time requested: (mins) 720
Job Prefix for results: job0
Queue: grid
SnB Run Parameters
• Invariants
Number of triplet invariants to use: 8400
• Trials To Process
Starting phases from: Random Atoms
Random seed (prime): 11909
Number of Trials: 1000
Starting Trial: 1
Input Phase File: none
Input Atom File: none
Keep complete (every trial) peak file? : Yes
• Cycles Information
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: 0.20
• Phase Refinement Method
SnB Setup
Done
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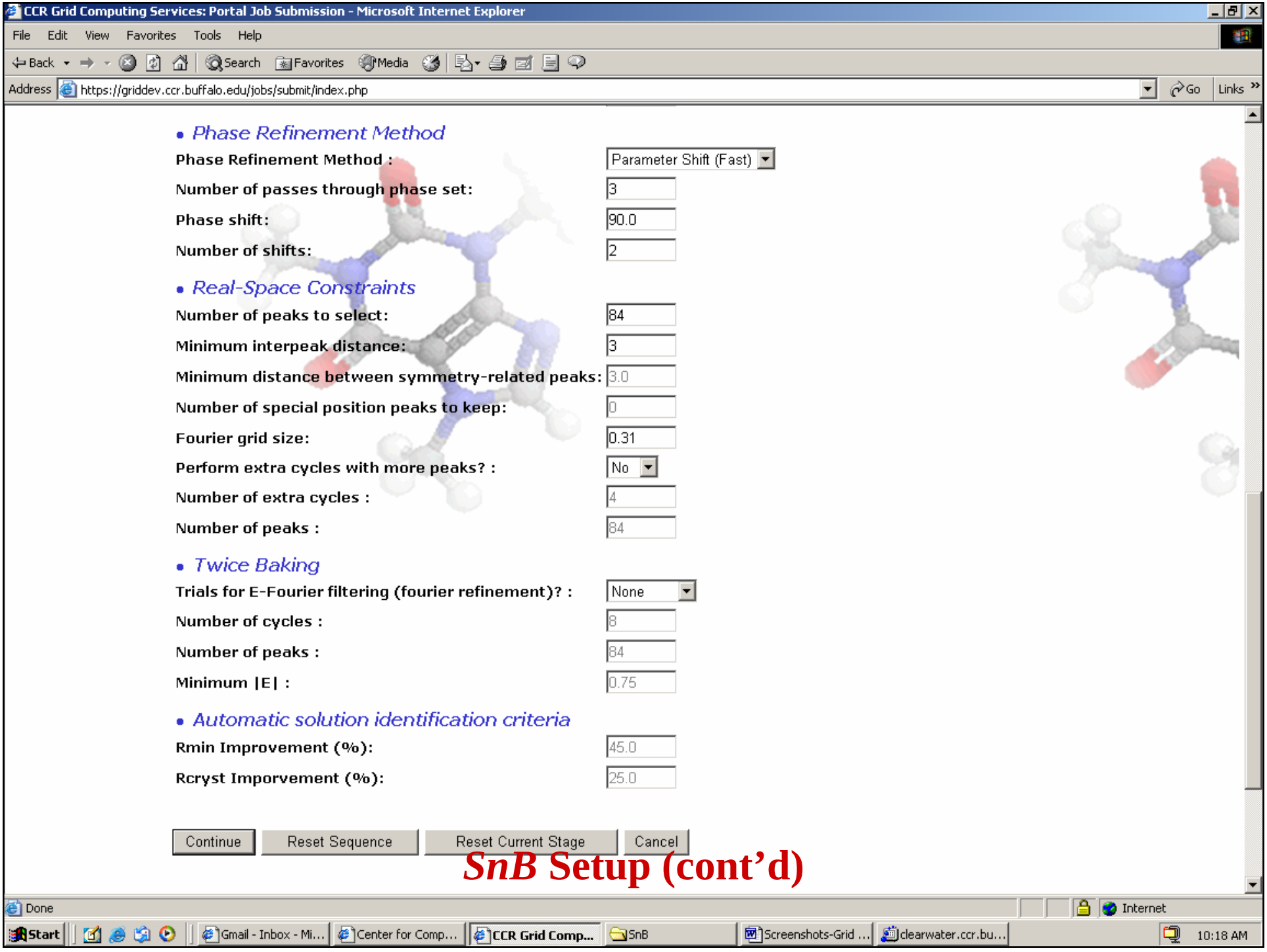
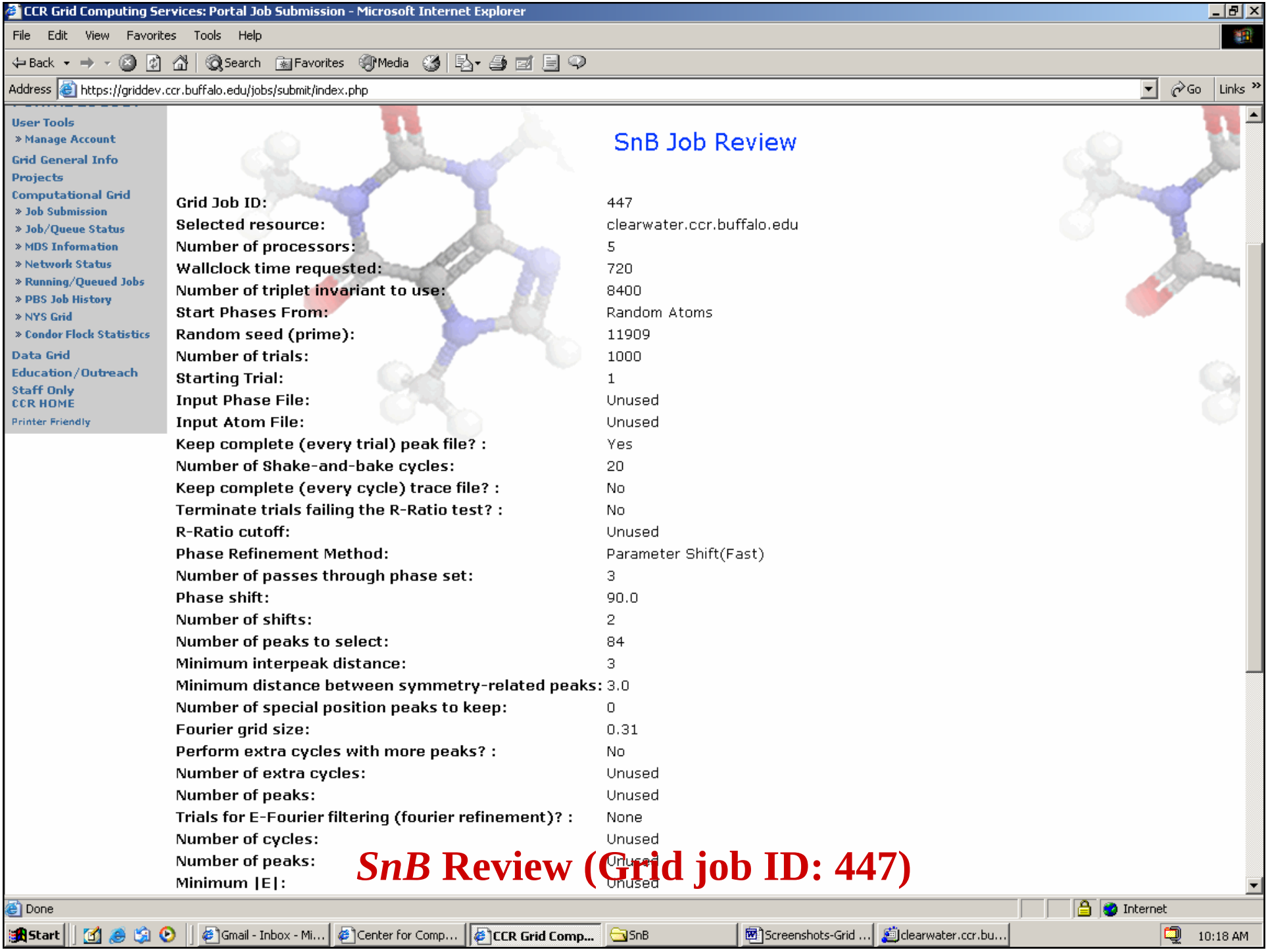


SnB Setup (cont'd)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SnB Job Review
Grid Job ID: 447
Selected resource: clearwater.ccr.buffalo.edu
Number of processors: 5
Wallclock time requested: 720
Number of triplet invariant to use: 8400
Start Phases From: Random Atoms
Random seed (prime): 11909
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)
Done
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Details for Grid Job 447 - iledhkl

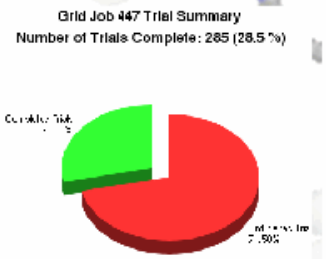
Job Detail Information

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

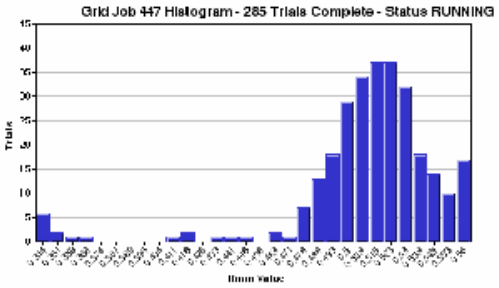
Best Trial Number: 34
Best Trial Rmin: 0.344
Processors: 5

Trial Summary



Walltime Summary

Grid Job Trial Histogram



Click on image for enlarged view.

Return to the Grid Job Menu

Graphical Representation of Intermediate Job Status

Advanced Center for Computational Research Data

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

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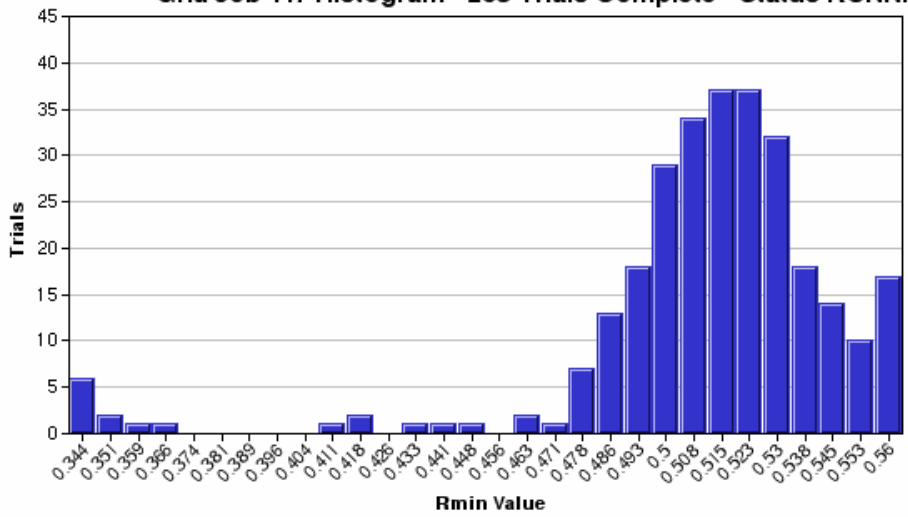
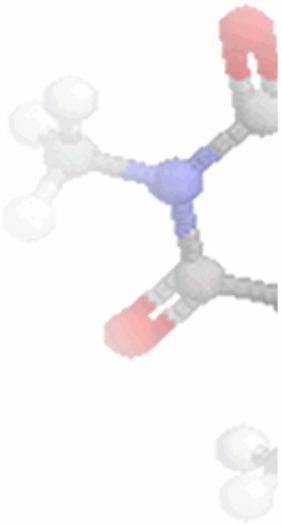
Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING





Return to Job Details

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Histogram of Completed Trial Structures

Advanced Center for Computational Research

Done

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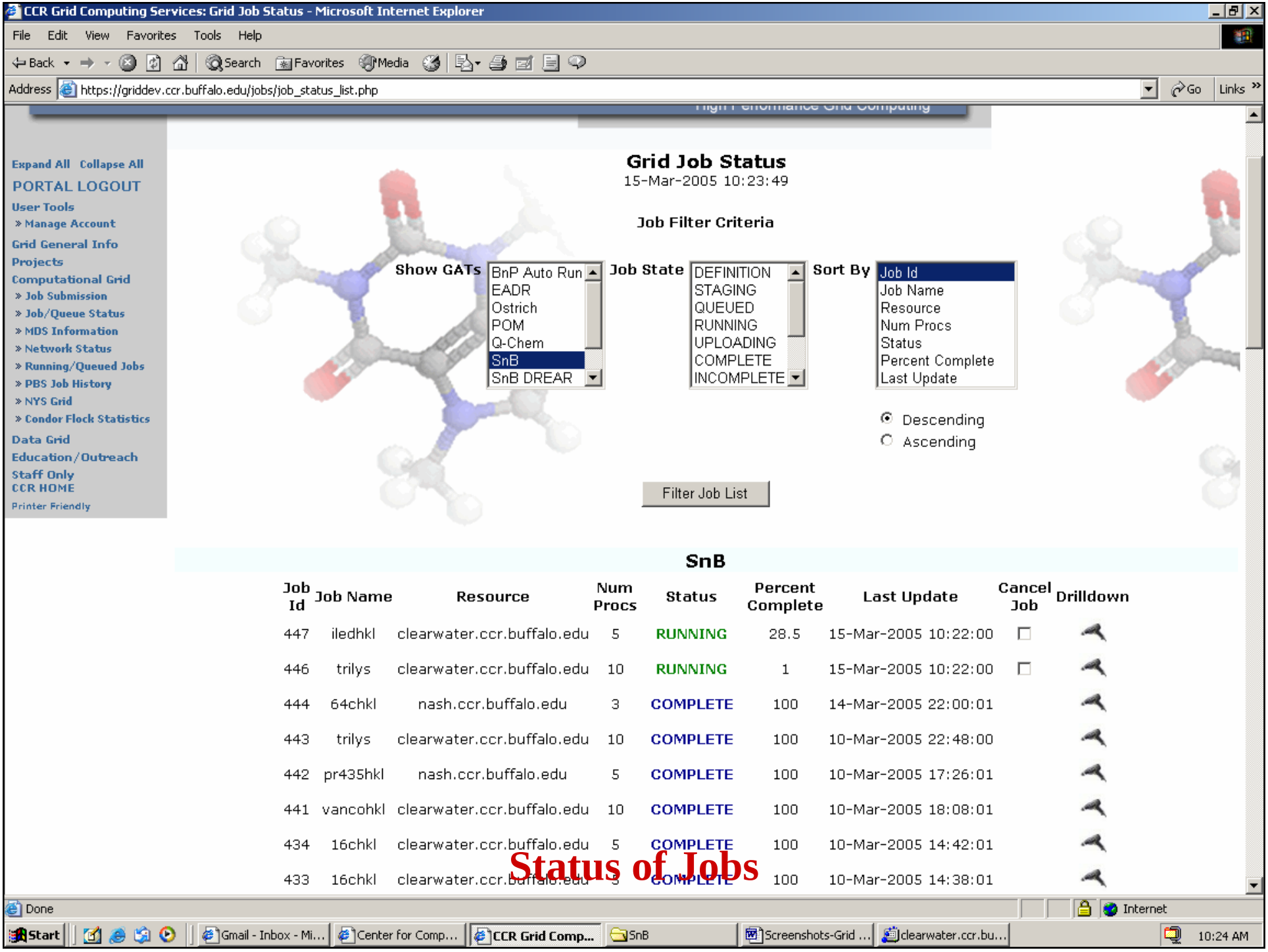
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Job Filter Criteria
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SnB DREAR
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RUNNING
UPLOADING
COMPLETE
INCOMPLETE
Sort By
Job Id
Job Name
Resource
Num Procs
Status
Percent Complete
Last Update
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
Done
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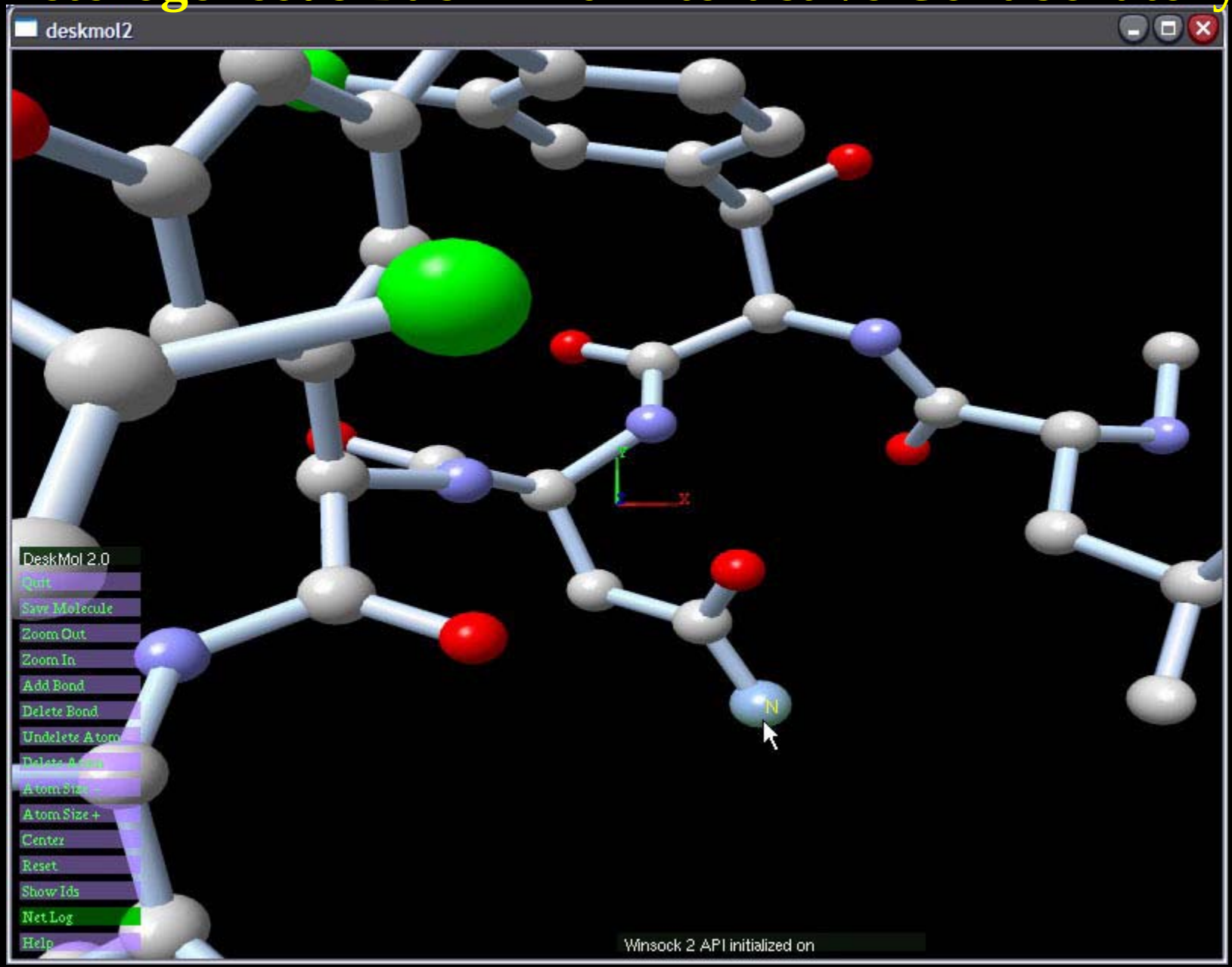
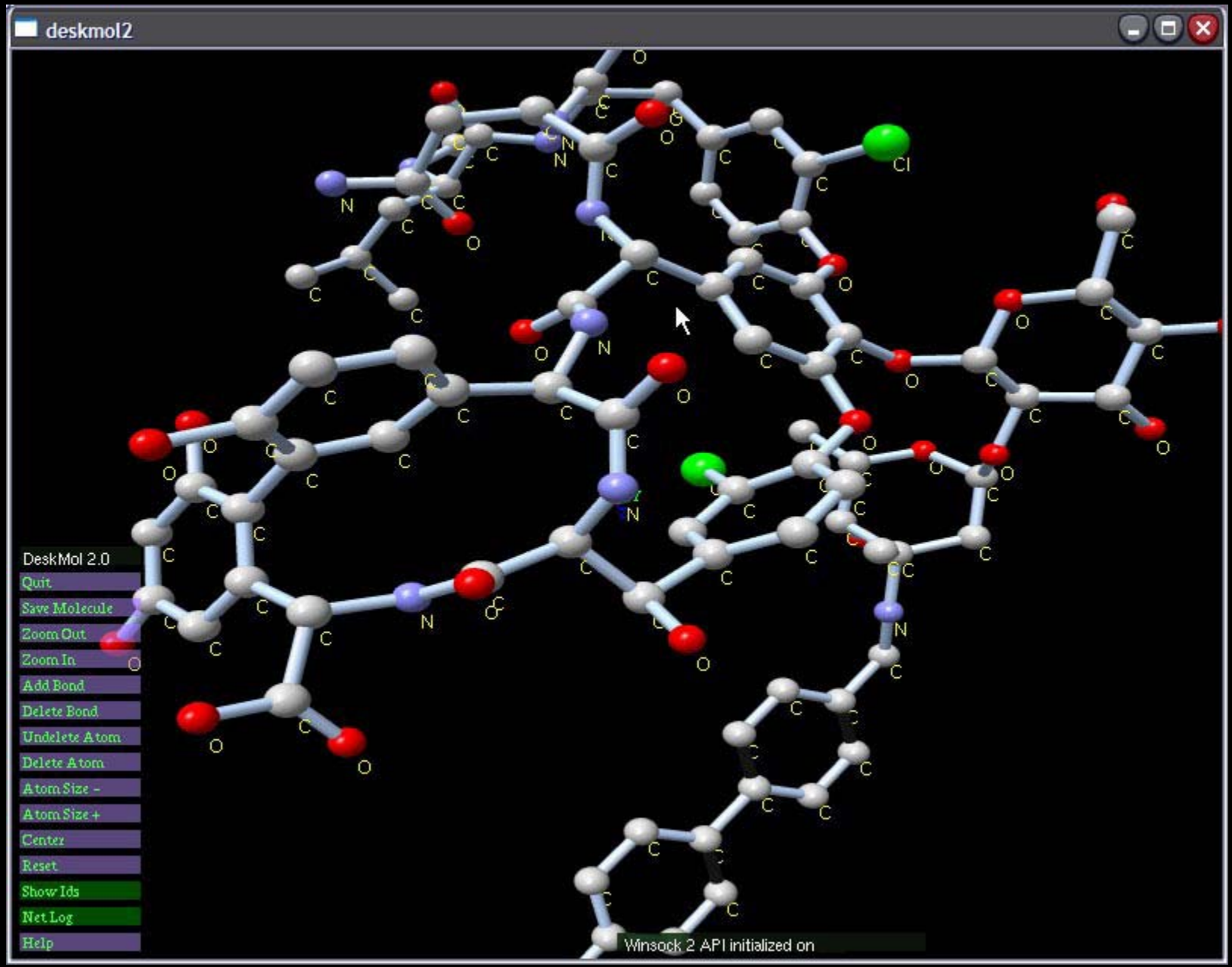
Heterogeneous Back-End Interactive Collaboratory



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
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- Cynthia Cornelius

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- Janet Penksa

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