

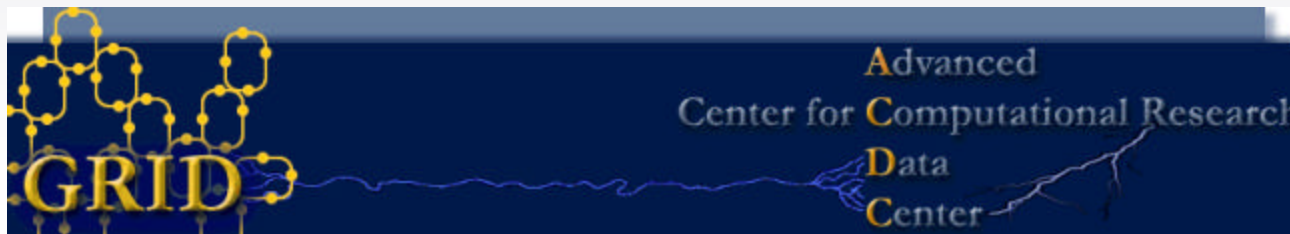
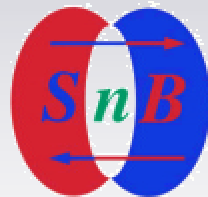
# High-Performance Computing in Buffalo

**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*

# 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
- Support HPC infrastructure, research, and applications
- 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

### □ ~140 Research Groups in 37 Depts

○ Physical Sciences

○ Life Sciences

○ Engineering

○ Scientific Visualization, Medical Imaging, Virtual Reality

### □ 13 Local Companies

### □ 10 Local Institutions

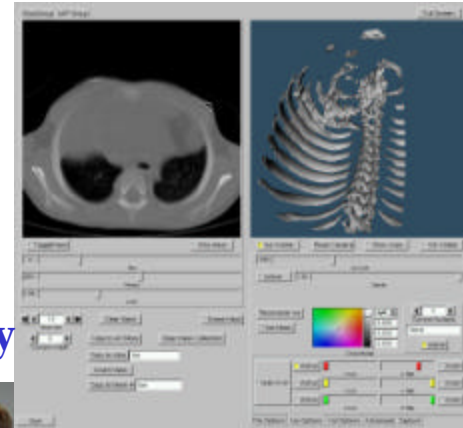
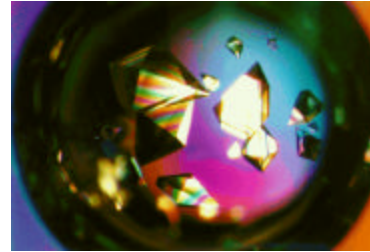
## ■ External Funding: \$300M+

## ■ Total Leveraged WNY: \$500M+

## ■ Deliverables

### □ 1100+ Publications

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



# 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

# Computational Projects

- **Archaeology**
- **Bioinformatics**
- **Computational Chemistry**
- **Computational Fluid Dynamics**
- **Data Mining**
- **Database**
- **Earthquake Engineering**
- **Environmental Modeling & Simulation**
- **Grid Computing**
- **Physics**

# 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



# Visualization Projects

## ■ Traffic Simulation

- Developed StreetScenes
- Meadowlands
- NYSTA
- DOTs

## ■ Urban Design

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

## ■ Media/Art

## ■ CAVE

## ■ Scientific Viz

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

## ■ MTV Monthly Show

## ■ Accident Reconstruction

## ■ Spin-off Companies



# 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

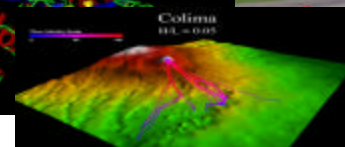
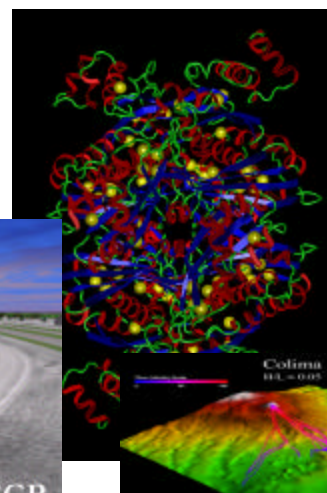
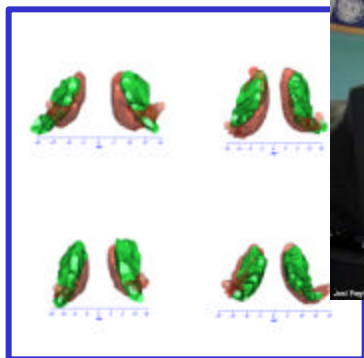
## ■ Current (New) Funding Model

- ❑ 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





# Peace Bridge Visualization

## ■ Proposed Options

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

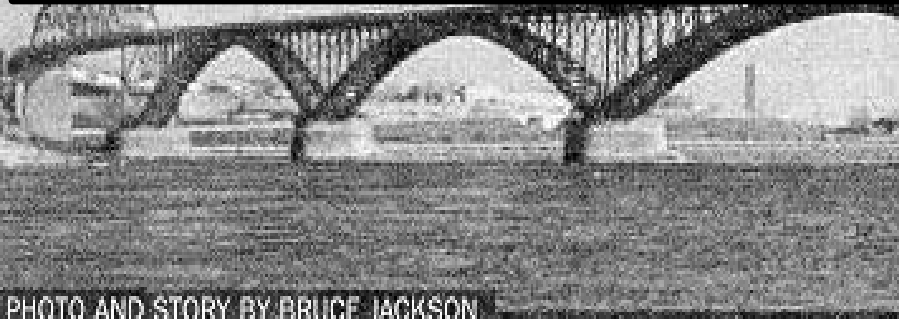


PHOTO AND STORY BY BRUCE JACKSON





# Public Forum





# Williamsville Toll Barrier Improvement Project



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



University at Buffalo

*The State University of New York*

Center for Computational Research

**CCR**

# Real-time Simulation

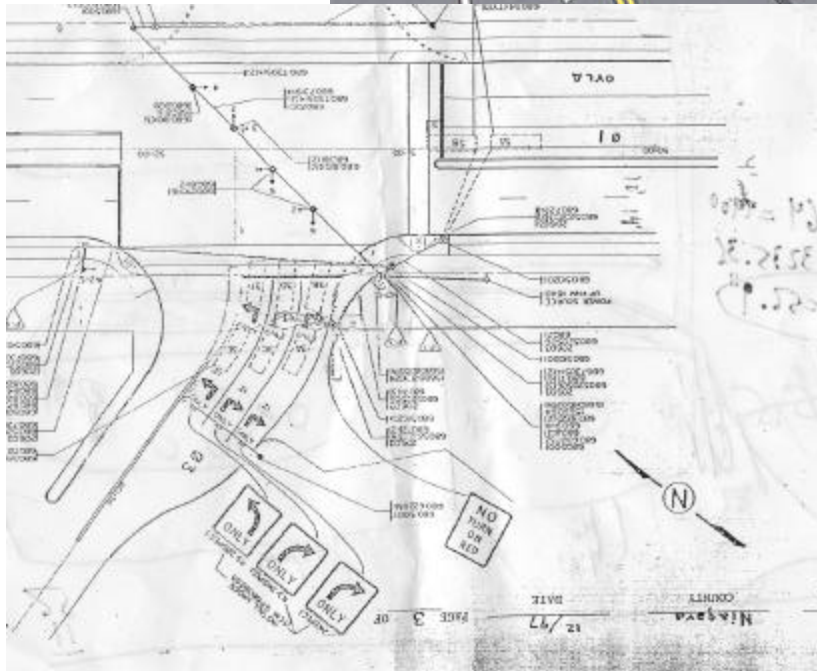
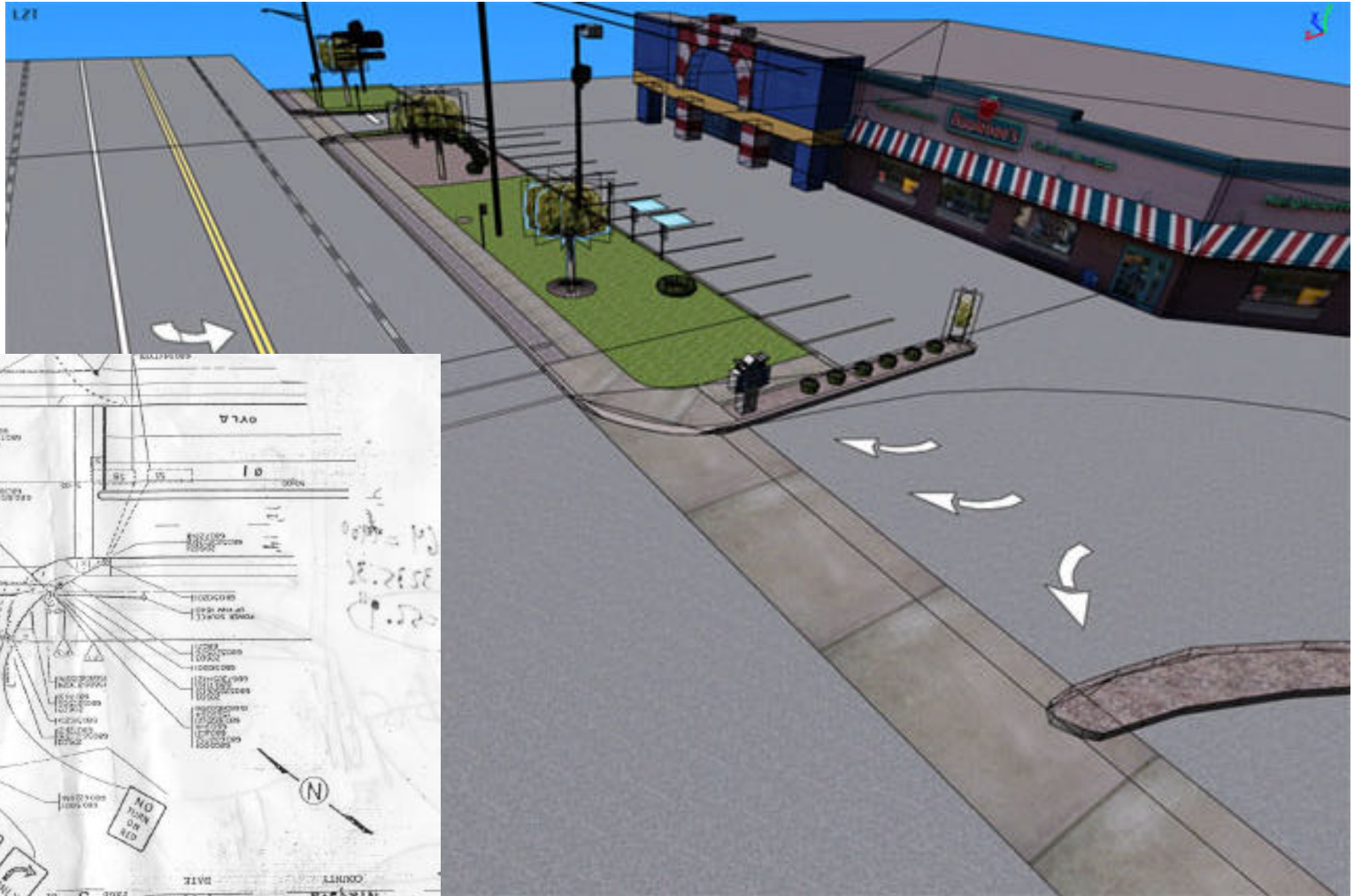


- Key Receptor Sites
- Multiple Viewpoints
- Fully Interactive
- Aerial Photography

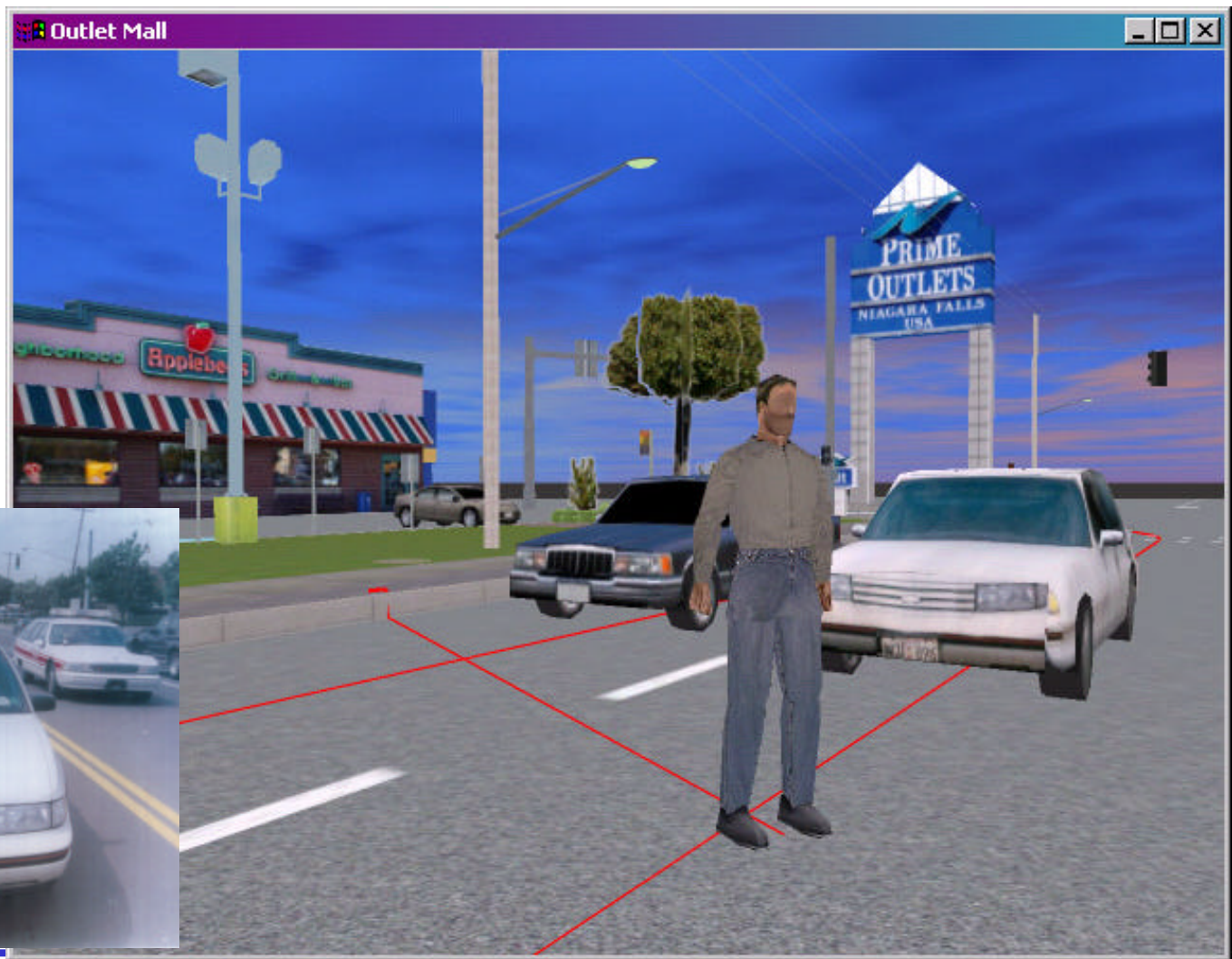




# Accident Reconstruction

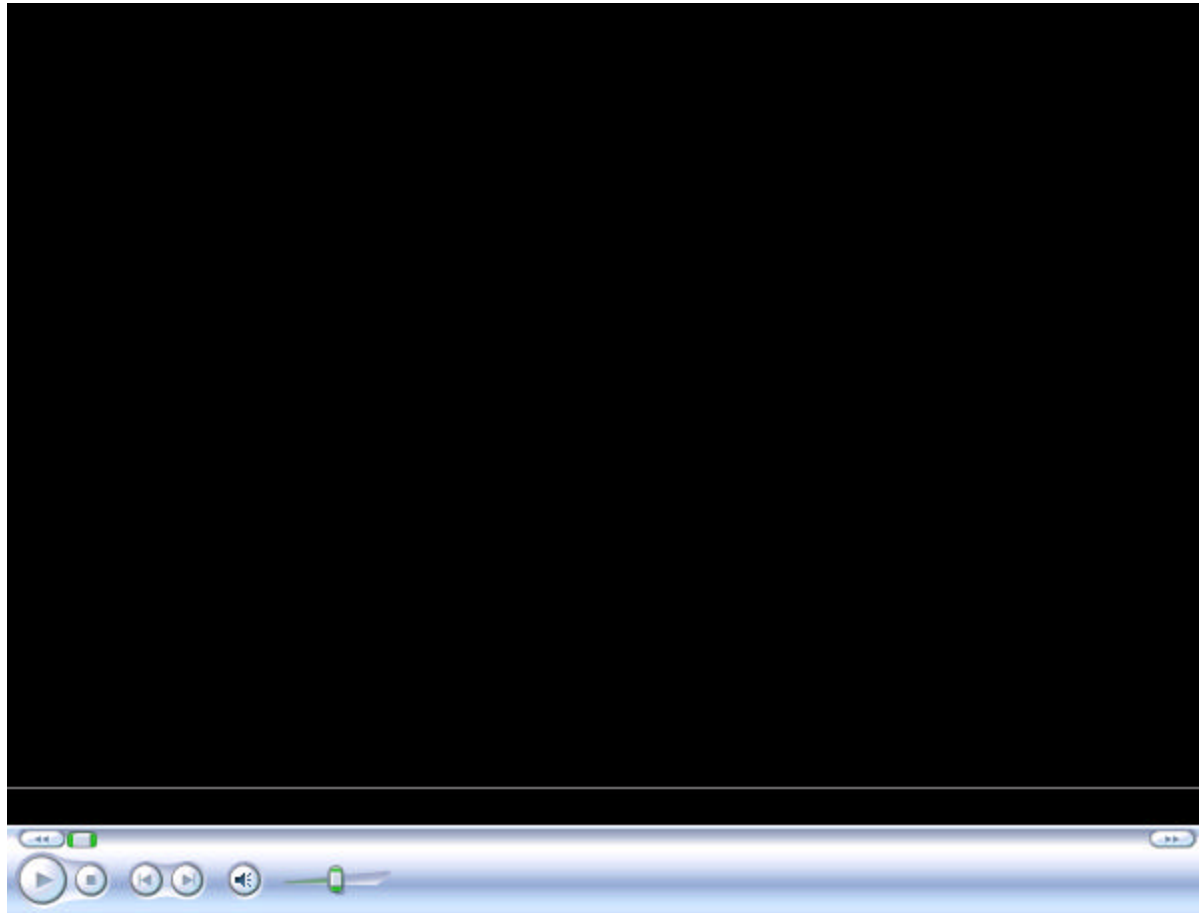


# The Accident





# Accident Animation (Driver's View)



# StreetScenes®

## 3D Traffic Simulation

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

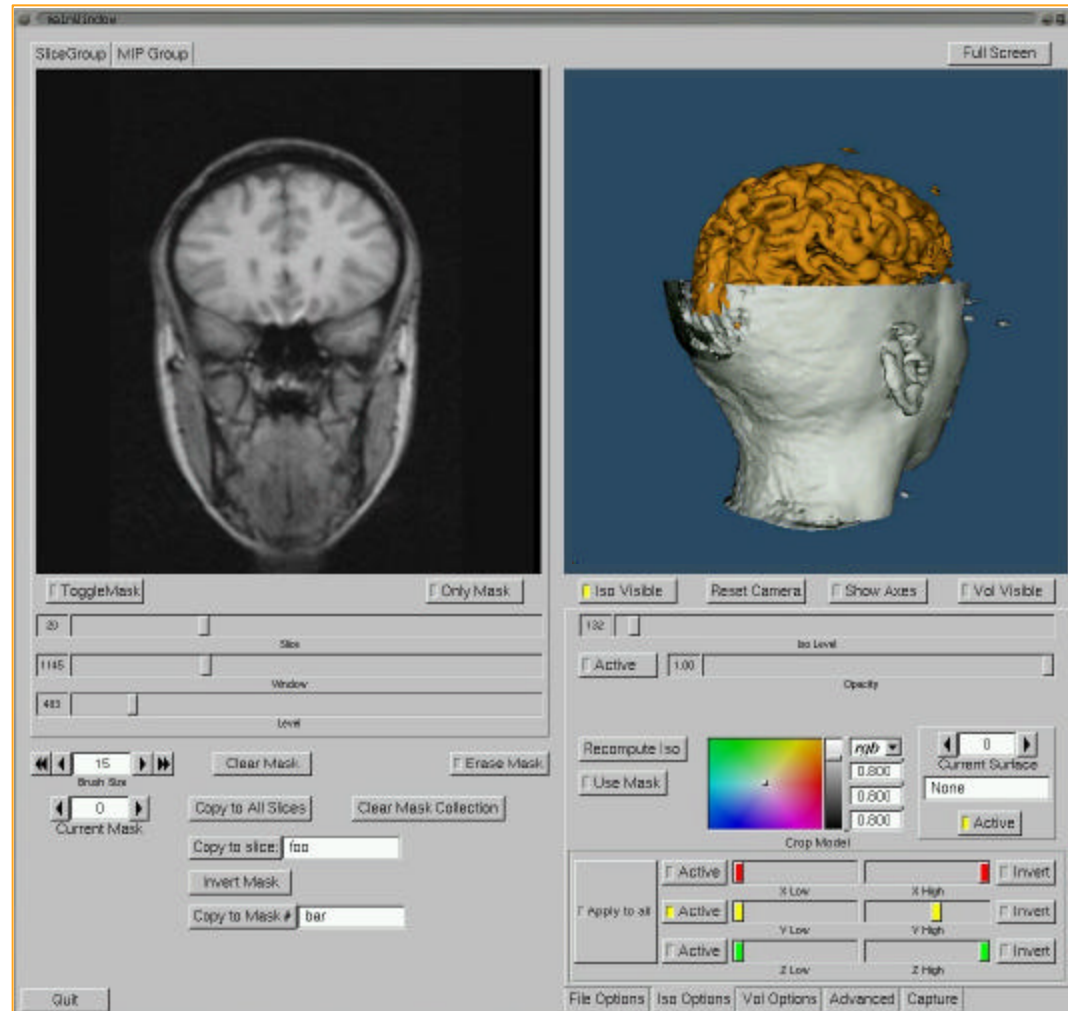


# Multiple Sclerosis Project

- Collaboration with Buffalo Neuroimaging Analysis Center (BNAC)

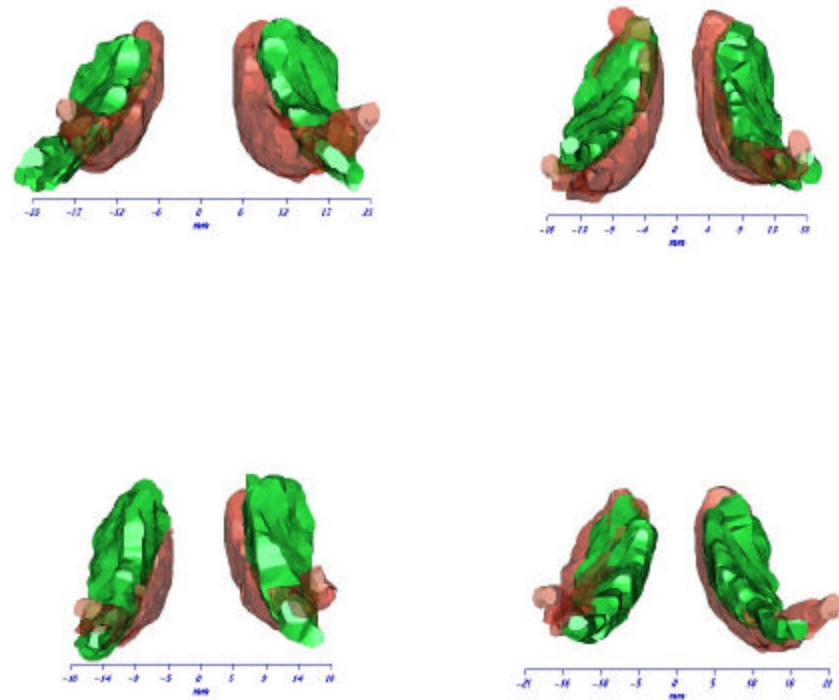
- Developers of Avonex, drug of choice for treatment of MS

- MS Project examines patients and compares scans to healthy volunteers



# Multiple Sclerosis Project

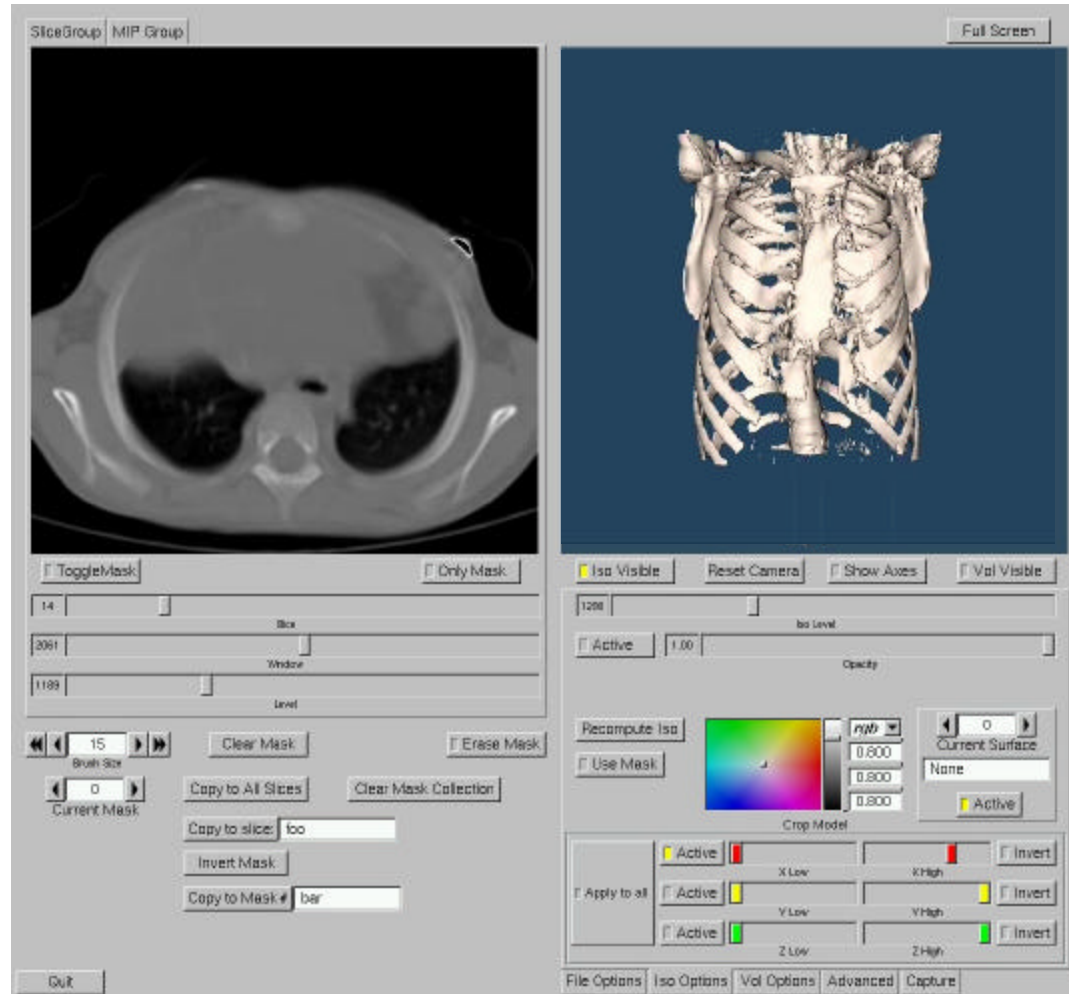
- Compare caudate nuclei between MS patients and healthy controls
- Looking for size as well as structure changes
  - Localized deformities
  - Spacing between halves
- Able to see correlation between disease progression and physical structure changes






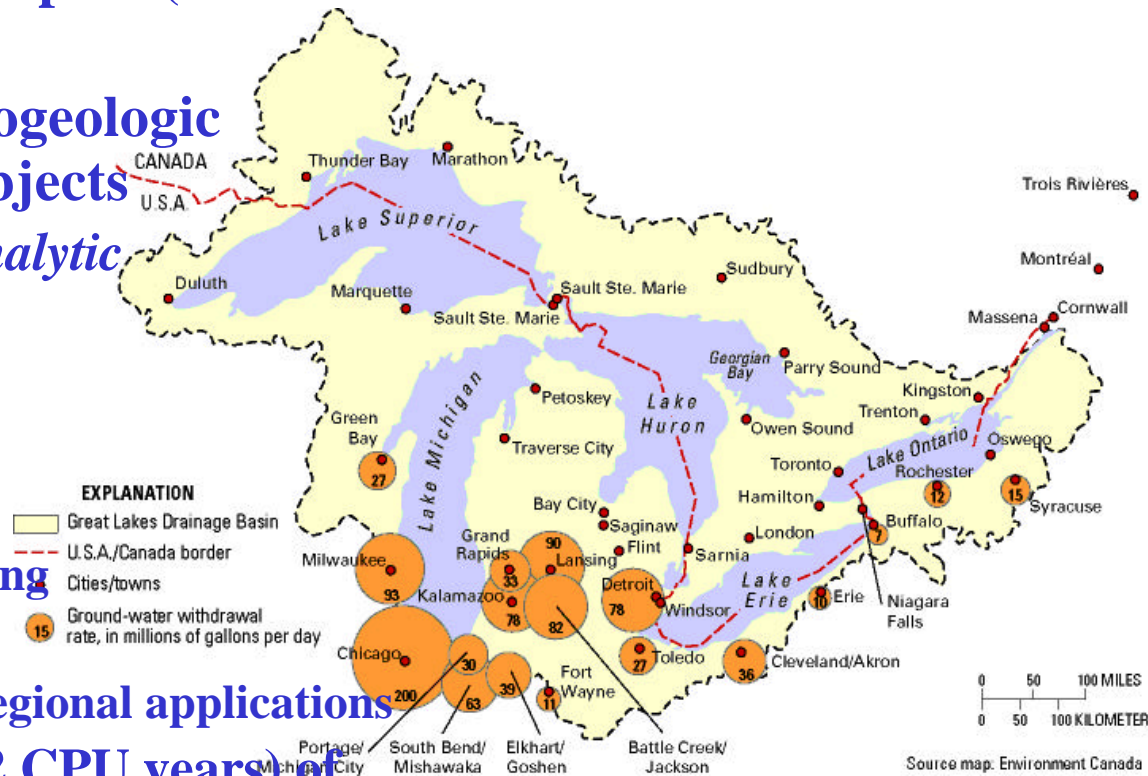
# 3D Medical Visualization App

- 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



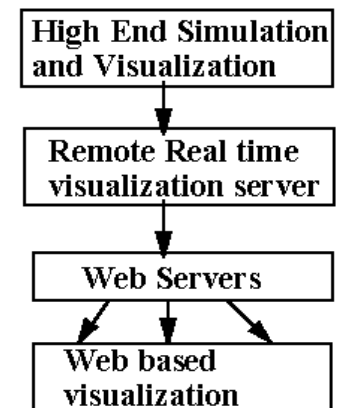
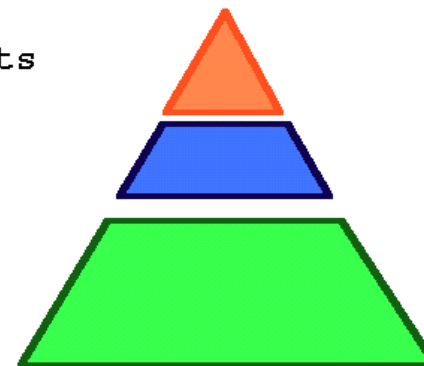
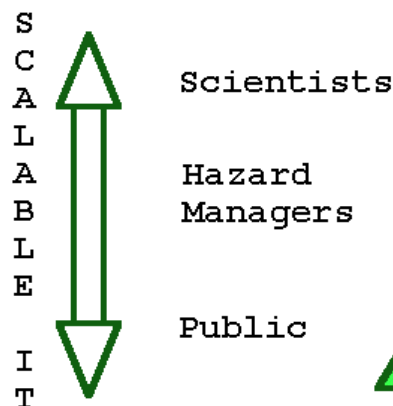
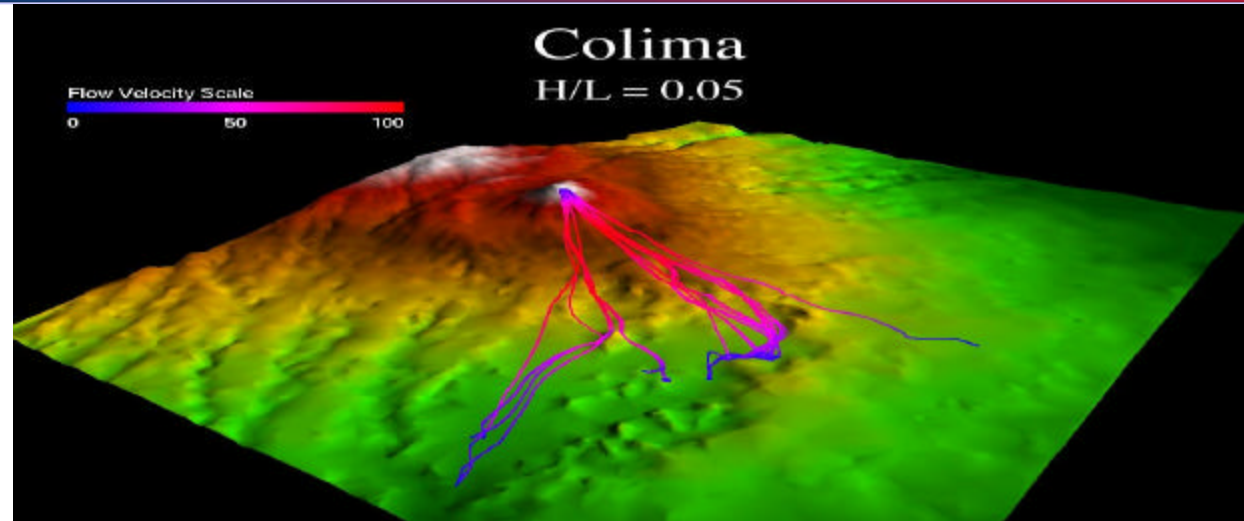
# Groundwater Flow Modeling

- **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**
- 
- The map shows the Great Lakes Drainage Basin, which includes Lake Superior, Lake Michigan, and Lake Huron. The U.S.A./Canada border is indicated by a dashed line. Cities/towns shown include Duluth, Marquette, Green Bay, Milwaukee, and Chicago. Ground-water withdrawal rates are indicated by orange circles with numbers inside, representing millions of gallons per day. The legend (EXPLANATION) defines the symbols: a yellow area for the Great Lakes Drainage Basin, a dashed line for the U.S.A./Canada border, a red dot for cities/towns, and an orange circle with a number for ground-water withdrawal rate.



# 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





# 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



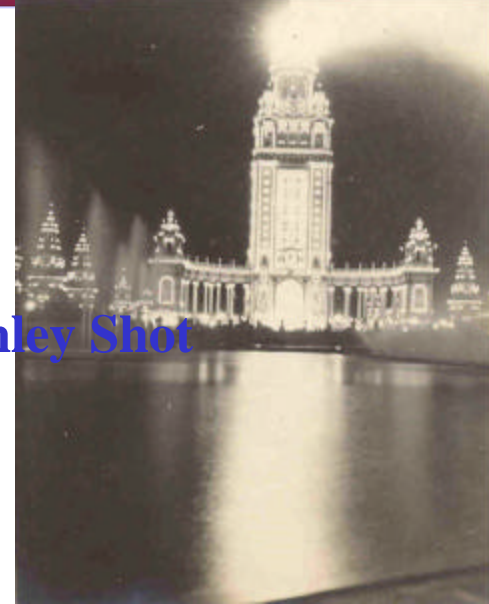




# Buffalo, New York



- The Queen City: 2<sup>nd</sup> Largest City in NYS
- Waterfront City: on North Coast of U.S.
- City of Lights
  - First city in U.S. to have electric street lights
  - Pan American Exposition (1901): Pres. McKinley Shot



- Architecture
  - Frederick Law Olmsted
  - Frank Lloyd Wright
- Underground Railroad: slaves escaped to freedom in Canada

- Four straight Super Bowl appearances

- Culinary Delights

- Pizzanwings
  - Wings invented at Anchor Bar, 1964
- Beef on Weck



- Two Seasons in Buffalo: Winter and July 4



# Recent Biomedical Advances (Buffalo, NY)

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

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

■ **Artificial Blood**

■ **Nicorette Gum**

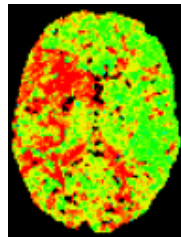
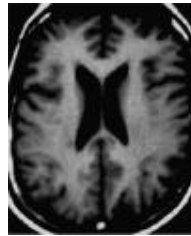
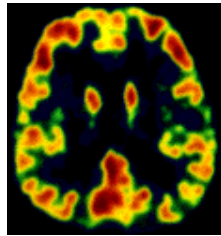
■ **Fetal Viability Test**

■ **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”**

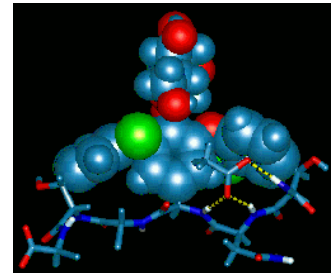
■ **Vancomycin**

■ **Gramacidin A**

■ **High Throughput Crystallization Method: Patented**

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

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

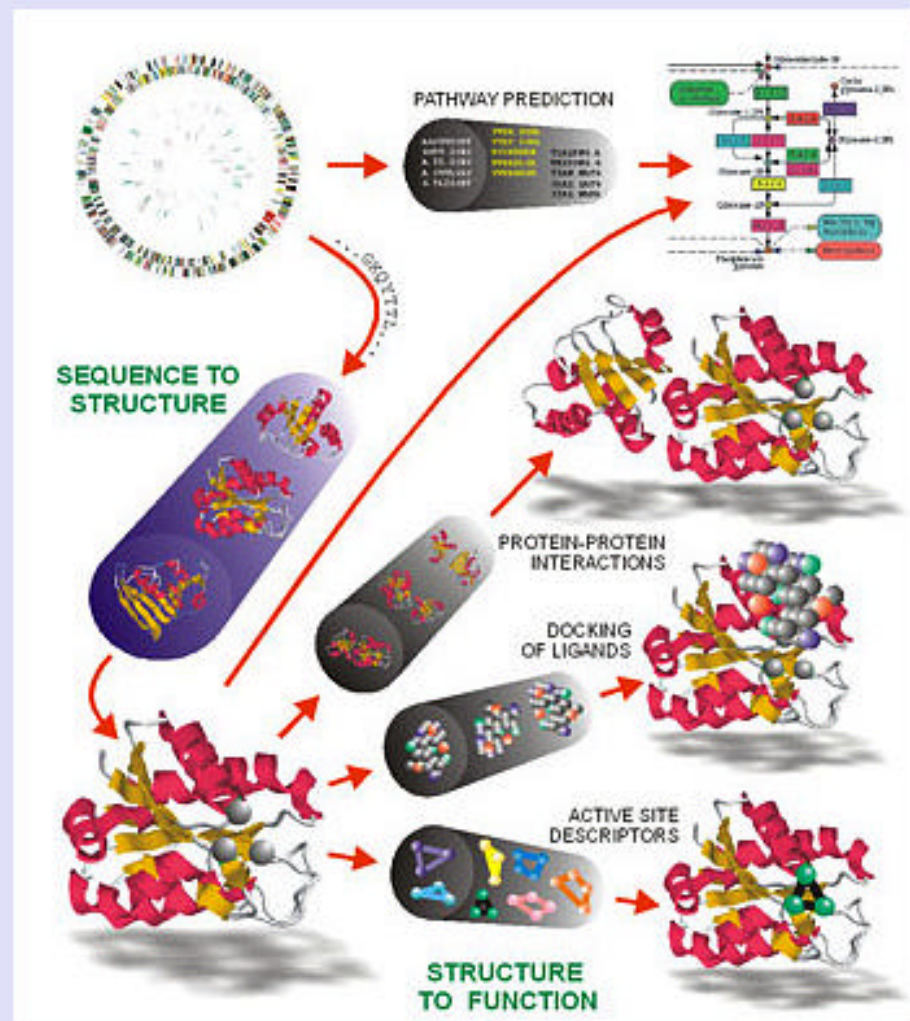




# Bioinformatics in Buffalo

## 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





# 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

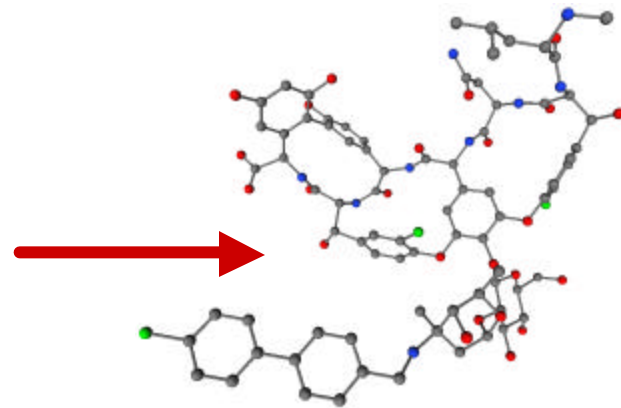
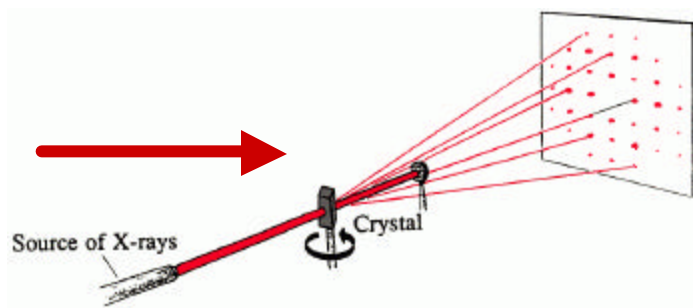
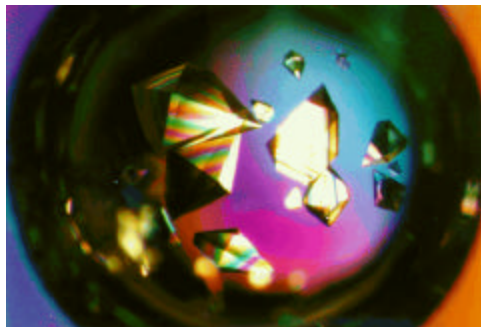
- ❑ Rational Drug Design
- ❑ Structural Biology
- ❑ Systems Biology

## ■ Vancomycin

- ❑ “Antibiotic of Last Resort”

## ■ Current Efforts

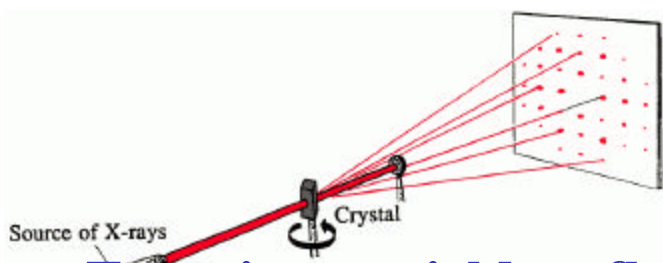
- ❑ Grid
- ❑ Collaboratory
- ❑ Intelligent Learning



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



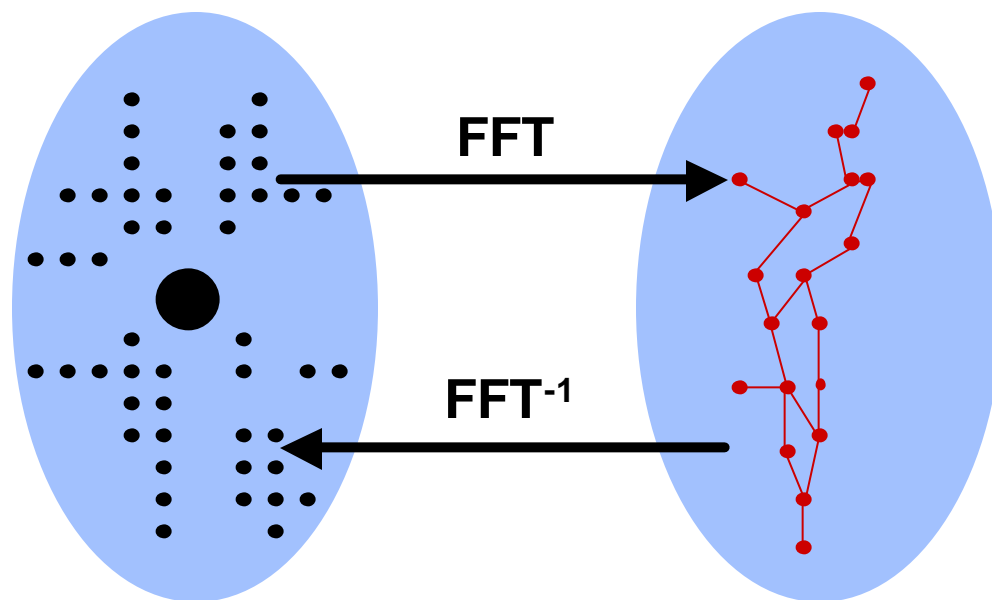
# X-Ray Data & Corresponding Molecular Structure



- 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



# Overview of Direct Methods

- Probability theory gives information about certain linear combinations of phases.
  - In particular, the triples  $f_H + f_K + f_{-H-K} = 0$  with high probability.
- Probabilistic estimates are expressed in terms of normalized structure factor magnitudes ( $|E|$ ).
- Optimization methods are used to extract the values of individual phases.
- A multiple trial approach is used during the optimization process.
- A suitable figure-of-merit is used to determine the trials that represent solutions.

# 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

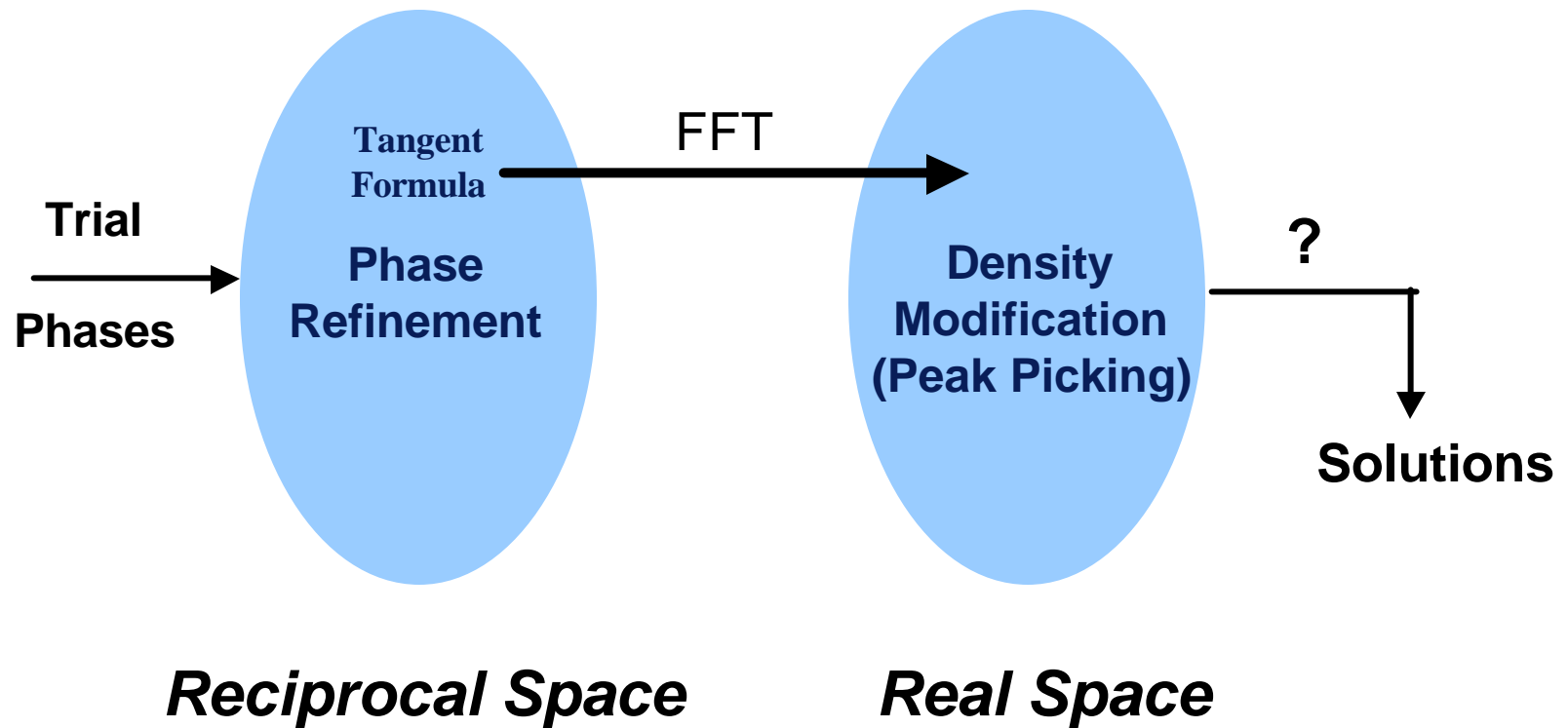
$$R(\mathbf{f}) = \frac{1}{\sum_{H,K} W_{HK}} \sum_{H,K} W_{HK} \left( \cos \Phi_{HK} - \frac{I_1(W_{HK})}{I_0(W_{HK})} \right)^2$$

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

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

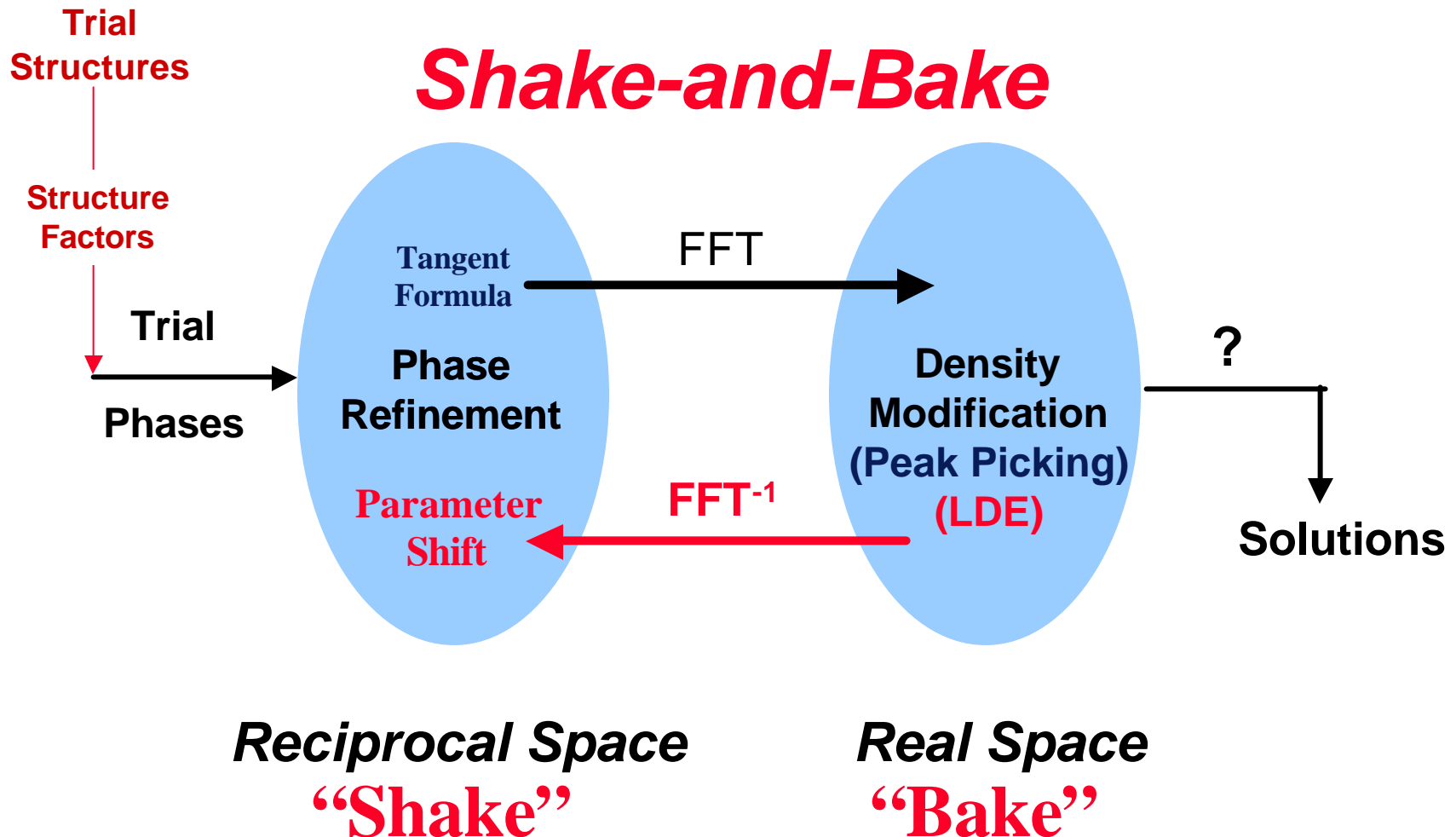
Weights :  $W_{HK} = A_{HK} = 2N^{-1/2} |E_H E_K E_{-H-K}|$

# Conventional Direct Methods

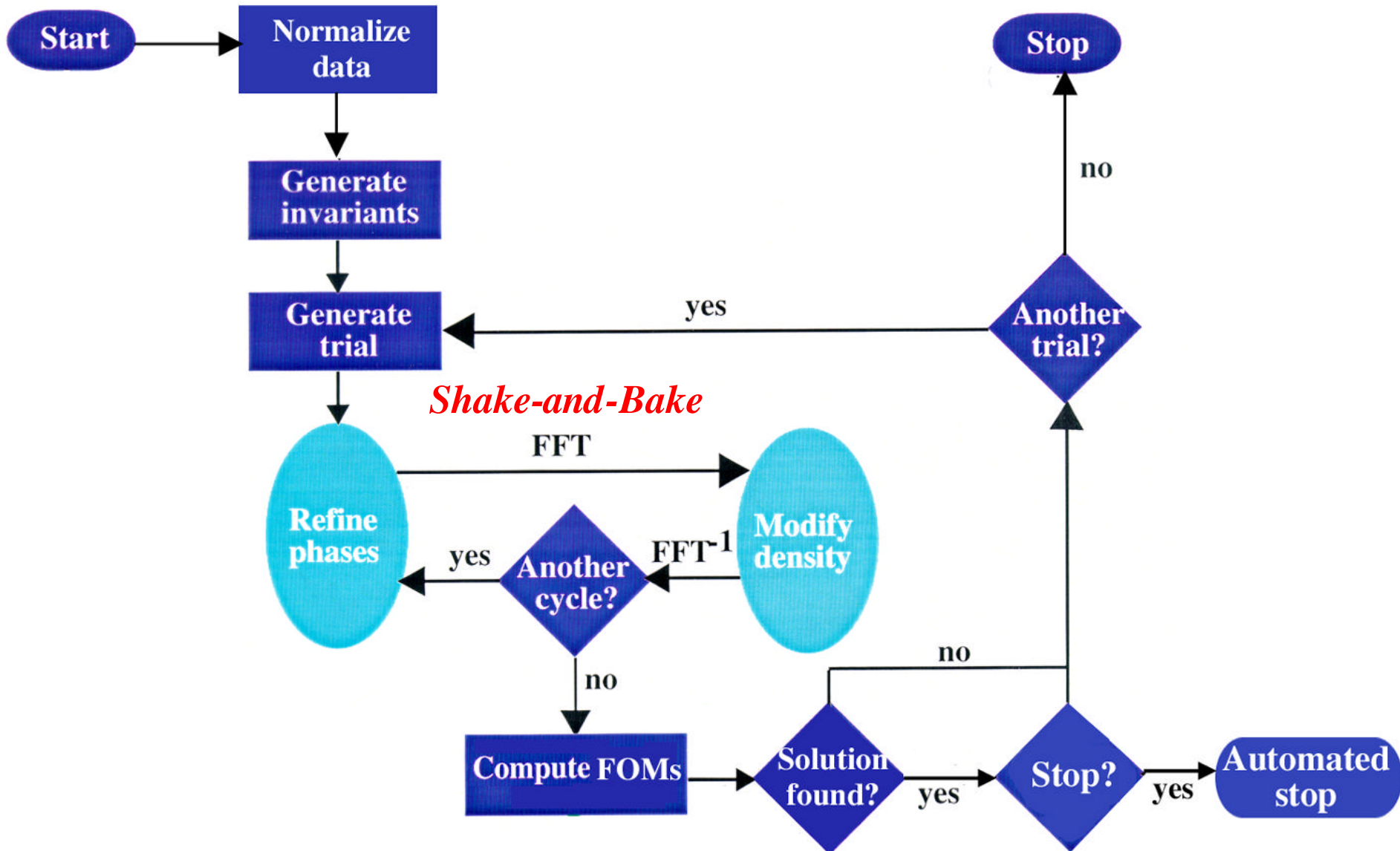




# Shake-and-Bake Method: Dual-Space Refinement



# A Direct Methods Flowchart



# *Shake-and-Bake Applications:* Structure Size and Data Resolution

## ■ Basic Data (Full Structure)

- ~750 unique non-H atoms (equal)
- ~2000 such atoms including 8 Fe's
- 1.1-1.2Å data (equal atom)
- 1.3-1.4Å data (unequal atoms, sometimes)

## ■ SAS or SIR Difference Data (substructures)

- 160 Se (567 kDa / ASU)
- 3-4Å data
- 5Å truncated data have also worked



# Phasing and Structure Size

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

Se-Met

190kDa

Multiple Isomorphous Replacement .....?

*Shake-and-Bake*

Conventional Direct Methods

Vancomycin

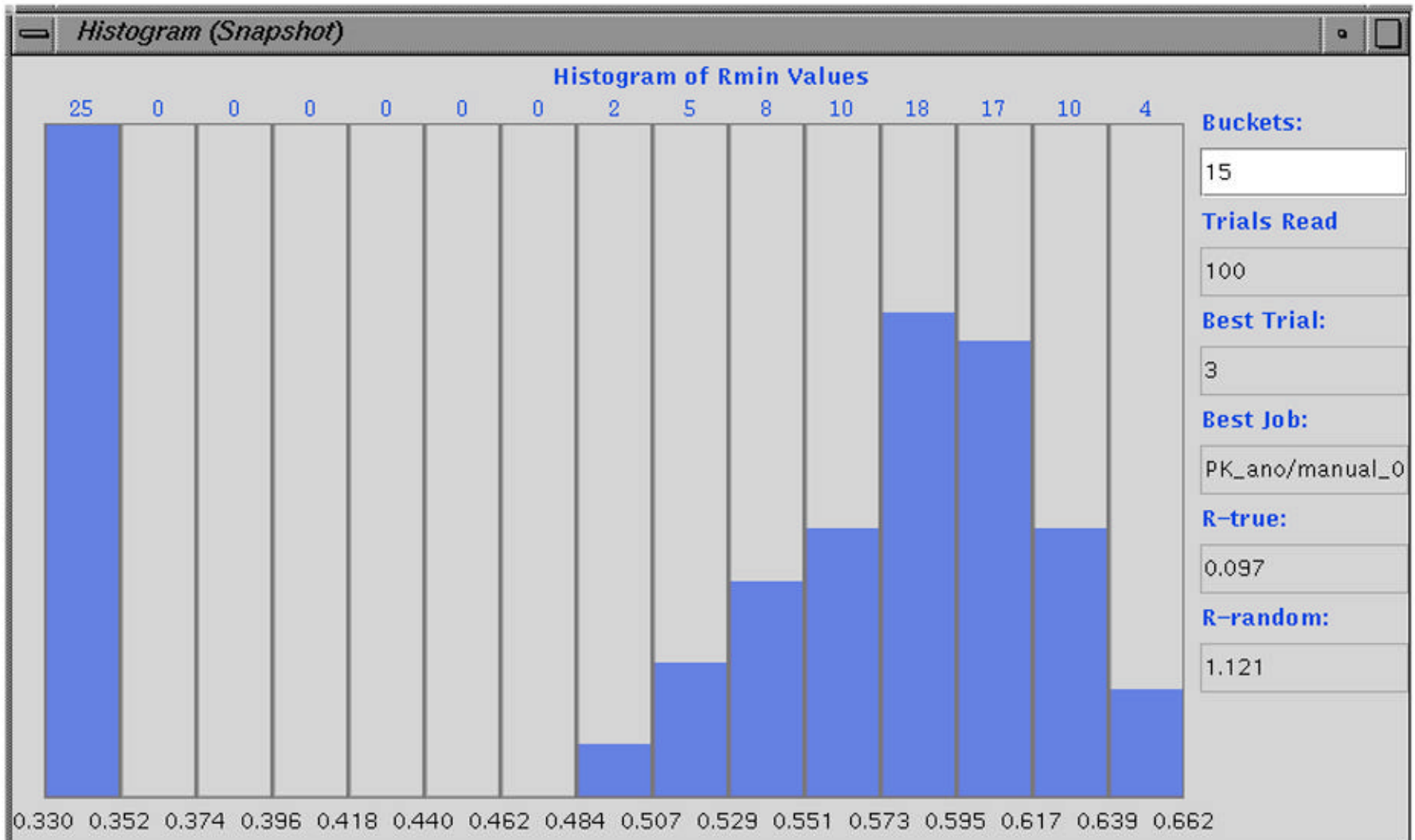


Number of Atoms in Structure

# Vancomycin

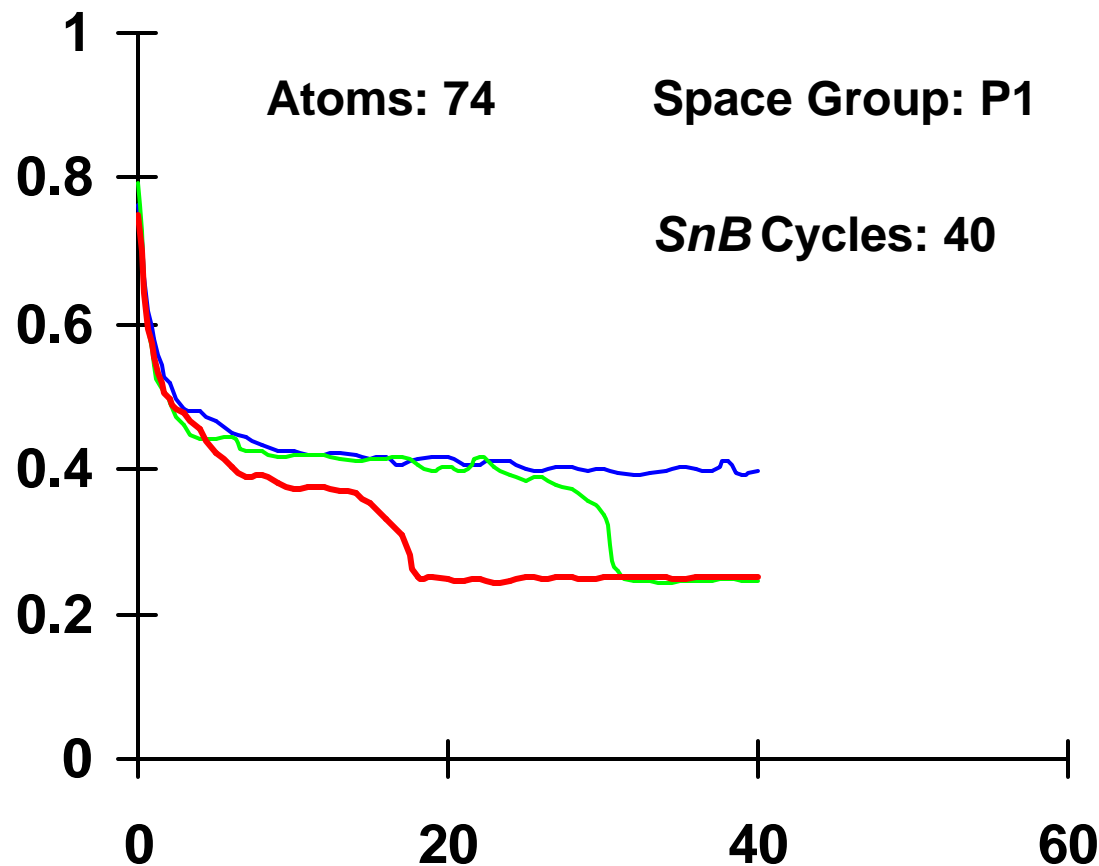
- Interferes with formation of bacterial walls
- *Last line of defense* against deadly
  - streptococcal and staphylococcal bacteria strains
- Vancomycin resistance exists (Michigan)
- Can't just synthesize variants and test
- Need structure-based approach to predict
- Solution with *SnB (Shake-and-Bake)*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

# Ph8755: SnB Histogram





# Ph8755: Trace of *SnB* Solution



# 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

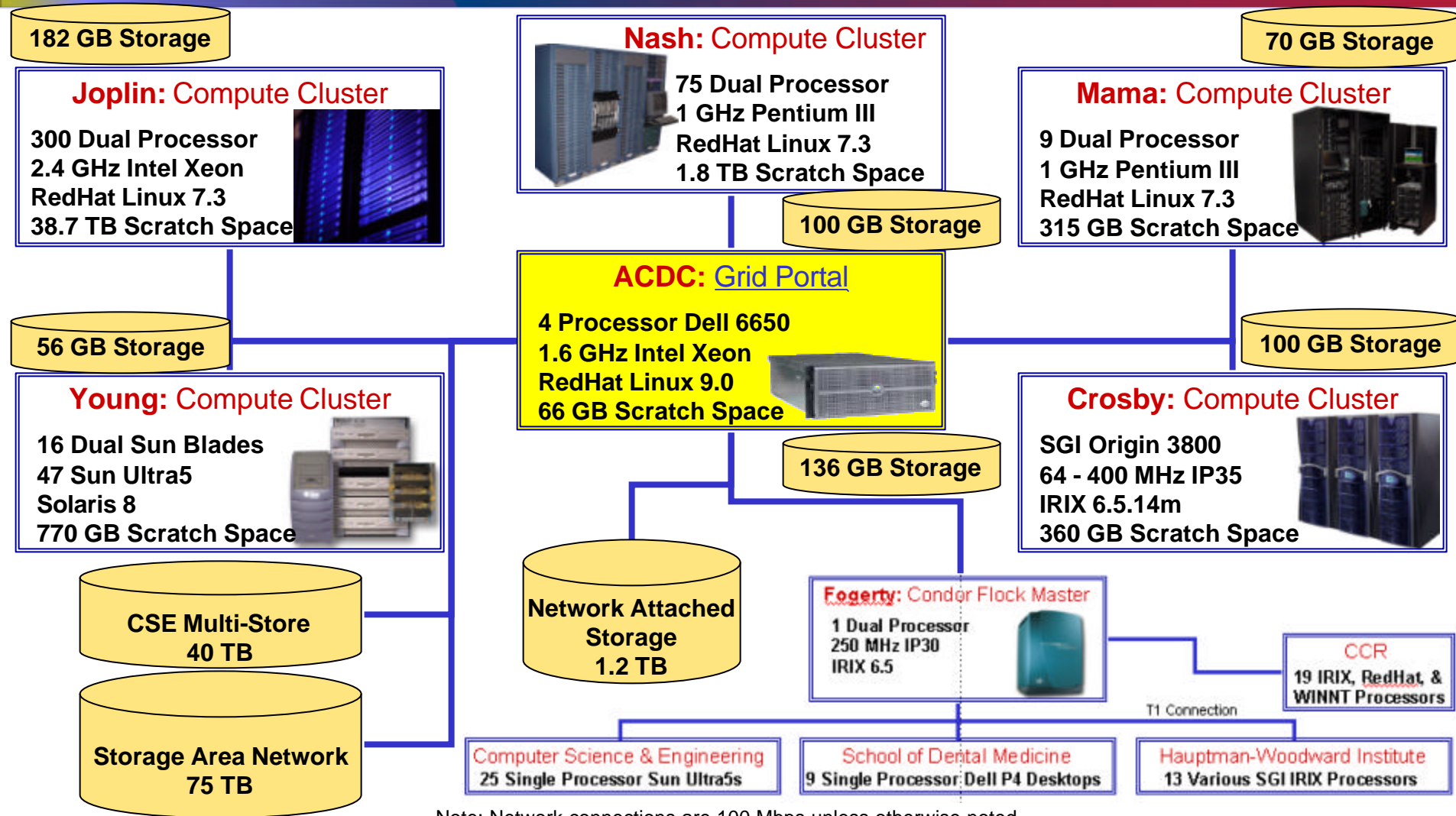
- Define quality of service estimates of job completion, by better estimating job runtimes by profiling users.

### ■ 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



# ACDC-Grid

CCR Grid Computing Services - Microsoft Internet Explorer

CCR University at Buffalo The State University of New York

## Center for Computational Research GRID PORTAL

High Performance Grid Computing

**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 Bioinformatics, 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.

Get your "Grid Computing Guide"?

CCR Grid Computing Services Data Management - Microsoft Internet Explorer

CCR University at Buffalo The State University of New York

## Center for Computational Research GRID PORTAL

High Performance Grid Computing

VIEW Group GROUP miller UserList rappleys

PORTAL LOGOUT

User Tools

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

reppleye

- KeyMaster
- Morpheus
  - Tank
  - Agent
  - Rabbit
  - Tank
  - Morpheus
  - Oracle.m
  - Nao

Browser view of "miller" group files published by user

CCR Grid Computing Services Grid Admin - Microsoft Internet Explorer

CCR University at Buffalo The State University of New York

## Center for Computational Research GRID PORTAL

High Performance Grid Computing

PORTAL LOGOUT

User Tools

- Manage Account
- Grid General Info
- Projects
- Resources
- Computational Grid
- Job Submission
- Job Queue Status
- Data Grid
- Network Status
- Running/Queued Jobs
- PBS Job History
- Grid Portal Statistics
- Cluster Fleet Statistics
- User Information
- 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 (MB)
miller	~1,815,000
griddev	~1,550,000
ccrstaff	~1,500,000
mgreen	~1,500,000

CCR Grid Computing Services Grid Admin - Microsoft Internet Explorer

CCR University at Buffalo The State University of New York

## Center for Computational Research GRID PORTAL

High Performance Grid Computing

PORTAL LOGOUT

User Tools

- Manage Account
- Grid General Info
- Projects
- Resources
- Computational Grid
- Job Submission
- Job Queue Status
- Data Grid
- Network Status
- Running/Queued Jobs
- PBS Job History
- Grid Portal Statistics
- Cluster Fleet Statistics
- User Information
- 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	mgreen	griddev	txt
2	56034	Cypher.sh	52858	10	mgreen	griddev	sh
3	56035	Oracle.asc	52958	10	mgreen	griddev	asc
4	56036	Cypher.sh	52634	10	mgreen	miller	sh
5	56037	Rabbit.dat	52830	10	mgreen	ccrstaff	dat
6	56038	Agent.exe	53064	10	mgreen	griddev	exe
7	56039	Dozer.sh	52852	10	mgreen	griddev	sh
8	56040	Nao.asc	52187	10	mgreen	mgreen	asc
9	56041	Agent.mpg	52833	10	mgreen	mgreen	mpg
10	56042	Tank.txt	52188	10	mgreen	mgreen	txt
11	56043	Smith.xls	52258	10	mgreen	ccrstaff	xls
12	56044	KeyMaster.csh	52186	10	mgreen	miller	csh
13	56045	Oracle.csh	52632	10	mgreen	griddev	csh
14	56046	Dozer.xls	52808	10	mgreen	mgreen	xls
15	56047	Cypher.exe	52204	10	mgreen	griddev	exe
16	56048	Rabbit.ppt	52861	10	mgreen	miller	ppt
17	56049	Nao.dat	52217	10	mgreen	ccrstaff	dat
18	56050	Cypher.asc	53086	10	mgreen	griddev	asc



# ACDC-Grid Administration

The collage displays four different pages from the CCR Grid Portal, all accessed via Microsoft Internet Explorer. The portal's header consistently shows the University at Buffalo logo and the text 'Center for Computational Research GRID PORTAL High Performance Grid Computing'.

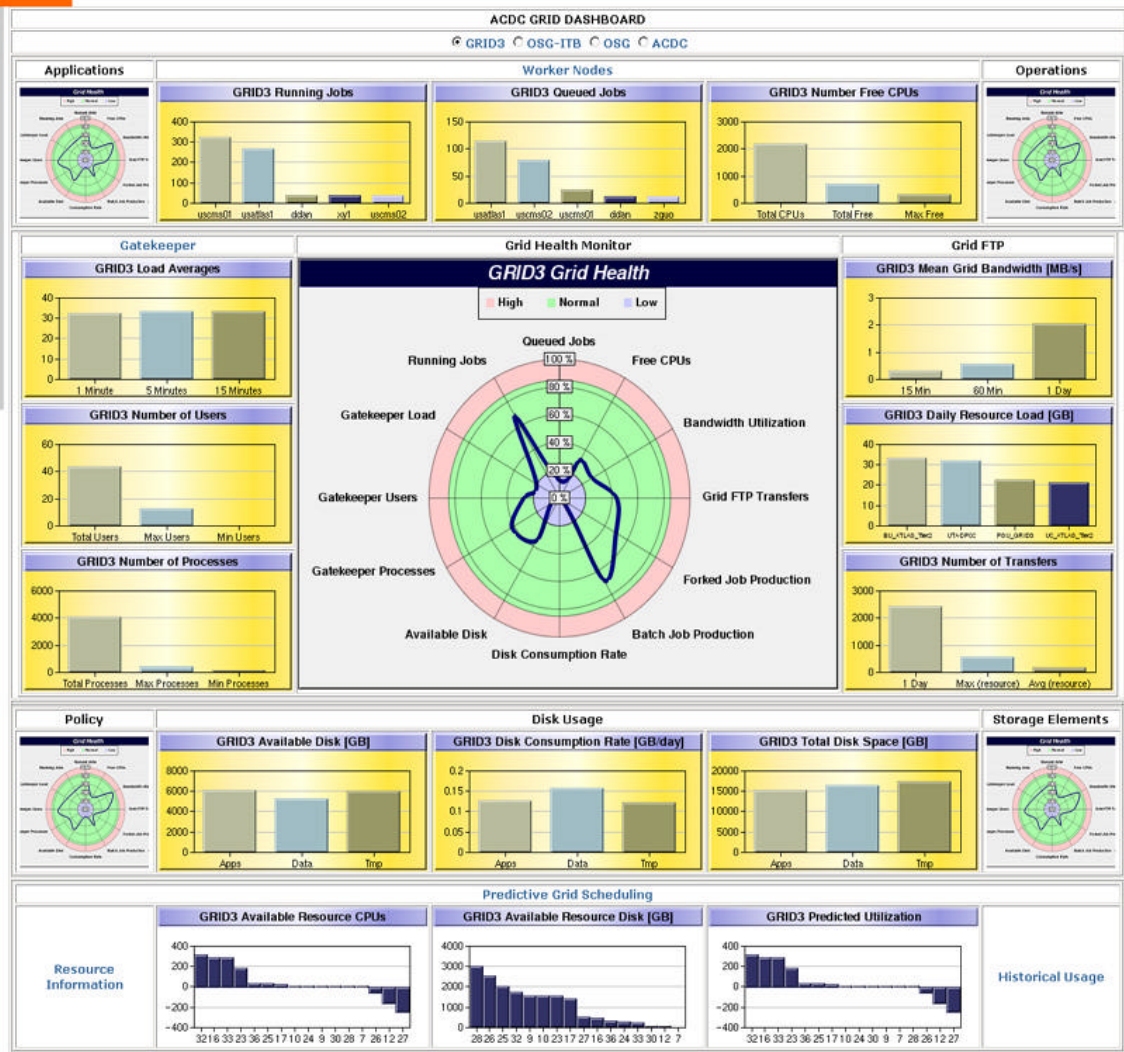
- Top Left:** The 'Grid Site Administration' page. It features a 'PORTAL LOGOUT' sidebar with links like 'Manage Account', 'Grid General Info', and 'Project Resources'. The main content area lists 'Users', 'Groups', 'Portal Event Log', and 'Database Job List'. Below these are sections for 'Organizations (add, edit, delete)', 'Resources (view, refresh, ping, delete, create host certificate)', and 'Globus Administration Reports (machine usage, user access to machines, etc.)'.
- Top Right:** The 'Generate Globus grid-mapfile' page. It includes a 'PORTAL LOGOUT' sidebar and a main section with instructions on specifying an optional include file and a grid-mapfile path. There are input fields for these and a checkbox for 'Do not stage the file to the grid nodes'.
- Bottom Left:** The 'Create New Database Job' page. It has a 'PORTAL LOGOUT' sidebar and a main section with a form to create a new database job. The form includes fields for 'Job Name', 'Full Path To Script', 'Accepts Arguments' (a dropdown menu), 'Run Script' (a dropdown menu), and 'Run As User' (a dropdown menu). There are 'Create Job' and 'Cancel' buttons at the bottom.
- Bottom Right:** The 'MDS Resource Update Status' page. It features a 'PORTAL LOGOUT' sidebar and a main section with a table showing the current time and a list of resources with their last update times and next update times. Below the table are links to return to the 'Grid Resource Admin menu' and the 'Grid Admin menu'.







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



# 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



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

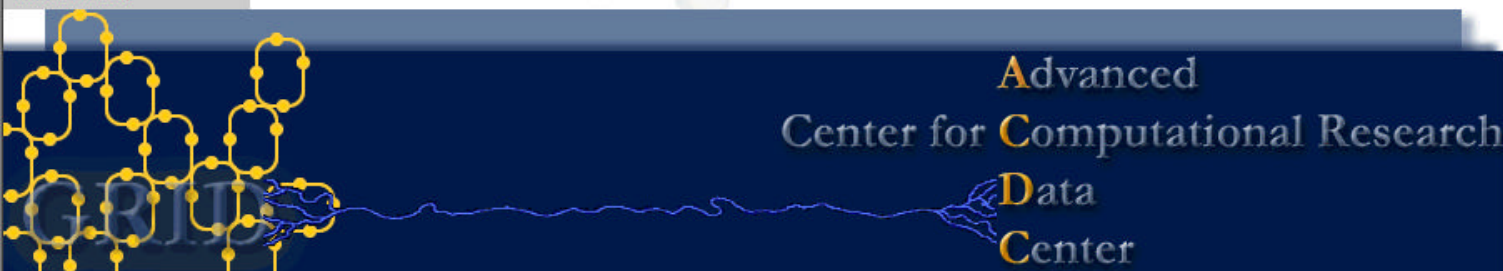
## Advanced Computational Data Center Grid Jobs

### 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.

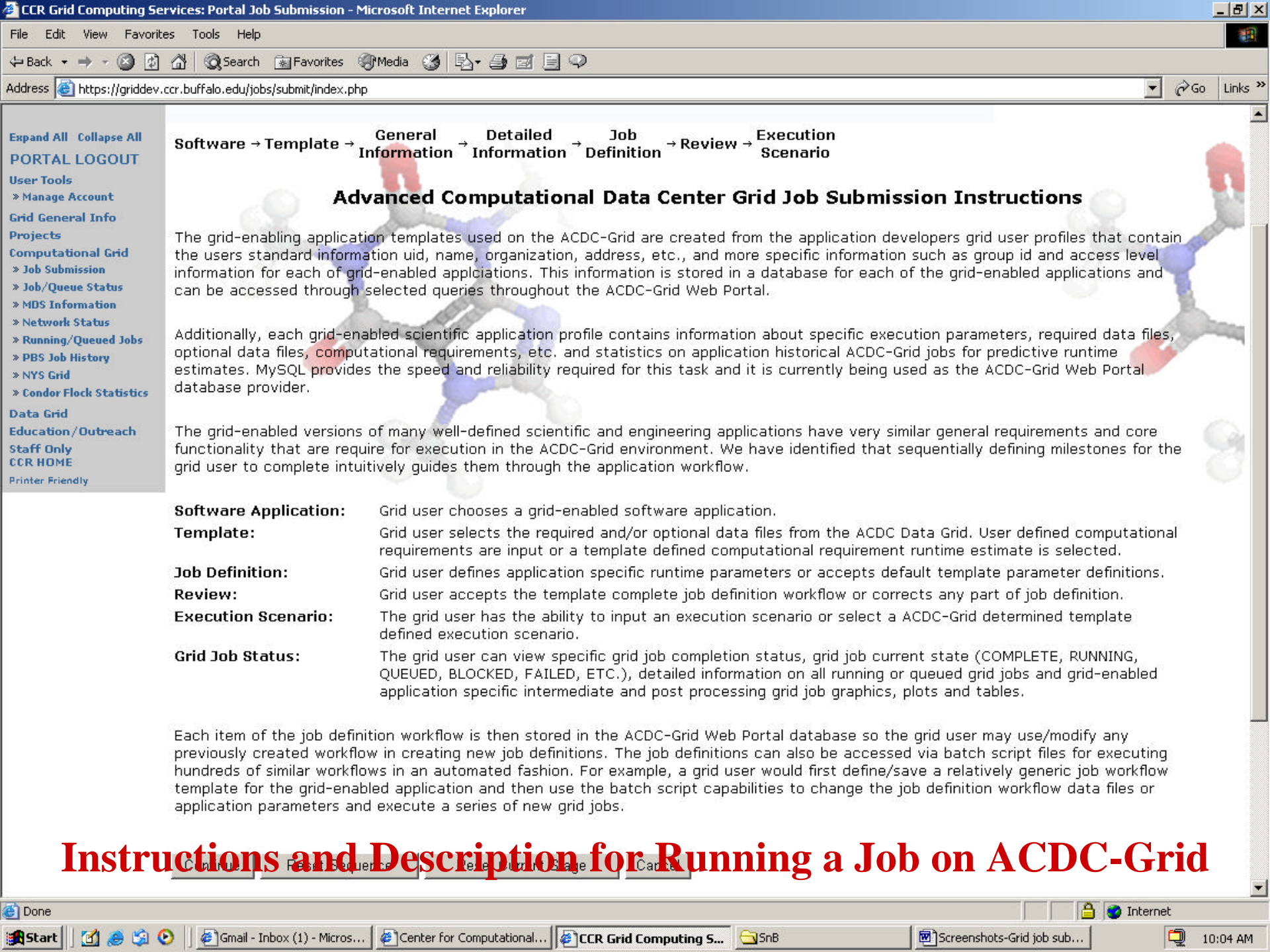
### Grid Job Status:

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**





Expand All Collapse All

PORTAL LOGOUT

User Tools

» Manage Account

Grid General Info

Projects

Computational Grid

» Job Submission

» Job/Queue Status

» MDS Information

» Network Status

» Running/Queued Jobs

» PBS Job History

» NYS Grid

» Condor Flock Statistics

Data Grid

Education/Outreach

Staff Only

CCR HOME

Printer Friendly

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

## Advanced Computational Data Center Grid Job Submission Instructions

The grid-enabling application templates used on the ACDC-Grid are created from the application developers grid user profiles that contain the users standard information uid, name, organization, address, etc., and more specific information such as group id and access level information for each of grid-enabled applications. This information is stored in a database for each of the grid-enabled applications and can be accessed through selected queries throughout the ACDC-Grid Web Portal.

Additionally, each grid-enabled scientific application profile contains information about specific execution parameters, required data files, optional data files, computational requirements, etc. and statistics on application historical ACDC-Grid jobs for predictive runtime estimates. MySQL provides the speed and reliability required for this task and it is currently being used as the ACDC-Grid Web Portal database provider.

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

- Software Application:** Grid user chooses a grid-enabled software application.
- Template:** Grid user selects the required and/or optional data files from the ACDC Data Grid. User defined computational requirements are input or a template defined computational requirement runtime estimate is selected.
- Job Definition:** Grid user defines application specific runtime parameters or accepts default template parameter definitions.
- Review:** Grid user accepts the template complete job definition workflow or corrects any part of job definition.
- Execution Scenario:** The grid user has the ability to input an execution scenario or select a ACDC-Grid determined template defined execution scenario.
- Grid Job Status:** The grid user can view specific grid job completion status, grid job current state (COMPLETE, RUNNING, QUEUED, BLOCKED, FAILED, ETC.), detailed information on all running or queued grid jobs and grid-enabled application specific intermediate and post processing grid job graphics, plots and tables.

Each item of the job definition workflow is then stored in the ACDC-Grid Web Portal database so the grid user may use/modify any previously created workflow in creating new job definitions. The job definitions can also be accessed via batch script files for executing hundreds of similar workflows in an automated fashion. For example, a grid user would first define/save a relatively generic job workflow template for the grid-enabled application and then use the batch script capabilities to change the job definition workflow data files or application parameters and execute a series of new grid jobs.

# Instructions and Description for Running a Job on ACDC-Grid

# CCR University at Buffalo The State University of New York

## Center for Computational Research GRID PORTAL

High Performance Grid Computing

Expand All Collapse All

PORTAL LOGOUT

User Tools

» Manage Account

Grid General Info

Projects

Computational Grid

» Job Submission

» Job/Queue Status

» MDS Information

» Network Status

» Running/Queued Jobs

» PBS Job History

» NYS Grid

» Condor Flock Statistics

Data Grid

Education/Outreach

Staff Only

CCR HOME

Printer Friendly

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

Select a GAT: BnP Auto Run

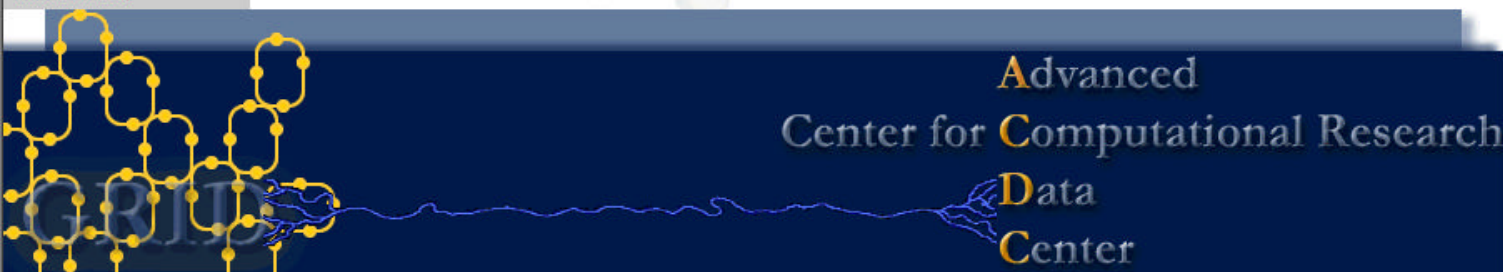
BnP Auto Run  
EADR  
Ostrich  
POM  
Q-Chem  
SnB  
SnB DREAR  
Split  
snb-dev

Continue

Reset Current Stage

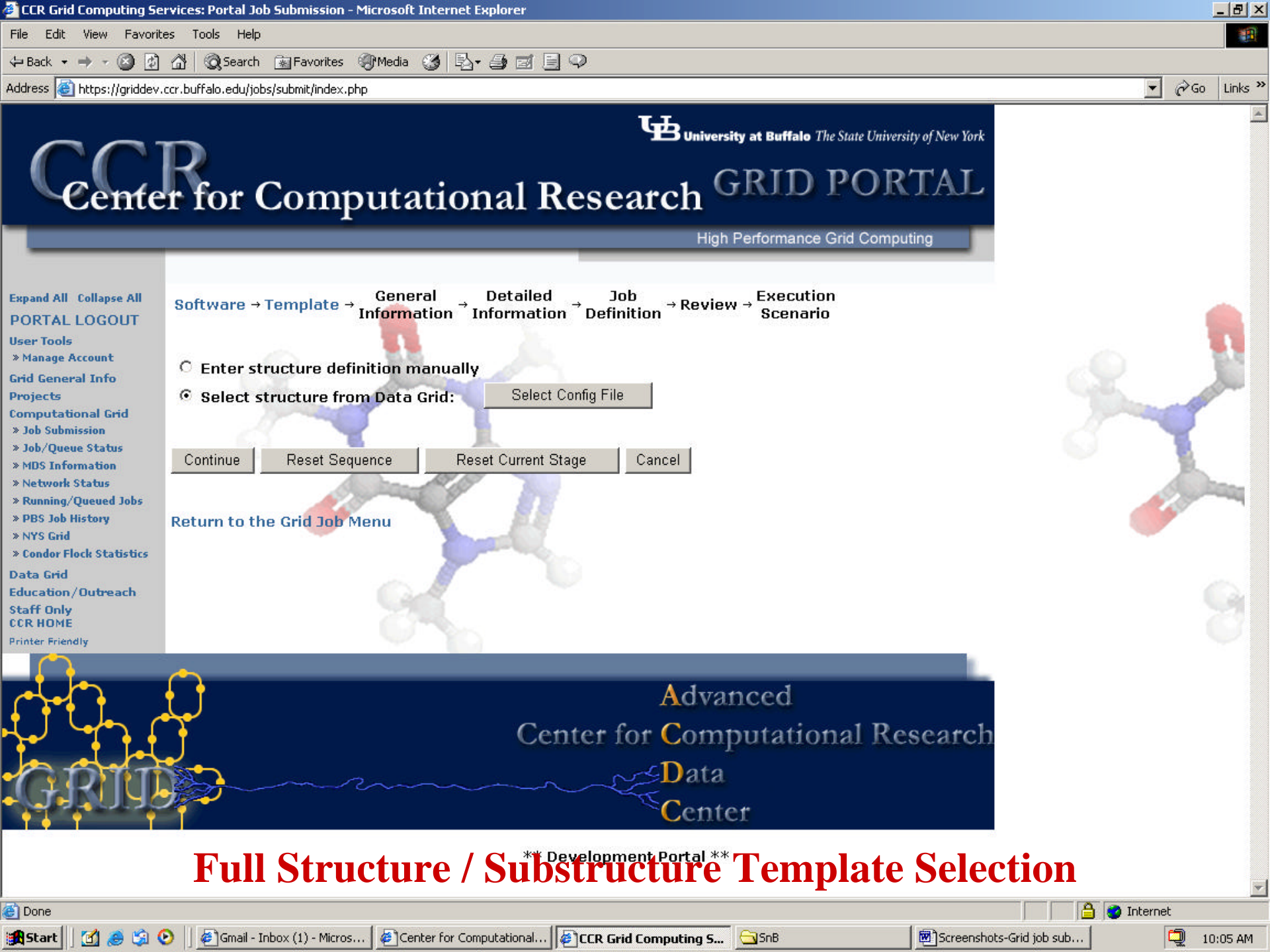
Cancel

Return to the



**Software Package Selection**







## 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

» Condo 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="text" value="Dataset 1"/>
Datasets	Dataset 1
Name (8 chars max)	

Default Parameters Based on Template

CCR Grid Computing Services: 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

Initial Data Sets

Add Dataset Delete Dataset

Select dataset to delete

DatasetsDataset 1

Name (8 chars max):iledhkl

Dataset Type:Native

File Name (\*.hkl):Browse

File Type:F, Sig(F)

Wavelength:1.5418

Max. Resolution:0.94

Anomalous Dispersion:Not Measured

Heavy Element Type:

Nat. Element Replaced:

No. Expected Sites:

F Prime (f'):

F Double Prime (f''):

ContinueReset SequenceReset Current StageCancel

Return to the Grid Job Menu

AdvancedCenter for Computational Research

Done

Start

Gmail - Inbox - Mi...

Center for Comp...

CCR Grid Comp...

Sn8

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
  - » 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)	

## 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

## Dreear 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 : 

## 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:

# 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
- » Conder Flock Statistics

#### Data Grid

- Education/Outreach
- Staff Only
- CCR HOME
- Printer Friendly

### 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**

CCR Grid Computing Services: 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 Improvement (%):

*SnB Setup (cont'd)*

Done

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

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

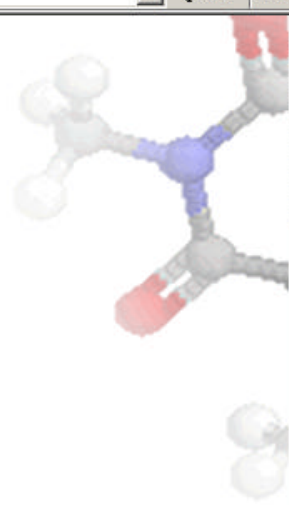
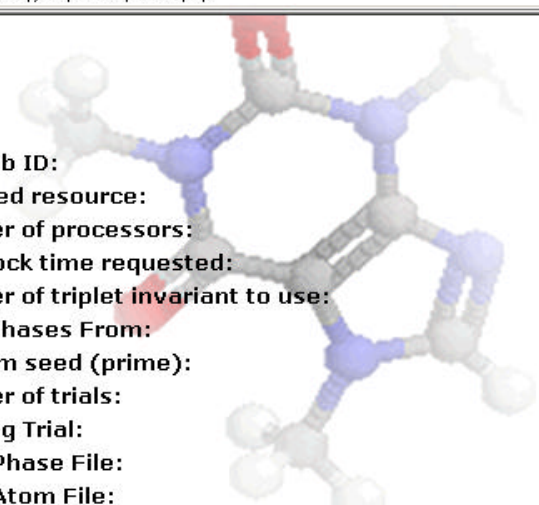
## Education/Outreach

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

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Media

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

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**  
Rmin Min: 0.344 Rmin Max: 0.56  
Last Updated: 15-Mar-2005 10:22:00

Total Trials: 1000  
Complete Trials: 285  
Resource: clearwater.ccr.buffalo.edu

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

Trial Summary

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

Walltime Summary

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

Grid Job Trial Histogram

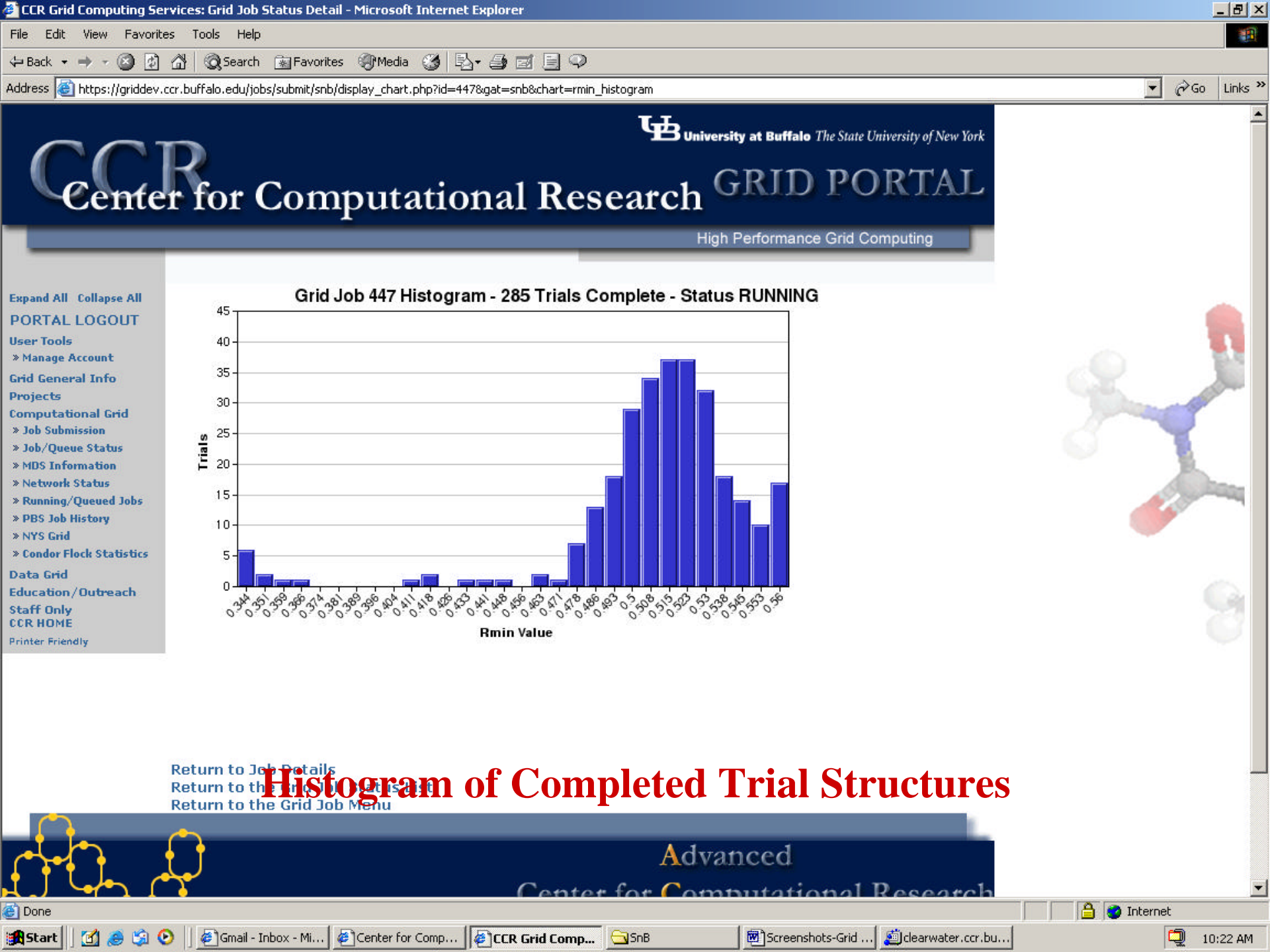
Grid Job 447 Histogram - 285 Trials Complete - Status RUNNING

Click on image for enlarged view.

Advanced  
Center for Computational Research  
Data

https://griddev.ccr.buffalo.edu/jobs/submit/snb/display\_chart.php?id=447&gat=snb&chart=rmin\_histogram

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





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

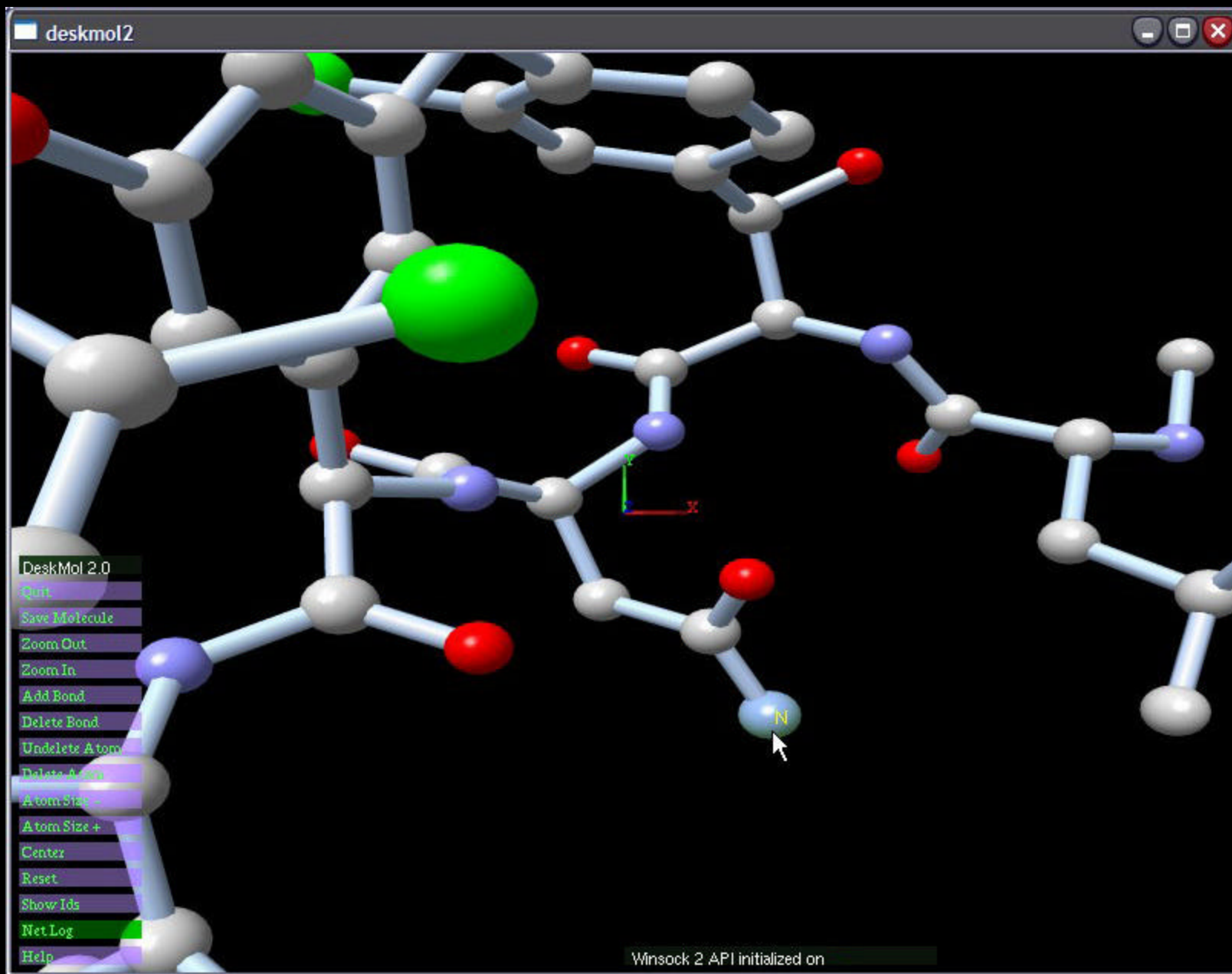
☒ Descending☐ Ascending

Filter Job List

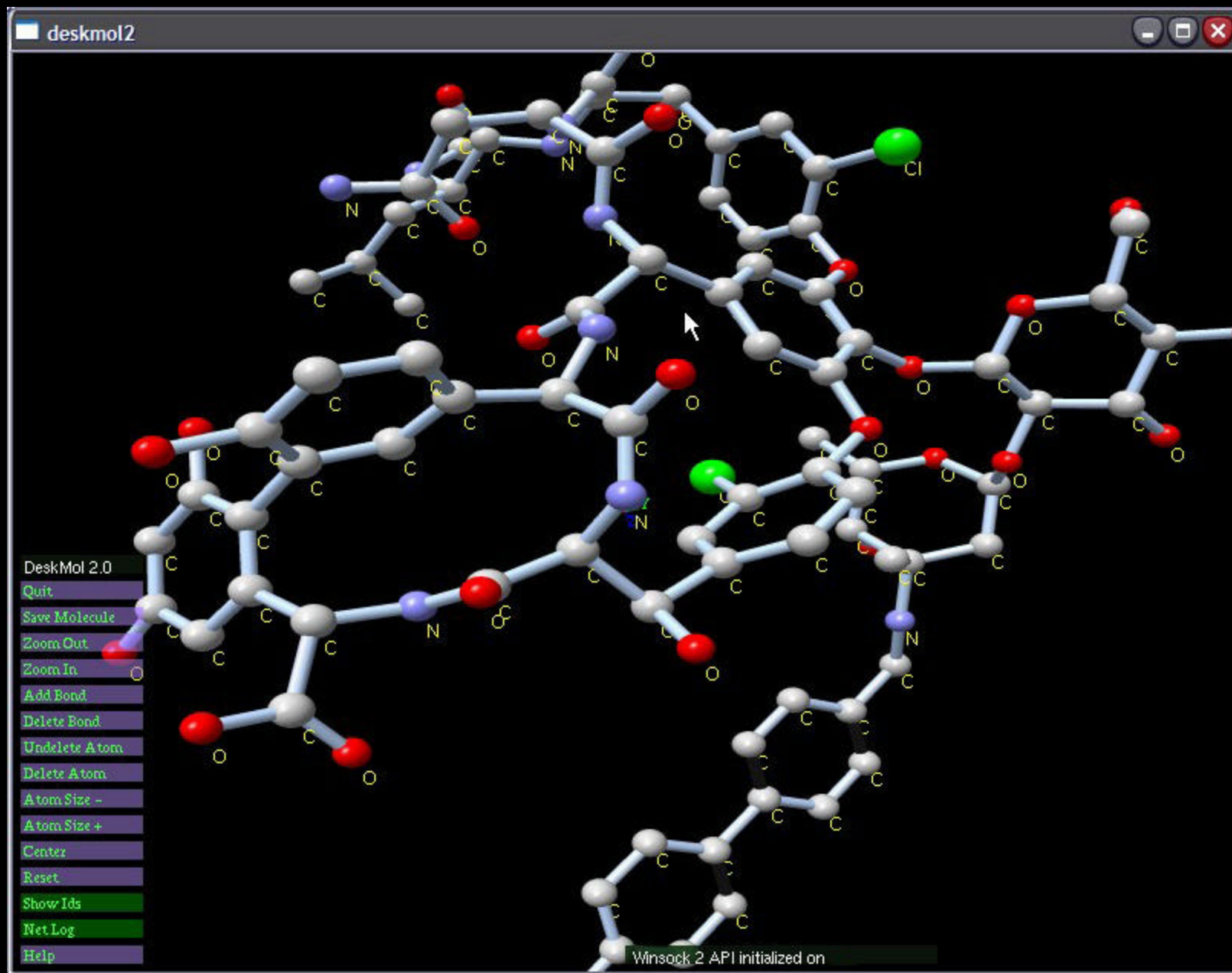
## SnB

Job Id	Job Name	Resource	Num Procs	Status	Percent Complete	Last Update	Cancel Job	Drilldown
447	iledhkl	clearwater.ccr.buffalo.edu	5	<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

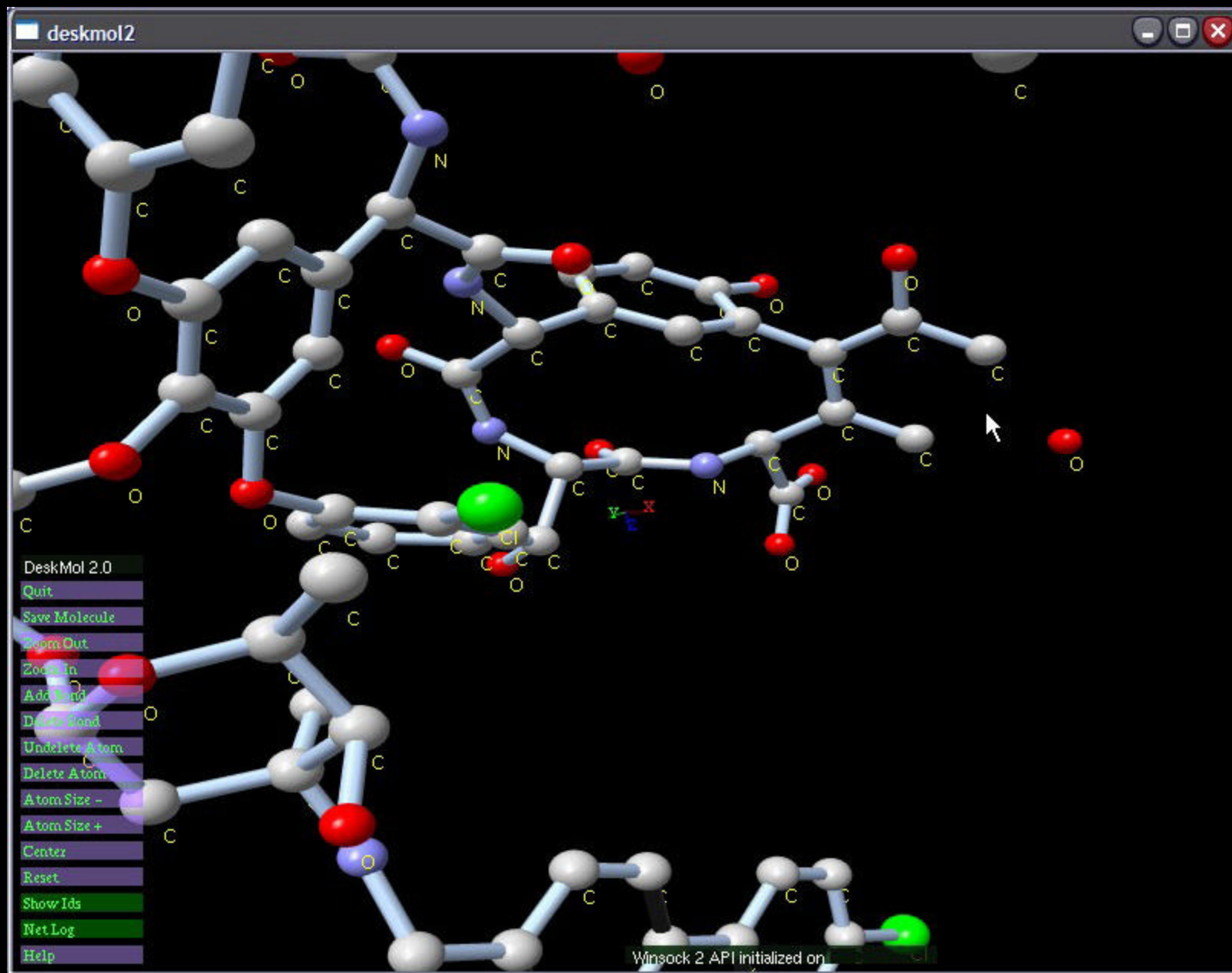


User starts up – default image of structure.

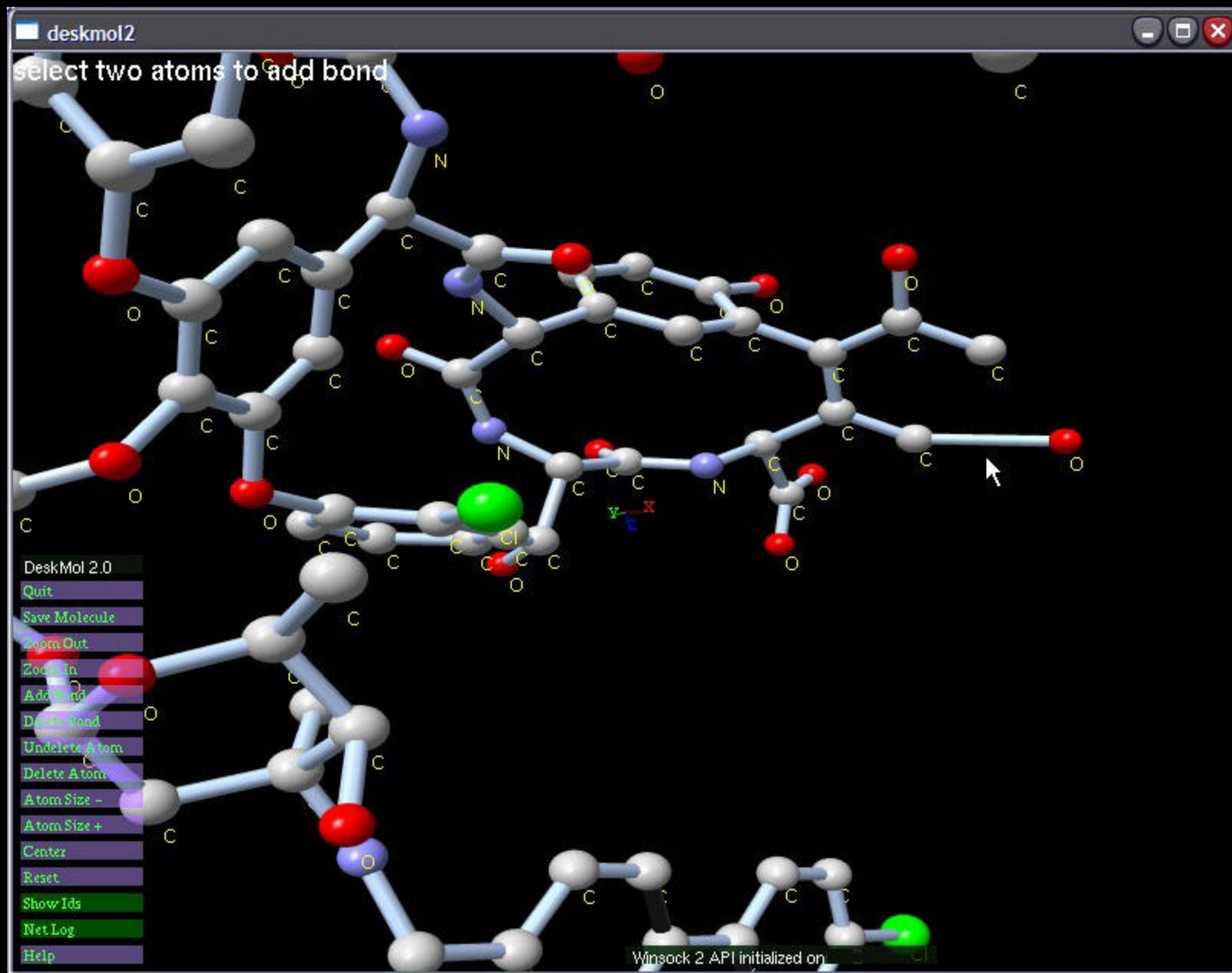


Molecule scaled, rotated, and labeled.





Remove Carbon Atoms (and Links)



User Adds Bond Between Atoms

# Outreach

- **HS Summer Workshops in Computational Science**
  - **Chemistry, Visualization, Bioinformatics**
  - **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

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

WED, SEPT 20  
10th Anniversary  
FEBRUARY 9 - 11, 2009 BUCKLE UP! 2009

## HMOs cut Medicare premiums

**BY ANTHONY CHAMBERLAIN**  
CHAMBERLAIN

The new rules of Independent Health and United Healthcare will become effective March 1, pushing the state's HMOs to cut Medicare premiums by 10 percent to 15 percent, according to the state's Department of Health. The changes are the result of the state's new Medicare program, which is set to begin in 2010.

The new rules of Independent Health and United Healthcare will become effective March 1, pushing the state's HMOs to cut Medicare premiums by 10 percent to 15 percent, according to the state's Department of Health. The changes are the result of the state's new Medicare program, which is set to begin in 2010.

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

**BY JAMES HALL**  
HALL

The Town of Aurora is considering a proposal for a new patio home development in the town's northern section. The development would consist of 100 units, each with a private patio and a two-car garage. The town's Board of Supervisors is expected to vote on the proposal in the coming weeks.

**Grammy: Designs on Buffalo**

**Ani DiFranco, art director up for award**

**BY JAMES HALL**  
HALL

It's not just the live show of Ani DiFranco's new album, "The Secret of the Secret," that has caught the attention of the Grammy Awards. It's the art direction of the album, designed by DiFranco's brother, Ani DiFranco Jr., that has earned him a nomination for Best Album Packaging.

**UB brings bioinformatics to a younger generation**

**BY JAMES HALL**  
HALL

Students at the University at Buffalo are getting a head start on the future of medicine and biology. The university has launched a new program in bioinformatics, which combines the fields of biology and computer science. The program is designed to prepare students for careers in the biotechnology industry.

**UNIVERSITY AT BUFFALO NEWS**  
EDUCATION

University at Buffalo undergraduate David Walsh works with Jaclyn Shaw, right, to demonstrate the "Next Generation Scientists" program. At left is Shannon O'Ryan.

## An early look at bioinformatics

**By EMMA D. SAPIRO**  
News Northern Bureau

For most of David Brown's educational career, science classes have been instructive but somewhat abstract. They've been steeped in theories and ideas that she left behind in the classroom.

But that's not the case anymore for the senior at Mount St. Mary's Academy. The world of science has come alive and is practical.

She's in her 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 Scientists: Training for Tomorrow's High School Teachers," merges life sciences and computational science. It is being taught at Mount St. Mary's, 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's. Attending were officials from UB and Versant, 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 Pitman, 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.

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."

emma.d.sapiro@buffalo.edu

**BUFFALO NEWS**  
EDUCATION

University at Buffalo undergraduate David Walsh works with Jaclyn Shaw, right, to demonstrate the "Next Generation Scientists" program. At left is Shannon O'Ryan.

## An early look at bioinformatics

**By EMMA D. SAPIRO**  
News Northern Bureau

For most of David Brown's educational career, science classes have been instructive but somewhat abstract. They've been steeped in theories and ideas that she left behind in the classroom.

But that's not the case anymore for the senior at Mount St. Mary's Academy. The world of science has come alive and is practical.

She's in her 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 Scientists: Training for Tomorrow's High School Teachers," merges life sciences and computational science. It is being taught at Mount St. Mary's, 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's. Attending were officials from UB and Versant, 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 Pitman, 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.

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."

emma.d.sapiro@buffalo.edu

# 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



