

# Data-Driven Computing: Storage, Processing, Networking, and Visualization

**Russ Miller**

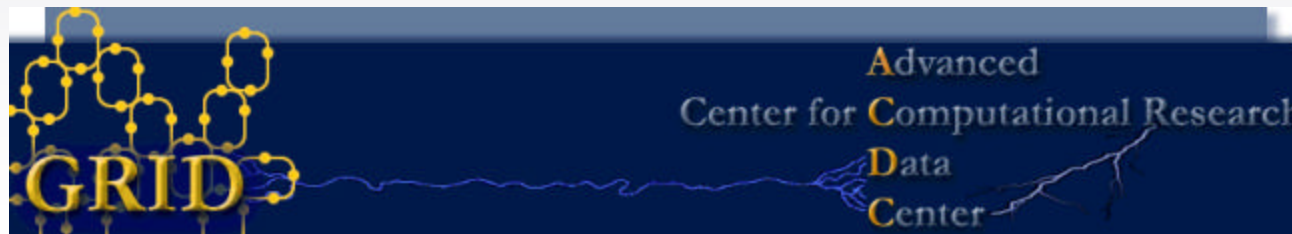
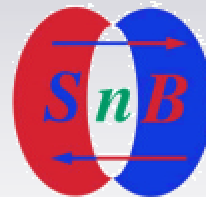
**Center for Computational Research**

**Computer Science & Engineering**

**SUNY-Buffalo**

**Hauptman-Woodward Medical Inst**

NSF, NIH, DOE  
NIMA, NYS, HP



**University at Buffalo**

*The State University of New York*

# Academia in the 21<sup>st</sup> Century

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

# Center for Computational Research 1998-2005 Snapshot

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

### □ ~100 Research Groups in 37 Depts

○ Physical Sciences

○ Life Sciences

○ Engineering

○ Scientific Visualization, Medical Imaging, Virtual Reality

### □ 13 Local Companies

### □ 10 Local Institutions

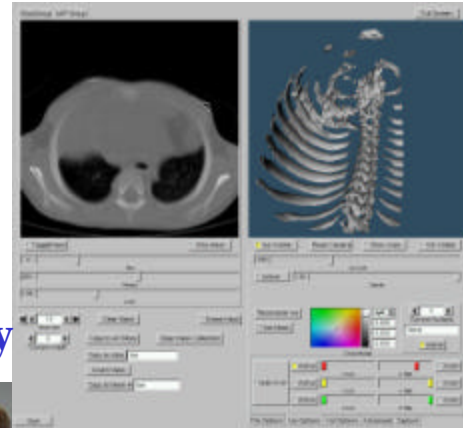
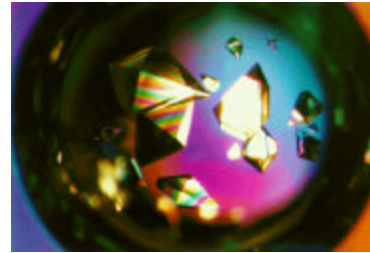
## ■ External Funding: \$300M+

## ■ Total Leveraged WNY: \$500M+

## ■ Deliverables

### □ 1100+ Publications

### □ Software, Media, Algorithms, Consulting, Training, CPU Cycles...



# CCR by the Numbers

## ■ Technical Staff: 13

- ❑ Associate Director
- ❑ Computational Scientist (3)
- ❑ Database Administrator
- ❑ Scientific Visualization
- ❑ System Administration (5)
- ❑ Storage Area Network Admin
- ❑ Multimedia

## ■ Support Staff: 3 FTE

- ❑ Financial/Contracts (2)
- ❑ Receptionist

## ■ Research Staff: 5 FTE

## ■ Initial 7-Year Funding Model

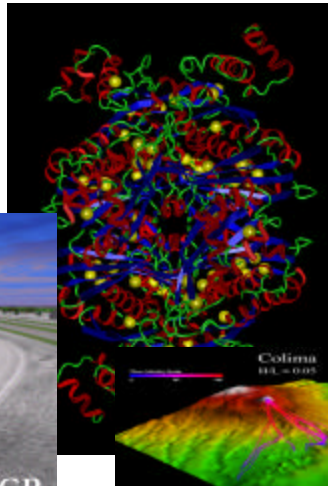
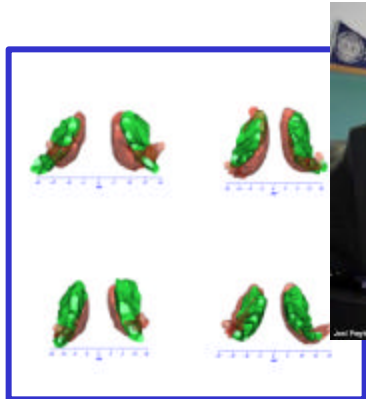
- ❑ SUNY-Buffalo Contribution: \$1.3M
  - Personnel: \$1.2M
  - Operating: \$0.1M
- ❑ User's Contributions: \$0.4M
- ❑ Annual Expend: ~\$2.4M
- ❑ Opportunistic Funding Model
  - Equipment, Maintenance, Licenses
- ❑ ROI: \$7M @ \$300M @ SUNY-B

## ■ Current (New) Funding Model

- ❑ Personnel + Operating: \$677K (2007)
- ❑ Increase Users Contributions
- ❑ Maintain Opportunistic Funding
- ❑ Move into Bioinformatics
- ❑ Provides "Stability"

# CCR Research & Projects

- Ground Water Modeling
- Computational Fluid Dynamics
- Molecular Structure Determination
- Protein Folding
- Digital Signal Processing
- Grid Computing
- Computational Chemistry
- Bioinformatics
- Real-time Simulations and Urban Visualization
- Accident Reconstruction
- Risk Mitigation (GIS)
- Medical Visualization
- High School Workshops
- Virtual Reality



# CCR-Supported Research at UB

## ■ Physical Sciences

- ❑ Autschbach (Chem), Coppens (Chem), Errington (CBE), Furlani (CCR), Han (Physics), Jones (CCR), King (Chem), Kinney (Physics), Kofke (CBE), Lund (CBE), Markelz (Physics), Ruckenstein (CBE), Sen (Physics), Swihart (CBE), Szyperski (Chem)

## ■ Life Sciences

- ❑ Almon (Biology), Andreadis (Chem Eng), Beal (CSE), DeTitta (Structural Biology), Halfon (Biochemistry), Gaile (Biostatistics), Hu (CCR), Hauptman (Structural Biology), Koffas (Chem Eng), Miller (CSE), Murphy (Medicine), Nowak (RPCI), Sullivan (Ophthalmology), Szyperski (Chem), Trevisan (Public Health), Weeks (Structural Biology), Willsky (Biochemistry), Zhang (CSE), Zhou (Physiology and Biophysics)

## ■ Engineering

- ❑ Atkinson (CSEE), Aref (CSEE), Bisantz (IE), Becker (Geology), Bucher (CCR), Bursik (Geology), Cartwright (EE), Dargush (CSEE), DesJardin (MAE), Flewelling (Geography), Green (CCR), Jankovic (CSEE), Jayaraman (CSE), Jones (CCR), Llinas (IE), Madnia (MAE), Nagi (IE), Patra (MAE), Pitman (Math), Qiao (CSE), Rabideau (CSEE), Reinhorn (CSEE), Sheridan (Geology), Singh (MAE), Upadhyaya (CSE), Zubrow (Anthropology)

## ■ Scientific Visualization, Medical Imaging, Virtual Reality

- ❑ Ansty (Media), Baker (Nuclear Med), Evans (Oral Bio), Geffan (Oral Bio), Hoffmann (Nuclear Med), Innus (CCR), Jones (CCR), Kesavadas (MAE), Lockwood (Neurology, Nuclear Med), Miletich (Nuclear Med), Pape (Media), Paley (Classics), Yao (Nuclear Med)



# Major Compute/Storage Resources

- **Dell Linux Cluster (10TF)**
  - ❑ 1600 Xeon EM64T Processors (3.2 GHz)
  - ❑ 2 TB RAM; 65 TB Disk
  - ❑ Myrinet / Force10
  - ❑ 30 TB EMC SAN
- **Dell Linux Cluster (2.9TF)**
  - ❑ 600 P4 Processors (2.4 GHz)
  - ❑ 600 GB RAM; 40 TB Disk; Myrinet
- **Dell Linux Cluster (6TF)**
  - ❑ 4036 Processors (PIII 1.2 GHz)
  - ❑ 2TB RAM; 160TB Disk; 16TB SAN
- **IBM BladeCenter Cluster (3TF)**
  - ❑ 532 P4 Processors (2.8 GHz)
  - ❑ 5TB SAN
- **SGI Intel Linux Cluster (0.1TF)**
  - ❑ 150 PIII Processors (1 GHz)
  - ❑ Myrinet
- **SGI Altix3700 (0.4TF)**
  - ❑ 64 Processors (1.3GHz ITF2)
  - ❑ 256 GB RAM
  - ❑ 2.5 TB Disk
- **Apex 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





# Peace Bridge Visualization

## ■ Proposed Options

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

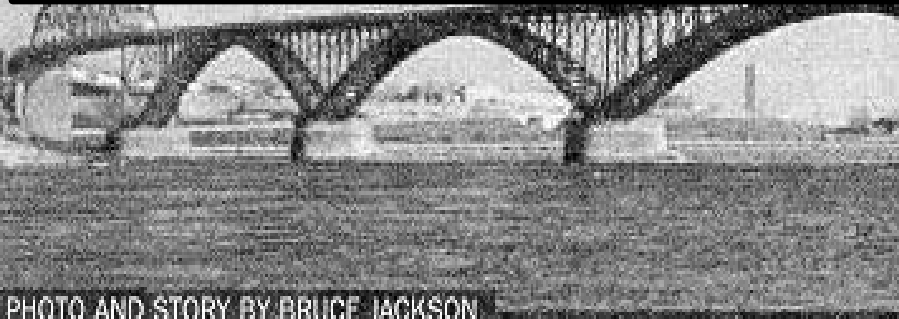
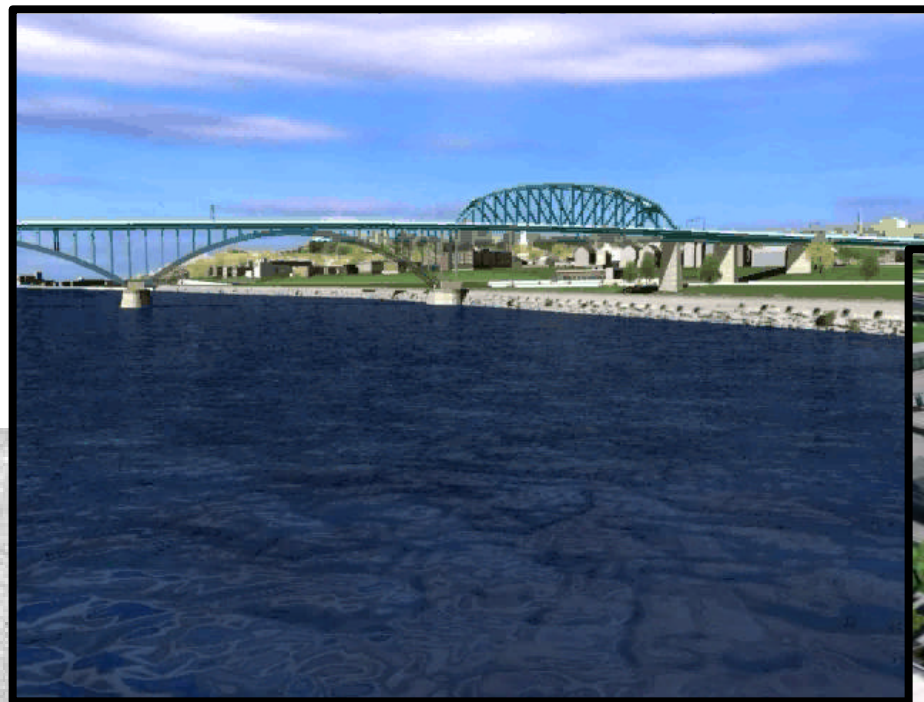


PHOTO AND STORY BY BRUCE JACKSON



# Public Forum

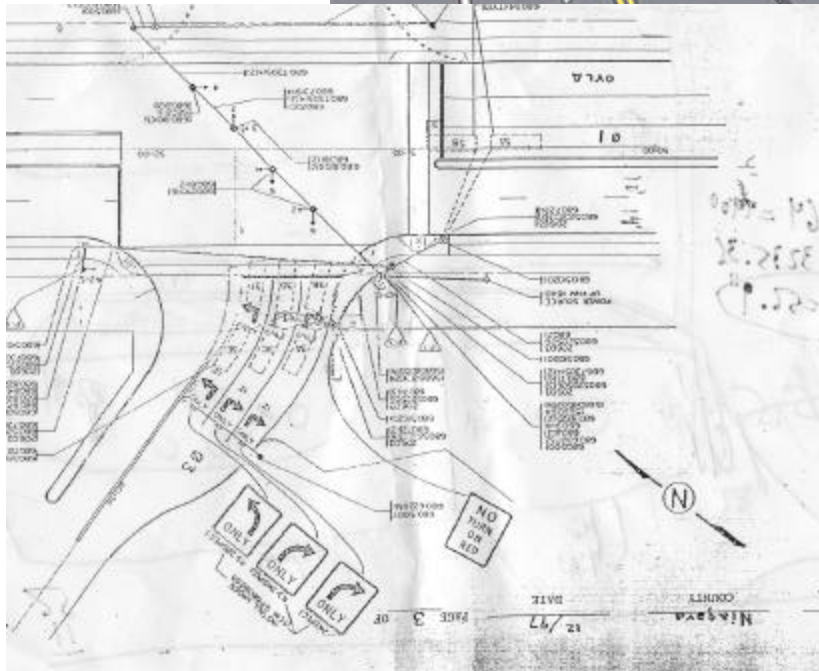
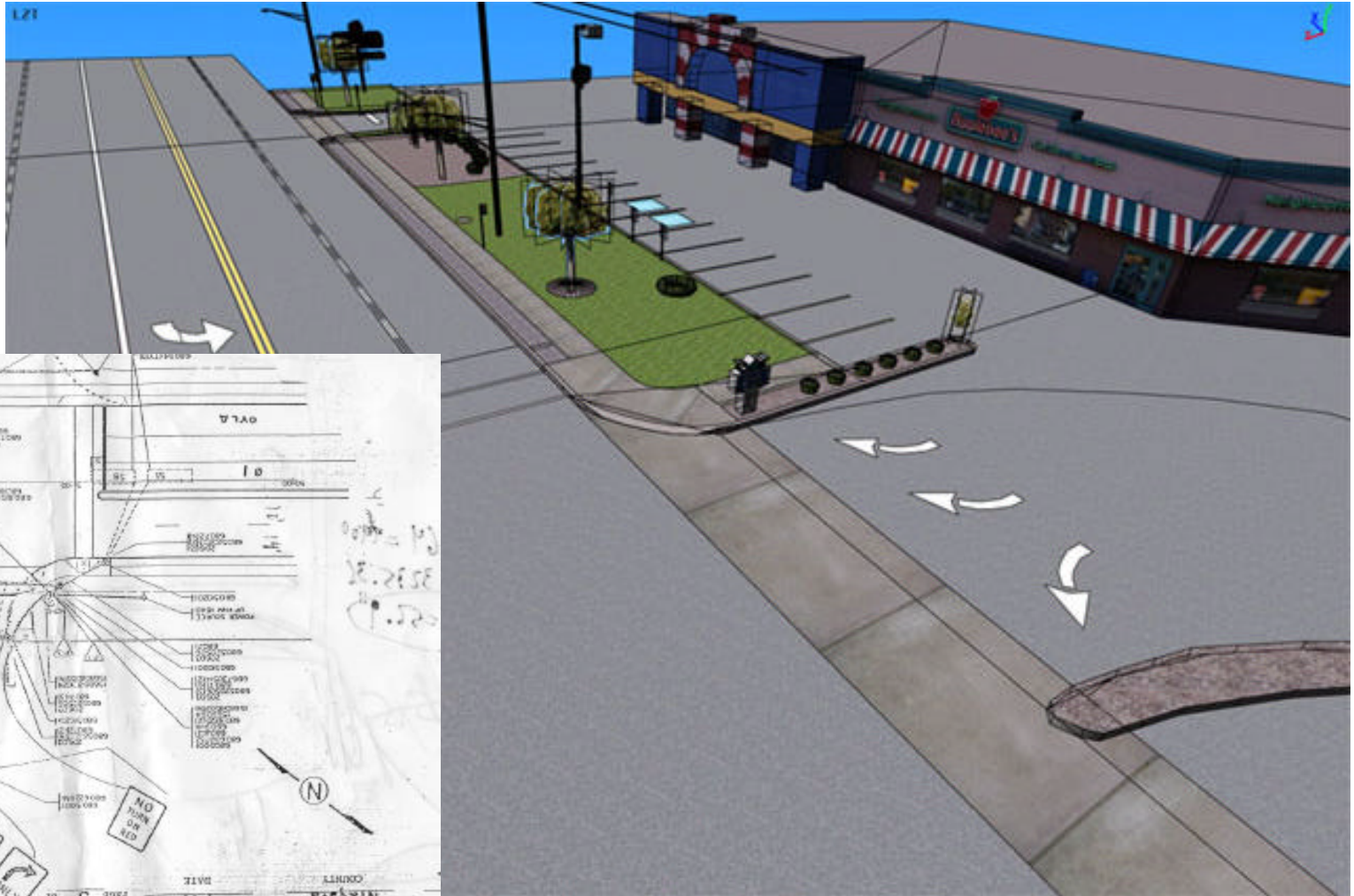


# Williamsville Toll Barrier Improvement Project

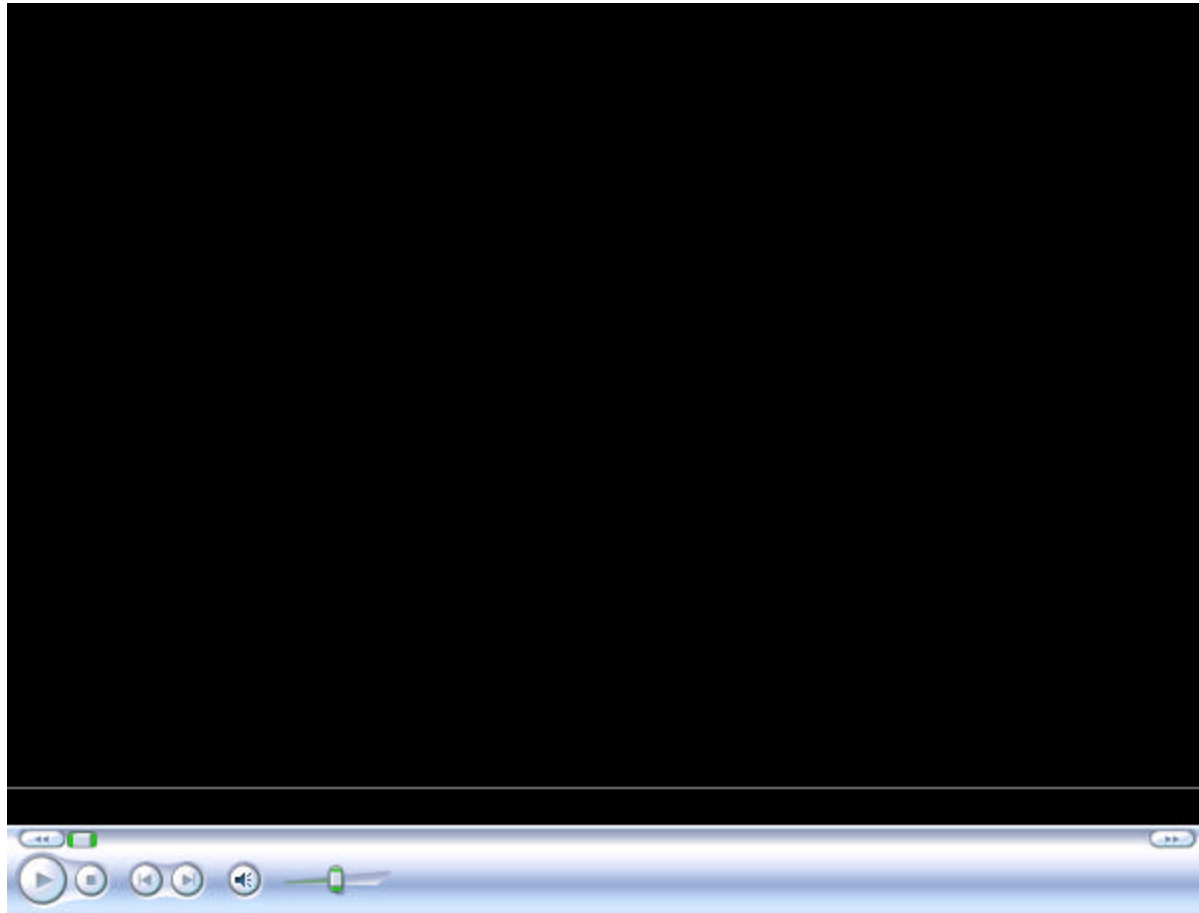


**Initial Photo Match incorporating real and computer-generated components**

# Accident Reconstruction



# Accident Animation (Driver's View)



# StreetScenes<sup>®</sup>

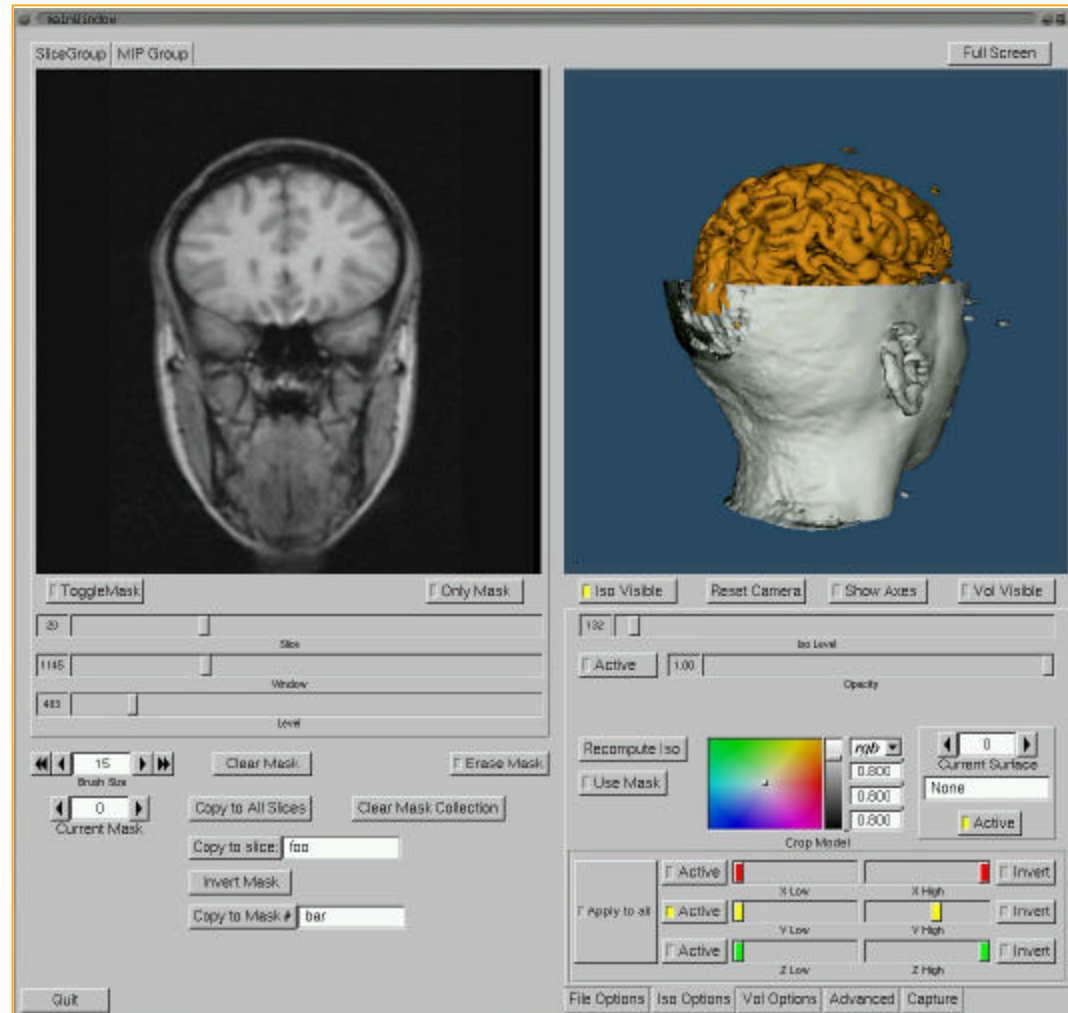
## 3D Traffic Simulation

- *StreetScenes*<sup>®</sup> is a Virtual Reality (VR) software solution for 3D visualization of surface traffic
- 3D model of proposed soccer stadium in Rochester
- Used *StreetScenes*<sup>®</sup> to import output file from Synchro traffic simulation



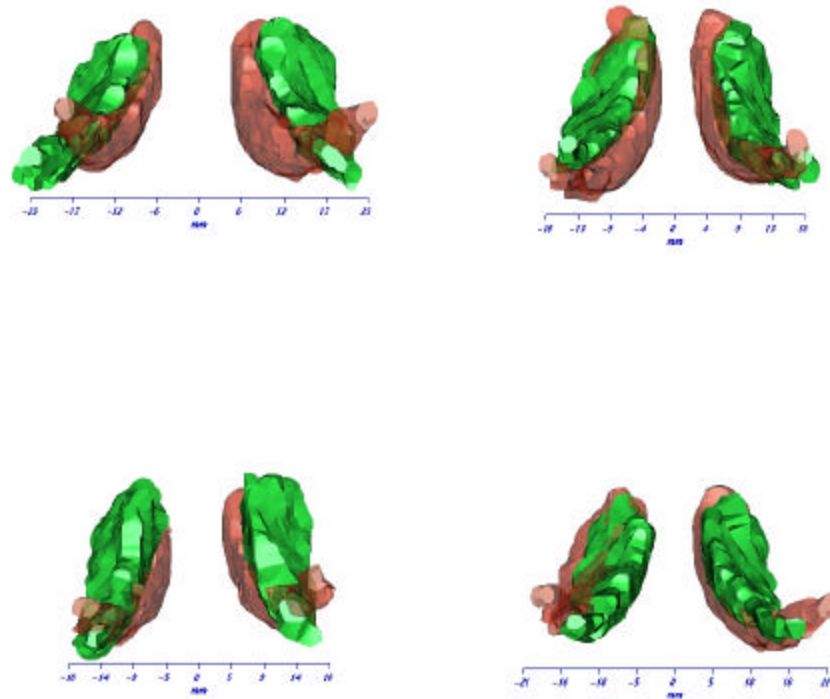
# Multiple Sclerosis Project

- 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



# Multiple Sclerosis Project

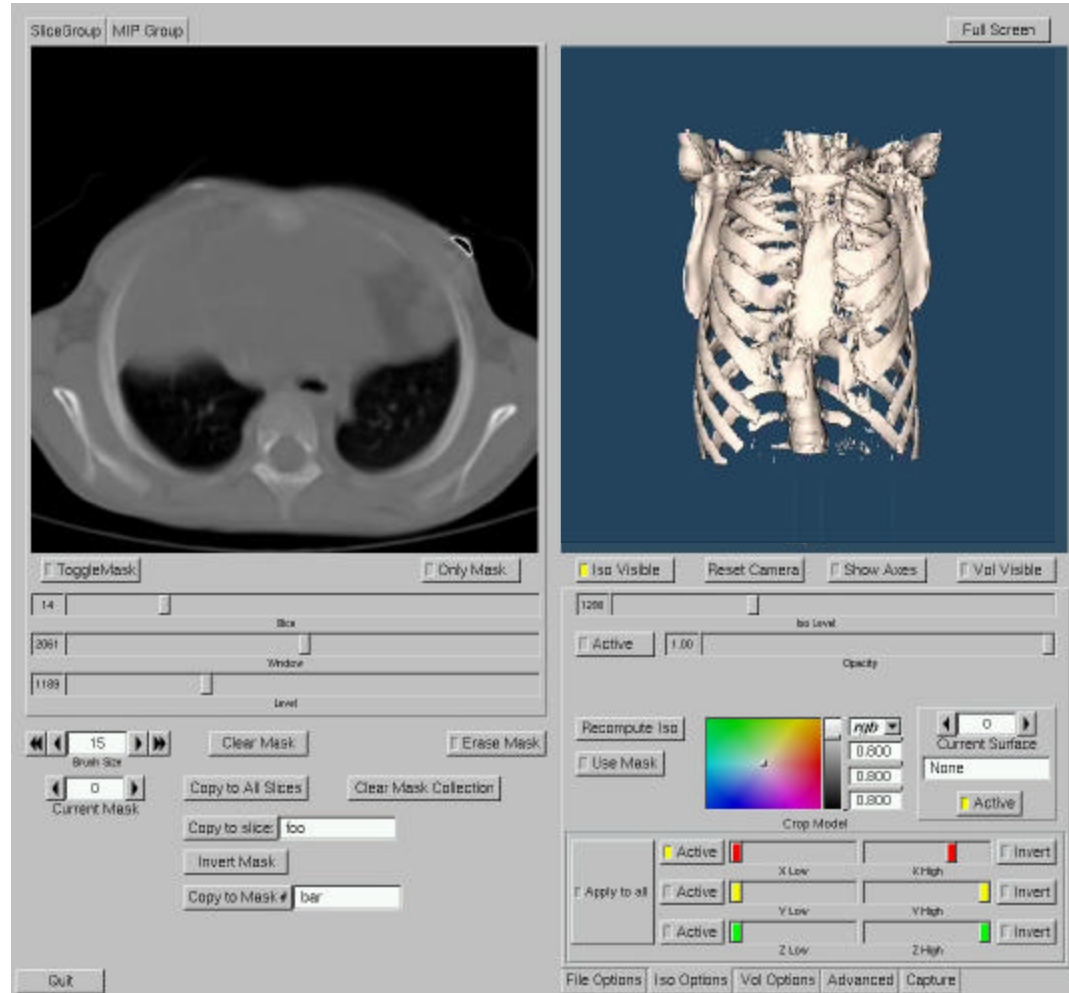
- Compare caudate nuclei between MS patients and healthy controls
- Looking for size as well as structure changes
  - Localized deformities
  - Spacing between halves
- Able to see correlation between disease progression and physical structure changes





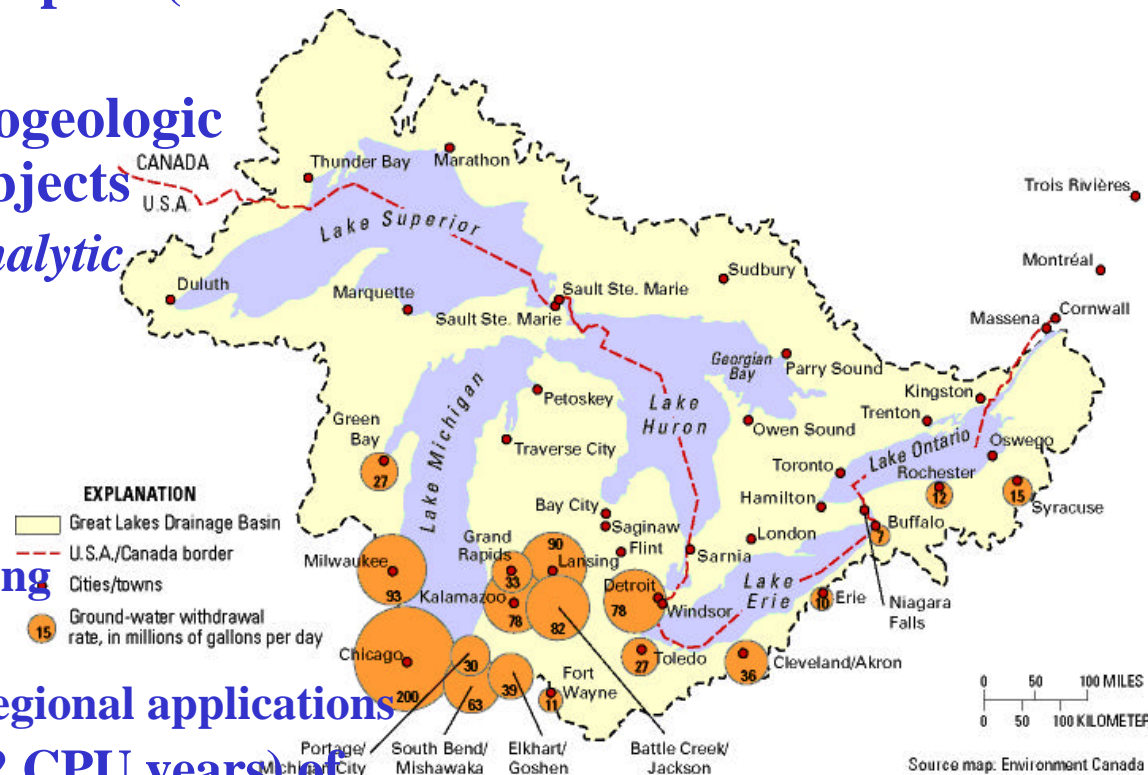
# 3D Medical Visualization App

- 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



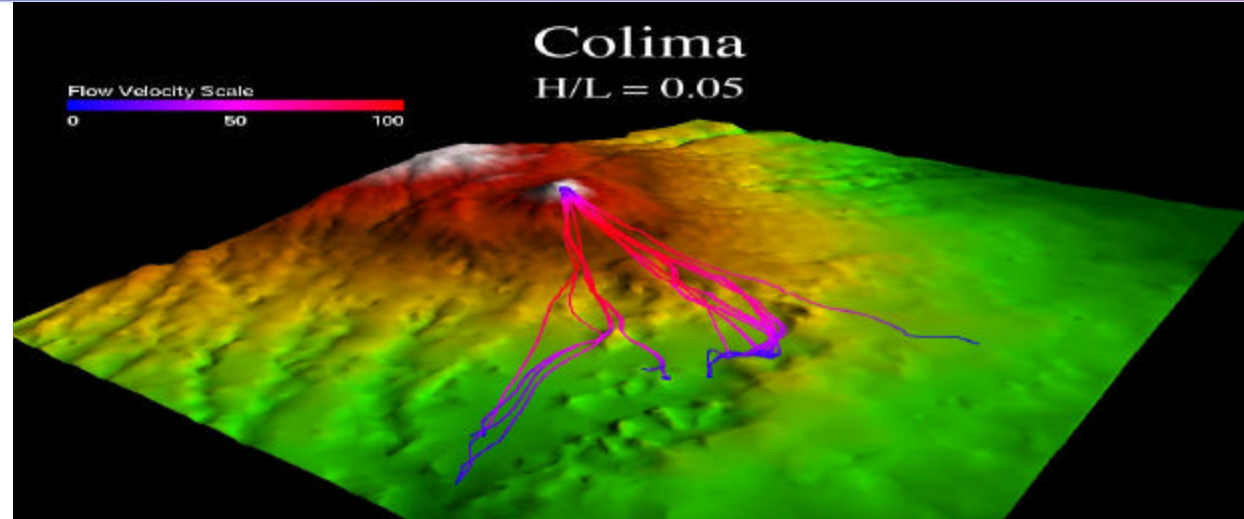
# Groundwater Flow Modeling

- 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

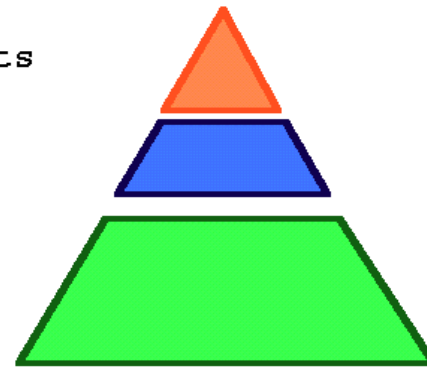


S  
C  
A  
L  
A  
B  
L  
E  
  
I  
T

Scientists

Hazard  
Managers

Public



High End Simulation  
and Visualization

Remote Real time  
visualization server

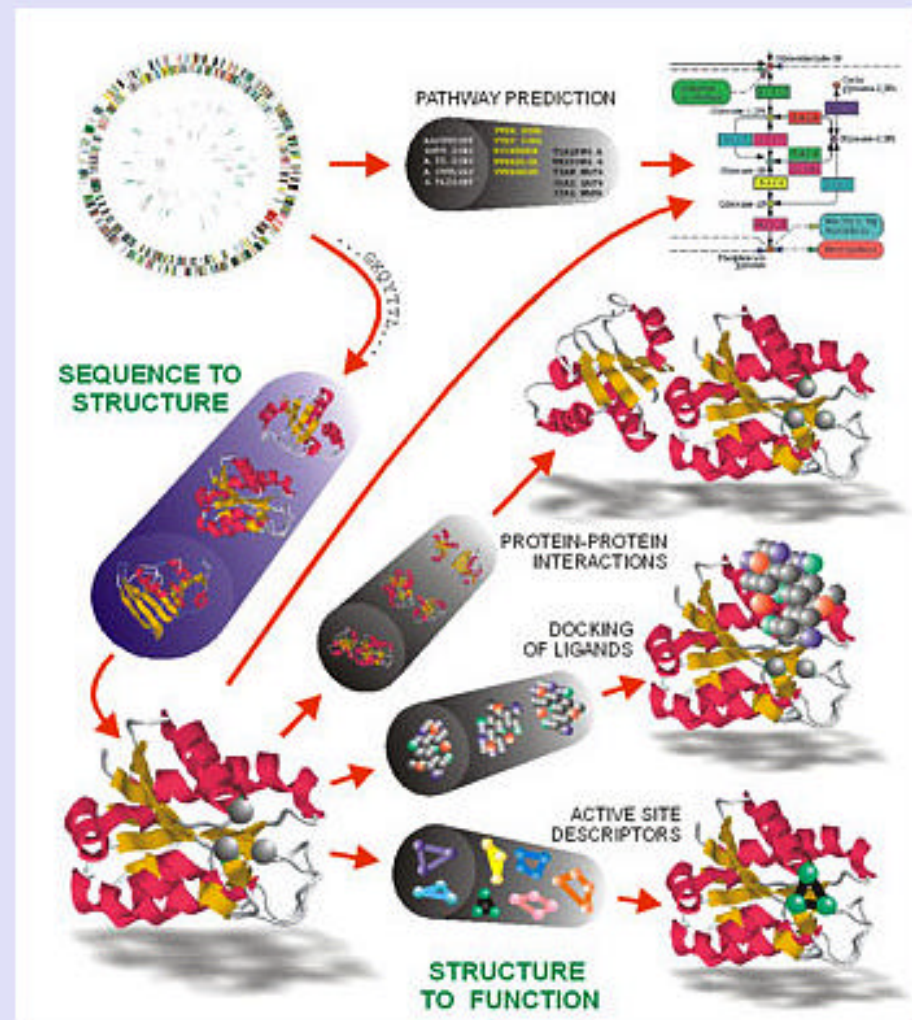
Web Servers

Web based  
visualization

# Bioinformatics in Buffalo

## A \$360M Initiative

- New York State: \$121M
- Federal Appropriations: \$13M
- Corporate: \$146
- Foundation: \$15M
- Grants & Contracts: \$64M
- Lead Institutions
  - SUNY-Buffalo
  - Roswell-Park Cancer Institute
  - Hauptman-Woodward Medical Research Institute



# Recent Biomedical Advances (Buffalo, NY)

■ **PSA Test (screen for Prostate Cancer)**

■ **Avonex: Interferon Treatment for Multiple Sclerosis**

■ **Artificial Blood**

■ **Nicorette Gum**

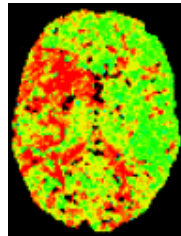
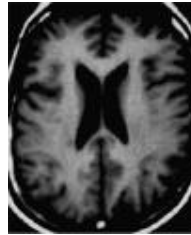
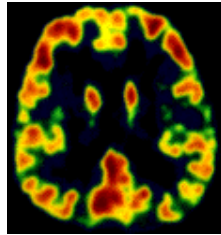
■ **Fetal Viability Test**

■ **Edible Vaccine for Hepatitis C**

■ **Timed-Release Insulin Therapy**

■ **Anti-Arrhythmia Therapy**

□ **Tarantula venom**



■ **Direct Methods Structure Determination**

□ **Listed on “Top Ten Algorithms of the 20<sup>th</sup> Century”**

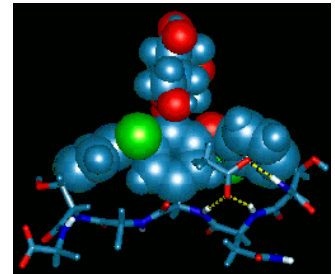
■ **Vancomycin**

■ **Gramacidin A**

■ **High Throughput Crystallization Method: Patented**

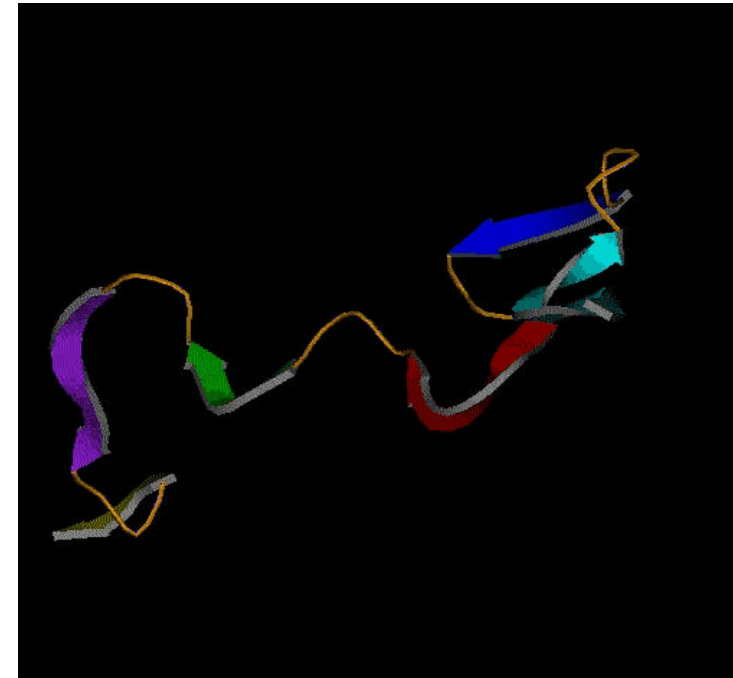
■ **NIH National Genomics Center: Northeast Consortium**

■ **Howard Hughes Medical Institute: Center for Genomics & Proteomics**



# Protein Folding

- Ability of proteins to perform biological function is attributed to their 3-D structure.
- Protein folding problem refers to the challenge of predicting 3-D structure from amino-acid sequence.
- Solving the protein folding problem will impact drug design.



# Northeast Structural Genomics Consortium

## ■ Consortium

- ❑ UB, Rutgers, Columbia, Cornell, PNNL, Yale, UToronto, Robert Wood Johnson Medical Center, Hauptman-Woodward Medical Research Center

## ■ Mission

- ❑ Develop integrated technologies for high-throughput (htp) protein production and 3D structure determination
- ❑ The goal is to determine 500 new protein structures over 5 years
- ❑ Combination of strong parallel efforts in both X-ray crystallography and solution-state NMR spectroscopy
- ❑ UB Professor Thomas Szyperski awarded Scientific American's Top 50 Scientists in 2003 for novel work in high-throughput structure determination with NMR

# Computational Chemistry

## ■ UB Software Development in Quantum Chemistry

- ❑ **Q-Chem** – development of parallel algorithms and combined QM/MM methods for large molecular systems
- ❑ **ADF** – development of algorithms to calculate magnetic and optical properties of molecules

## ■ Used to determine

- ❑ Molecular Structure
- ❑ Electronic Spectra
- ❑ Chemical Reactivity

## ■ Applications

- ❑ Pharmaceutical Drug Design
- ❑ Industrial Catalysis
- ❑ Materials Science
- ❑ Nanotechnology
- ❑ Solution Phase Chemistry
- ❑ Chemical Kinetics





# Western New York Health Information Project

## Goals:

- Build a secure community-wide healthcare database
- Develop an electronic patient medical record that “follows the patient”
- Provide care providers with real-time patient information wherever they are
- Provide a tool to aid agencies in community safety, epidemiology, resource allocation, and bioterrorism response
- Improve the overall quality of healthcare while reducing costs

## Selected Participants:

- SUNY-Buffalo (CCR, School of Informatics, School of Medicine, Health Science Library)
- Buffalo Academy of Medicine
- Erie County DoH
- New York State DoH
- WNY HealtheNet
- Involvement from Kaleida Health, ECMC, Catholic Health System, Independent Health, HealthNow, and Univera Healthcare



# Molecular Structure Determination via *Shake-and-Bake*

## ■ *SnB* Software by UB/HWI

- ❑ “Top Algorithms of the Century”

## ■ Worldwide Utilization

## ■ Critical Step

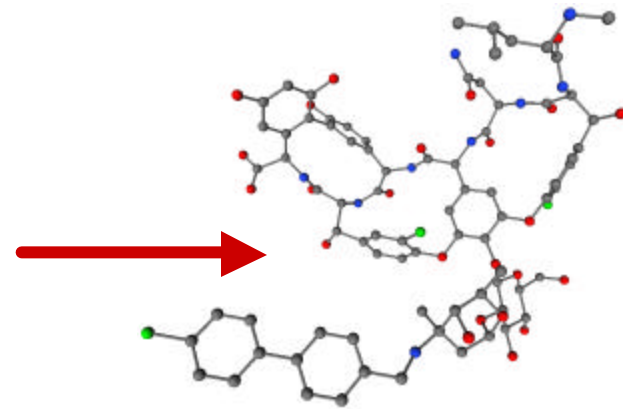
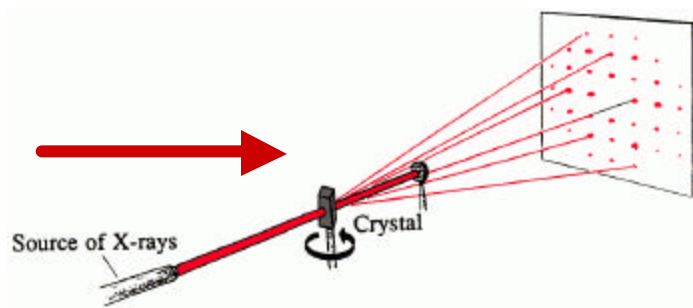
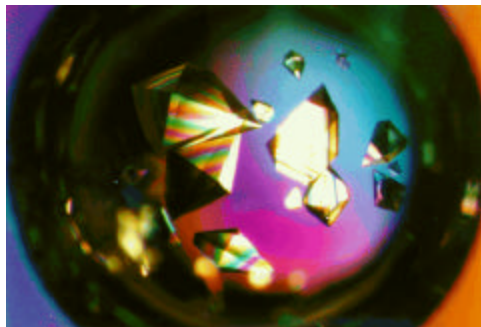
- ❑ Rational Drug Design
- ❑ Structural Biology
- ❑ Systems Biology

## ■ Vancomycin

- ❑ “Antibiotic of Last Resort”

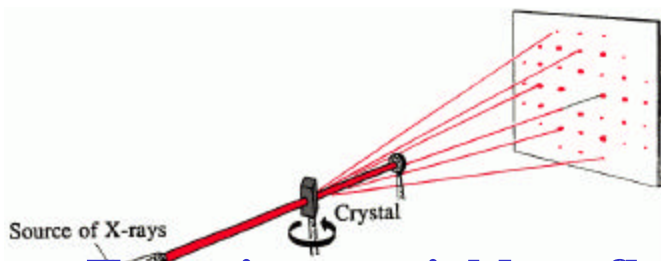
## ■ Current Efforts

- ❑ Grid
- ❑ Collaboratory
- ❑ Intelligent Learning



1. Isolate a single crystal    2. Perform the X-Ray diffraction experiment    3. Determine the crystal structure

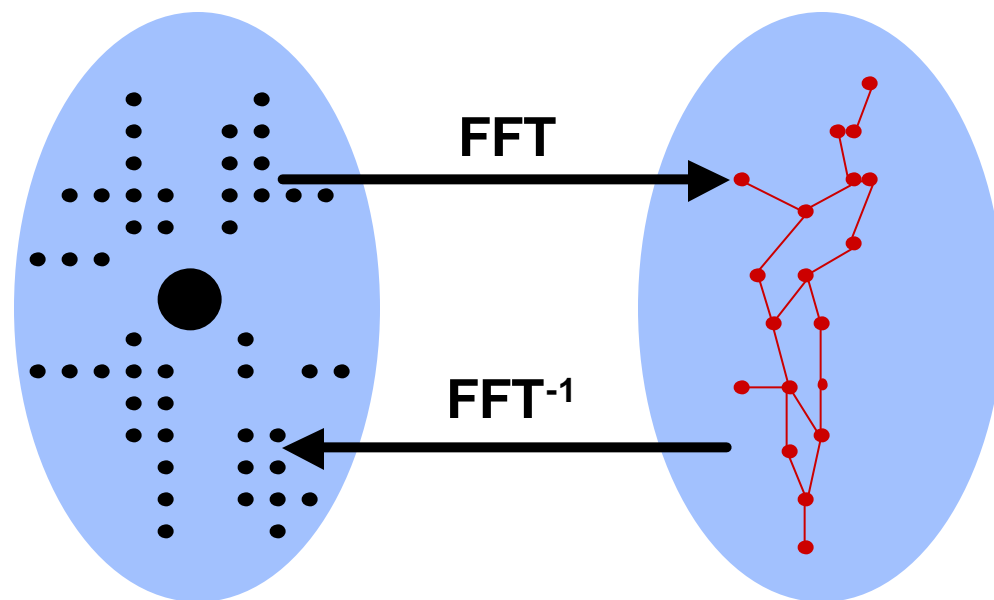
# X-Ray Data & Corresponding Molecular Structure



- 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

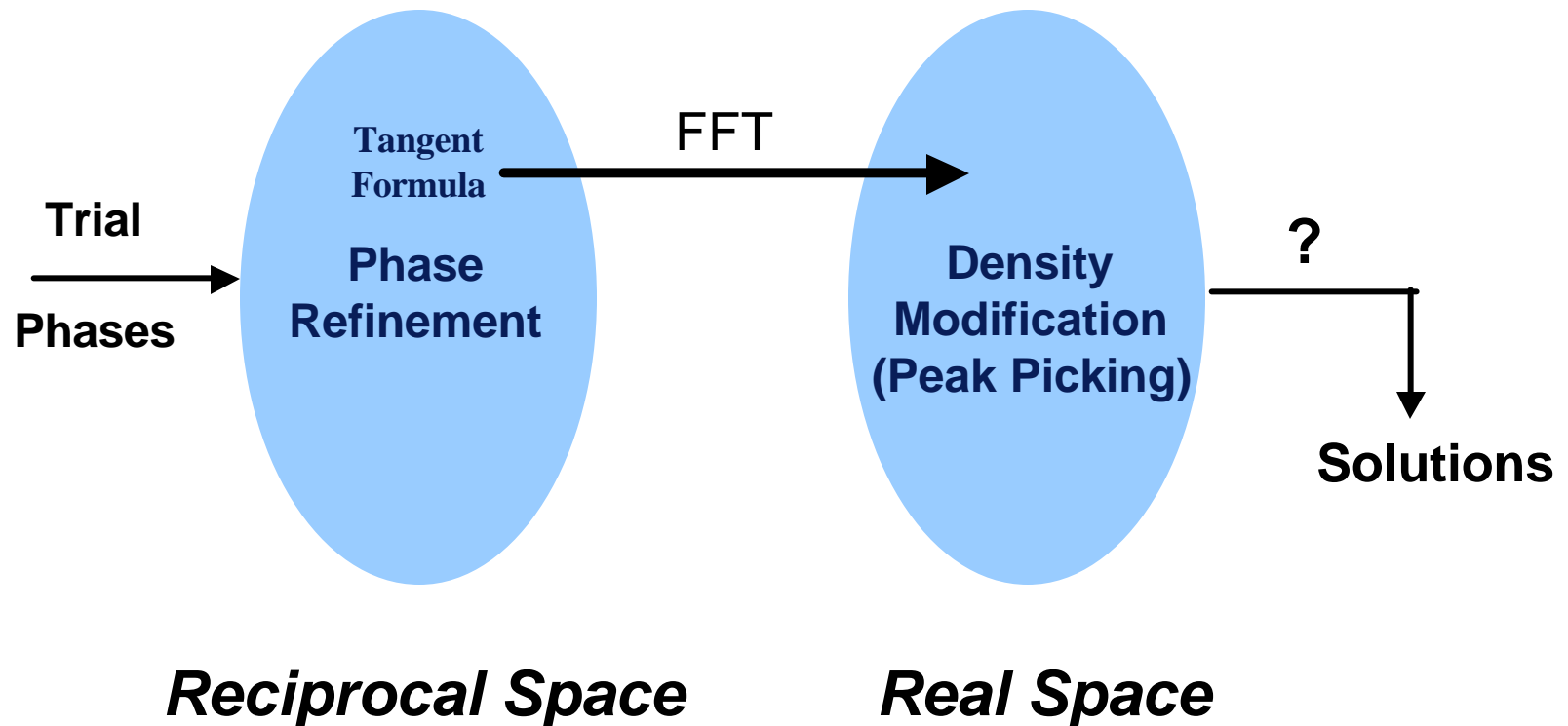
Real Space



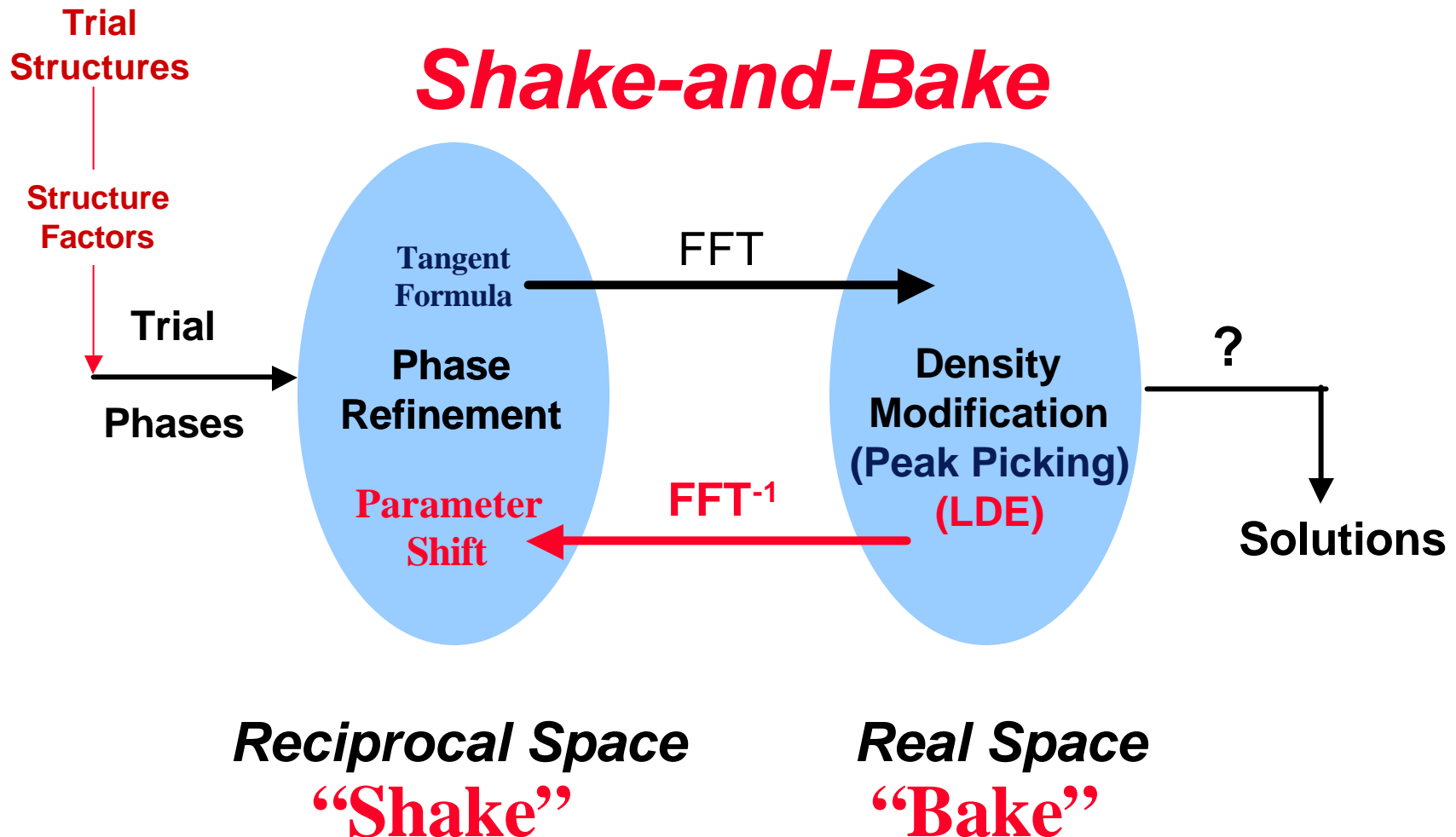
*X-Ray Data*

*Molecular Structure*

# Conventional Direct Methods



# Shake-and-Bake Method: Dual-Space Refinement



# 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

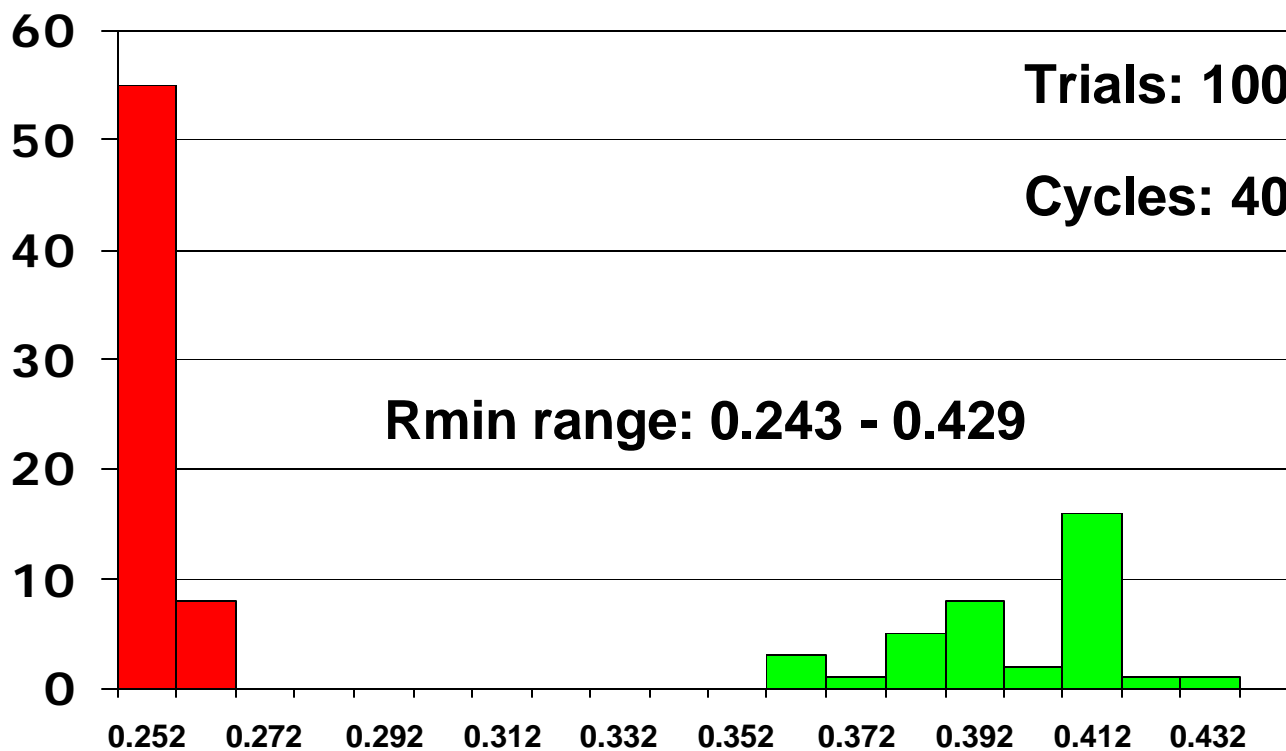
Invariants :  $\Phi_{HK} = \mathbf{f}_H + \mathbf{f}_K + \mathbf{f}_{-H-K} \approx 0$

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

# Ph8755: *SnB* Histogram

**Atoms: 74**  
**Space Group: P1**

**Phases: 740**  
**Triples: 7,400**



# Phasing and Structure Size

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

Se-Met

190kDa

Multiple Isomorphous Replacement .....?

*Shake-and-Bake*

Conventional Direct Methods

Vancomycin



Number of Atoms in Structure



# Vancomycin

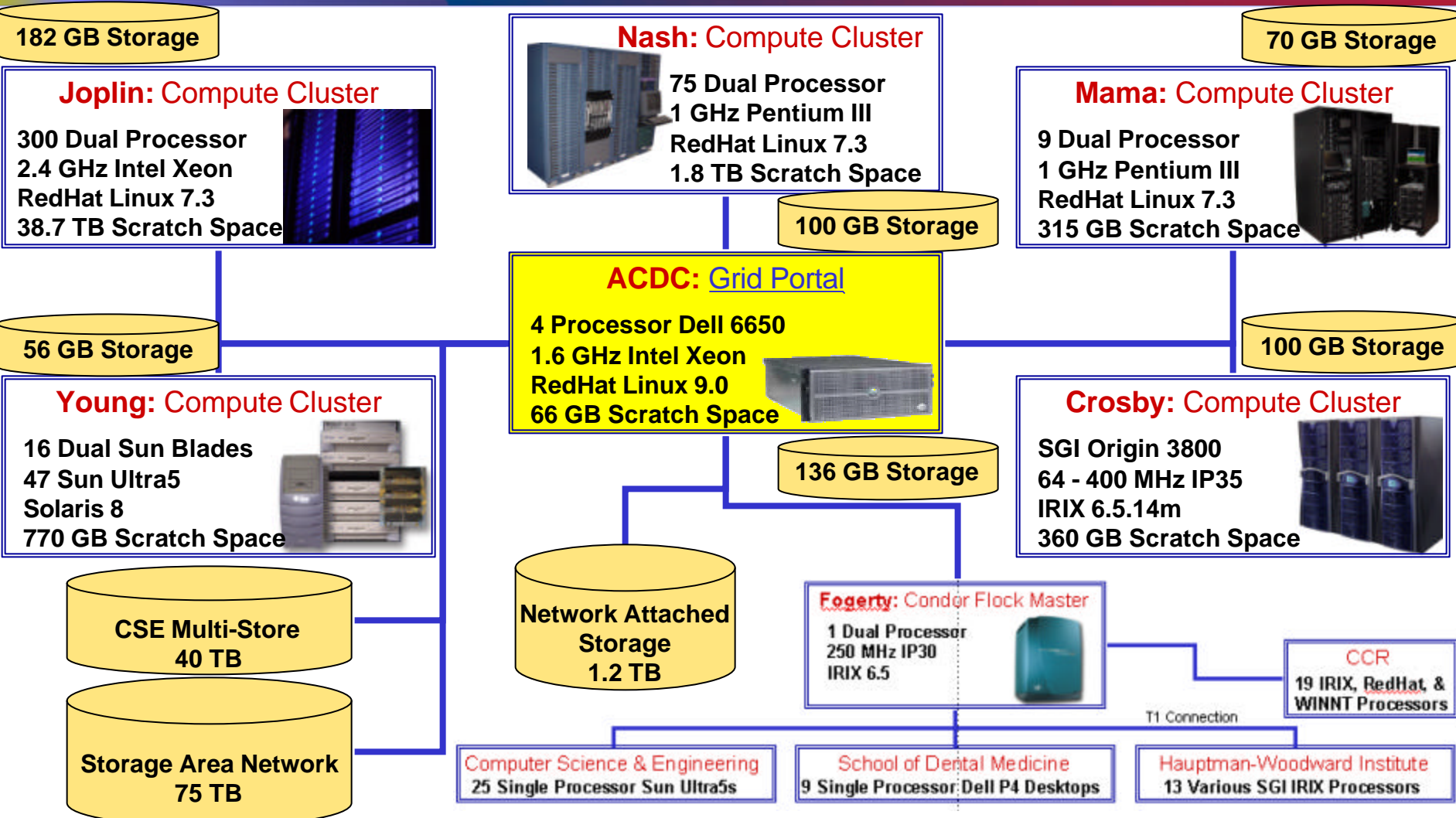
- Interferes with formation of bacterial walls
- *Last line of defense* against deadly
  - streptococcal and staphylococcal bacteria strains
- Vancomycin resistance exists (Michigan)
- Can't just synthesize variants and test
- Need structure-based approach to predict
- Solution with *SnB (Shake-and-Bake)*
  - Pat Loll
  - George Sheldrick

# ACDC-Grid Cyber-Infrastructure

- **Integrated Data Grid**
  - Automated Data File Migration based on profiling users.
- **High-Performance Grid-Enabled Data Repositories**
  - Develop automated procedures for dynamic data repository creation and deletion.
- **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.

# ACDC Data Grid Overview

## (Grid-Available Data Repositories)



Note: Network connections are 100 Mbps unless otherwise noted.

# ACDC-Grid Collaborations

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



# 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

# ACDC-Grid

CCR Grid Computing Services - Microsoft Internet Explorer

Center for Computational Research GRID PORTAL  
High Performance Grid Computing

PORTAL LOGIN  
Grid General Info  
About ACDC Grid  
Computational Grid  
Data Grid  
Makuboot  
Technical Pages  
Presentations  
Contact Us  
Grid Account Request  
Grid Account Support  
Events  
News  
Projects  
Resources  
Education/Outreach  
Staff Only  
CCR HOME

University at Buffalo The State University of New York

Welcome to Grid Computing Services

University at Buffalo Center for Computational Research is currently forming the first Western New York computational grid. The computational grid consist of many supercomputers located at the Center and several other networked supercomputers throughout the Western New York region. These resources will be shared by many researchers from several departments working on a diverse suite of problems including Biomimetics, Computational Chemistry, and Medical Imaging to name a few.

We also provide grid computing support for the University's Center for Computational Research learning, teaching and research activities plus the infrastructure for both high performance computing and grid enabled software.

Got your "Grid Computing Guide"?



CCR Grid Computing Services Data Management - Microsoft Internet Explorer

Center for Computational Research GRID PORTAL  
High Performance Grid Computing

PORTAL LOGOUT  
User Tools  
Manage Account  
Grid General Info  
Projects  
Resources  
Computational Grid  
Job Submissions  
Data Grid  
Network Status  
Pending/Queued Jobs  
PBS Job History  
Grid Portal Statistics  
Leader/Flock Statistics  
User Info  
Education/Outreach  
Staff Only  
CCR HOME

VIEW Group GROUP:miller UserList:ropplaye

reppleye  
KeyMaster  
Morpheus  
Tank  
Agent  
Rabbit  
Tank  
Morpheus  
Oracle.m  
Neo

Browser view of "miller" group files published by user

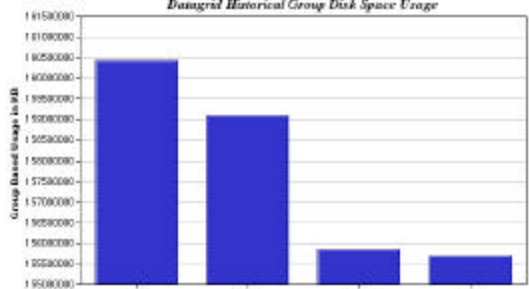
CCR Grid Computing Services Grid Admin - Microsoft Internet Explorer

Center for Computational Research GRID PORTAL  
High Performance Grid Computing

PORTAL LOGOUT  
User Tools  
Manage Account  
Grid General Info  
Projects  
Resources  
Computational Grid  
Job Submissions  
Data Grid  
Network Status  
Pending/Queued Jobs  
PBS Job History  
Grid Portal Statistics  
Leader/Flock Statistics  
User Info  
Education/Outreach  
Staff Only  
CCR HOME

View statistics for: disk\_space  
Data based on: group  
from starting date: January 1 2000  
to ending date: September 13 2003 inclusive  
for: Grid Portal resources OK

Baagrid Historical Group Disk Space Usage



Group	Disk Space Usage (KB)
miller	~1,950,000
griddev	~1,850,000
ccrstaff	~1,550,000
mlgreen	~1,500,000

CCR Grid Computing Services: Grid Admin - Microsoft Internet Explorer

Center for Computational Research GRID PORTAL  
High Performance Grid Computing

PORTAL LOGOUT  
User Tools  
Manage Account  
Grid General Info  
Projects  
Resources  
Computational Grid  
Job Submissions  
Data Grid  
Network Status  
Pending/Queued Jobs  
PBS Job History  
Grid Portal Statistics  
Leader/Flock Statistics  
User Info  
Education/Outreach  
Staff Only  
CCR HOME

View statistics for: disk\_space  
Data based on: user  
from starting date: January 1 2000  
to ending date: September 13 2003 inclusive  
for: Grid Portal resources OK

File_num	File_ID	Filename	Dir_ID	Resource_ID	Owner	Groupname	Type
1	56033	Cypher.txt	52831	10	mlgreen	griddev	txt
2	56034	Cypher.sh	52858	10	mlgreen	griddev	sh
3	56035	Oracle.asc	52958	10	mlgreen	griddev	asc
4	56036	Cypher.sh	52634	10	mlgreen	miller	sh
5	56037	Rabbit.dat	52830	10	mlgreen	ccrstaff	dat
6	56038	Agent.exe	53064	10	mlgreen	griddev	exe
7	56039	Dozer.sh	52852	10	mlgreen	griddev	sh
8	56040	Neo.asc	52187	10	mlgreen	mlgreen	asc
9	56041	Agent.mpg	52833	10	mlgreen	mlgreen	mpg
10	56042	Tank.txt	52188	10	mlgreen	mlgreen	txt
11	56043	Smith.xls	52258	10	mlgreen	ccrstaff	xls
12	56044	KeyMaster.csh	52186	10	mlgreen	miller	csh
13	56045	Oracle.csh	52622	10	mlgreen	griddev	csh
14	56046	Dozer.xls	52808	10	mlgreen	mlgreen	xls
15	56047	Cypher.exe	52204	10	mlgreen	griddev	exe
16	56048	Rabbit.ppt	52861	10	mlgreen	miller	ppt
17	56049	Neo.dat	52217	10	mlgreen	ccrstaff	dat
18	56050	Cypher.asc	53086	10	mlgreen	griddev	asc



# 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**

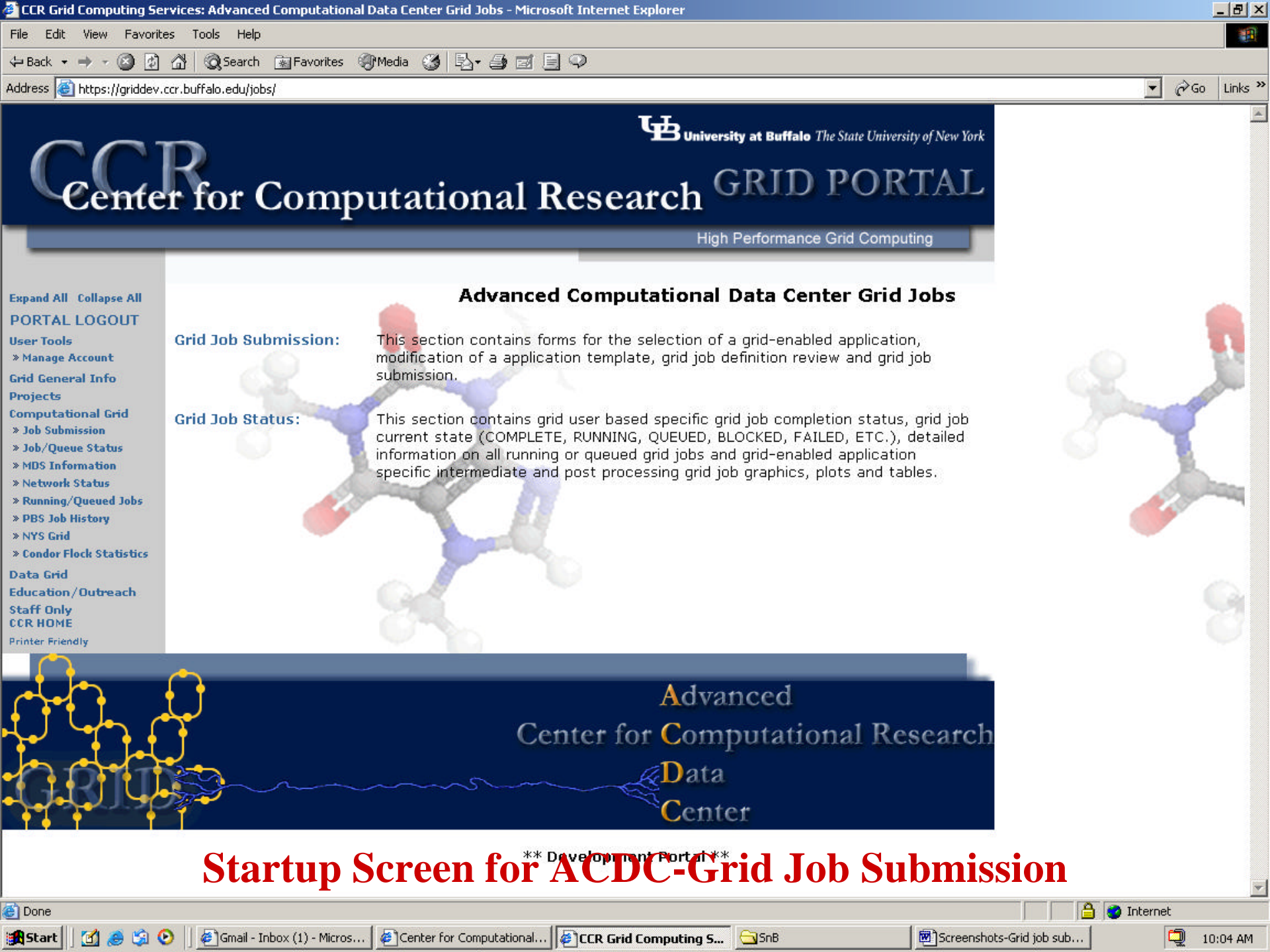
Current Time: 16-September-2003 10:59:12

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





# CCR Center for Computational Research GRID PORTAL

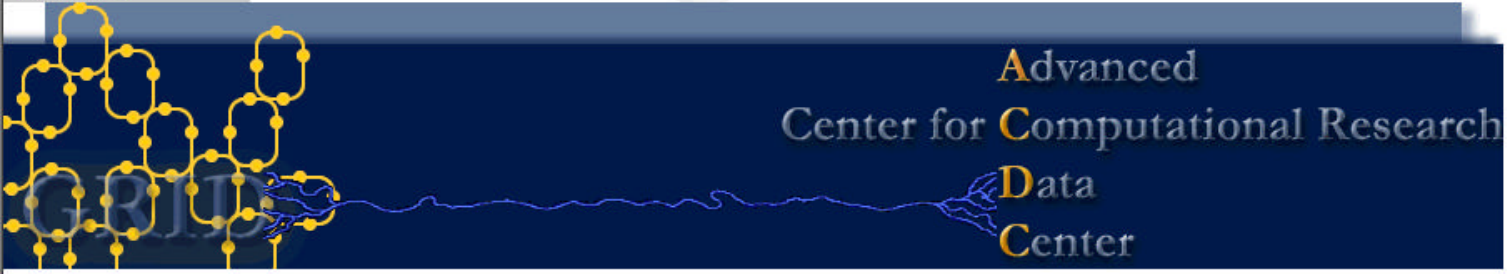
High Performance Grid Computing

- 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

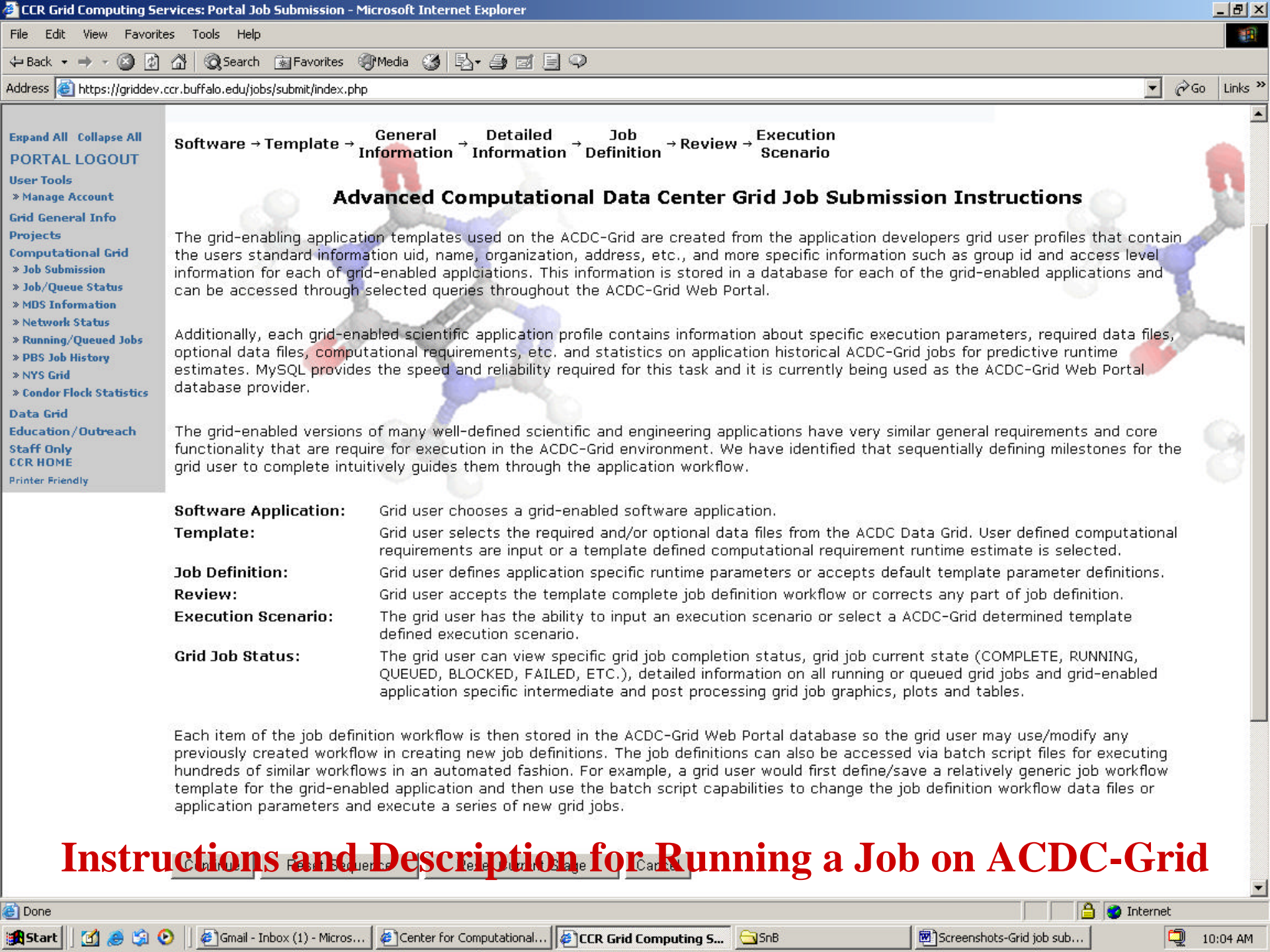
**Grid Job Submission:** This section contains forms for the selection of a grid-enabled application, modification of a application template, grid job definition review and grid job submission.

**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


**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
  - » 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:

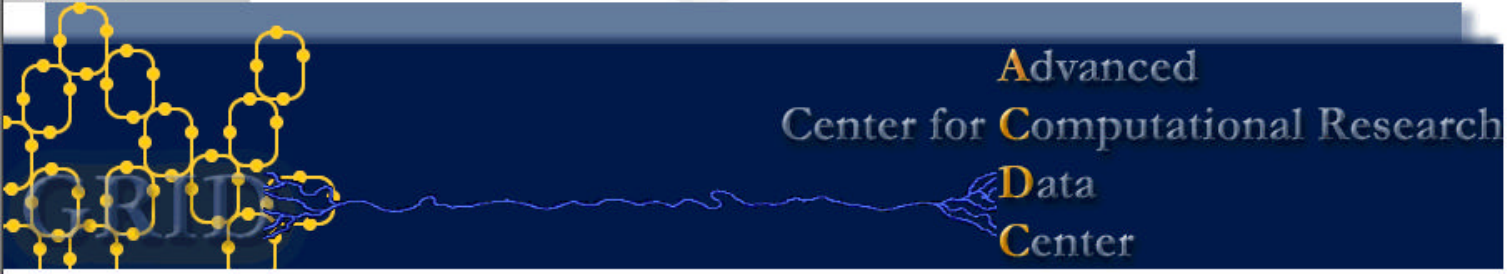
- BnP Auto Run
- BnP Auto Run
- EADR
- Ostrich
- POM
- Q-Chem
- SnB**
- SnB DREAR
- Split
- snb-dev

Continue

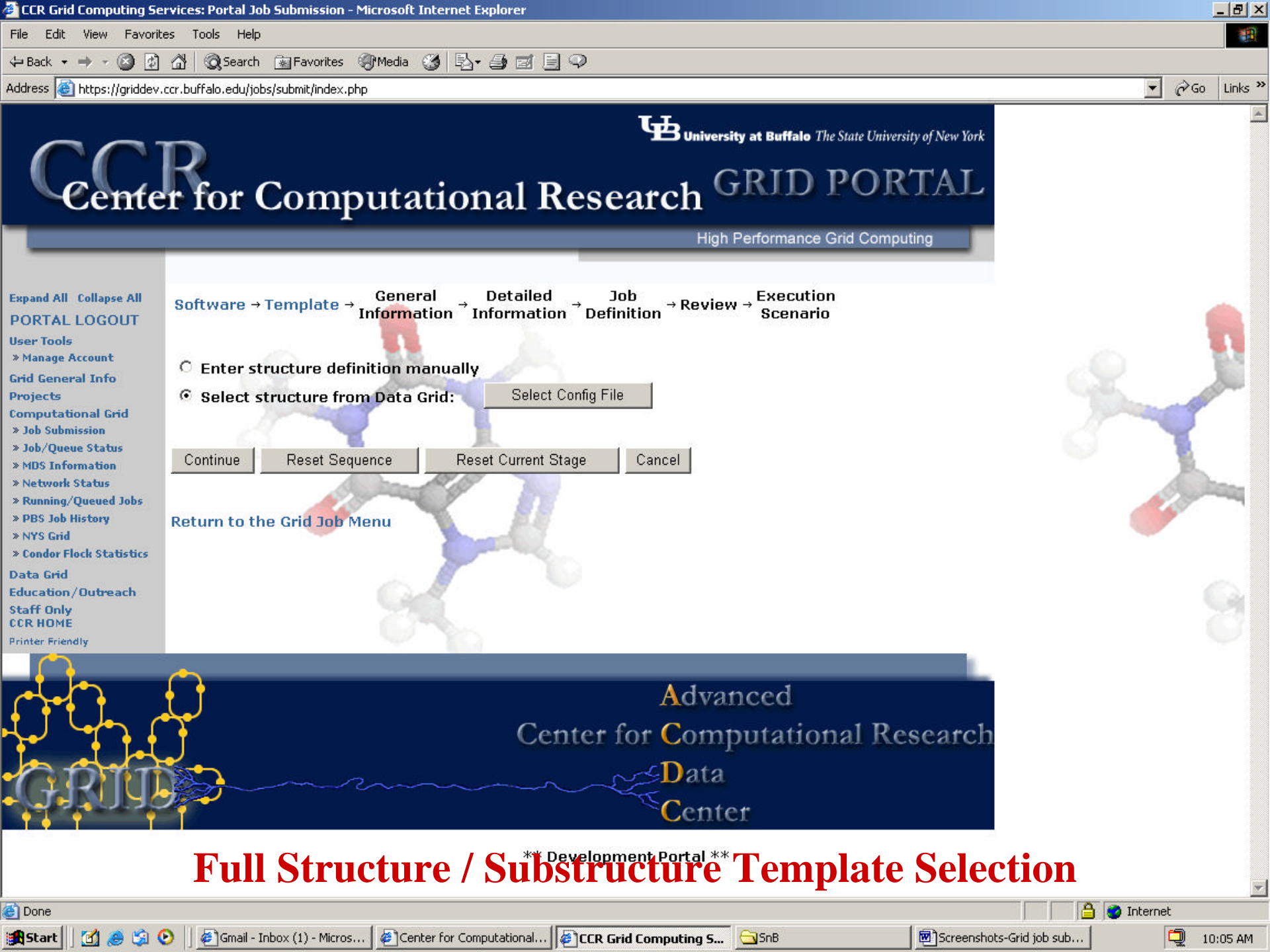
Reset Current Stage

Cancel

Return to the



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



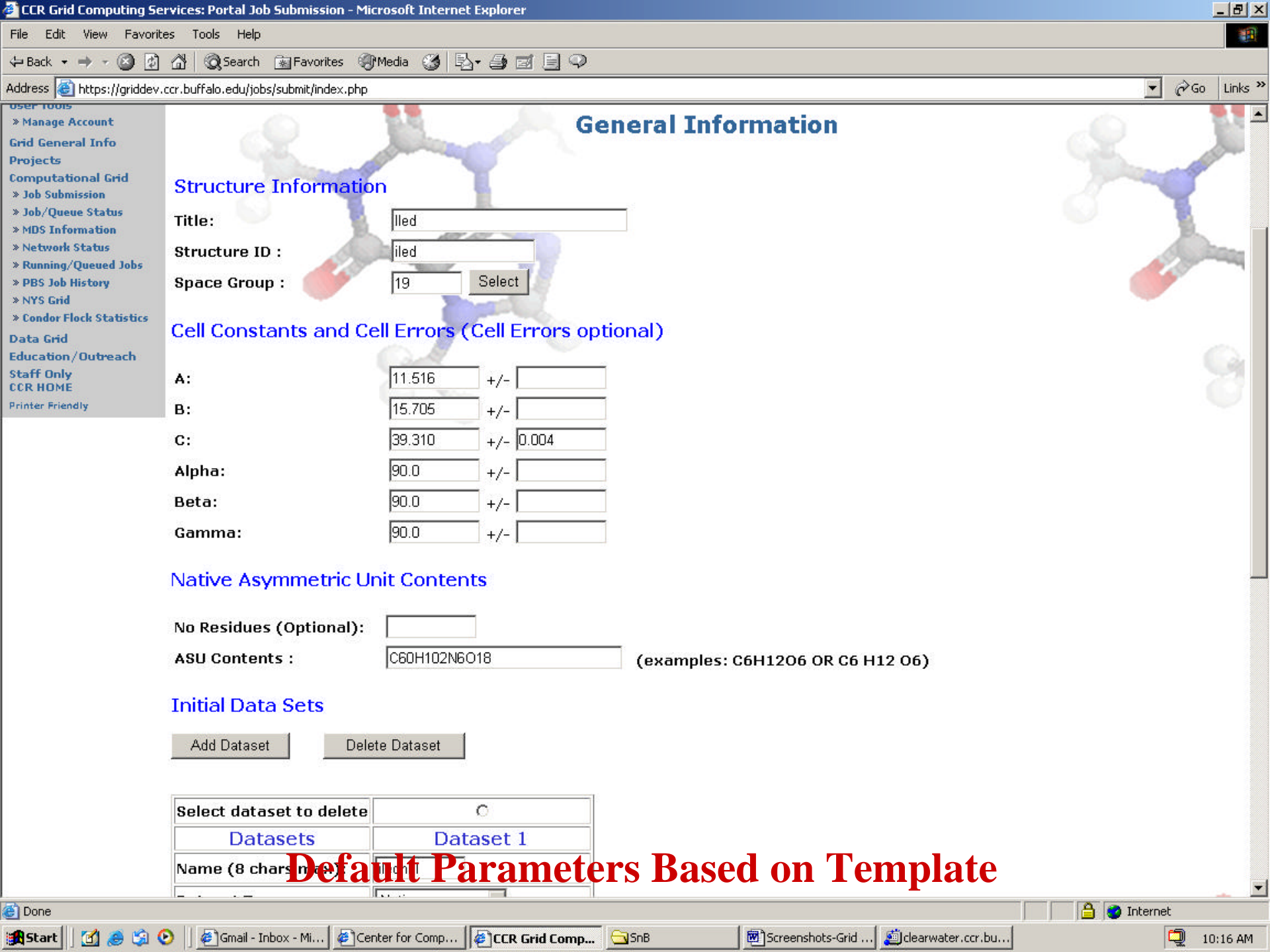
Software → **Template** → General Information → Detailed Information → Job Definition → Review → Execution Scenario

Enter structure definition manually  
 Select structure from Data Grid:

[Return to the Grid Job Menu](#)

**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
- > Condon 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

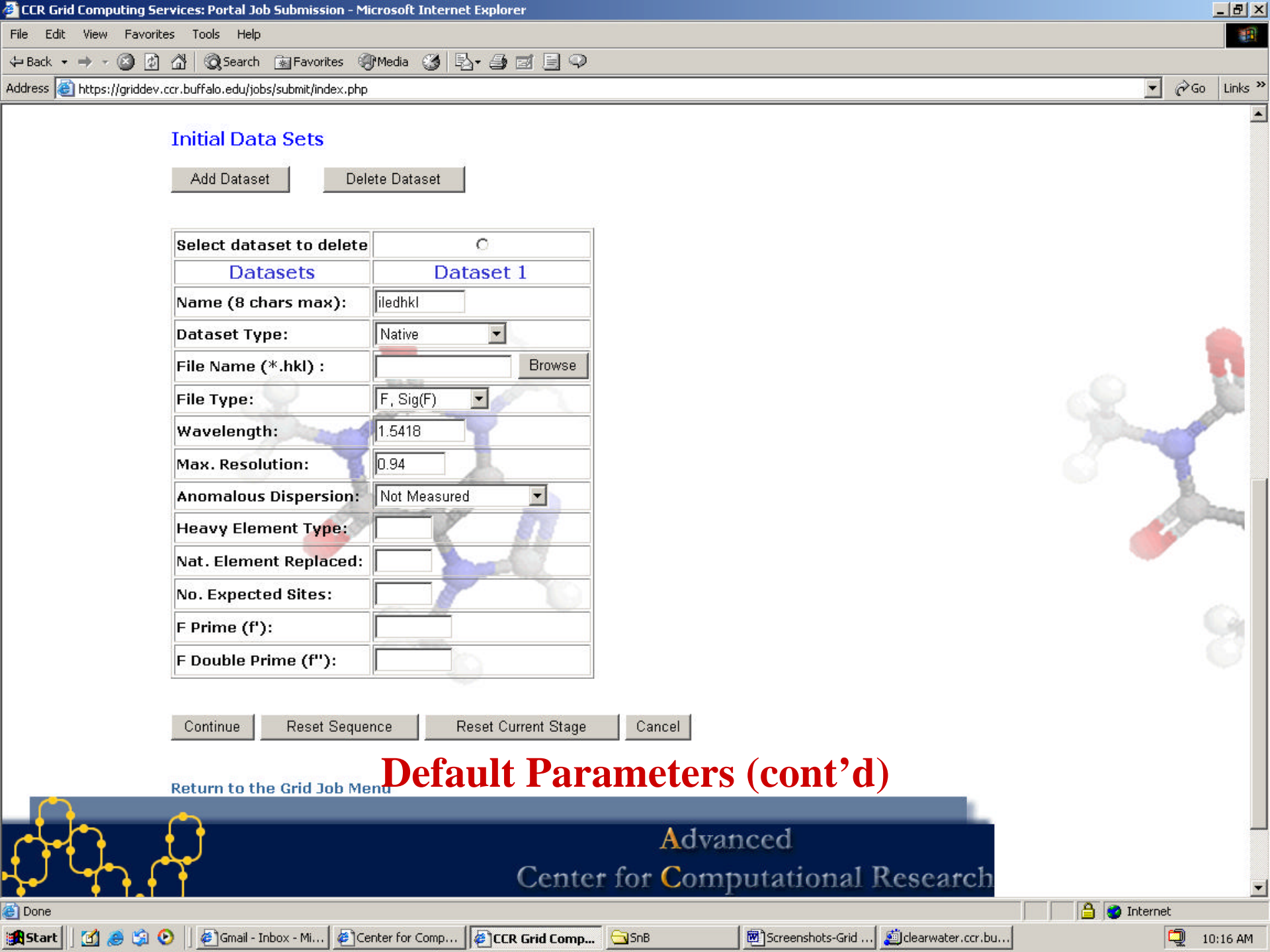
No Residues (Optional):

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

### Initial Data Sets

Select dataset to delete	
<a href="#">Datasets</a>	<a href="#">Dataset 1</a>
Name (8 chars max)	

**Default Parameters Based on Template**



## Initial Data Sets

Add Dataset

Delete Dataset

Select dataset to delete	Dataset 1
<b>Datasets</b>	<b>Dataset 1</b>
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

Done

Start

Gmail - Inbox - Mi...

Center for Comp...

CCR Grid Comp...

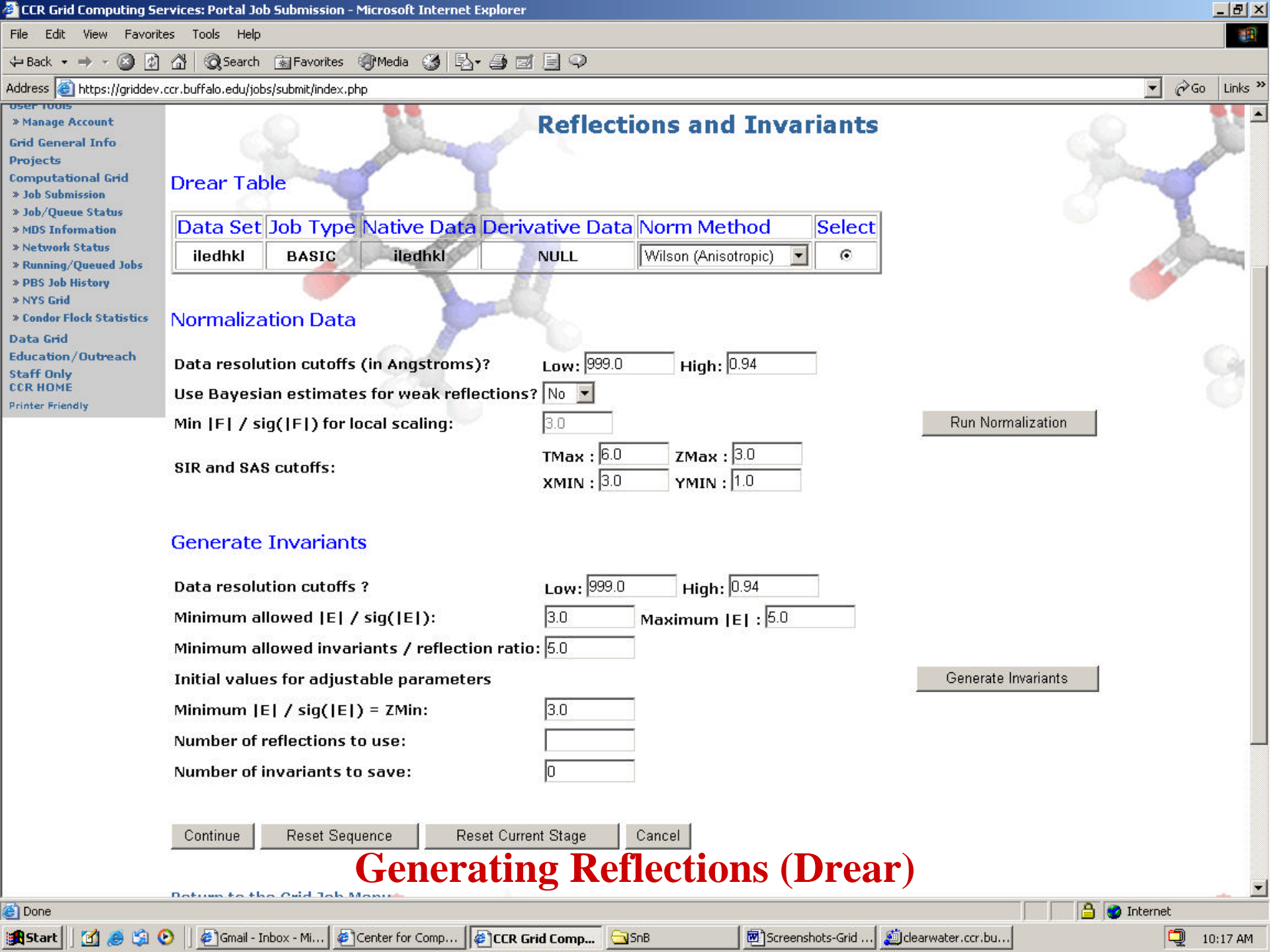
SnB

Screenshots-Grid ...

clearwater.ccr.bu...

Internet

10:16 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

## 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 :

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

**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:

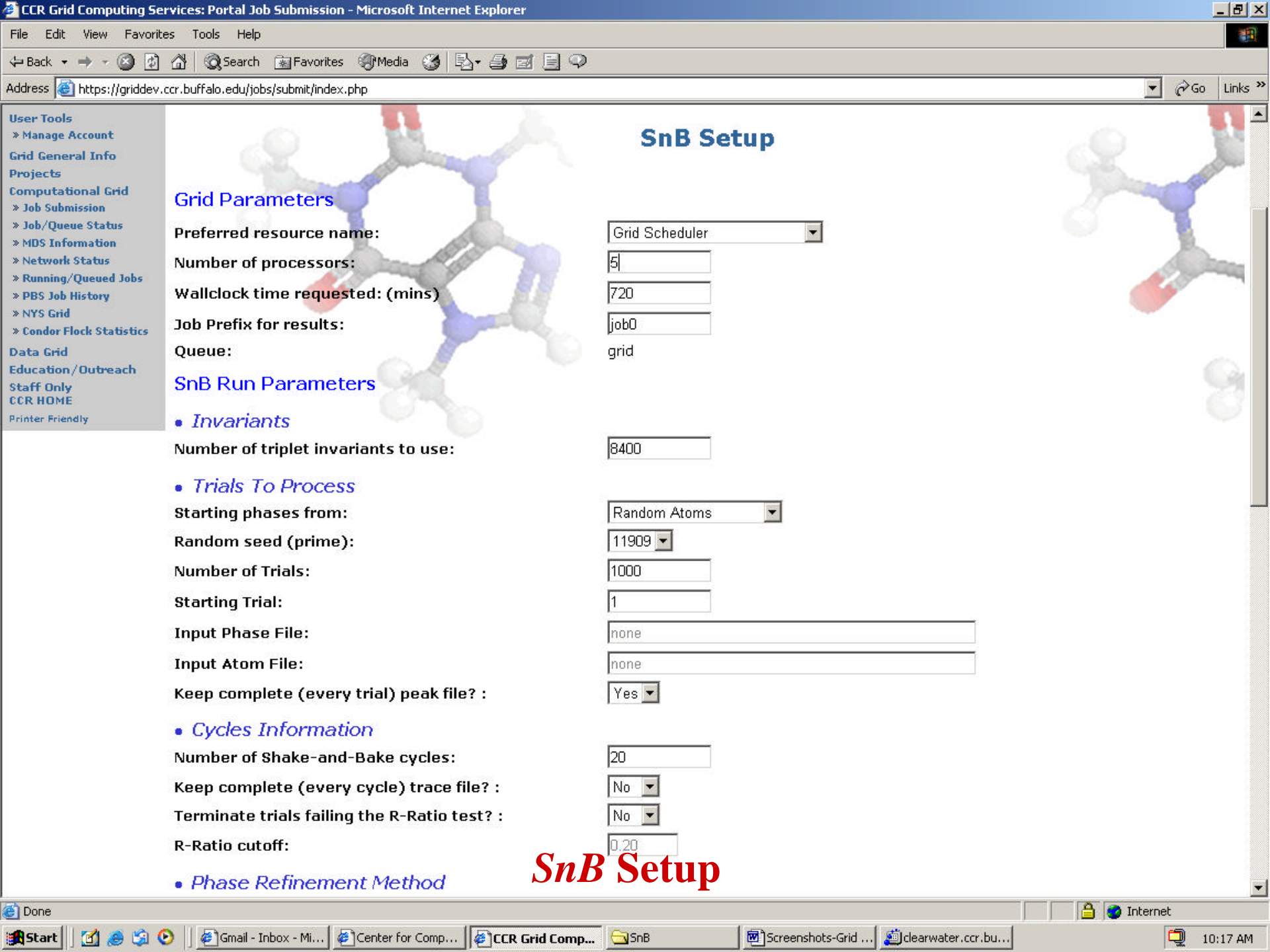
Number of reflections to use:

Number of invariants to save:

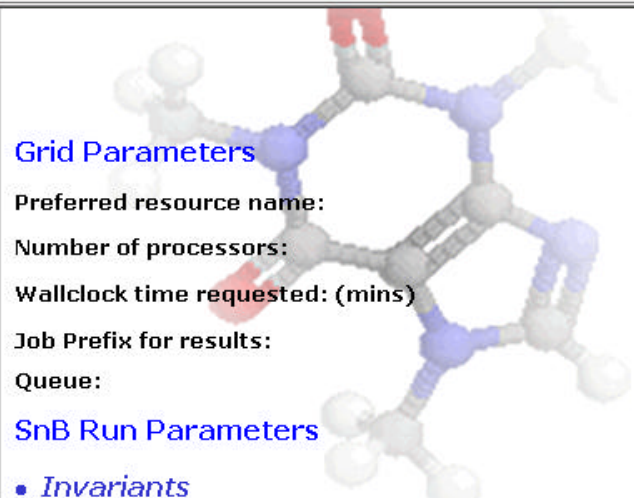
Generate Invariants

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

Back Forward Stop Home Search Favorites Media

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

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>

**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

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

# SnB Review (Grid job ID: 447)

Done

Start

Gmail - Inbox - Mi...

Center for Comp...

CCR Grid Comp...

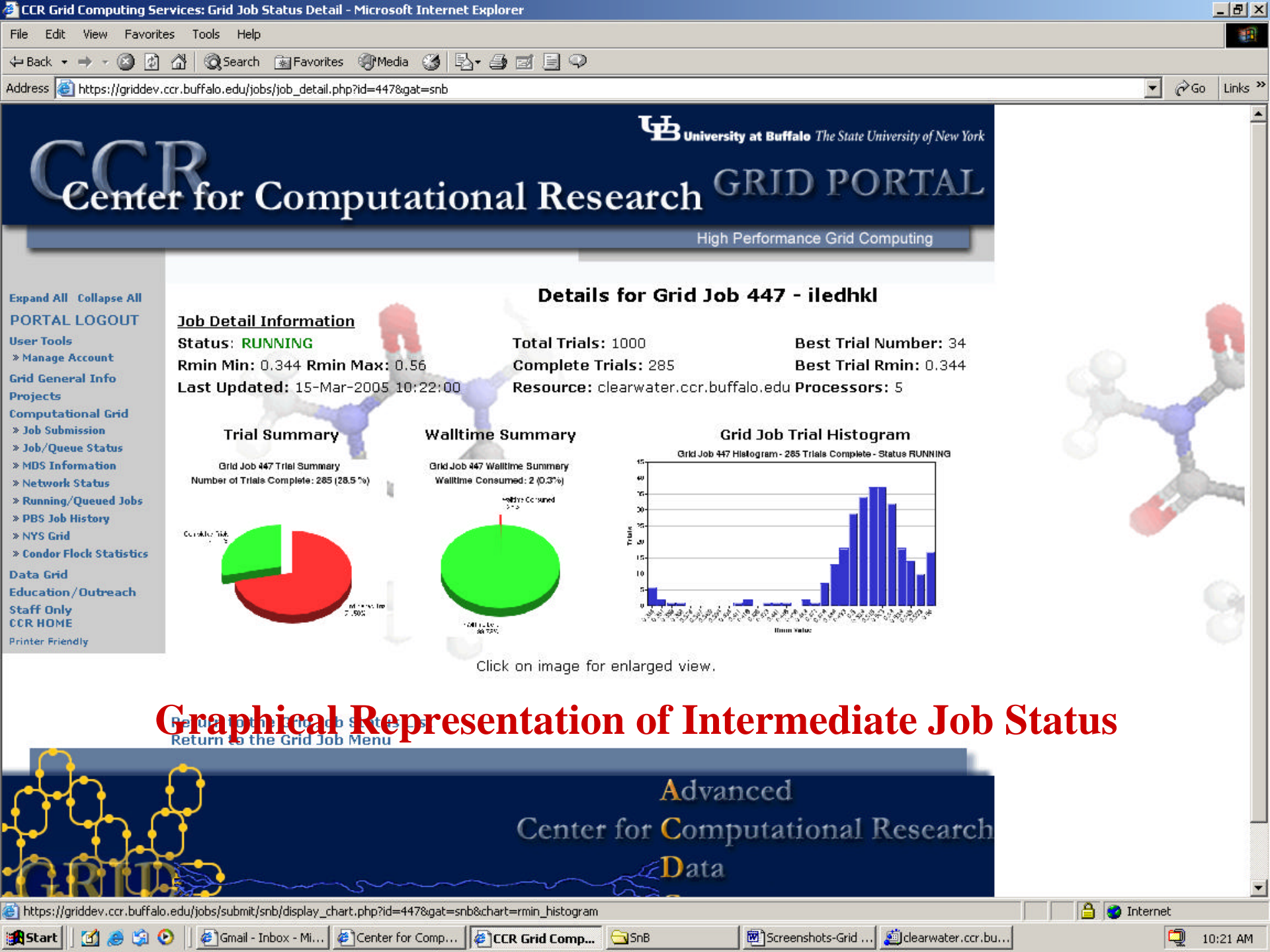
SnB

Screenshots-Grid ...

clearwater.ccr.bu...

Internet

10:18 AM



# CCR 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

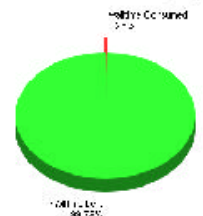
### Trial Summary

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



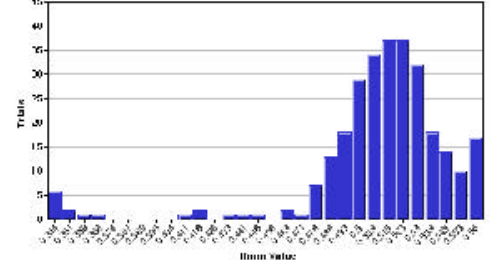
### Walltime Summary

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



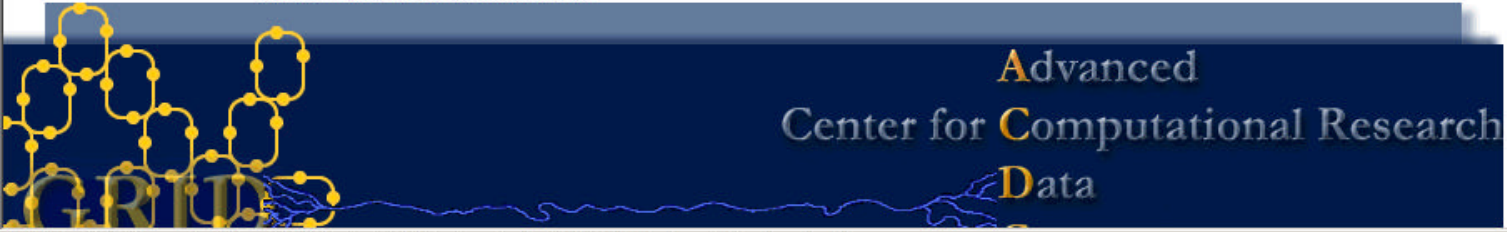
### Grid Job Trial Histogram

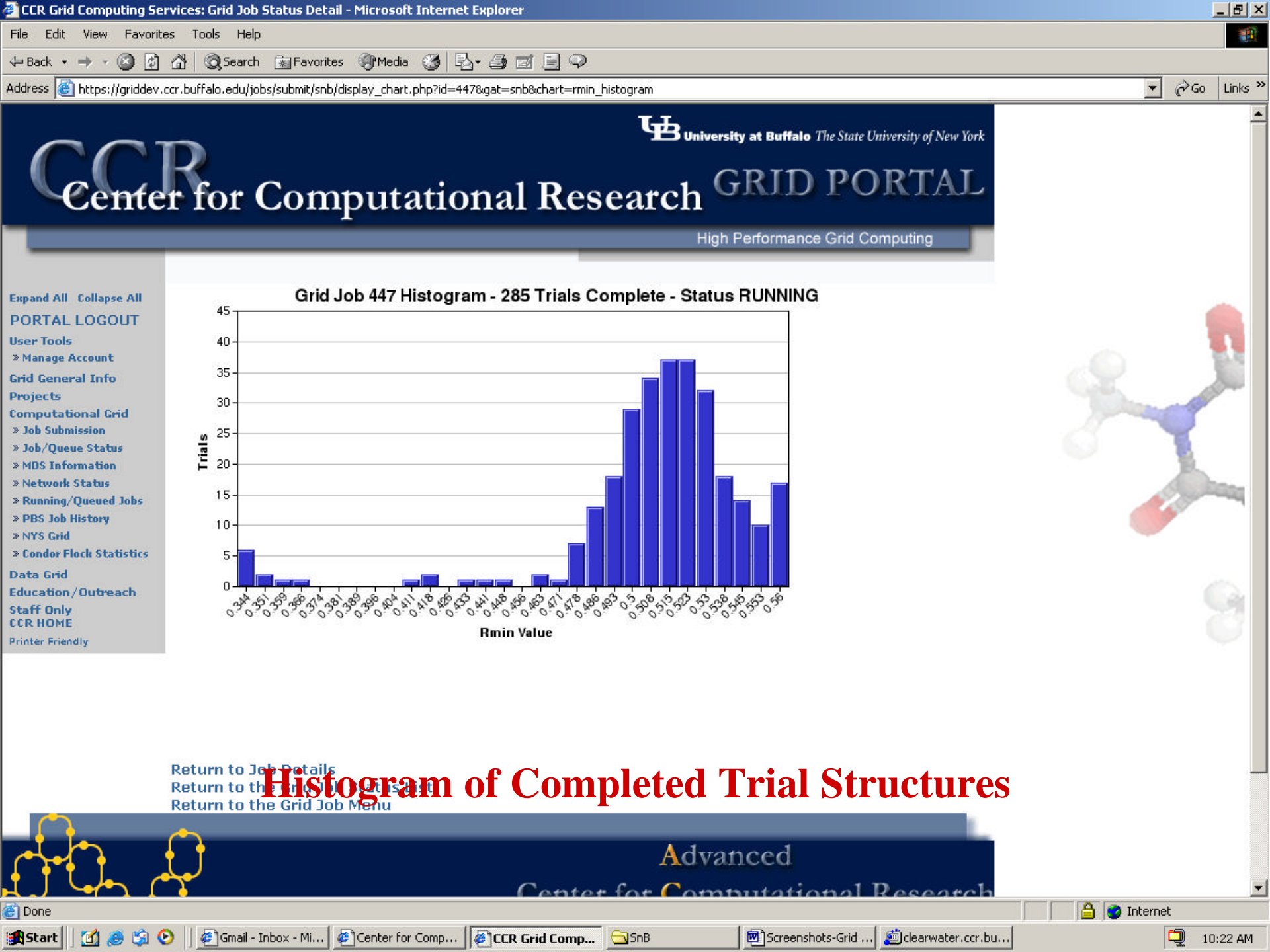
Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING



Click on image for enlarged view.

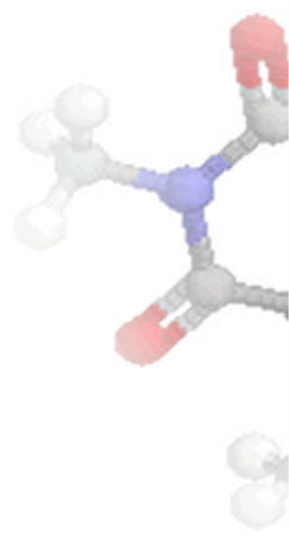
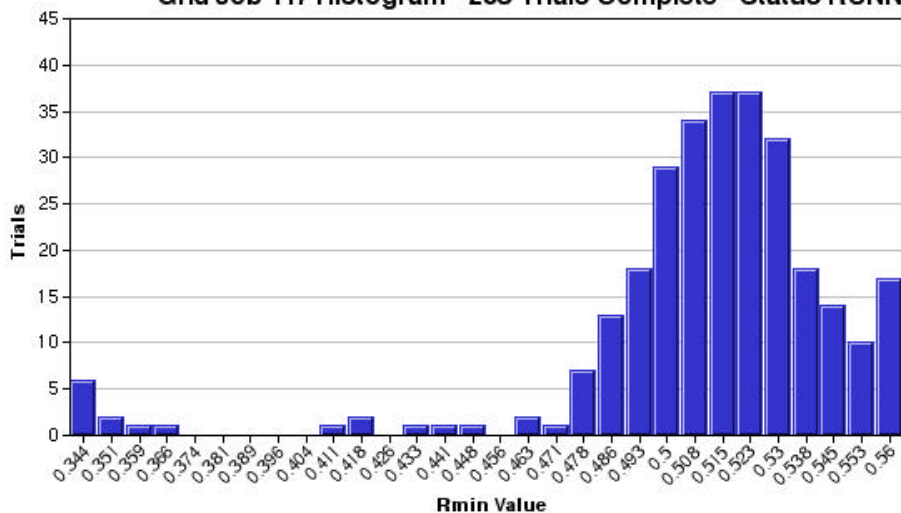
# Graphical Representation of Intermediate Job Status





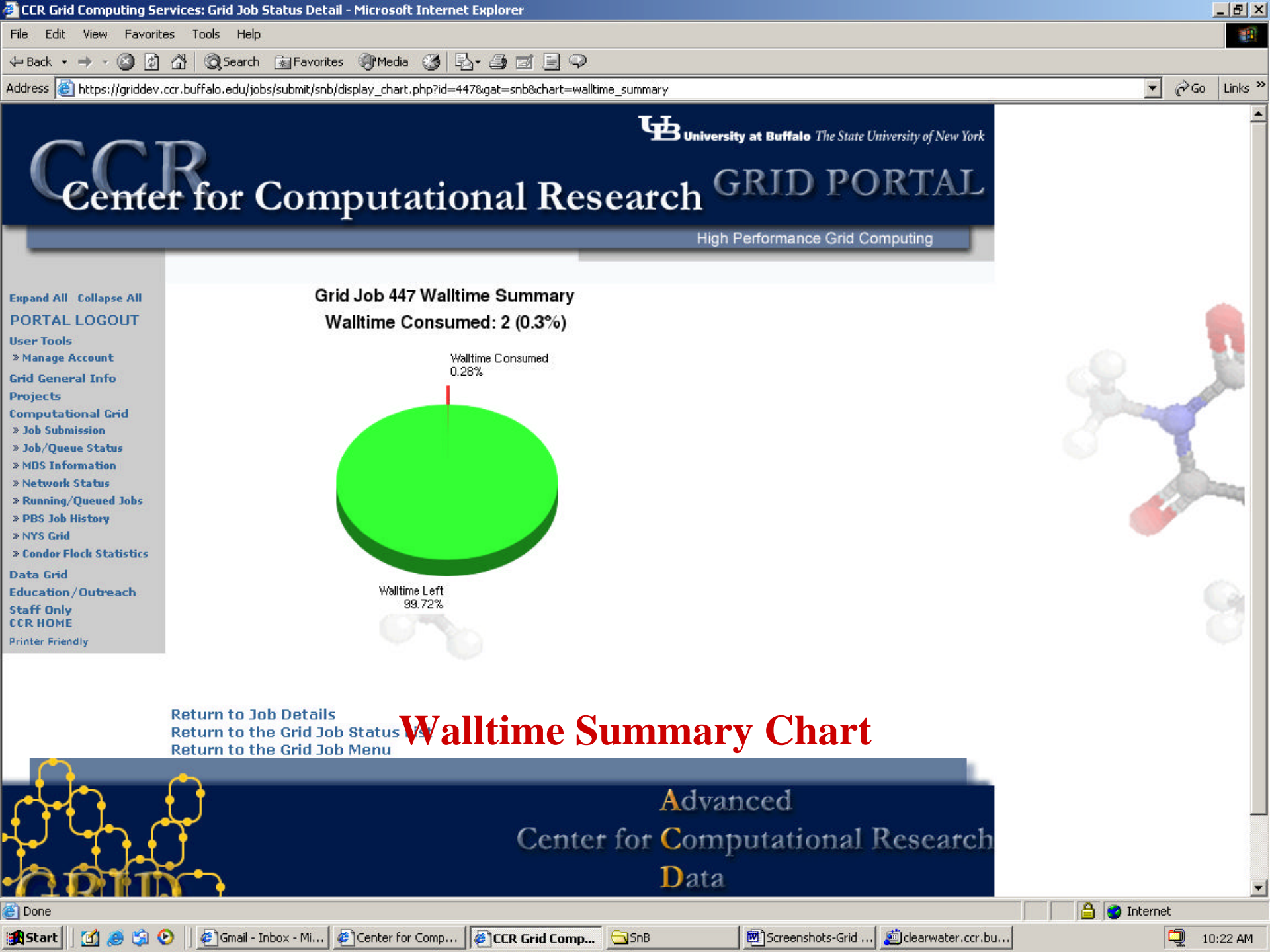
- Expand All Collapse All
- PORTAL LOGOUT
- User Tools
  - » Manage Account
- Grid General Info
- Projects
- Computational Grid
  - » Job Submission
  - » Job/Queue Status
  - » MDS Information
  - » Network Status
  - » Running/Queued Jobs
  - » PBS Job History
  - » NYS Grid
  - » Condor Flock Statistics
- 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 List  
 Return to the Grid Job Menu

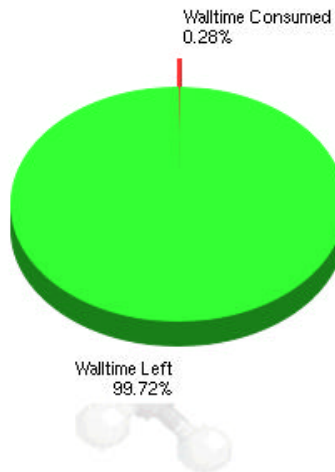
**Histogram of Completed Trial Structures**



# CCR Center for Computational Research GRID PORTAL

High Performance Grid Computing

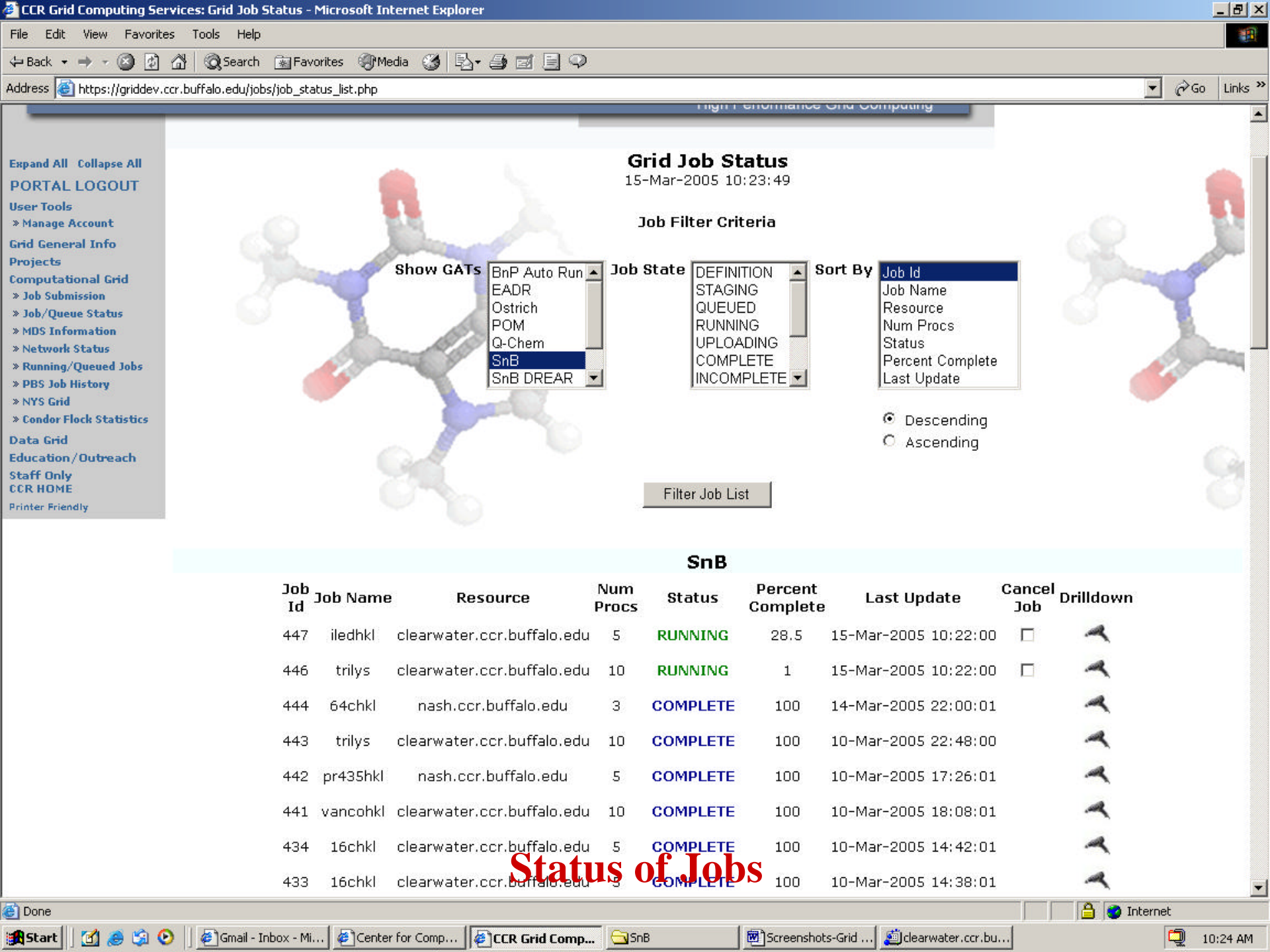
## Grid Job 447 Walltime Summary Walltime Consumed: 2 (0.3%)



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

## Walltime Summary Chart

Advanced  
Center for Computational Research  
Data



## 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

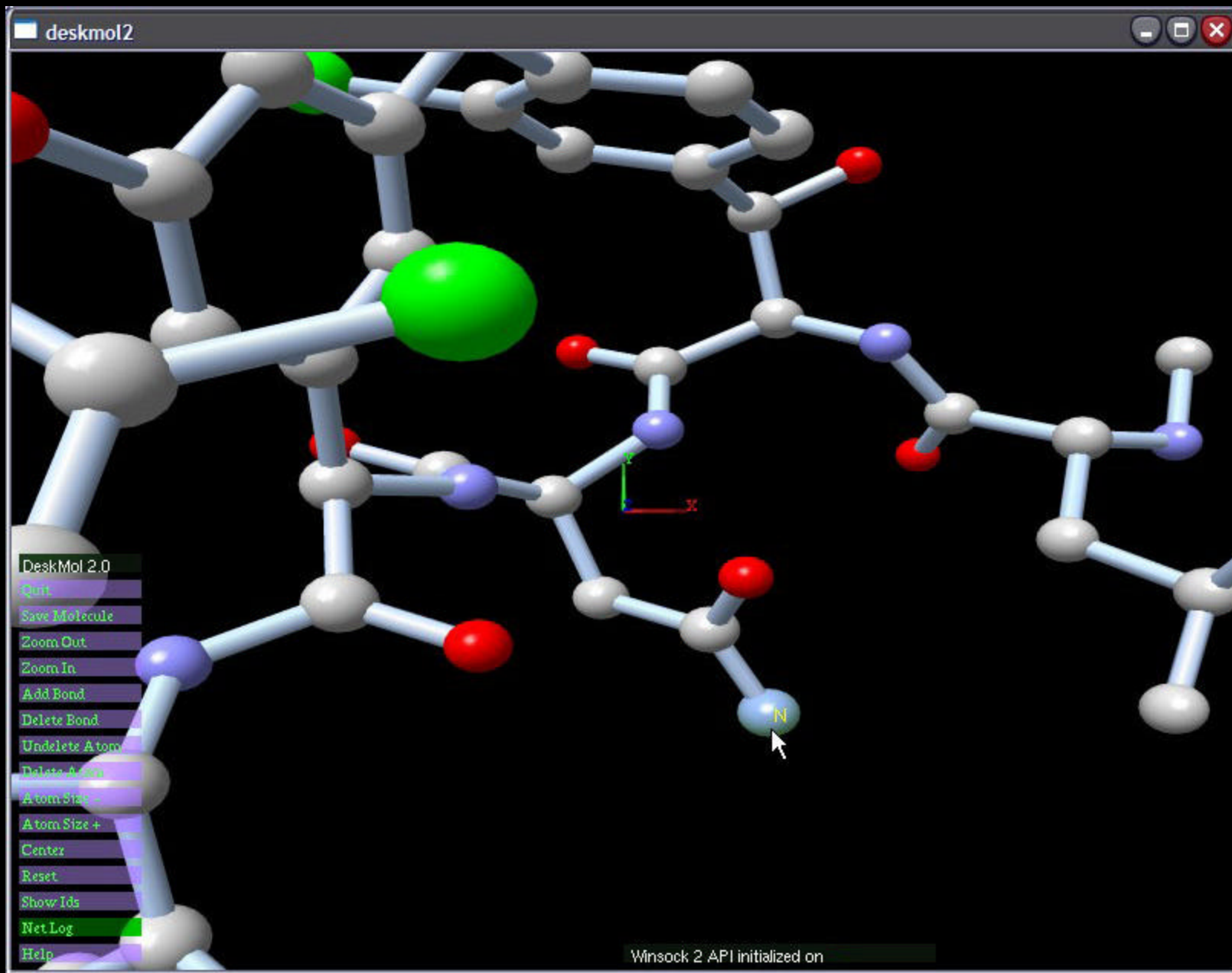
- Descending
- Ascending

Filter Job List

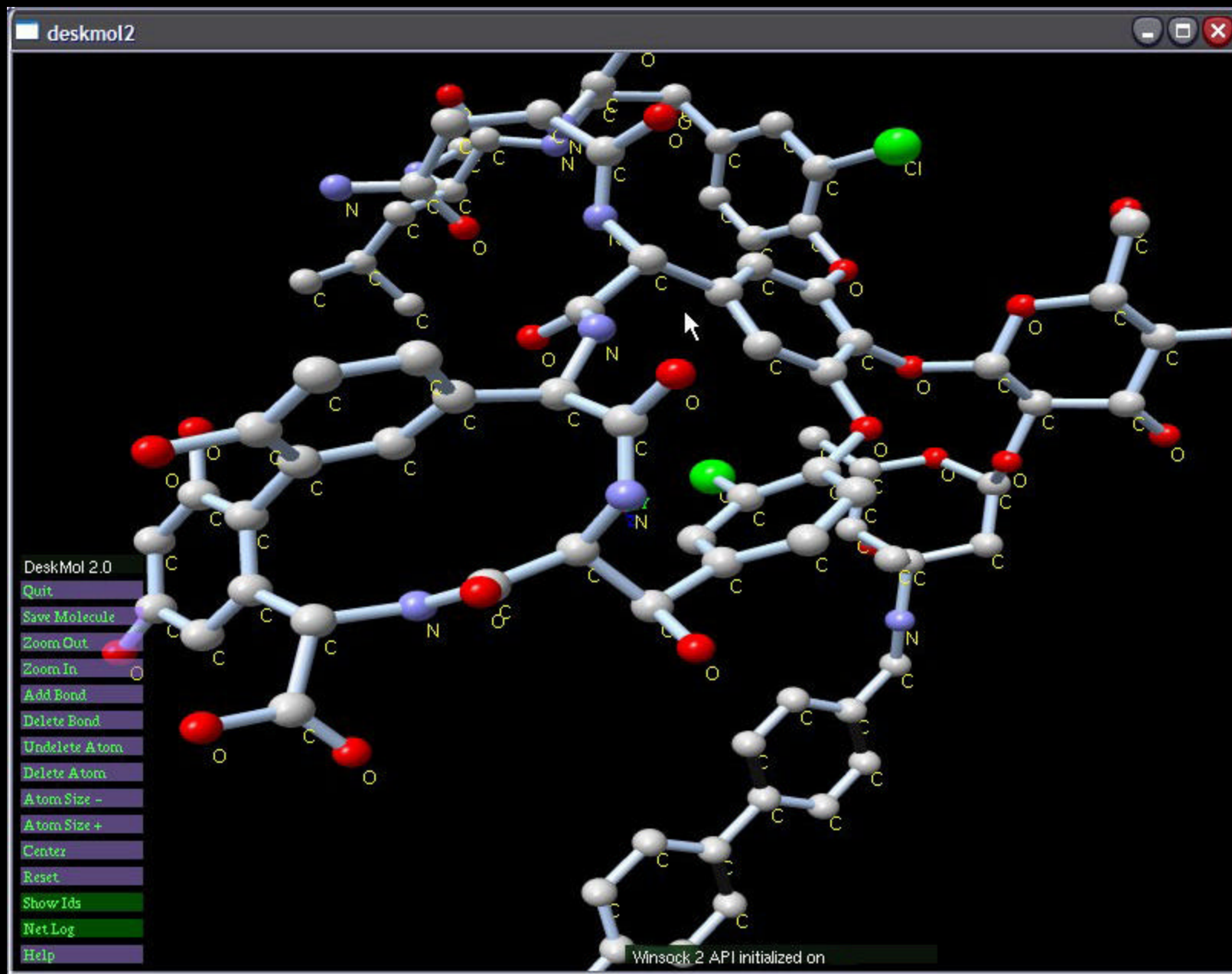
### SnB

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

Status of Jobs

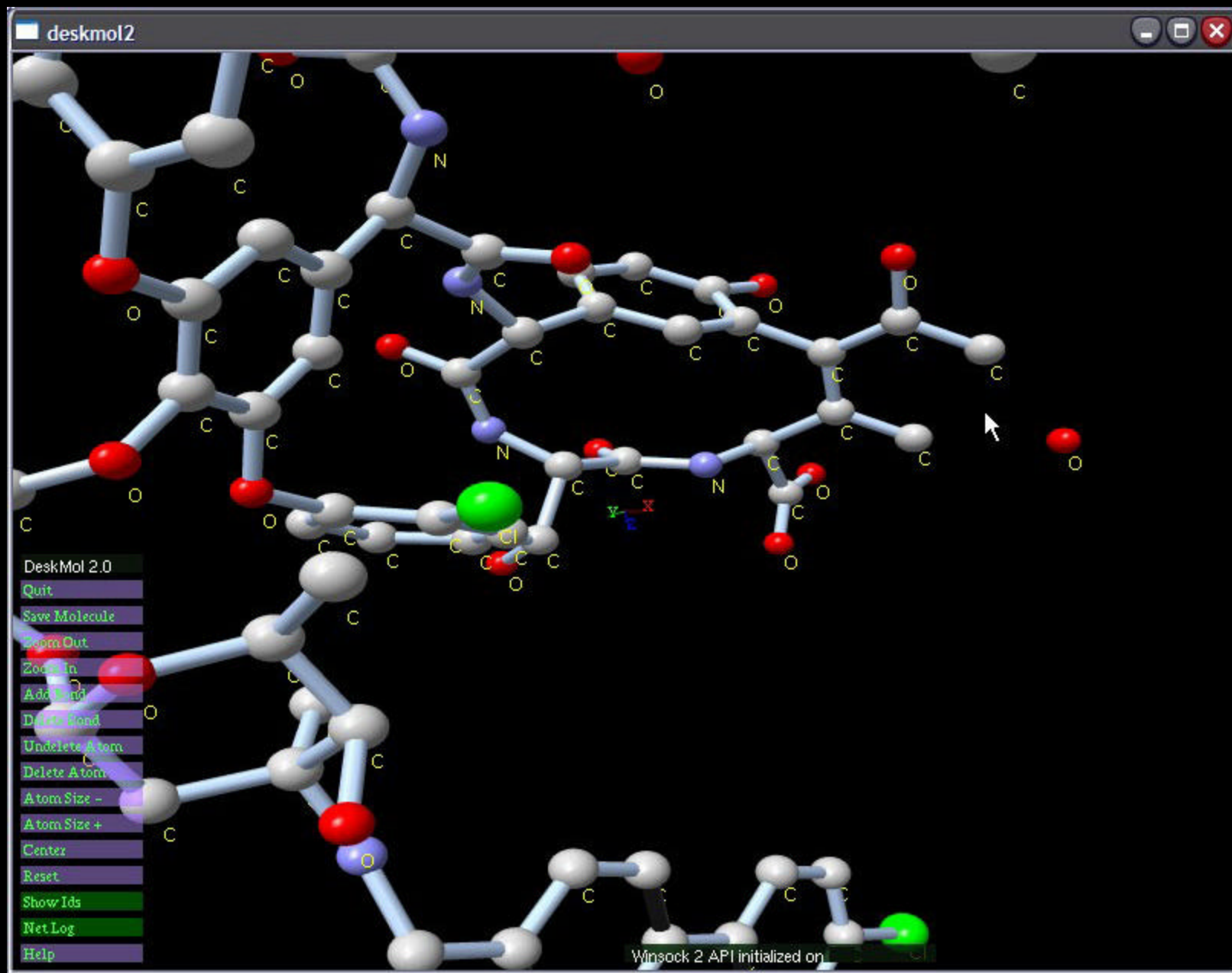


User starts up – default image of structure.

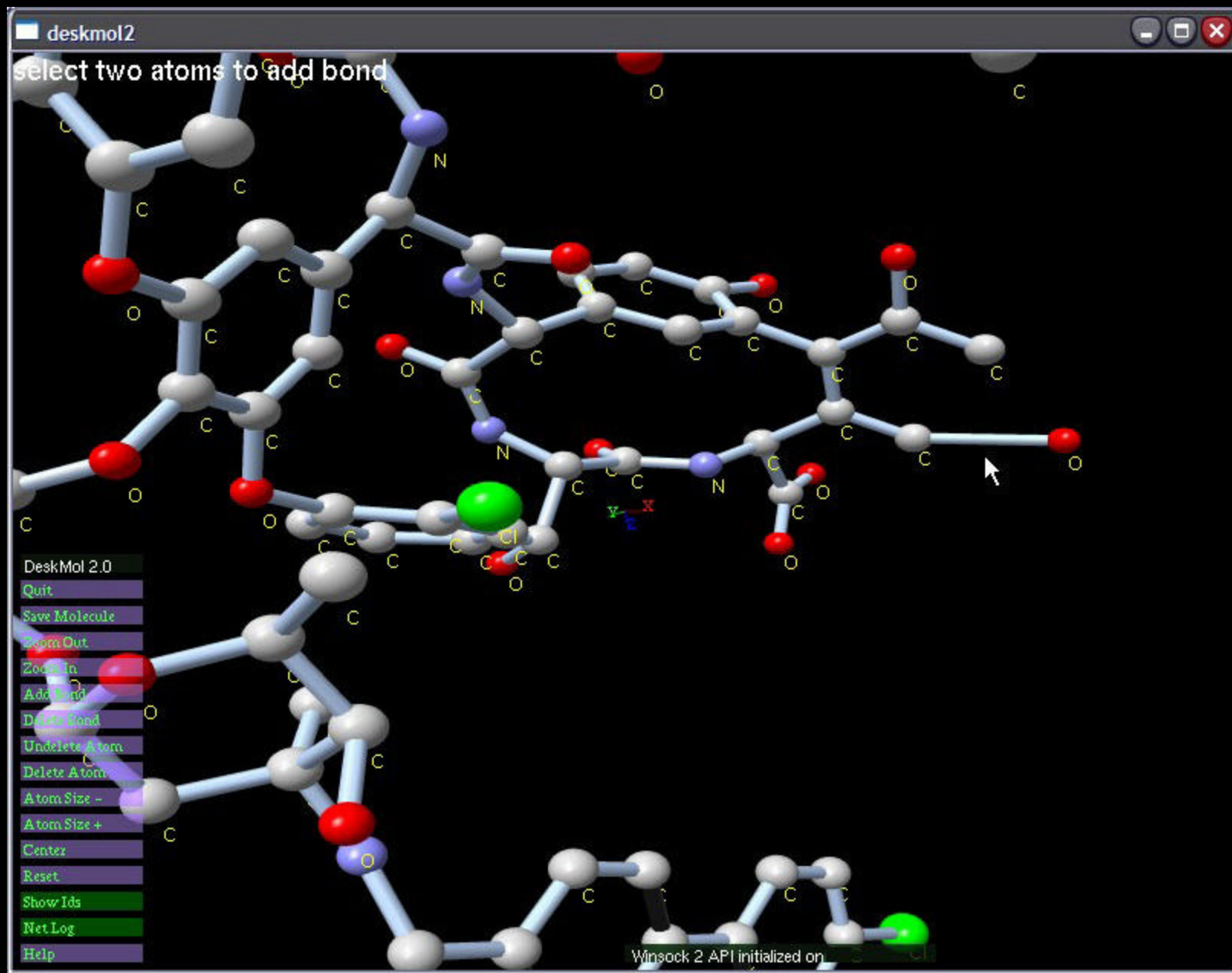


Molecule scaled, rotated, and labeled.





Remove Carbon Atoms (and Links)



User Adds Bond Between Atoms

# Outreach

- **HS Summer Workshops in Computational Science**
  - **Chemistry, Bioinformatics, Visualization**
  - **10-14 HS Students Participate Each Summer for 2 weeks**
  - **Project-Based Program**



# Outreach

## ■ Pilot HS Program in Computational Science

- Year long extracurricular activity at Mount St. Mary's, City Honors, and Orchard Park HS
- Produce next generation scientists and engineers
- Students learn Perl, SQL, Bioinformatics
- \$50,000 startup funding from Verizon, PC's from HP



# Media Coverage

**20th Year**

**BUSINESS FIRST ONLINE**

Go online to access the full text of this article at [buffalo.bizjournals.com](http://buffalo.bizjournals.com)

---

**THIS WEEK**

**COLLECTOR AGENCIES**  
Facing a RPT system  
Page 11

---

**THE CITY**

**Patio home development proposed for Town of Aurora**  
By Anna Lisa  
Page 1

---

**PROJ. DEVELOPMENT**

**Is new construction being up to the standards of fall in Western New York?**  
Page 7

---

**HOUSING PROBLEMS & THE ENVIRONMENT**

**Living here today, with people tomorrow in the region: energy and housing.**  
Page 17

---

**REAL ESTATE**

**Local market shows softening of the market.**  
Page 4

**BUFFALO Business First**  
Western New York's Business Newspaper

---

**HMOs cut Medicare premiums**

The new rules of Independent Health and United HealthCare will decrease the rate of Medicare premiums for those who are 65 and older. The change is an expansion of the Medicare standard cap for Medicare. *Staff Writer*

---


**Patio home development proposed for Town of Aurora**

**Grammy: Designs on Buffalo**


Ani DiFranco, art director up for award

**UB brings bioinformatics to a younger generation**

Darcy Brown, a senior at Mount St. Mary Academy, learned about bioinformatics during a summer workshop at the UB Center for Computational Research.



**EDUCATION**



**An early look at bioinformatics**

University at Buffalo undergraduate David Walsh works with Jaclyn Shaw, right, to demonstrate the "Next Generation Science" program. At left is Swarnan D'Avry.

By EMMA D. SAPIRO  
*News Staff/News Bureau*

For most of Darcy Brown's educational career, science classes have been instructive but somewhat abstract. They've been taught in lecture halls and labs, but she felt behind in the classroom.

That that's not the case anymore for the senior at Mount St. Mary Academy, learned about bioinformatics during a summer workshop at the UB Center for Computational Research.

Bioinformatics is the job that she pursued to become her.

"Most of the students of my generation work from textbooks that contained the same information, but it was not a great experience. A new program implemented at these two high schools for the workshop at Buffalo is changing the way we learn.

"So in my second year of a University at Buffalo Center for Computational Research bioinformatics program geared to high school students. And when she studies DNA in biology class, she can bring that lesson to life by writing a DNA program.

The innovative and rigorous pilot program, called "Next Generation Science: Training for Students and Teachers," merges life sciences and computational science. It is being taught at Mount St. Mary, Orchard Park High School and City Honors School. About two dozen students are involved in the program; they work on smaller versions of the computers used at the research center.

Brown and the three other students in the program demonstrated and spoke about the program Thursday at Mount St. Mary. Awarding were officials from UB and Vermont, which funded the program with a \$50,000 grant.

"When you take science in school, it's really not practical," Brown said. "Bioinformatics has shown me how to apply science in real life. It has really opened doors for me."

E. Bruce Pomeroy, associate dean for research and sponsored programs at UB, said the program also is being implemented in high schools by developing a curriculum and training teachers in opening years.

The students work with a couple of selected teachers in their schools who also are receiving training and three UB undergraduate students.

Senior Courtney Kowalski, who plans to major in mechanical engineering at Clarkson University, said bioinformatics has prepared her for her field of study. She said it's "going to give me a stronger background in engineering."

Because the students are all graduating, Brown said they are trying to recruit students for the program.

"Bioinformatics is really a different experience," she said. "You think of computers and computer programs and the way they are, and now you know the work that goes behind them."

Contact Emma D. Sapiro at [esapiro@buffalo.com](mailto:esapiro@buffalo.com)

# 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**
- **Bruce Holm**
- **Janet Penksa**
- **NSF, NIH, NYS,  
NIMA, NTA, Oishei,  
Wendt, DOE**



www.ccr.buffalo.edu