Shake-and-Bake, Grid Computing, and Visualization

Russ Miller

Center for Computational Research

Computer Science & Engineering
SUNY-Buffalo

Hauptman-Woodward Medical Inst

NSF, NIH, DOE
NIMA, NYS, HP

Grid3 2003

SnB

GRID

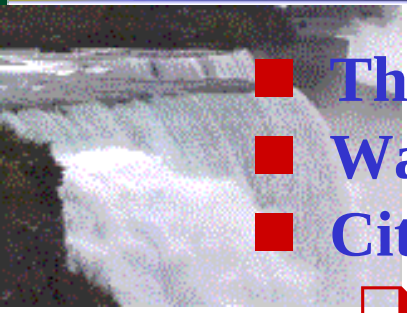
Advanced
Center for Computational Research
Data
Center

University at Buffalo

The State University of New York

Buffalo, New York

Two Seasons: Winter and July 4



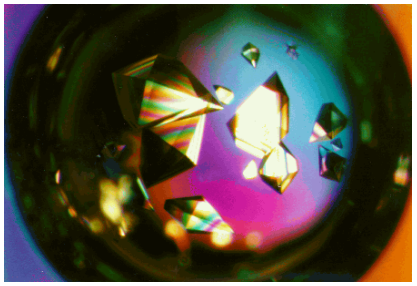
- The Queen City: 2nd Largest City in NYS
- Waterfront City: on North Coast of U.S.
- City of Lights
  - First U.S. city to have electric street lights
  - Pan American Exposition (1901)
    - Pres. McKinley Shot
- Architecture
  - Frederick Law Olmsted
  - Frank Lloyd Wright
- Underground Railroad: slaves escaped to freedom in Canada
- Four straight Super Bowl appearances
- Culinary Delights
  - (Buffalo) Wings: Anchor Bar, 1964
  - Beef on Weck

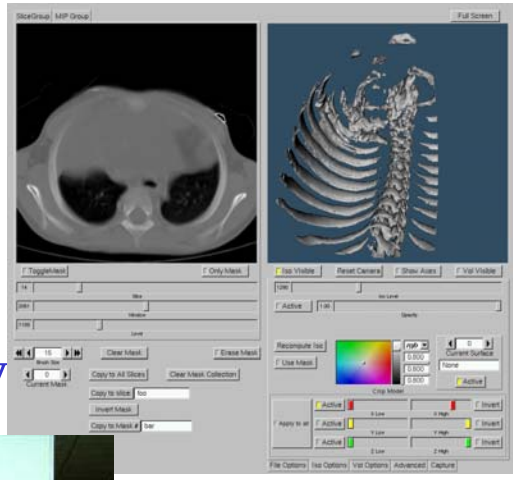
Academia in the 21st Century

- Embrace digital data-driven society
- Empower students to compete in knowledge-based economy
- Support research, scholarship, education, and outreach
  - Computational Science & Engineering: Simulation & Modeling
    - Complements Theory & Experimentation
    - Can lead to generation of *new* knowledge
  - High-Performance Computing & High-End Visualization
- 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 Overview

- **High-End Computing, Storage, Networking, and Visualization**
  - **~140 Research Groups in 37 Depts**
    - **Physical Sciences**
    - **Life Sciences**
    - **Engineering**
    - **Scientific Visualization, Medical Imaging, Virtual Reality**
  - **13 Local Companies**
  - **10 Local Institutions**
- **External Funding: $300M+**
- **Total Leveraged WNY: $500M+**
- **1100+ Publications**
- **EOT, Economic Development, Software, Media, Algorithms, Consulting, Training, CPU Cycles…**





CCR by the Numbers (2005)

- Current Technical Staff: 20→13
  - Seven (7) Contracted & Univ Tech Staff cut by Provost
  - 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

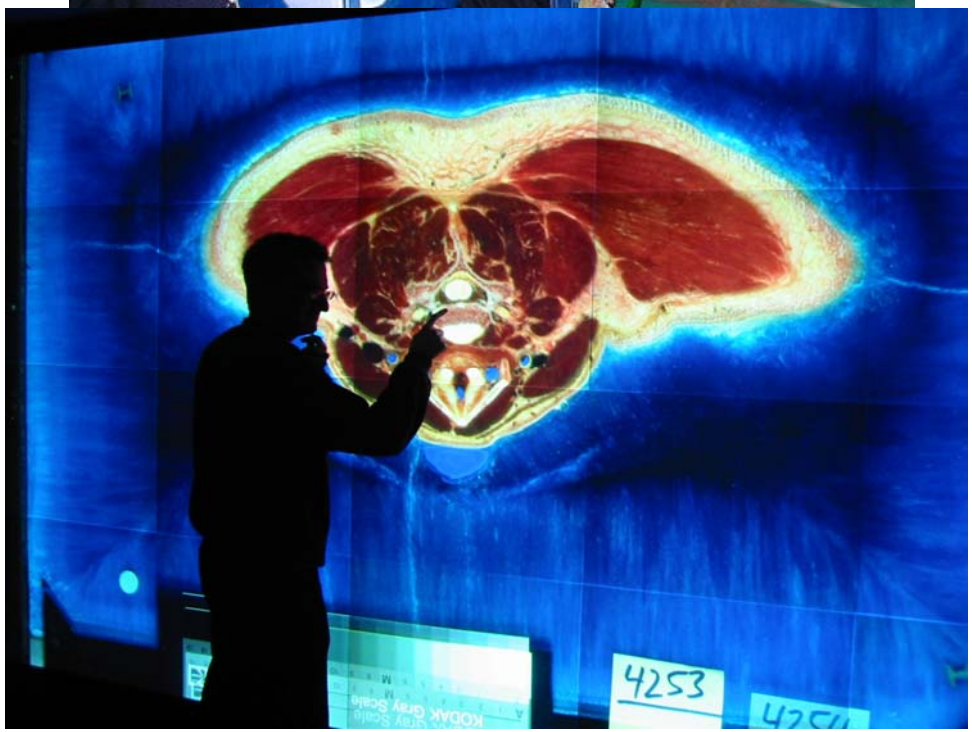
- Initial 7-Year Funding Model
  - SUNY-Buffalo Contribution: $1.3M
    - Personnel: $1.2M
    - Operating: $0.1M
  - User's Contributions: $0.4M
  - Annual Expend: ~$2.4M
  - Opportunistic Funding Model
    - Equipment, Maintenance, Licenses
  - **ROI: $7M → $300M @ SUNY-B**
- New Administration's Model
  - Moved into Bioinformatics
  - Move 30 mins from Main Campus
  - 50% Additional Reduction in Personnel & Operating in Addition to Current Cuts
  - Maintain Opportunistic Funding
  - Provost Rationale
    - Will Increase Users Contributions
    - "Provides Stability"

Major Compute/Storage Resources

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

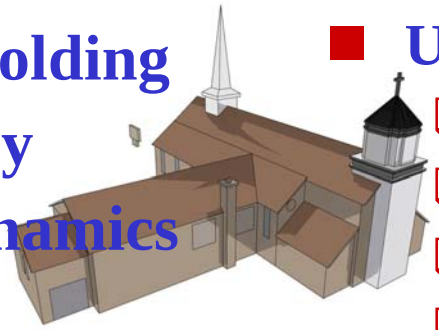
CCR Visualization Resources

- **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'×7'
  - Dell PCs with Myrinet2000
- **Access Grid Nodes (2)**
  - Group-to-Group Communication
  - Commodity components
- **SGI Reality Center 3300W**
  - Dual Barco's on 8'×4' screen
  - Onyx300: 10 R14000 @ 500MHz
  - 2 IR4 Pipes; 1 GB texture mem per pipe

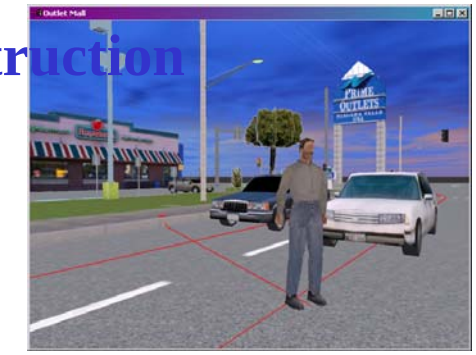


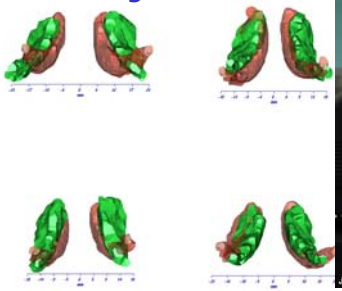
CCR Research & Projects

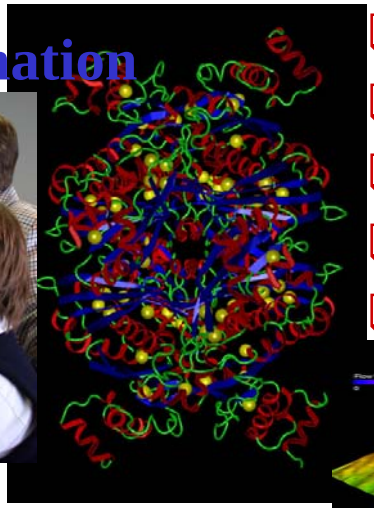
- Archaeology
- Bioinformatics/Protein Folding
- Computational Chemistry
- Computational Fluid Dynamics
- Data Mining/Database
- Earthquake Engineering
- Environ Modeling & Simulation
- Grid Computing
- Molecular Structure Determination
- Physics

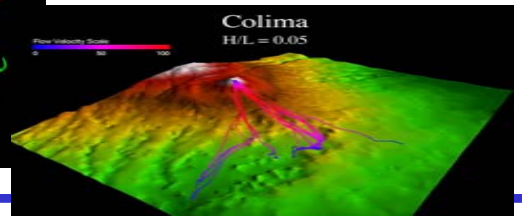


- Videos: MTV
- Urban Simulation and Viz
  - StreetScenes
  - I-90 Toll Barrier
  - Medical Campus
  - Peace Bridge
- Accident Reconstruction
- Scientific Viz
  - Dental
  - Surgery
  - MRI/CT Scan
  - Confocal Microscopy
  - Crystallization Wells
  - Collaboratories





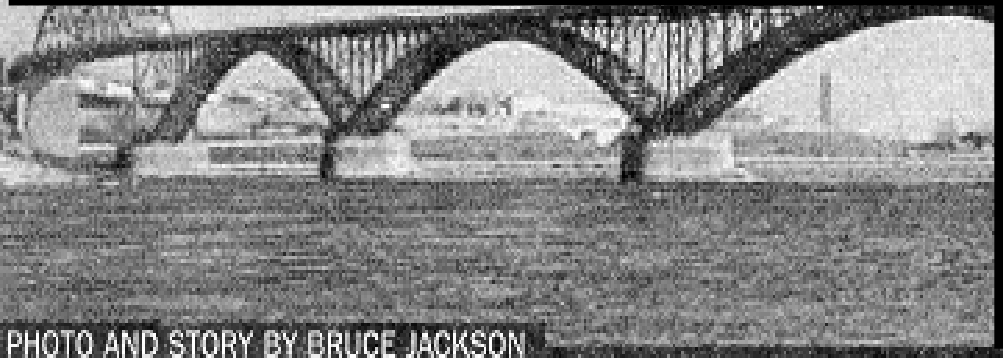




StreetScenes: Real-Time 3D Traffic Simulation

- Accurate local landmarks: Bridges, Street Signs, Business, Homes
- Can be viewed from driver's perspective
- Real-Time Navigation
- Works with
  - Corsim
  - Synchro
- Generate AVI & MOV
- Multiple Simultaneous
  - Traffic Loads
  - Simulation
  - Varying POV

Peace Bridge Visualization: Animation & Simulation



- **Proposed Options**
  - **Relocate US plaza**
  - **Build a 3-lane companion span & rehab existing bridge**

Public Forum

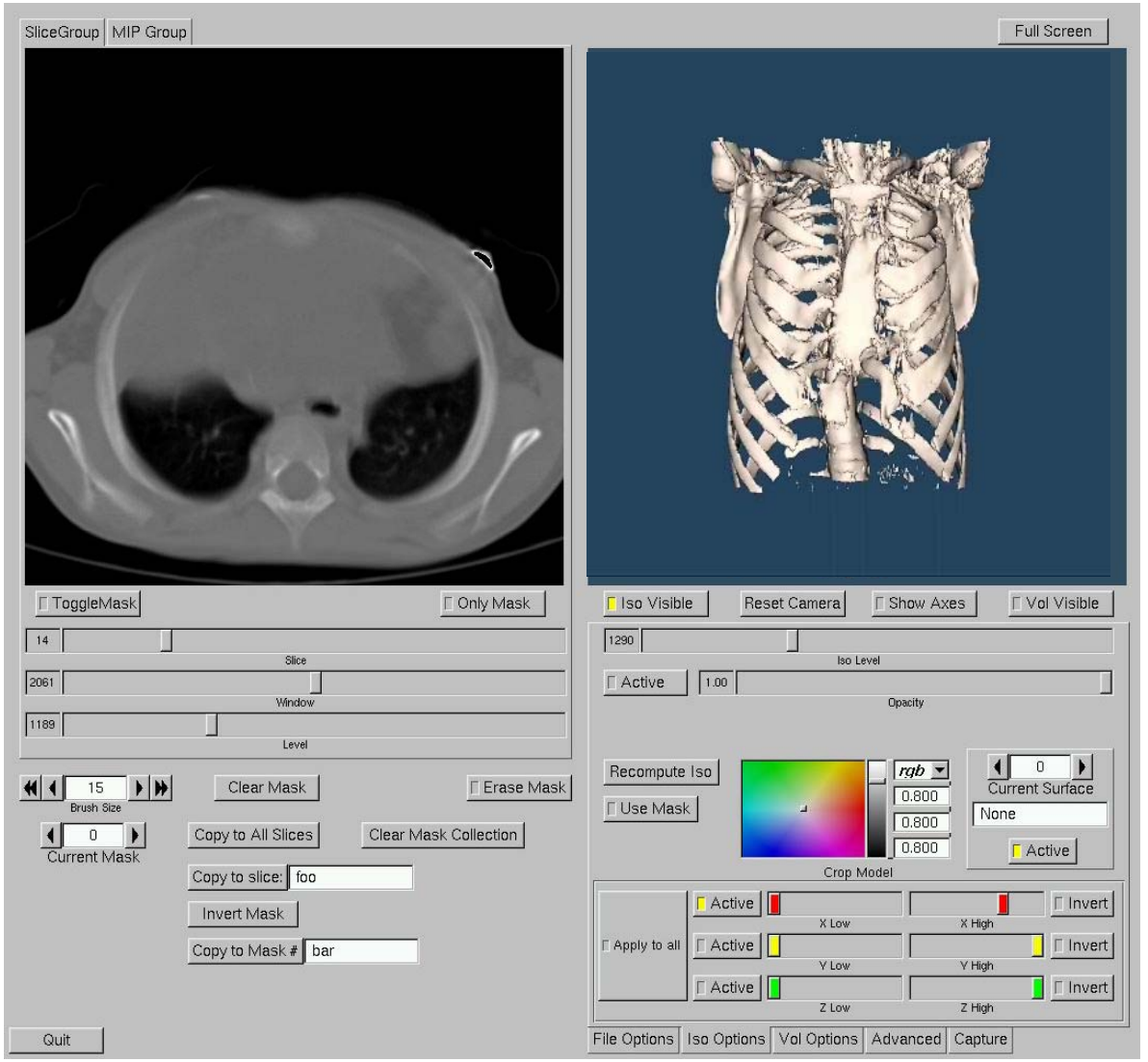
MTV

IBC Digital & CCR

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

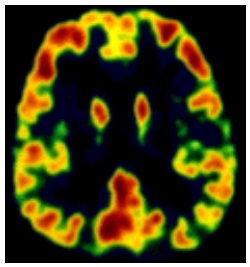
3D Medical Visualization App

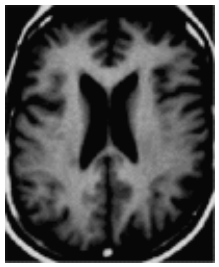
- Collaboration with Children's Hospital
  - Leading miniature access surgery center
- Application reads data output from a CT Scan
- Visualize multiple surfaces and volumes
- Export images, movies or CAD representation of model

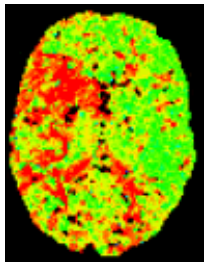


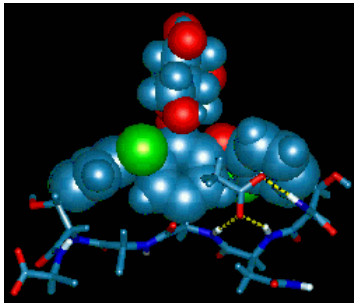
Recent Biomedical Advances (Buffalo, NY)

- 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-Arrythmia Therapy
  - Tarantula venom





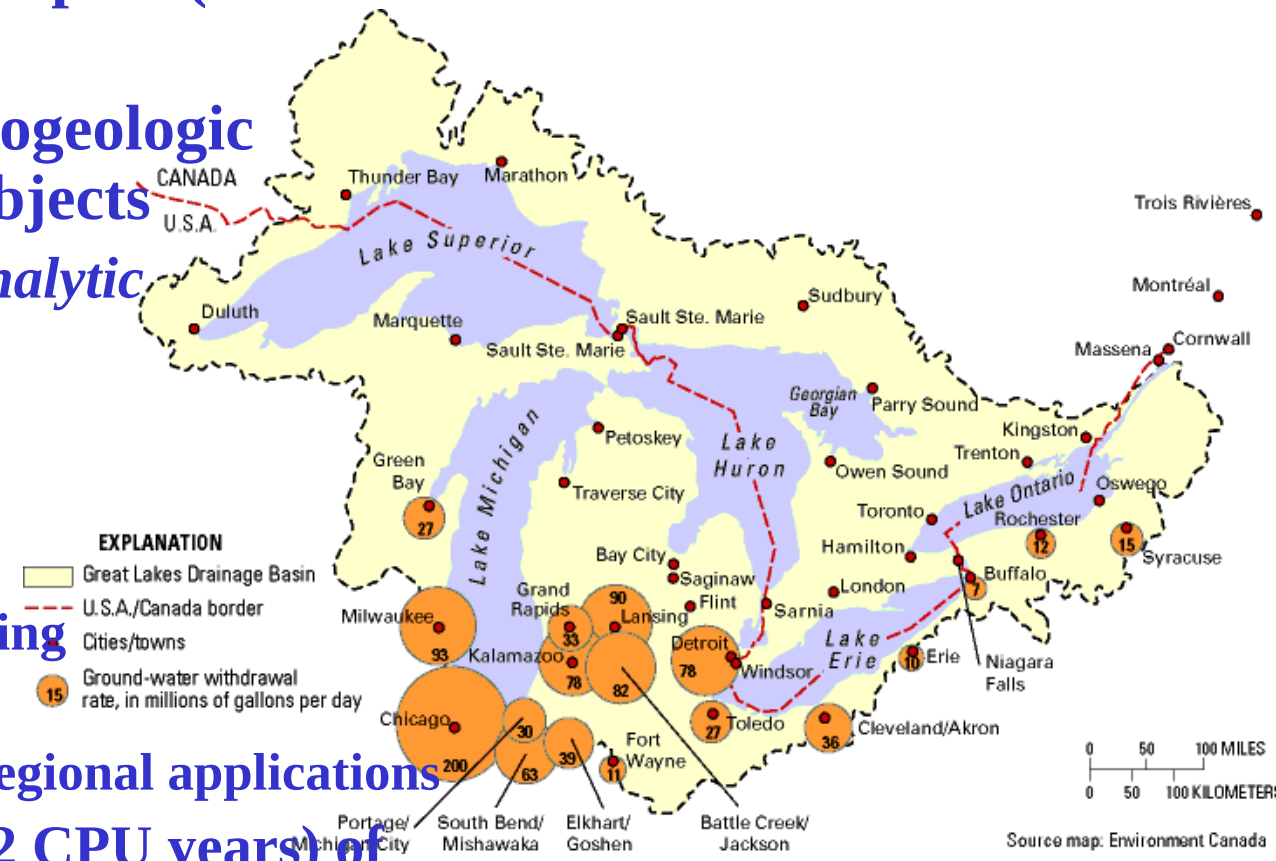




- Direct Methods Structure Determination
  - Listed on "Top Ten Algorithms of the 20th Century"
  - Vancomycin & Gramacidin A
- High Throughput Crystallization Method
- NIH National Genomics Center: Northeast Consortium
- HHMI: Center for Genomics & Proteomics
- NYSCOEBLS: $360M with RPCI & HWI

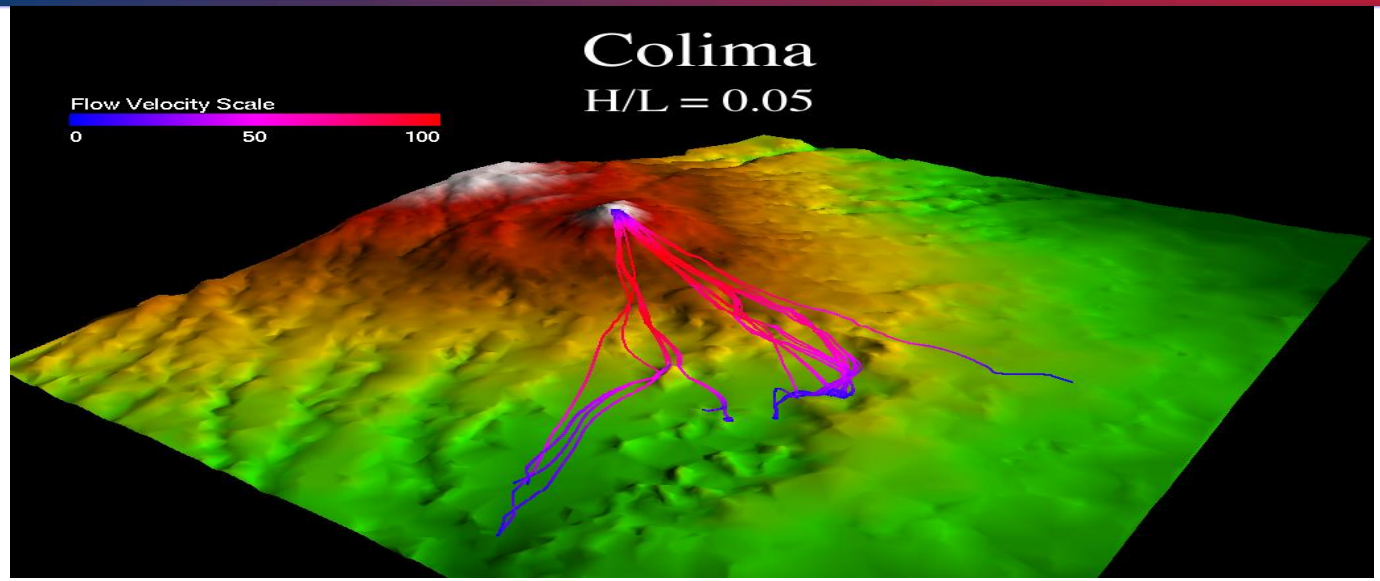
Groundwater Flow Modeling

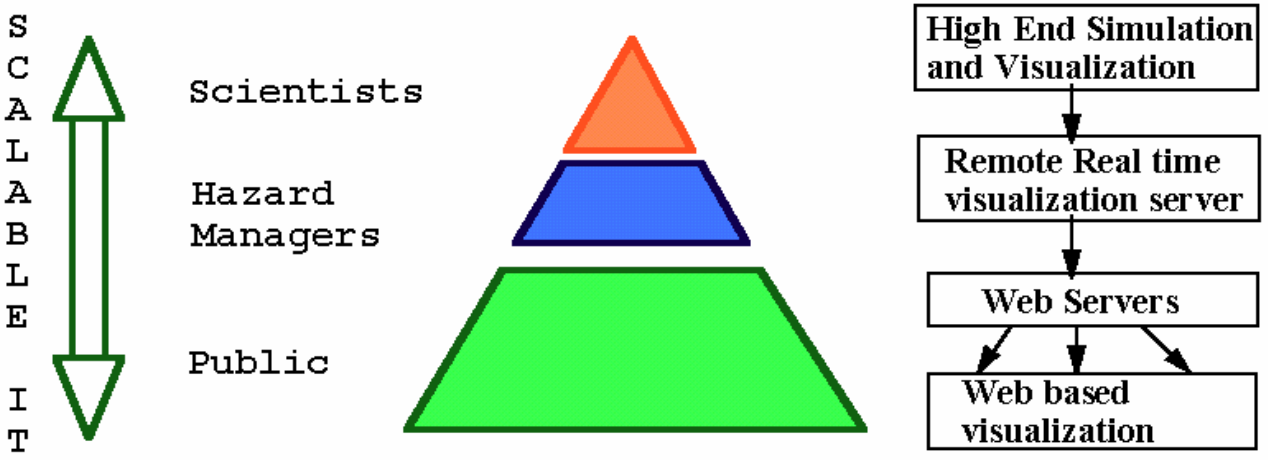
- **Regional-scale modeling of groundwater flow and contaminant transport (Great Lakes Region)**
- **Ability to include all hydrogeologic features as independent objects**
- **Current work is based on *Analytic Element Method***
- **Key features:**
  - **High precision**
  - **Highly parallel**
  - **Object-oriented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

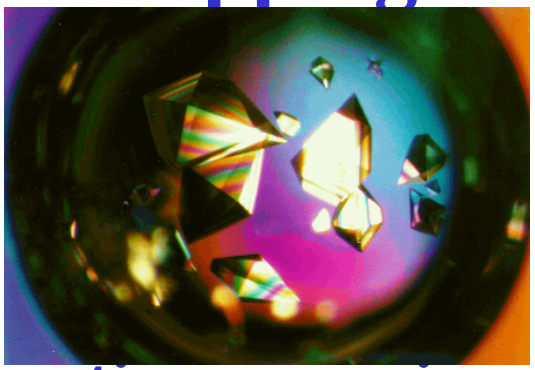
- Modeling of Volcanic Flows, Mud flows (flash flooding), and Avalanches
- Integrate information from several sources
  - Simulation results
  - Remote sensing
  - GIS data
- Develop realistic 3D models of mass flows
- Present information at appropriate level



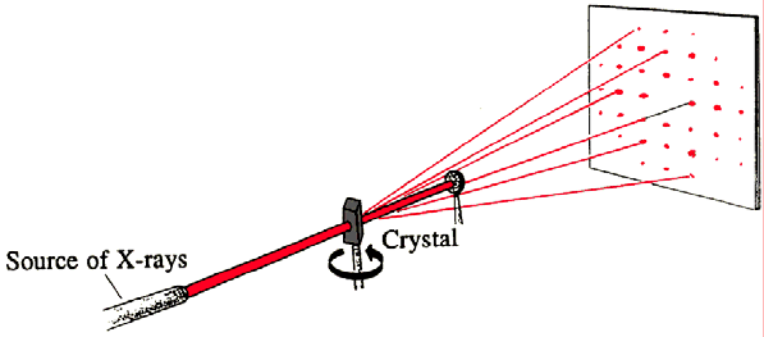


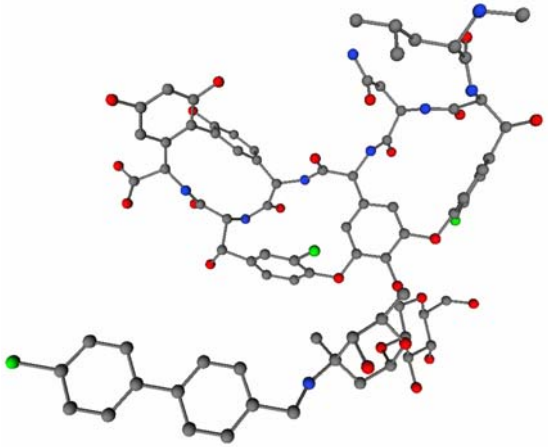
X-Ray Crystallography

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



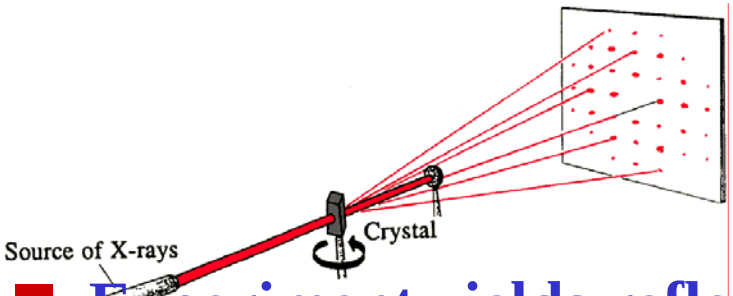
- **Procedure:**
  1. **Isolate a single crystal.**
  2. **Perform the X-Ray diffraction experiment.**



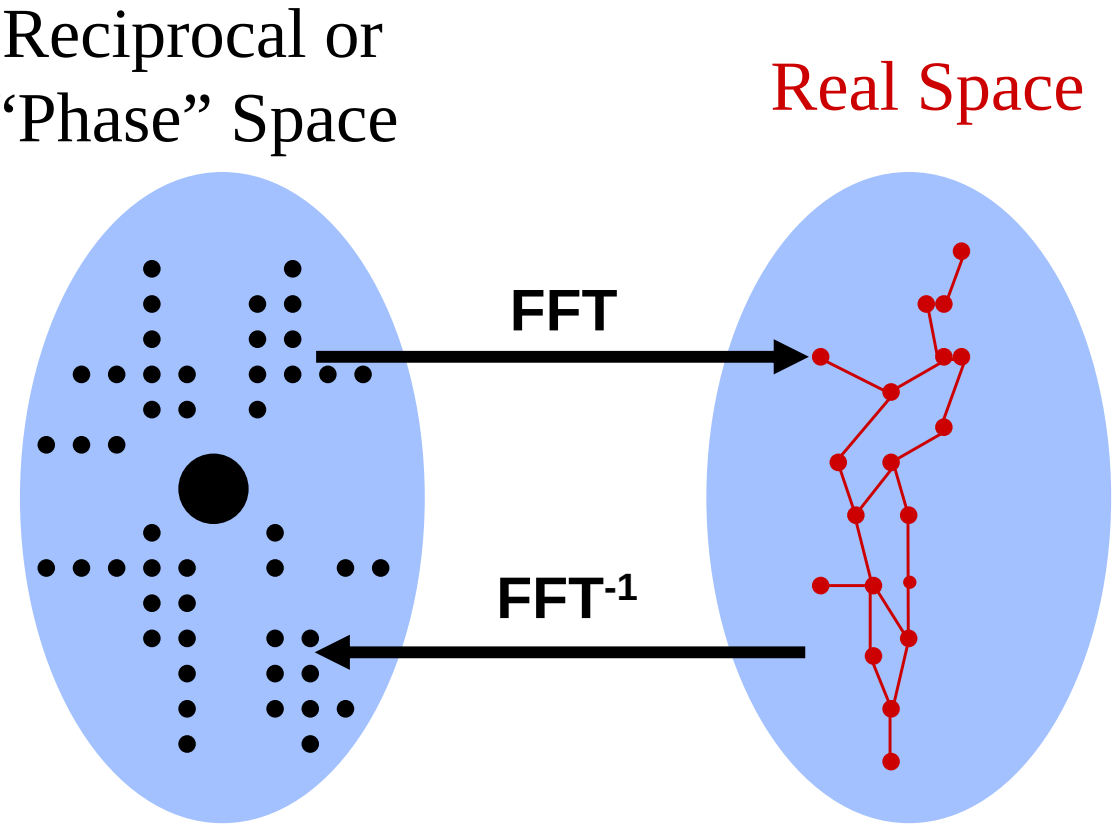


  3. **Determine molecular structure that agrees with diffration data.**

X-Ray Data & Corresponding Molecular Structure



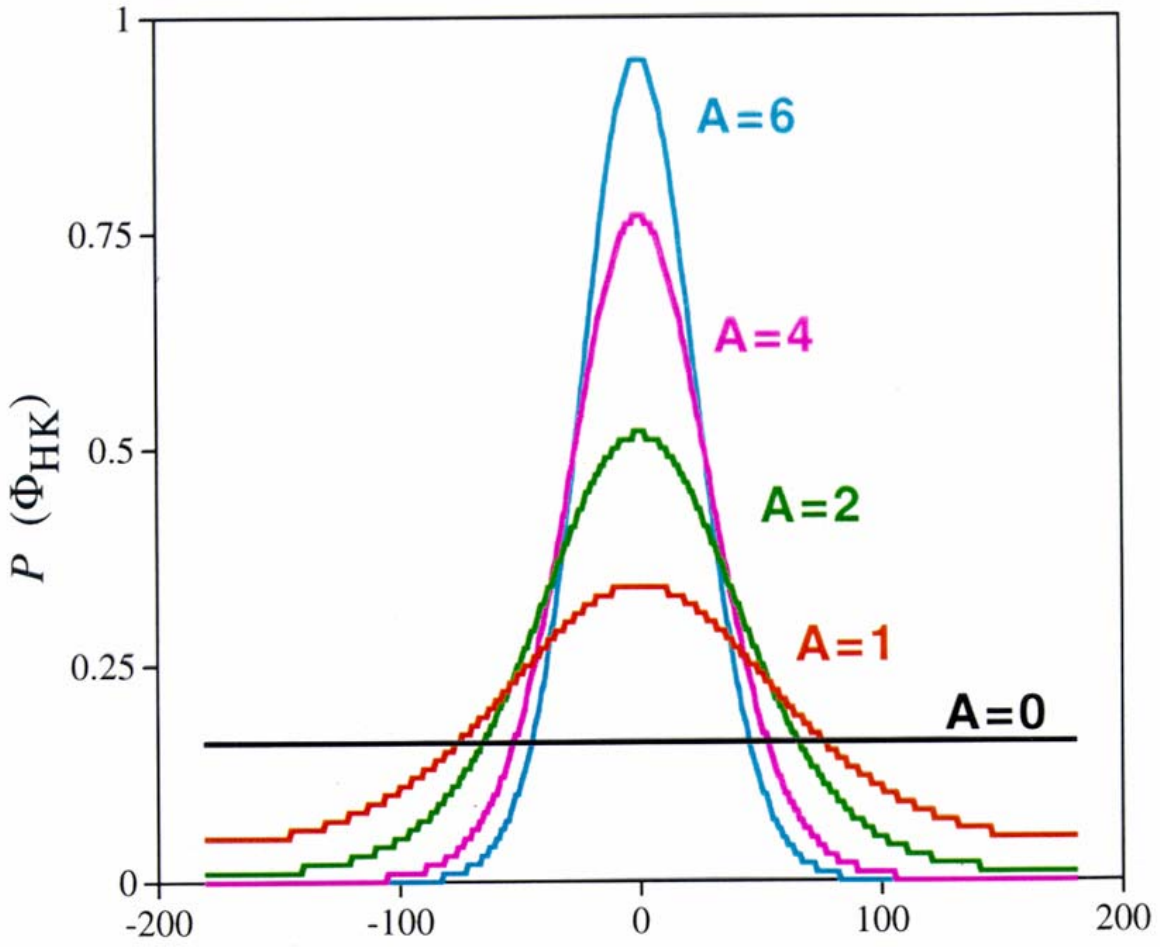
- **Experiment yields reflections and associated intensities.**
- **Underlying atomic arrangement is related to the reflections by a 3-D Fourier transform.**
- ***Phase angles are lost in experiment.***
- ***Phase Problem*: Determine the set of phases corresponding to the reflections.**



Overview of Direct Methods

- **Probability theory gives information about certain linear combinations of phases.**
  - **In particular, the triples $\phi_H + \phi_K + \phi_{-H-K} = 0$ 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.**

Cochran Distribution



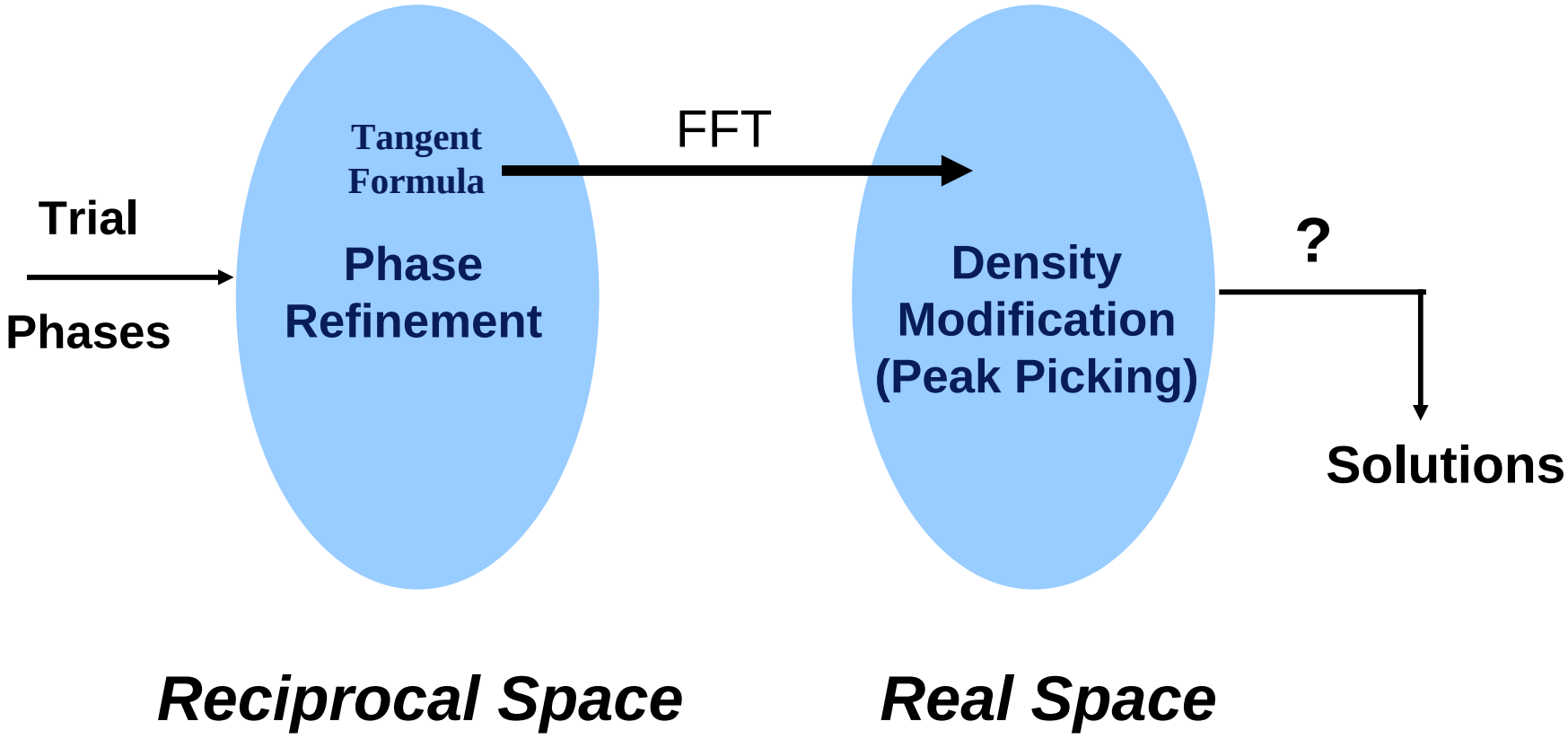
$\Phi_{HK}=\phi_H+\phi_K+\phi_{-H-K}$

- *N*=non-H atoms in unit cell
- Each triplet of phases or structure invariant, Φ_{HK}, has an associated parameter

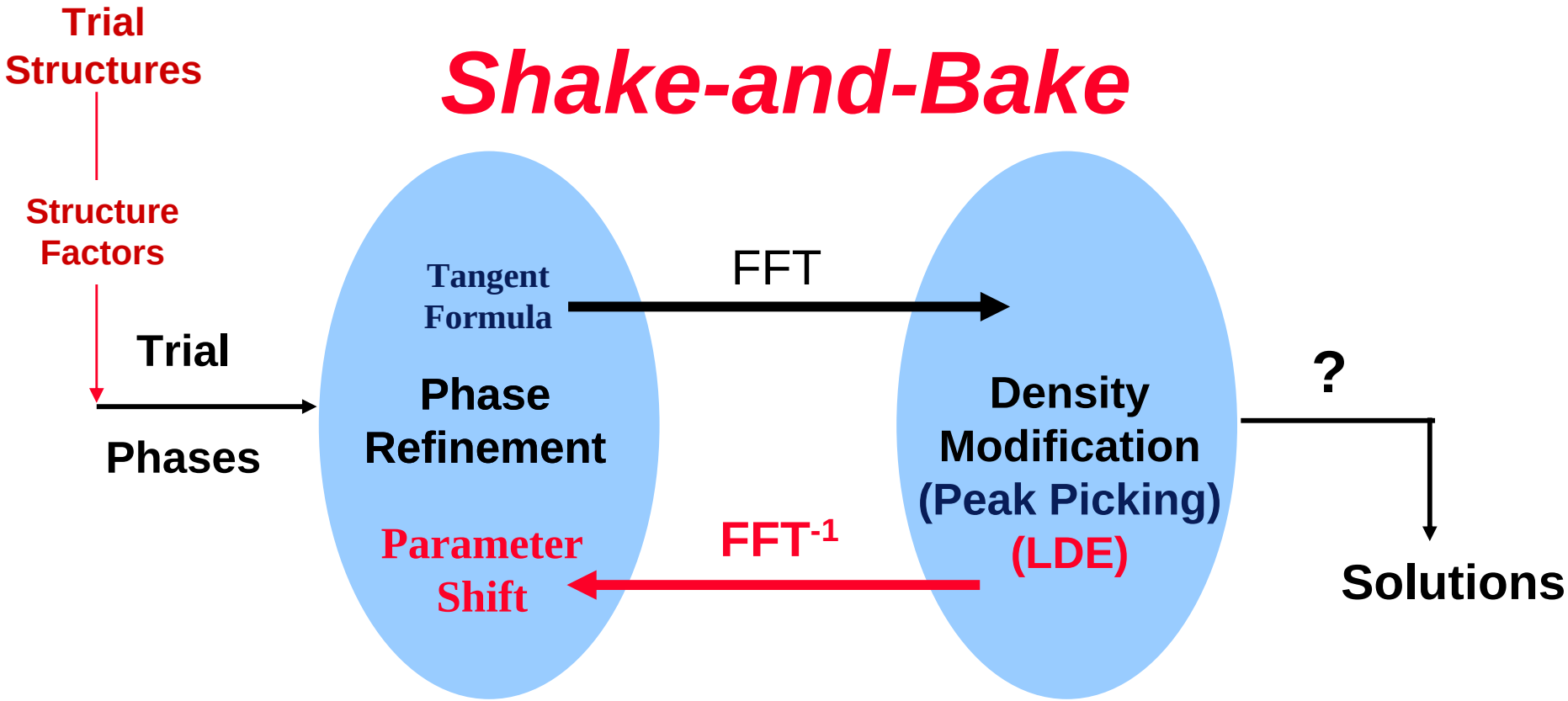
$$A_{HK}=2|E_H E_K E_{-H-K}|/N^{1/2}$$

- A_{HK} is large if
  - $|E_H|$, $|E_K|$, $|E_{-H-K}|$ are large
  - *N* is small
- If A_{HK} is large, $\Phi_{HK}\approx 0$

Conventional Direct Methods



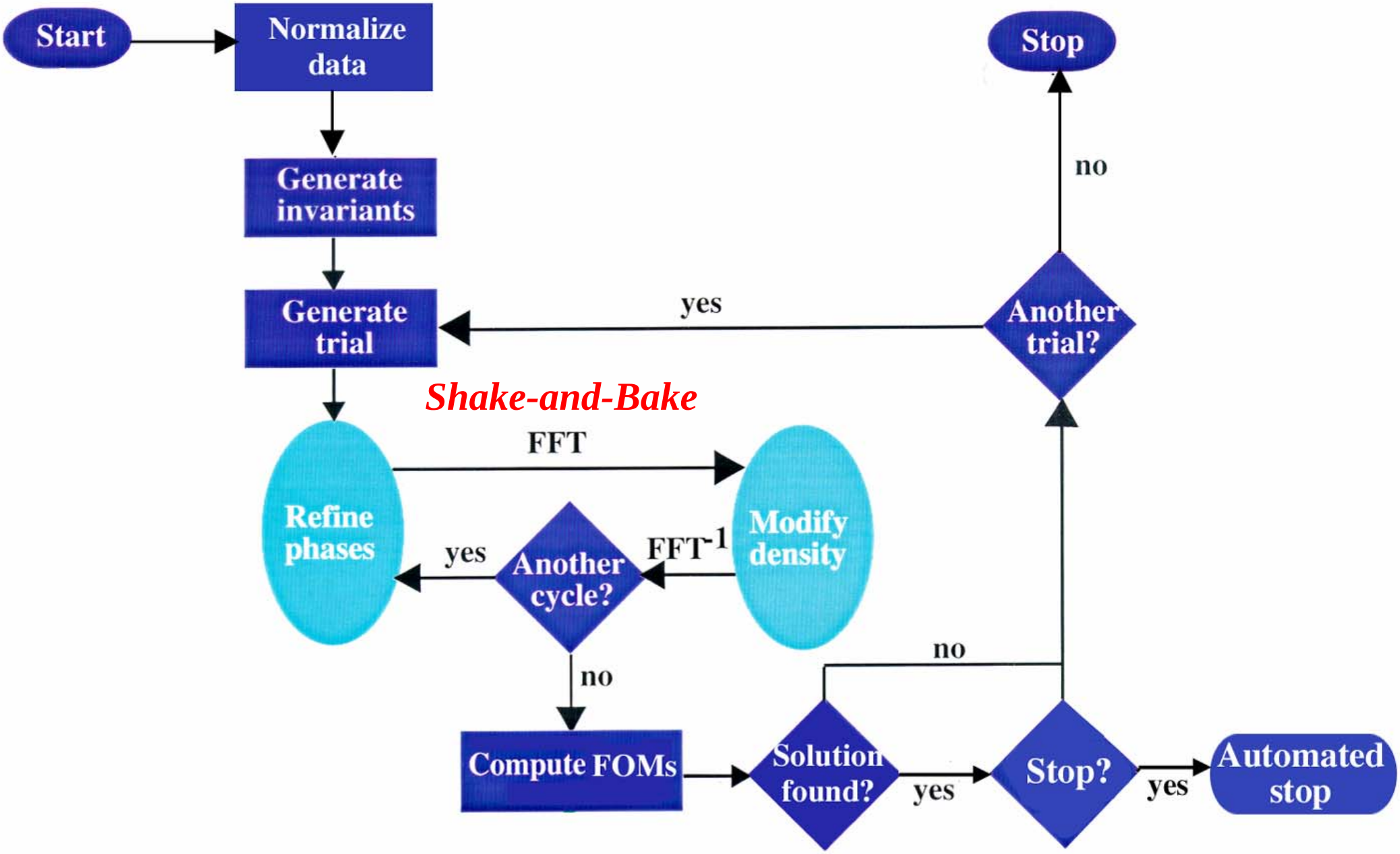
Shake-and-Bake Method: Dual-Space Refinement



Reciprocal Space
"Shake"

Real Space
"Bake"

A Direct Methods Flowchart



Generate Triplet Invariants

Reflections

Rank	h	k	l	|E|
1	0	3	4	4.65
2	0	7	30	3.67
3	5	1	1	3.67
4	8	8	5	3.26
5	6	0	1	3.15
⋮	⋮	⋮	⋮	⋮
10n=840	7	0	3	1.33
841	2	4	30	1.33

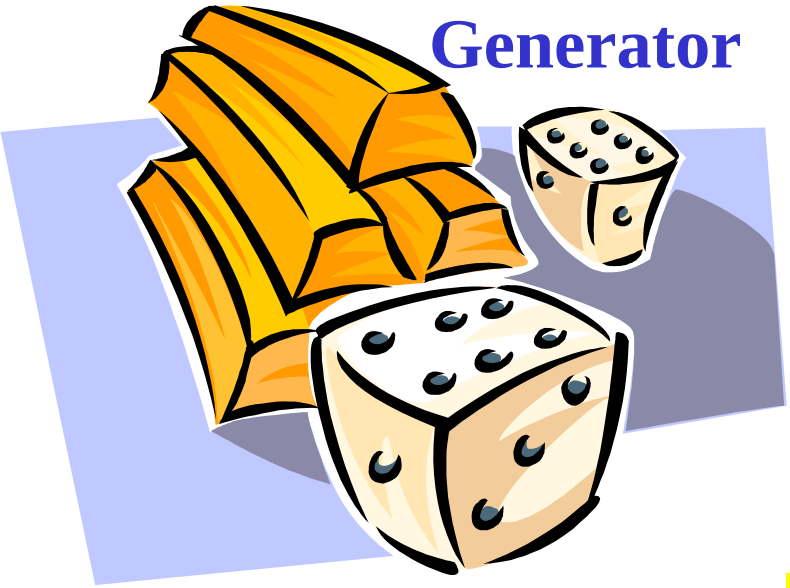
Triplets

Rank	H	K	-H-K	A
1	1	4	45	3.90
2	1	3	165	3.52
3	3	5	17	3.37
4	1	3	289	3.16
5	1	28	40	3.09
⋮	⋮	⋮	⋮	⋮
100n=840	19	259	734	0.71
8401	142	179	283	0.71

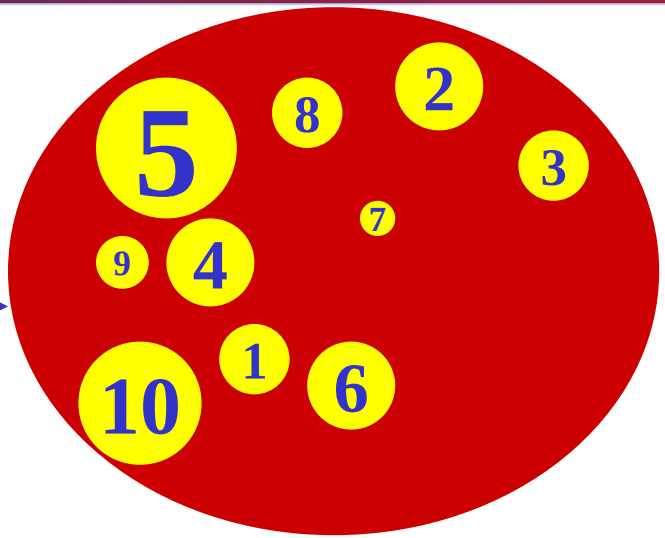
n = 84 unique atoms

Getting Started: Random Atoms

Random Number Generator



n = 10 atoms
(30 coordinates)



Structure Factor Calculation

ϕ_1 ϕ_2
ϕ_3 ϕ_4
ϕ_5 ϕ_6
ϕ_7 ϕ_8
ϕ_9 ϕ_{10}

Useful Relationships for Multiple Trial Phasing

Tangent Formula

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

Parameter Shift Optimization

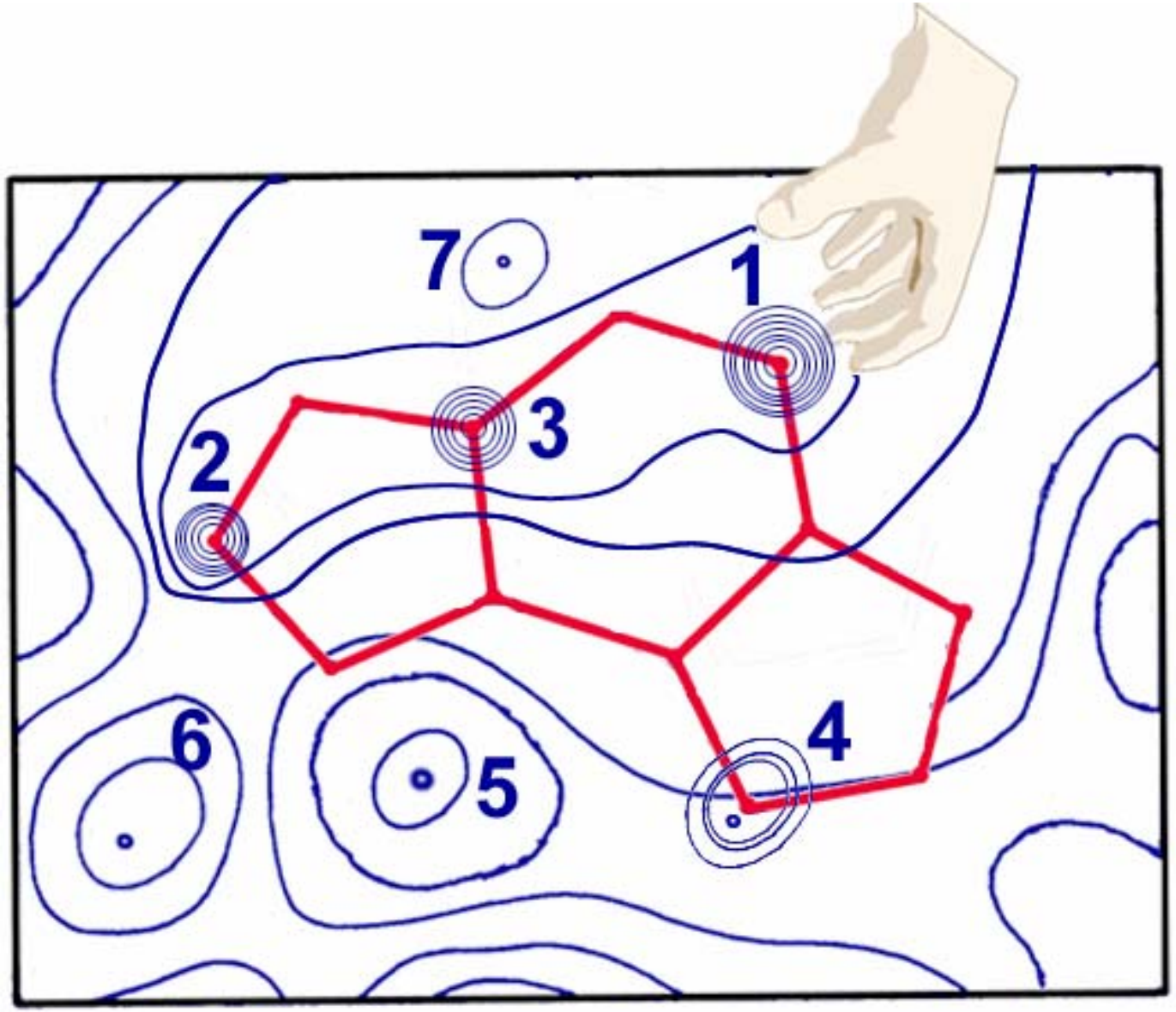
$$R(\phi) = \frac{1}{\sum_{H,K} W_{HK}} \sum_{H,K} W_{HK} \left(\cos\Phi_{HK} - \frac{I_1(W_{HK})}{I_0(W_{HK})} \right)^2$$

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

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

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

Peak Picking



Sorted Trials

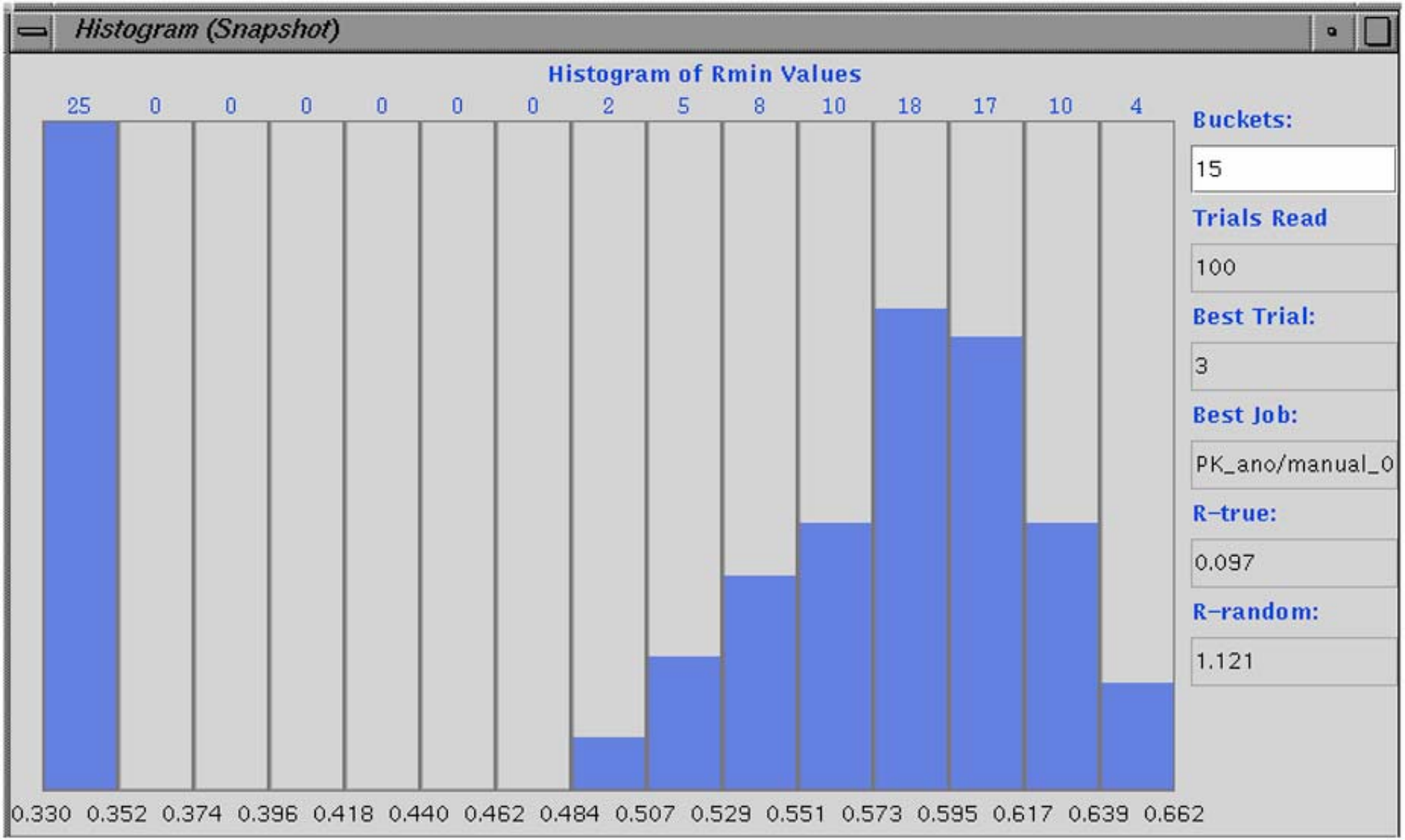
Sorted Trial Data

Trial	Cycle	Refl Phased	R Rmin	R Cryst.	CC	R Ratio	Peak Ratio
97	56	836	0.349	0.27	0.45	0.05	1.2
51	56	836	0.350	0.26	0.43	0.03	1.1
82	56	836	0.350	0.26	0.44	0.03	1.1
30	56	836	0.351	0.26	0.45	0.03	1.0
56	56	836	**0.351**	**0.27**	**0.48**	0.03	1.1
93	56	836	**0.506**	**0.36**	**0.36**	0.08	1.0
81	56	836	0.515	0.38	0.37	0.18	2.3
69	56	836	0.522	0.37	0.39	0.21	2.6
63	56	836	0.523	0.37	0.39	0.21	2.5
16	56	836	0.525	0.39	0.43	0.21	2.7

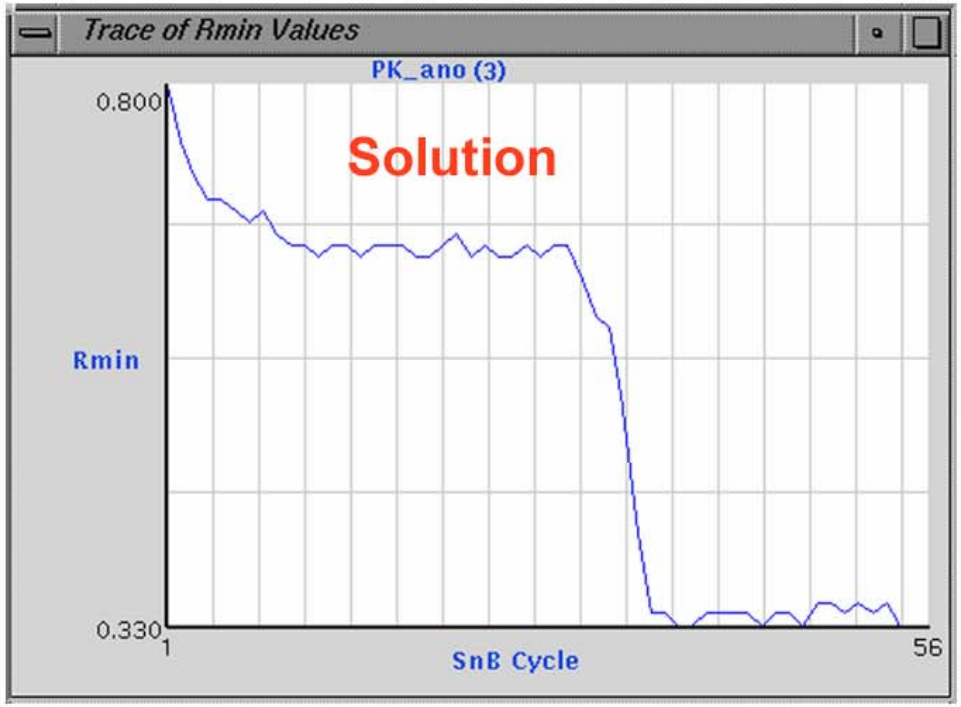
Solutions

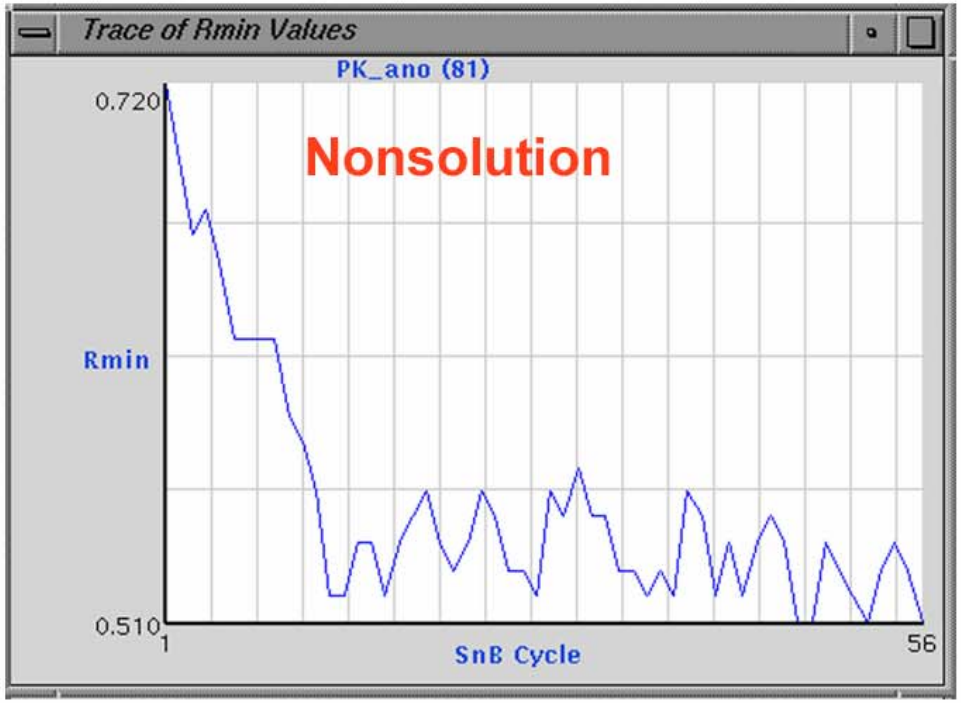
Nonsolutions

Ph8755: *SnB* Histogram

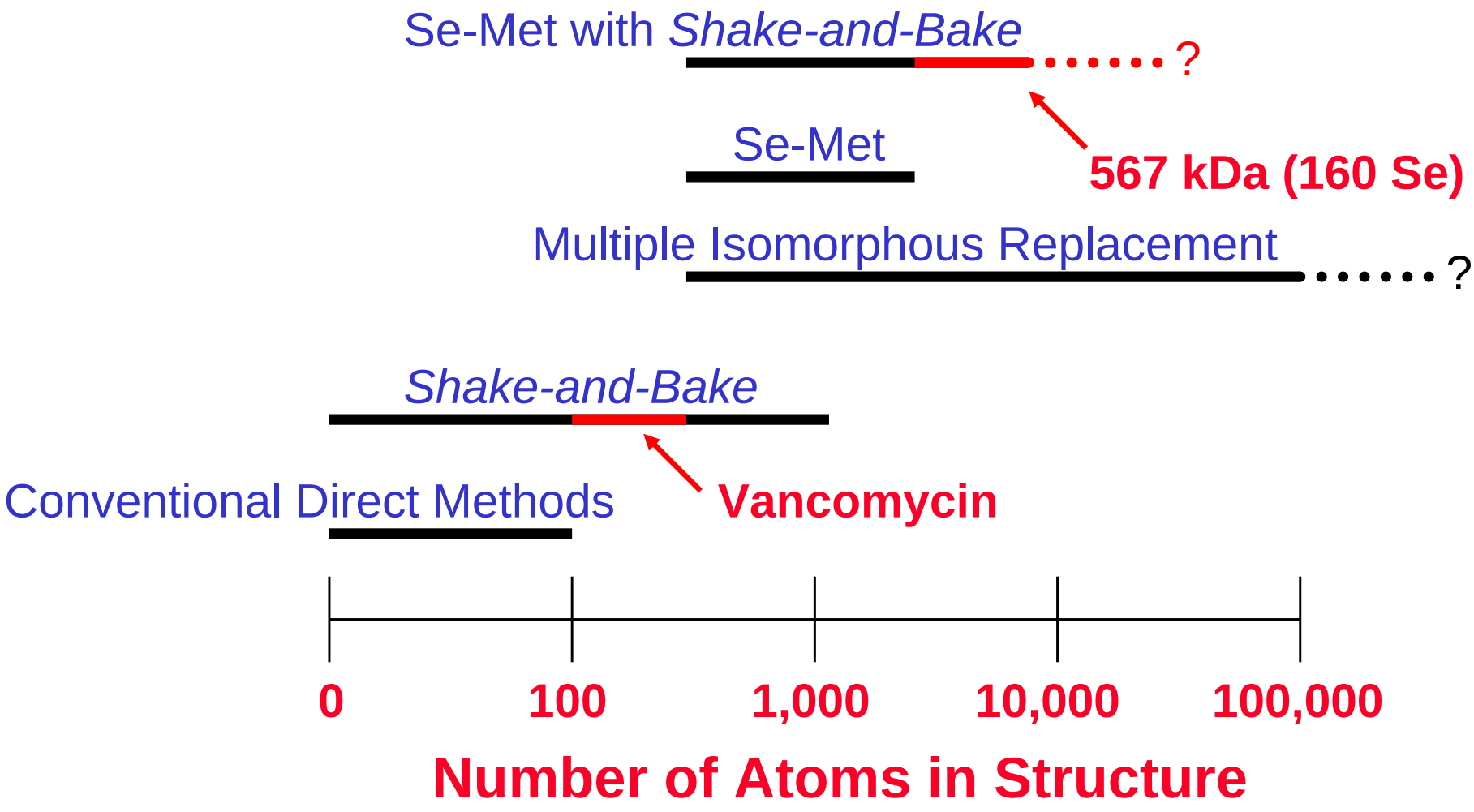


Minimal Function Traces





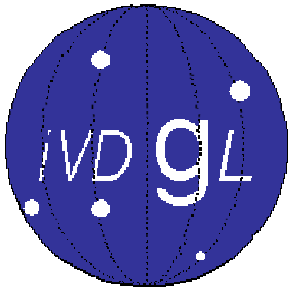
Phasing and Structure Size

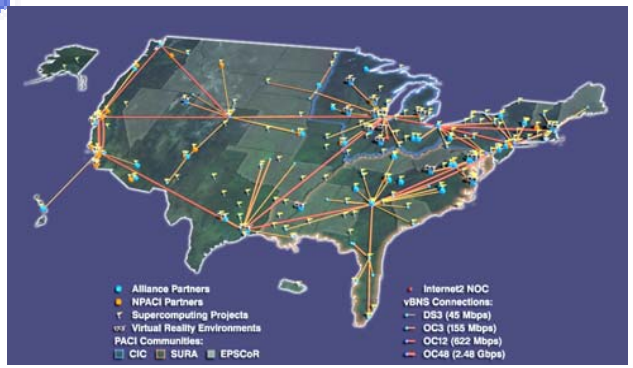


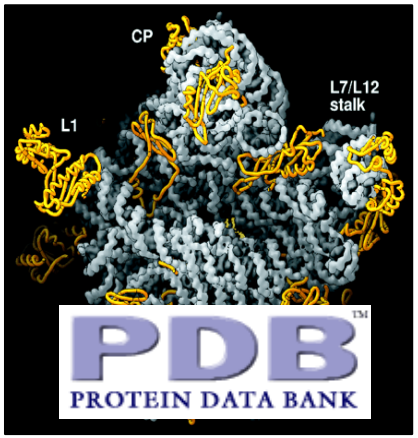
Shake-and-Bake Applications: Structure Size and Data Resolution

- **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**

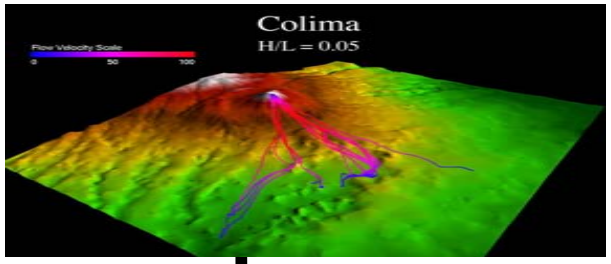
Grid Computing



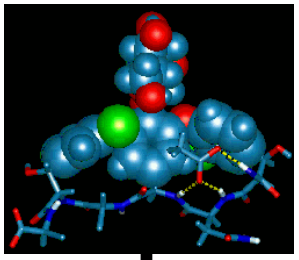




Grid Computing Overview



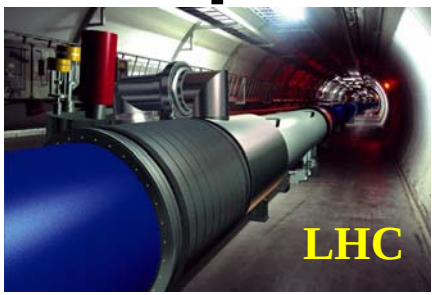
Data Acquisition

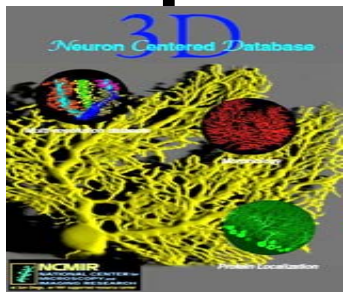


Advanced Visualization

Analysis

Imaging Instruments



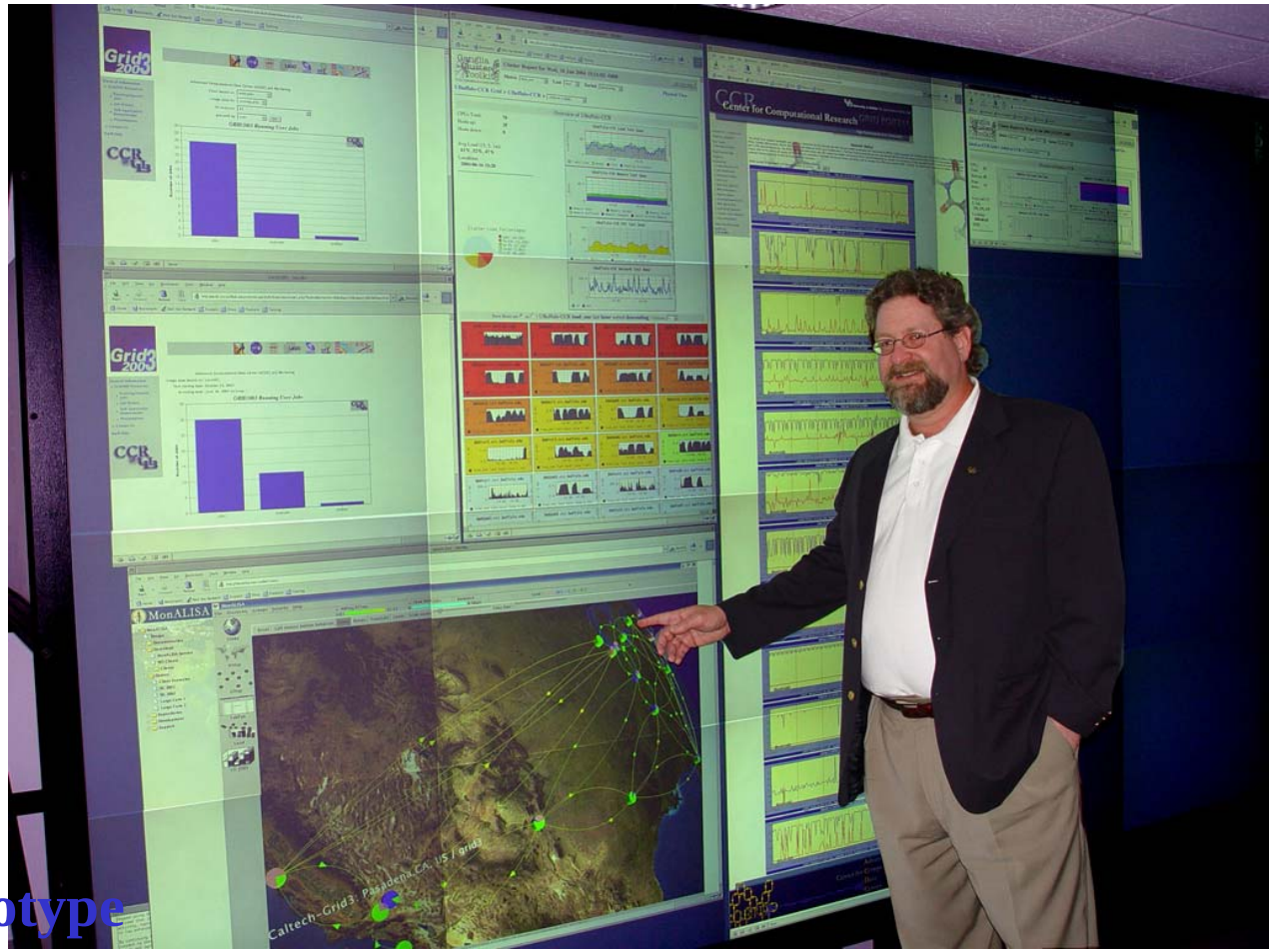


Large-Scale Databases

- Coordinate Computing Resources, People, Instruments in Dynamic Geographically-Distributed Multi-Institutional Environment
- Treat Computing Resources like Commodities
  - Compute cycles, data storage, instruments
  - Human communication environments
- No Central Control; No Trust

ACDC-Grid Collaborations

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



ACDC Data Grid Overview
(Grid-Available Data Repositories)

182 GB Storage

Joplin: Compute Cluster

300 Dual Processor
2.4 GHz Intel Xeon
RedHat Linux 7.3
38.7 TB Scratch Space

Nash: Compute Cluster

75 Dual Processor
1 GHz Pentium III
RedHat Linux 7.3
1.8 TB Scratch Space

100 GB Storage

70 GB Storage

Mama: Compute Cluster

9 Dual Processor
1 GHz Pentium III
RedHat Linux 7.3
315 GB Scratch Space

56 GB Storage

ACDC: Grid Portal

4 Processor Dell 6650
1.6 GHz Intel Xeon
RedHat Linux 9.0
66 GB Scratch Space

100 GB Storage

Young: Compute Cluster

16 Dual Sun Blades
47 Sun Ultra5
Solaris 8
770 GB Scratch Space

136 GB Storage

Crosby: Compute Cluster

SGI Origin 3800
64 - 400 MHz IP35
IRIX 6.5.14m
360 GB Scratch Space

CSE Multi-Store
40 TB

Storage Area Network
75 TB

Network Attached Storage
1.2 TB

Fogerty: Condor Flock Master

1 Dual Processor
250 MHz IP30
IRIX 6.5

CCR
19 IRIX, RedHat, & WINNT Processors

T1 Connection

Computer Science & Engineering
25 Single Processor Sun Ultra5s

School of Dental Medicine
9 Single Processor Dell P4 Desktops

Hauptman-Woodward Institute
13 Various SGI IRIX Processors

Note: Network connections are 100 Mbps unless otherwise noted.

ACDC-Grid Cyber-Infrastructure

- **Integrated Data Grid**
  - **Automated Data File Migration based on profiling users.**
- **Lightweight Grid Monitor (Dashboard)**
- **Predictive Scheduler**
  - **Define quality of service estimates of job completion, by better estimating job runtimes by profiling users.**
- **Dynamic Resource Allocation**
  - **Develop automated procedures for dynamic computational resource allocation.**
- **High-Performance Grid-Enabled Data Repositories**
  - **Develop automated procedures for dynamic data repository creation and deletion.**

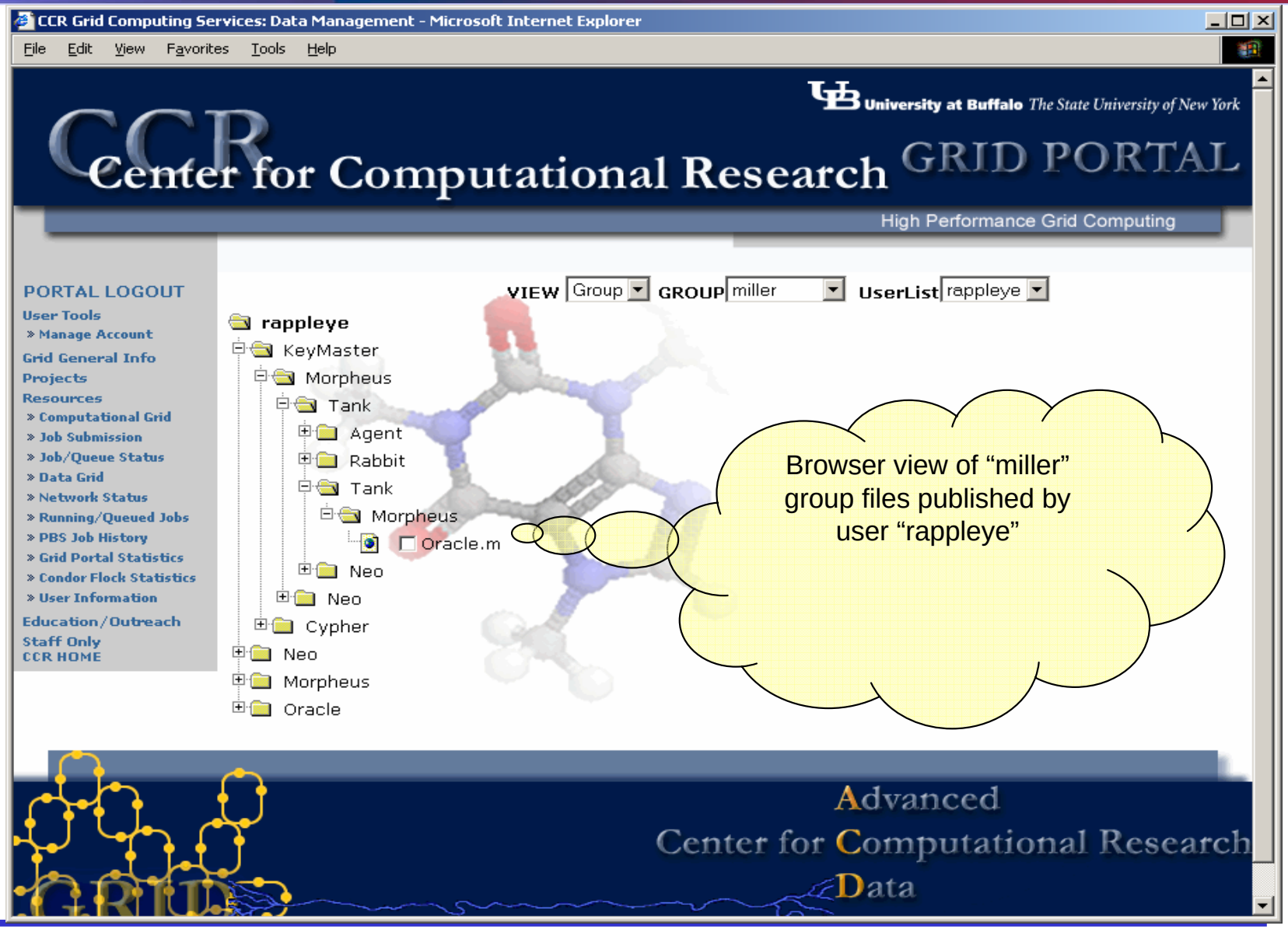
Data Grid

- **Motivation:**
  - **Large data collections are emerging as important community resources.**
  - **Data Grids complement Computational Grids.**
- **Definition:** ***A data grid is a network of distributed storage resources, including archival systems, caches, and databases, which are linked logically to create a sense of global persistence.***
- **Goal: Design and implement transparent management of data distributed across heterogeneous resources.**

ACDC-Grid Data Grid Functionality

- **Basic file management functions are accessible via a platform-independent web interface.**
- **User-friendly menus/interface.**
- **File Upload/Download to/from the Data Grid Portal.**
- **Simple Web-based file editor.**
- **Efficient search utility.**
- **Logical display of files (user/ group/ public).**
- **Ability to logically display files based on metadata (file name, size, modification date, etc.)**

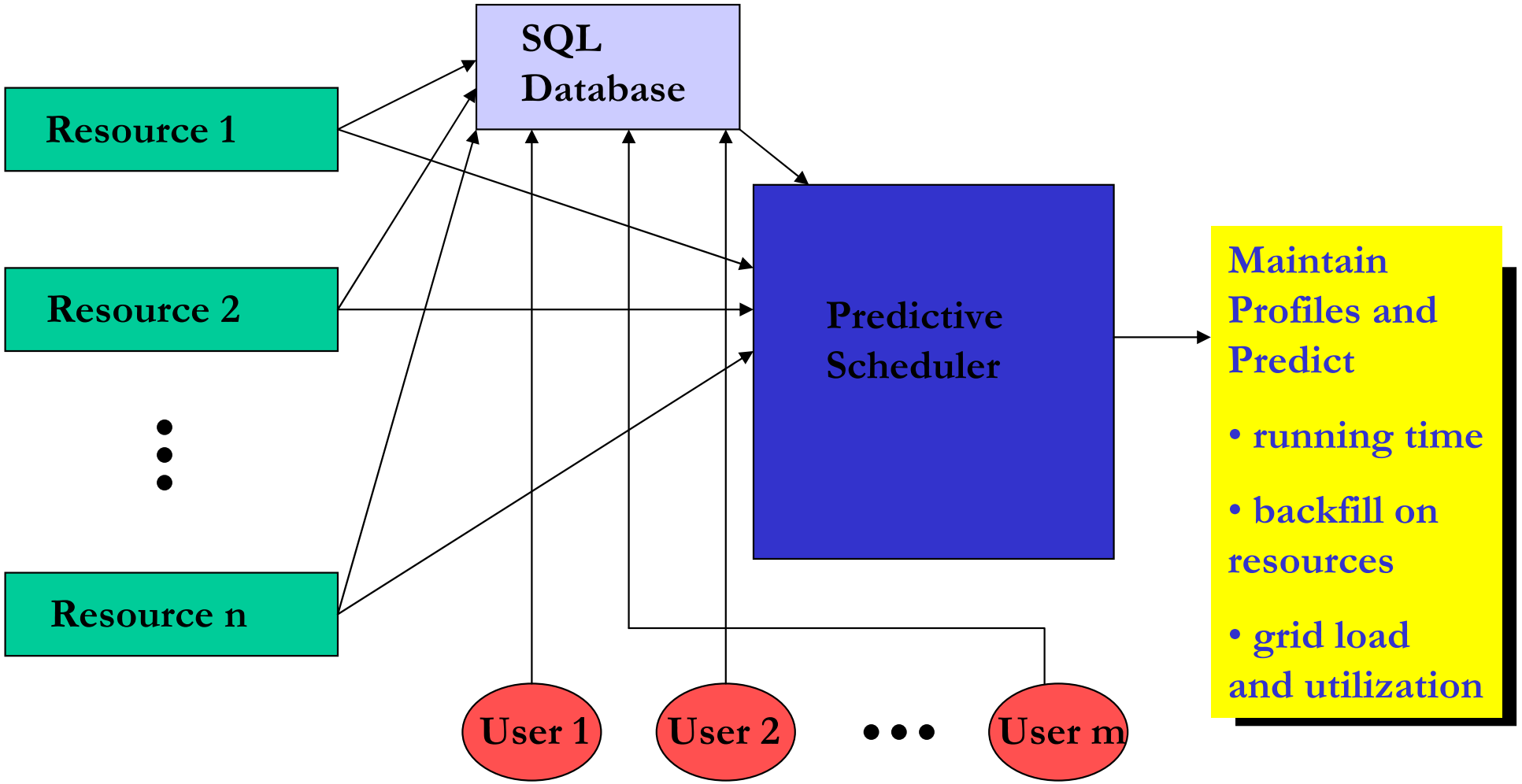
ACDC-Grid Data Grid



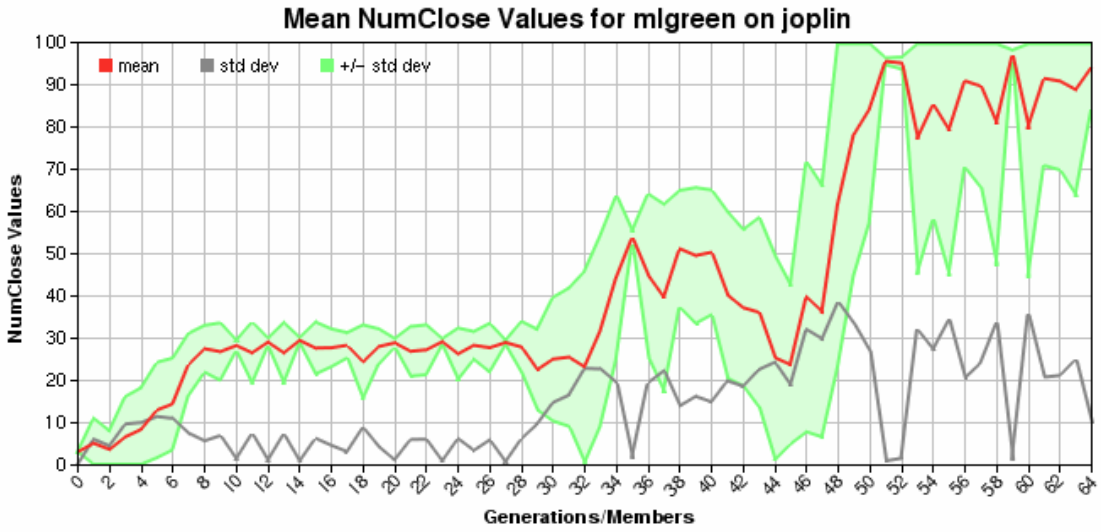
Predictive Scheduler

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

System Diagram

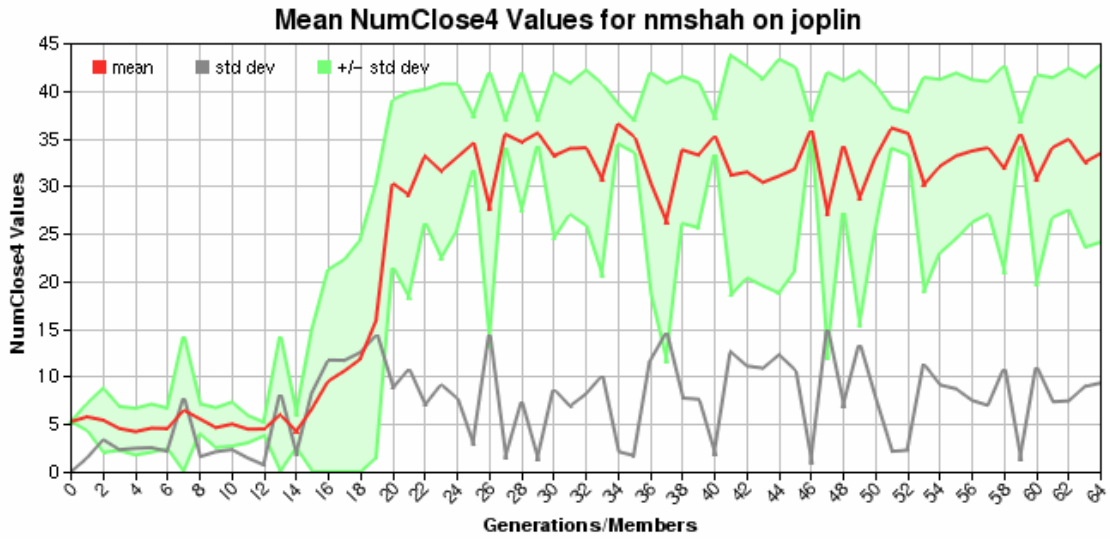


Preliminary GA results



Percent of estimates within 5% of actual values

Percent of estimates within 20% of actual values

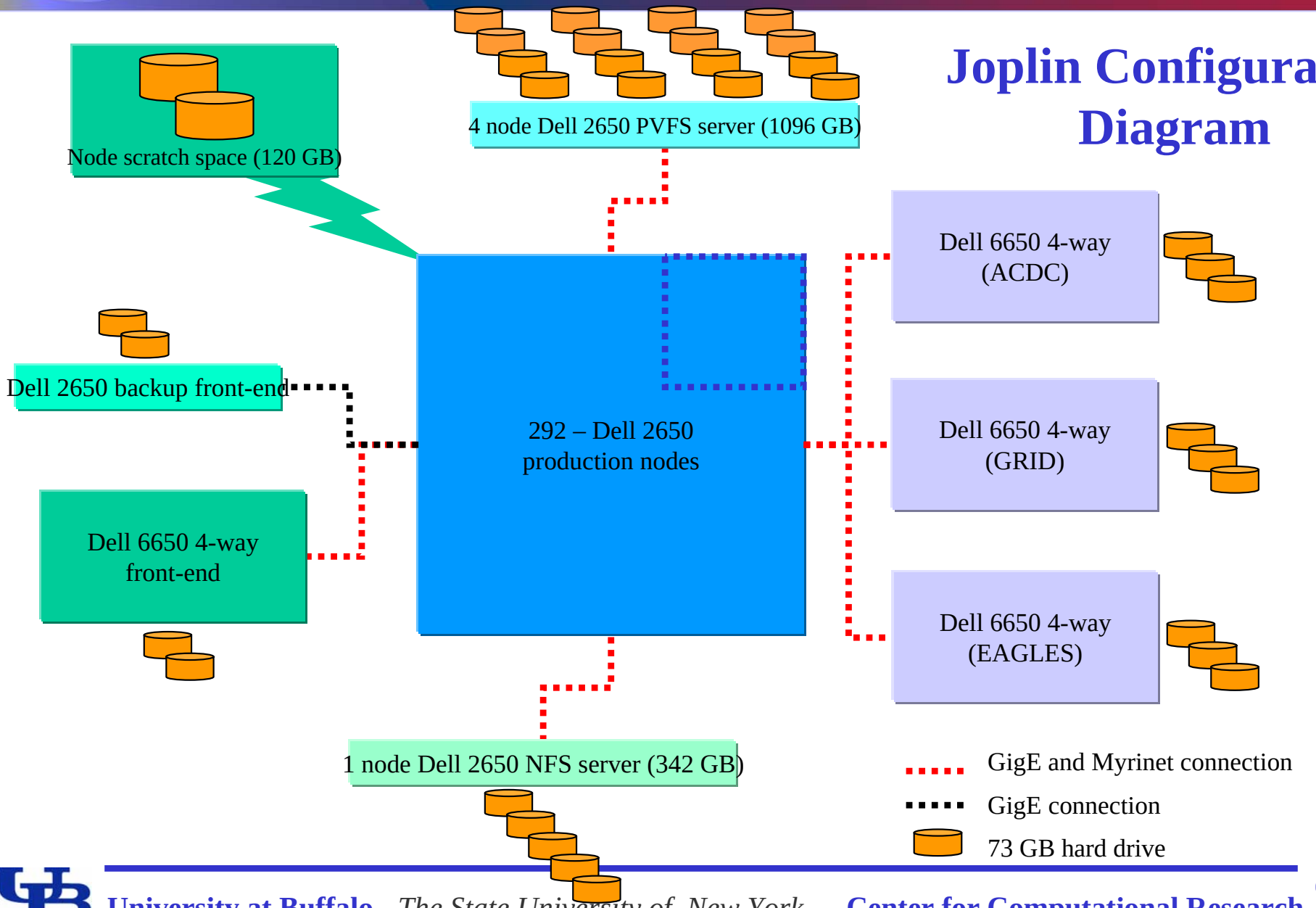


ACDC-Grid Dynamic Resource Allocation at SC03 with Grid3

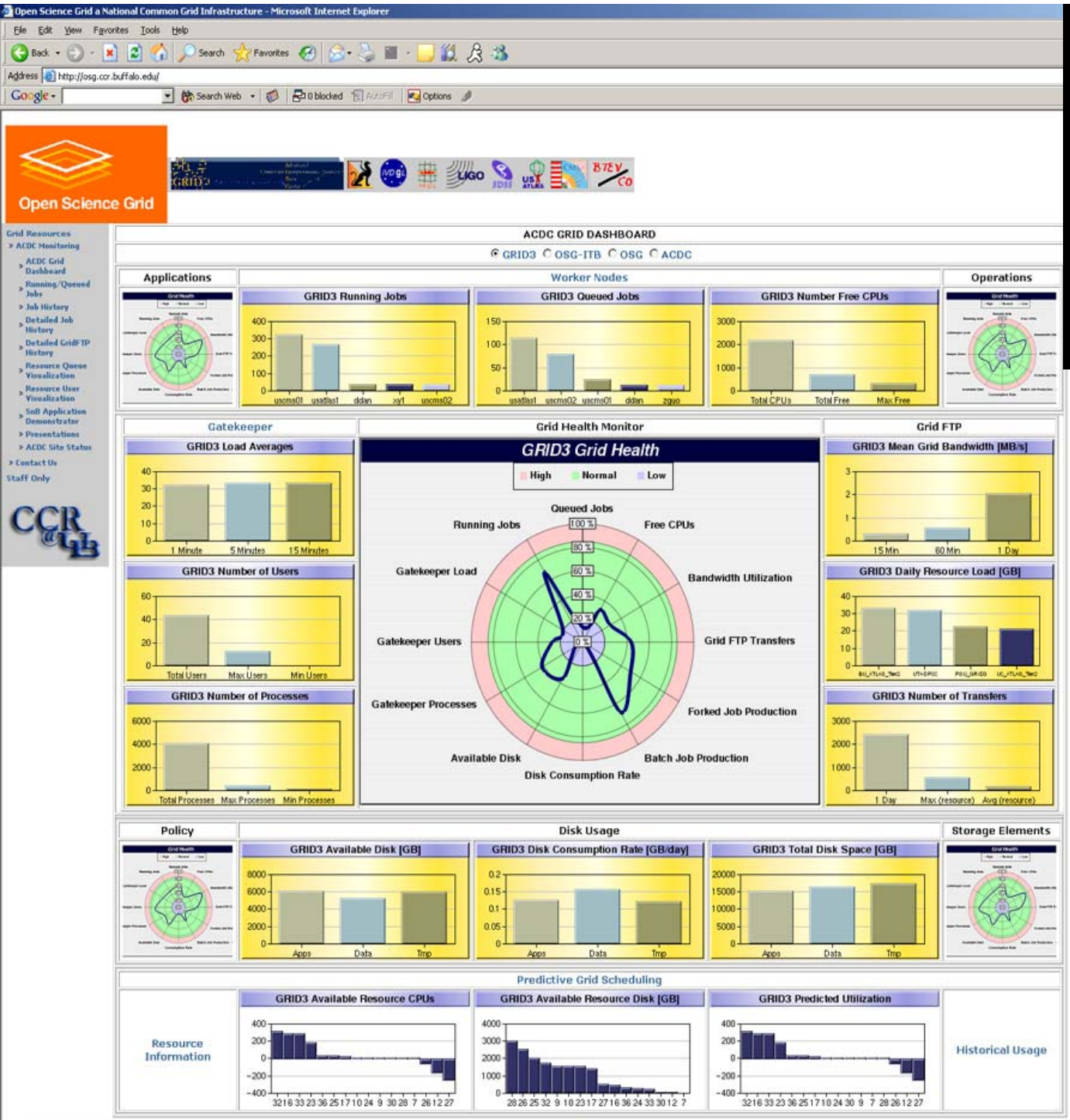
- **Small number (40) of CPUs were dedicated at night**
- **An additional 400 CPUs were dynamically allocated during the day**
- **No human intervention was required**
- **Grid applications were able to utilize the resources and surpassed the Grid3 goals**

ACDC-Grid Dynamic Resource Allocation

Joplin Configuration Diagram

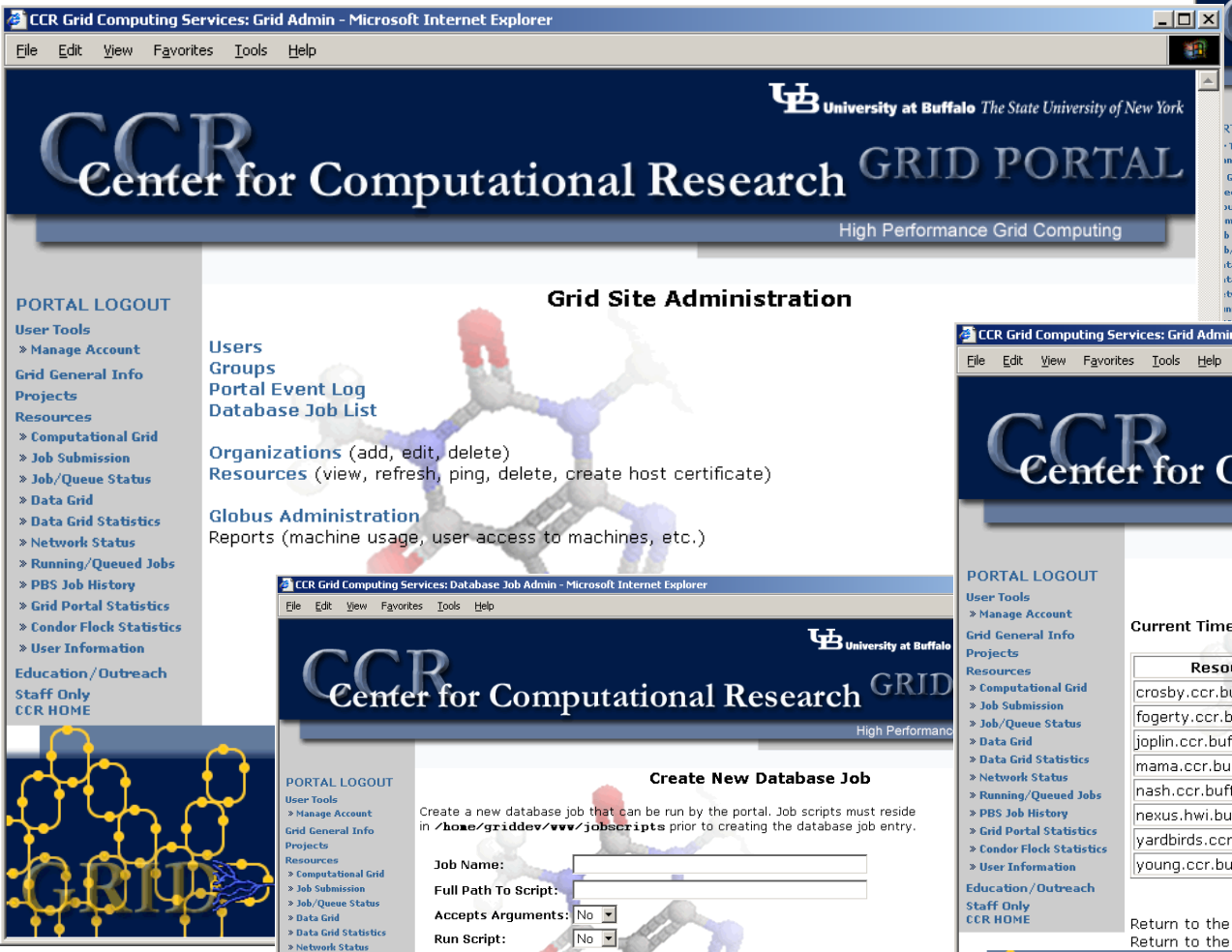


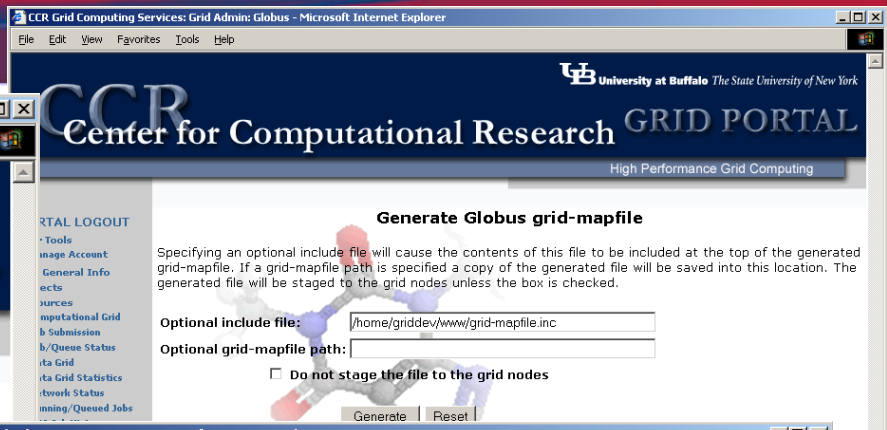
ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD

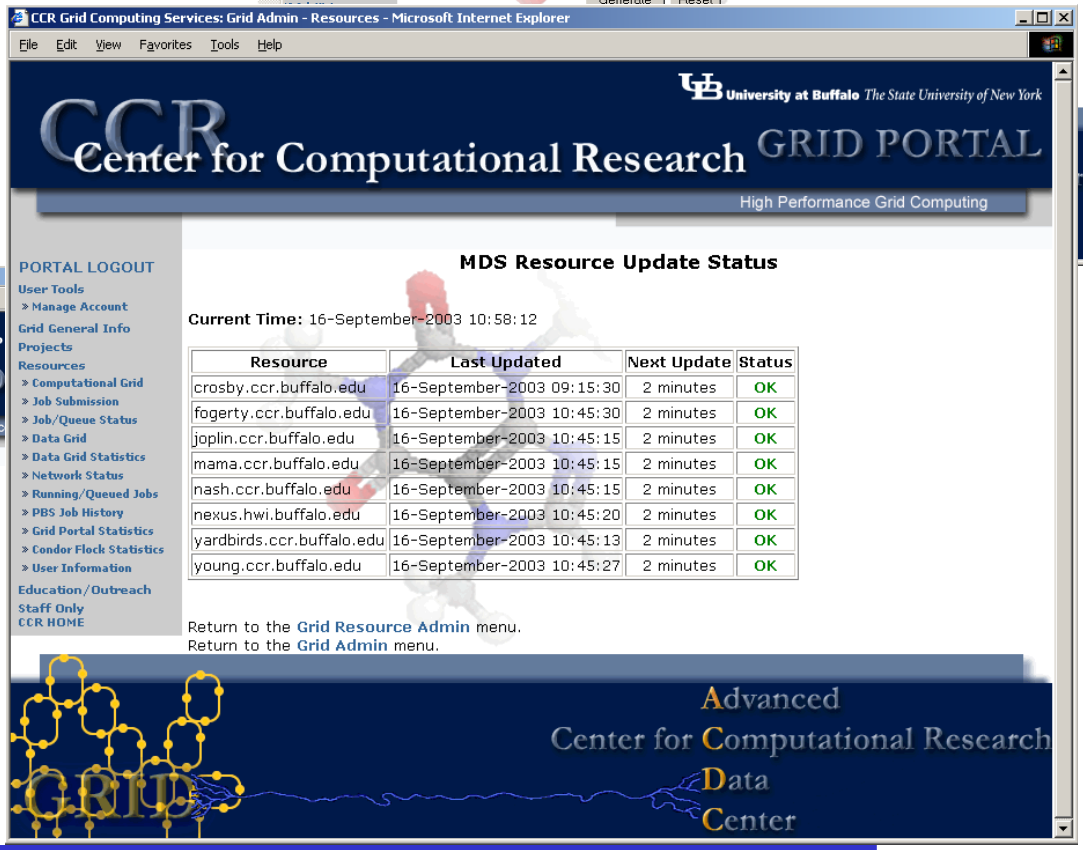


http://osg.ccr.buffalo.edu

ACDC-Grid Administration







Grid-Enabling Application Templates (GATs)

- **Structural Biology**
  - ***SnB* and *BnP* for Molecular Structure Determination/Phasing**
- **Groundwater Modeling**
  - ***Ostrich*: Optimization and Parameter Estimation Tool**
  - ***POMGL*: Princeton Ocean Model Great Lakes for Hydrodynamic Circulation**
  - ***Split*: Modeling Groundwater Flow with Analytic Element Method**
- **Earthquake Engineering**
  - ***EADR*: Evolutionary Aseismic Design and Retrofit; Passive Energy Dissipation System for Designing Earthquake Resilient Structures**
- **Computational Chemistry**
  - ***Q-Chem*: Quantum Chemistry Package**
- **Geographic Information Systems & BioHazards**
  - ***Titan*: Computational Modeling of Hazardous Geophysical Mass Flows**

Grid Enabled *SnB*

- **Problem Statement**
  - Use all available resources for determining a single structure
- **Grid Enabling Criteria**
  - Run on heterogeneous set of resources
  - Store results in *SnB* database
  - Mine database (and automagically deploy new jobs) to improve parameter settings
- **Runtime Parameters Transparent to User**
  - Assembling Necessary Files
  - Number of Processors
  - Trials per Processor
  - Appropriate Queue and Running Times

Grid Services and Applications

ACDC-Grid Computational Resources

Applications

Shake-and-Bake | Apache | MySQL | Oracle

Globus Toolkit | **High-level Services and Tools** | NWS

MPI | MPI-IO | C, C++, Fortran, PHP | globusrun

Core Services

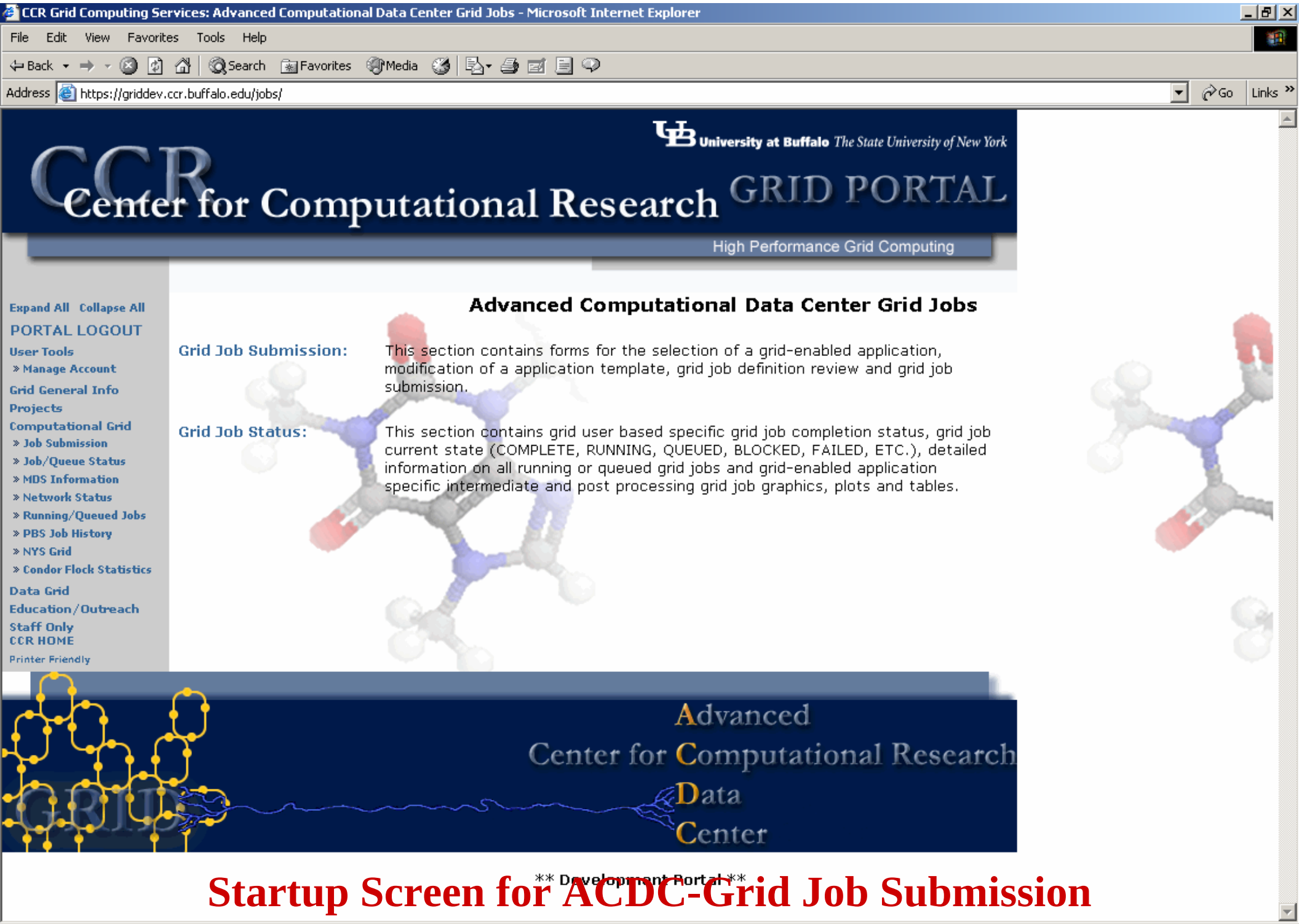
Metacomputing Directory Service | Globus Security Interface | GRAM | GASS

ACDC-Grid Data Resources

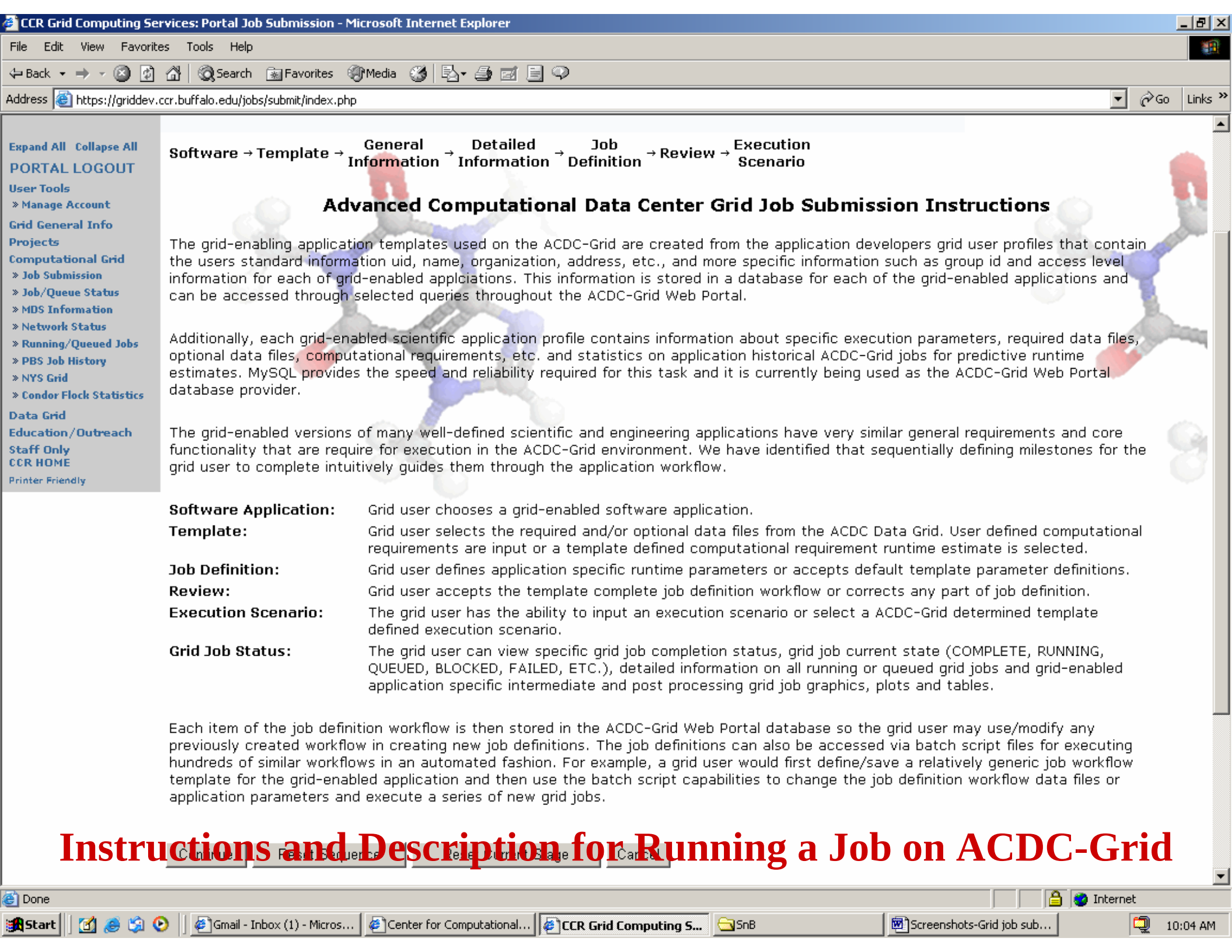
Condor | Stork | MPI | **Local Services** | RedHat Linux | WINNT

LSF | PBS | Maui Scheduler | TCP | UDP | Irix | Solaris

Adapted from Ian Foster and Carl Kesselman



Startup Screen for ACDC-Grid Job Submission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» MDS Information
» Network Status
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» PBS Job History
» NYS Grid
» Condor Flock Statistics
Data Grid
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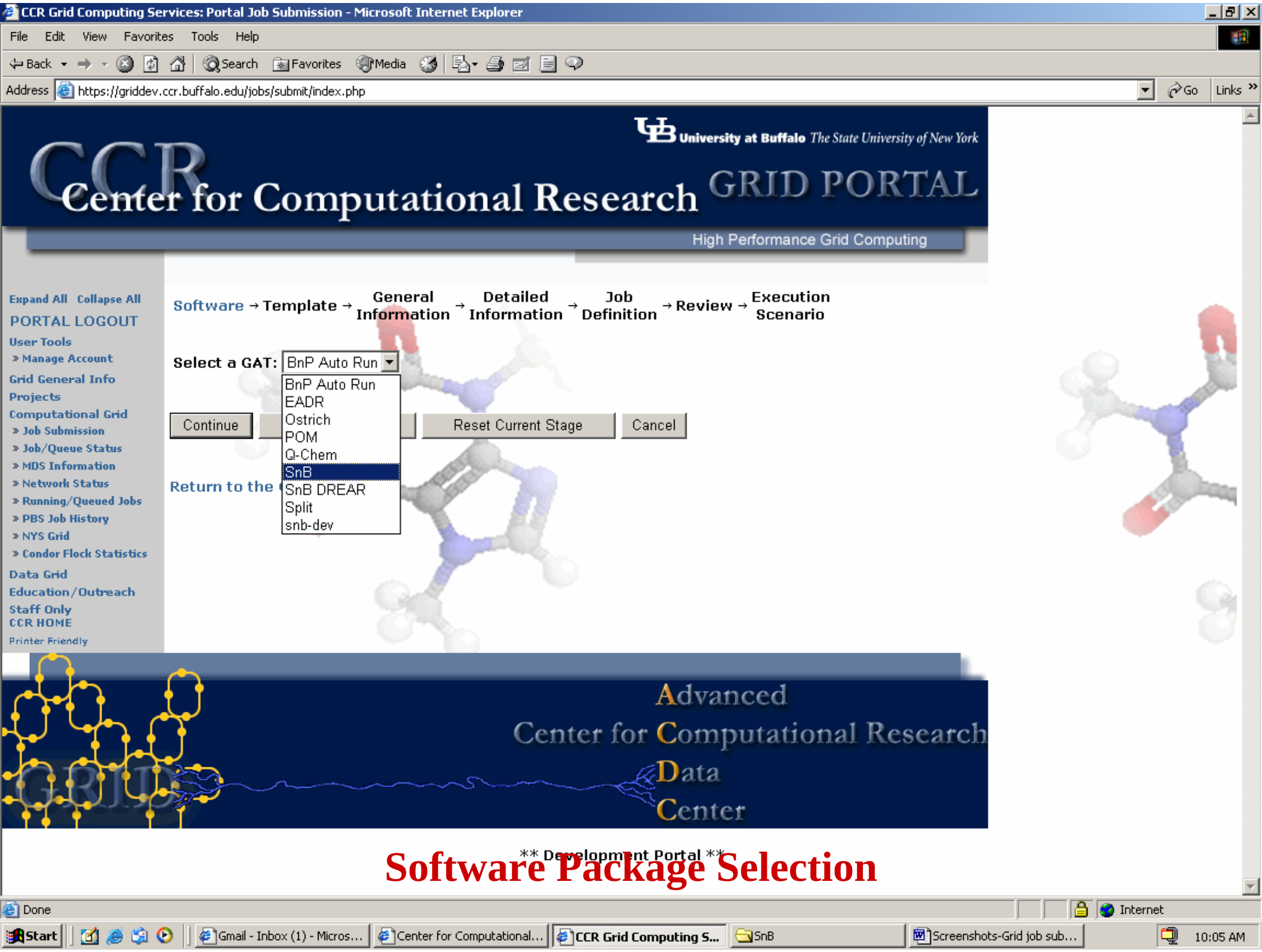
CCR HOME
Printer Friendly
Software → Template → General Information → Detailed Information → Job Definition → Review → Execution Scenario
Advanced Computational Data Center Grid Job Submission Instructions
The grid-enabling application templates used on the ACDC-Grid are created from the application developers grid user profiles that contain the users standard information uid, name, organization, address, etc., and more specific information such as group id and access level information for each of grid-enabled applciations. This information is stored in a database for each of the grid-enabled applications and can be accessed through selected queries throughout the ACDC-Grid Web Portal.
Additionally, each grid-enabled scientific application profile contains information about specific execution parameters, required data files, optional data files, computational requirements, etc. and statistics on application historical ACDC-Grid jobs for predictive runtime estimates. MySQL provides the speed and reliability required for this task and it is currently being used as the ACDC-Grid Web Portal database provider.
The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are require for execution in the ACDC-Grid environment. We have identified that sequentially defining milestones for the grid user to complete intuitively guides them through the application workflow.
Software Application: Grid user chooses a grid-enabled software application.
Template: Grid user selects the required and/or optional data files from the ACDC Data Grid. User defined computational requirements are input or a template defined computational requirement runtime estimate is selected.
Job Definition: Grid user defines application specific runtime parameters or accepts default template parameter definitions.
Review: Grid user accepts the template complete job definition workflow or corrects any part of job definition.
Execution Scenario: The grid user has the ability to input an execution scenario or select a ACDC-Grid determined template defined execution scenario.
Grid Job Status: The grid user can view specific grid job completion status, grid job current state (COMPLETE, RUNNING, QUEUED, BLOCKED, FAILED, ETC.), detailed information on all running or queued grid jobs and grid-enabled application specific intermediate and post processing grid job graphics, plots and tables.
Each item of the job definition workflow is then stored in the ACDC-Grid Web Portal database so the grid user may use/modify any previously created workflow in creating new job definitions. The job definitions can also be accessed via batch script files for executing hundreds of similar workflows in an automated fashion. For example, a grid user would first define/save a relatively generic job workflow template for the grid-enabled application and then use the batch script capabilities to change the job definition workflow data files or application parameters and execute a series of new grid jobs.
Instructions and Description for Running a Job on ACDC-Grid
Done
Internet
Start
Gmail - Inbox (1) - Micros...
Center for Computational...
CCR Grid Computing S...
SnB
Screenshots-Grid job sub...
10:04 AM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Go Links
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
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» MDS Information
» Network Status
» Running/Queued Jobs
» PBS Job History
» NYS Grid
» Condor Flock Statistics
Data Grid
Education/Outreach
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CCR HOME
Printer Friendly
Software → Template → General Information → Detailed Information → Job Definition → Review → Execution Scenario
Select a GAT: BnP Auto Run
BnP Auto Run
EADR
Ostrich
POM
Q-Chem
SnB
SnB DREAR
Split
snb-dev
Continue
Reset Current Stage
Cancel
Return to the
Advanced
Center for Computational Research
Data
Center
** Development Portal **
Software Package Selection
Done
Internet
Start
Gmail - Inbox (1) - Micros...
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CCR Grid Computing S...
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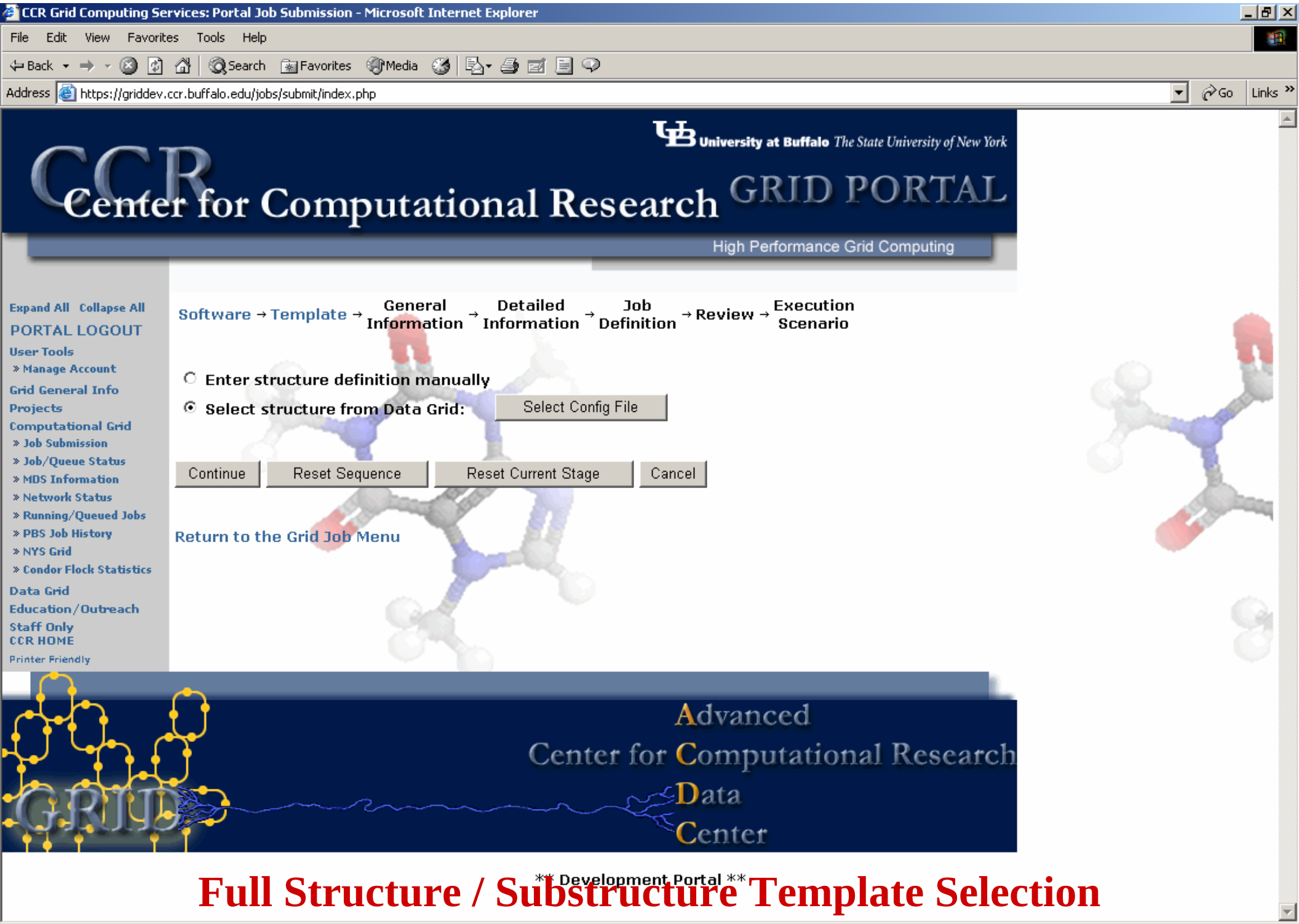
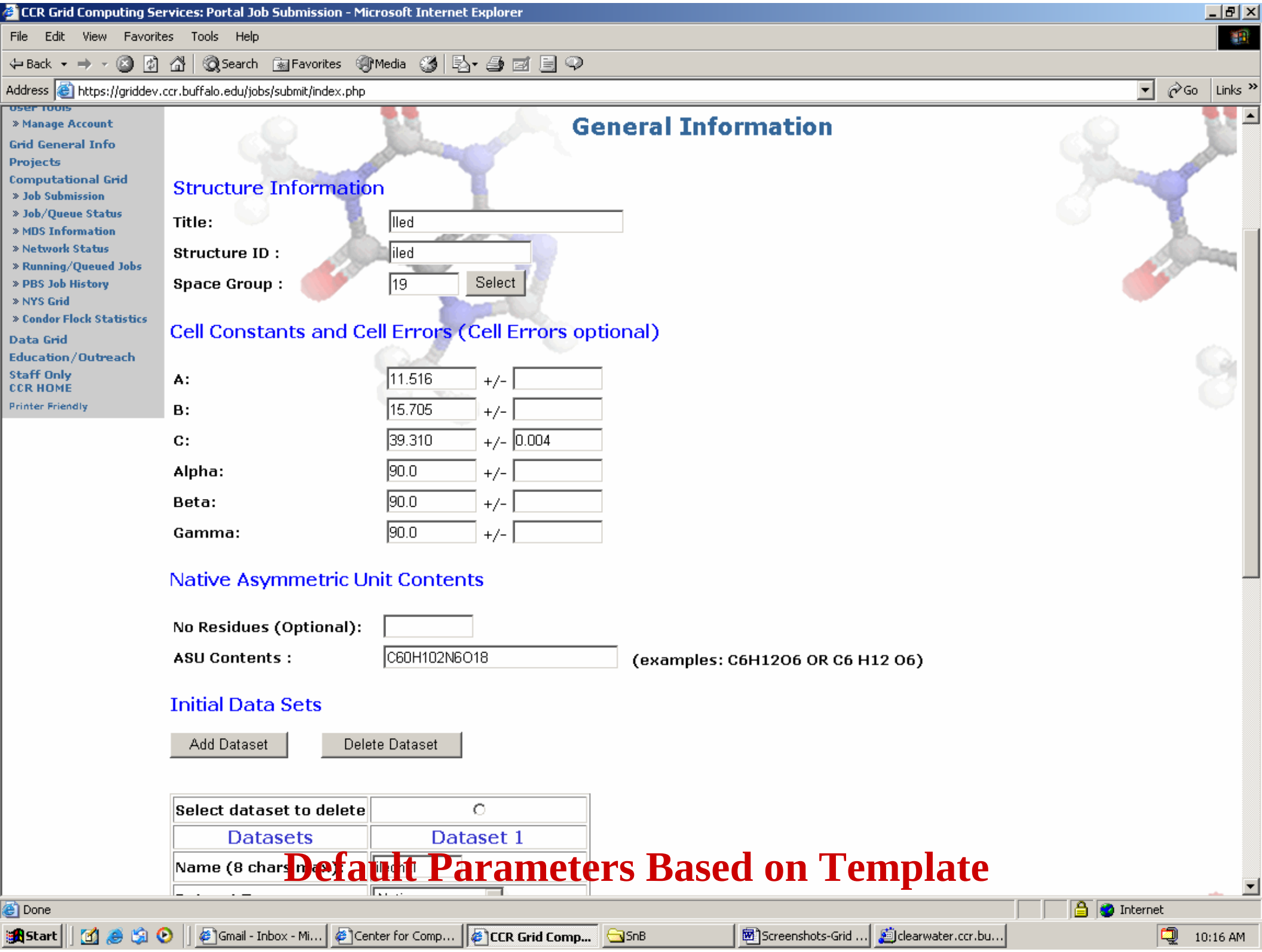


Full Structure / Substructure Template Selection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General Information
Structure Information
Title: lled
Structure ID : iled
Space Group : 19 Select
Cell Constants and Cell Errors (Cell Errors optional)
A: 11.516 +/-
B: 15.705 +/-
C: 39.310 +/- 0.004
Alpha: 90.0 +/-
Beta: 90.0 +/-
Gamma: 90.0 +/-
Native Asymmetric Unit Contents
No Residues (Optional):
ASU Contents : C60H102N6O18 (examples: C6H12O6 OR C6 H12 O6)
Initial Data Sets
Add Dataset
Delete Dataset
Select dataset to delete
Datasets Dataset 1
Name (8 chars max)
Default Parameters Based on Template
Done
Internet
Start
Gmail - Inbox - Mi...
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CCR Grid Comp...
SnB
Screenshots-Grid ...
clearwater.ccr.bu...
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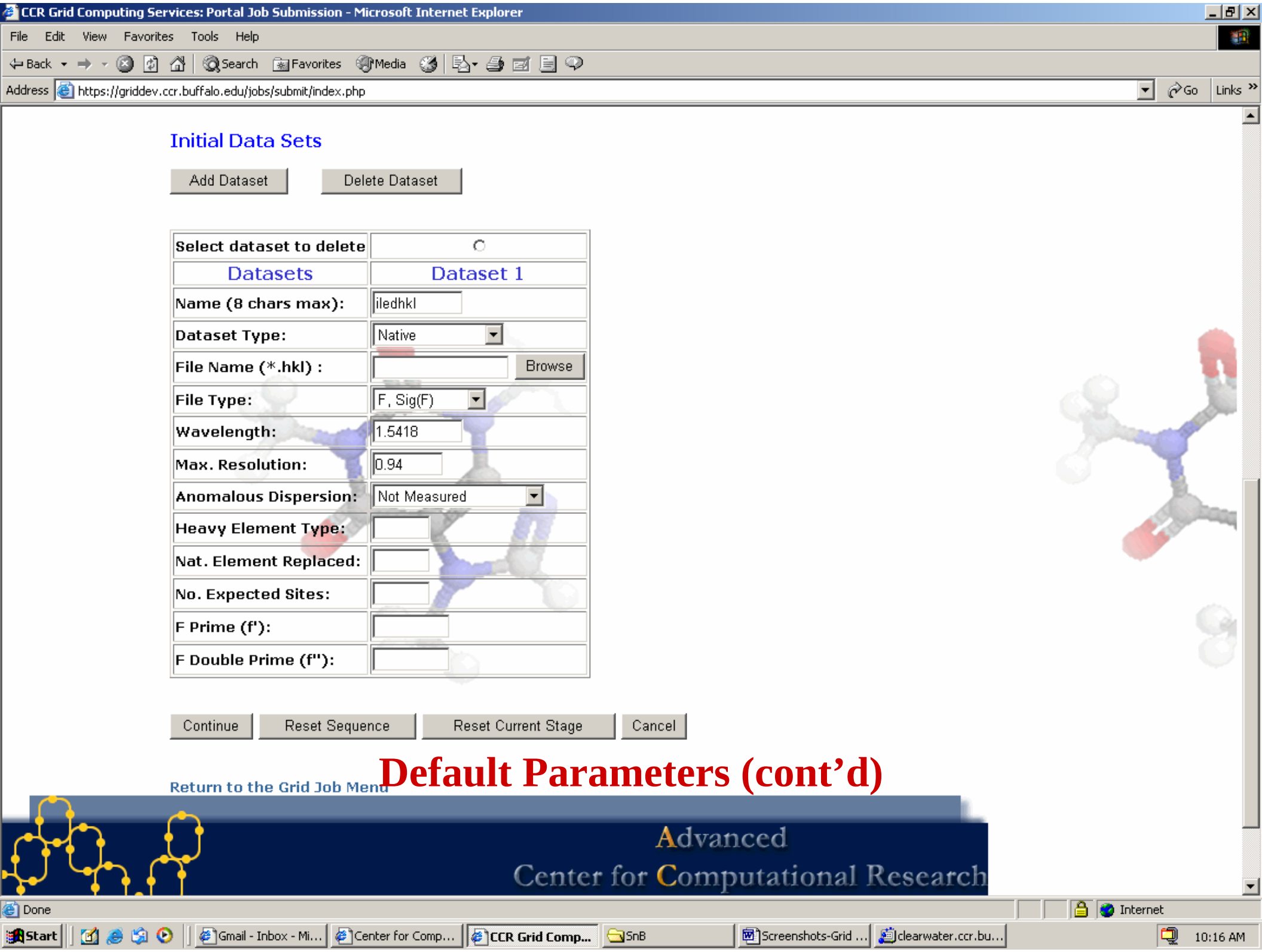
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Go Links
Initial Data Sets
Add Dataset
Delete Dataset
Select dataset to delete
Datasets
Dataset 1
Name (8 chars max):
iledhkl
Dataset Type:
Native
File Name (*.hkl) :
Browse
File Type:
F, Sig(F)
Wavelength:
1.5418
Max. Resolution:
0.94
Anomalous Dispersion:
Not Measured
Heavy Element Type:
Nat. Element Replaced:
No. Expected Sites:
F Prime (f'):
F Double Prime (f''):
Continue
Reset Sequence
Reset Current Stage
Cancel
Return to the Grid Job Menu
Default Parameters (cont'd)
Advanced
Center for Computational Research
Done
Internet
Start
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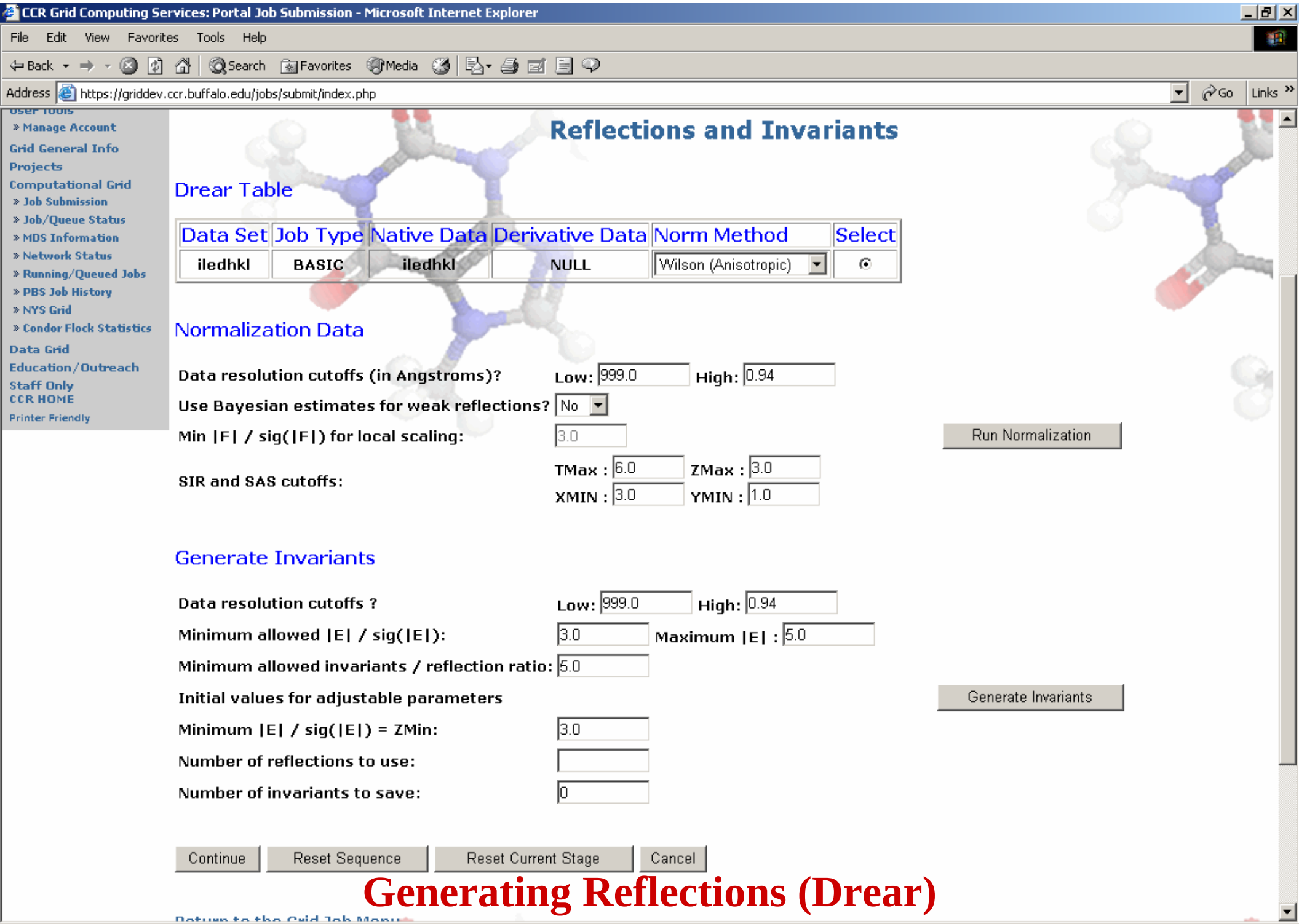
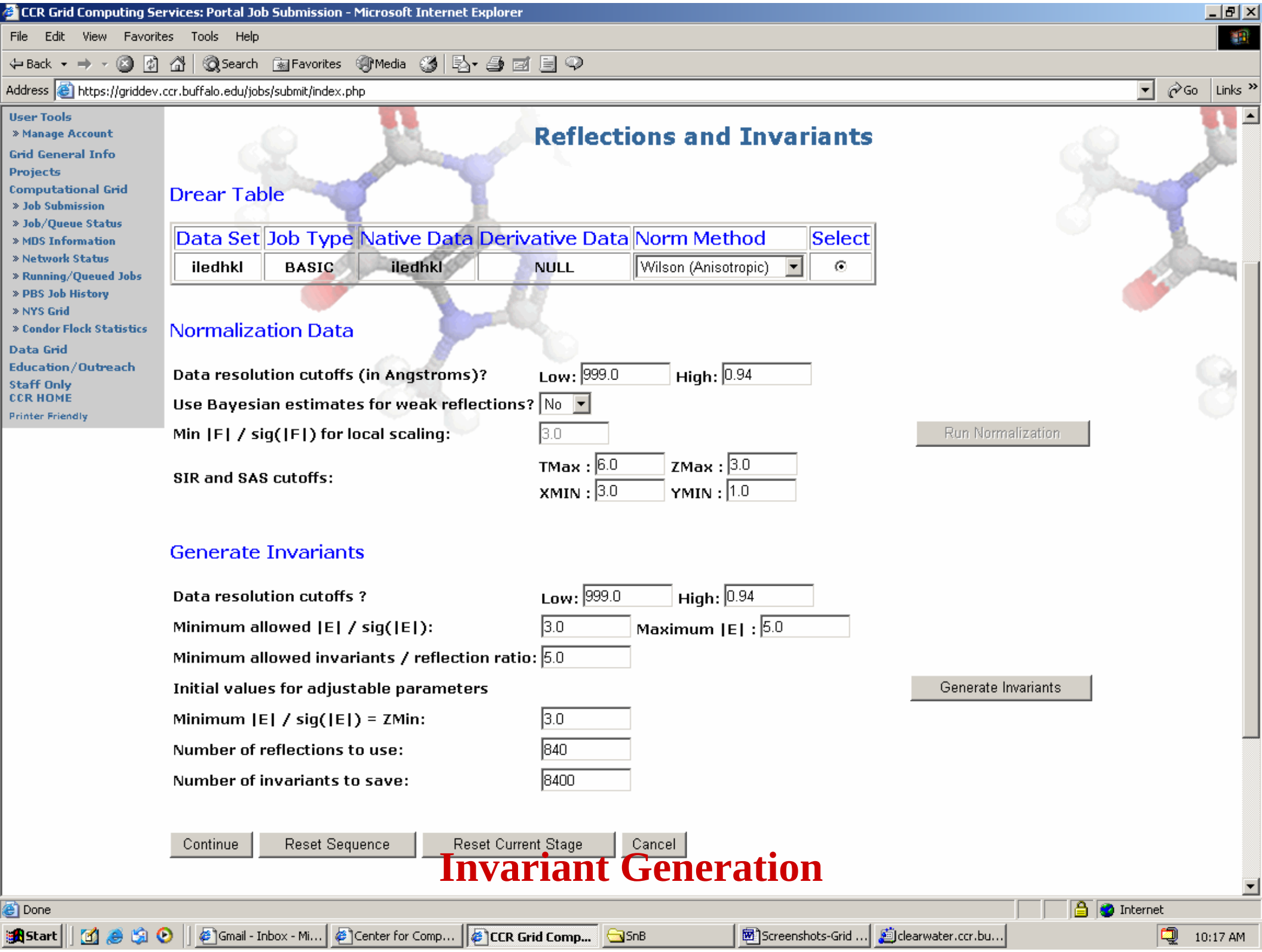


Generating Reflections (Drear)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Printer Friendly
Reflections and Invariants
Drear Table
Data Set
Job Type
Native Data
Derivative Data
Norm Method
Select
iledhkl
BASIC
iledhkl
NULL
Wilson (Anisotropic)
Normalization Data
Data resolution cutoffs (in Angstroms)?
Low: 999.0
High: 0.94
Use Bayesian estimates for weak reflections?
No
Min |F| / sig(|F|) for local scaling:
3.0
Run Normalization
SIR and SAS cutoffs:
TMax : 6.0
ZMax : 3.0
XMIN : 3.0
YMIN : 1.0
Generate Invariants
Data resolution cutoffs ?
Low: 999.0
High: 0.94
Minimum allowed |E| / sig(|E|):
3.0
Maximum |E| : 5.0
Minimum allowed invariants / reflection ratio:
5.0
Initial values for adjustable parameters
Generate Invariants
Minimum |E| / sig(|E|) = ZMin:
3.0
Number of reflections to use:
840
Number of invariants to save:
8400
Continue
Reset Sequence
Reset Current Stage
Cancel
Invariant Generation
Done
Internet
Start
Gmail - Inbox - Mi...
Center for Comp...
CCR Grid Comp...
SnB
Screenshots-Grid ...
clearwater.ccr.bu...
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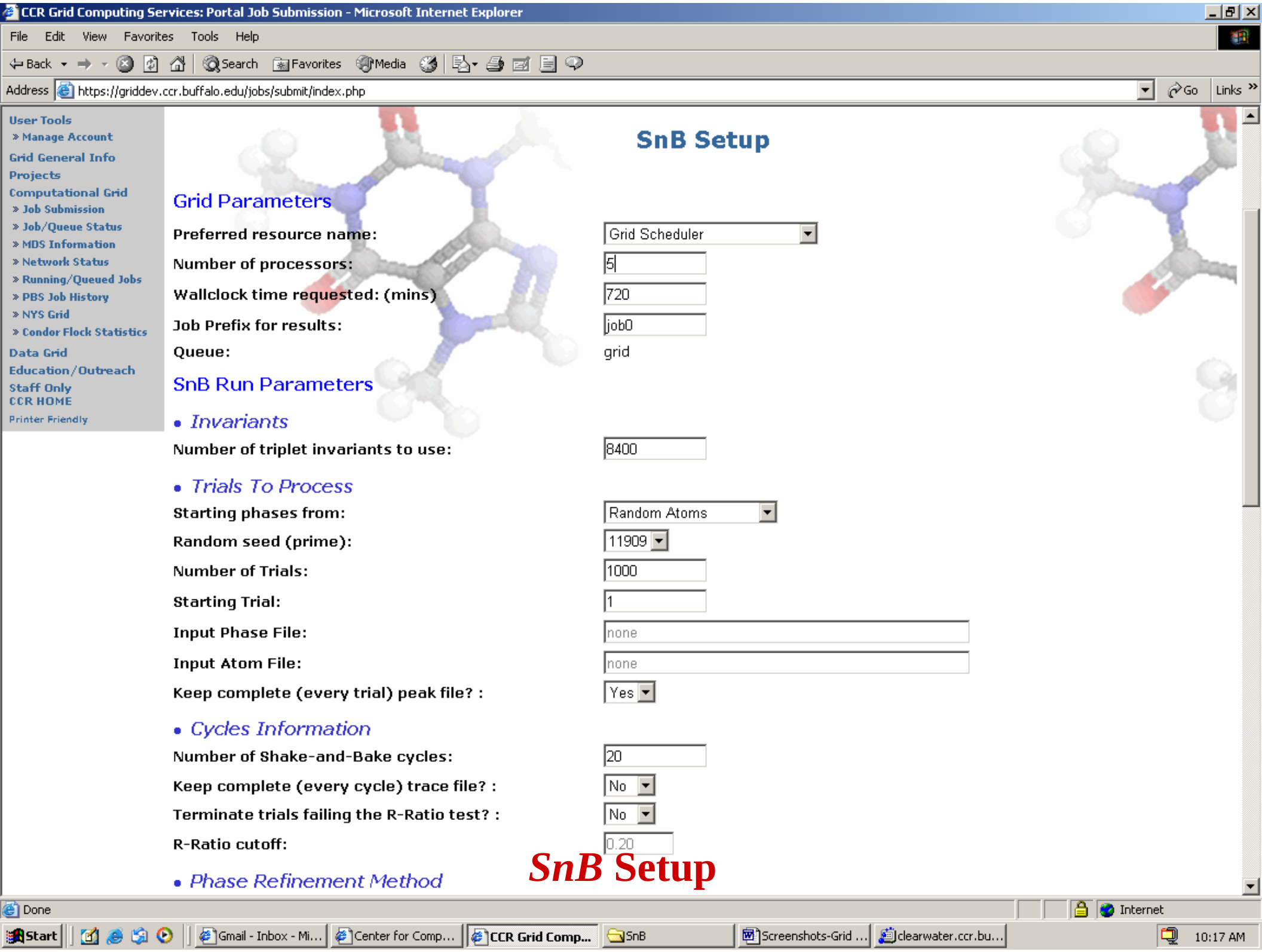
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» PBS Job History
» NYS Grid
» Condor Flock Statistics
Data Grid
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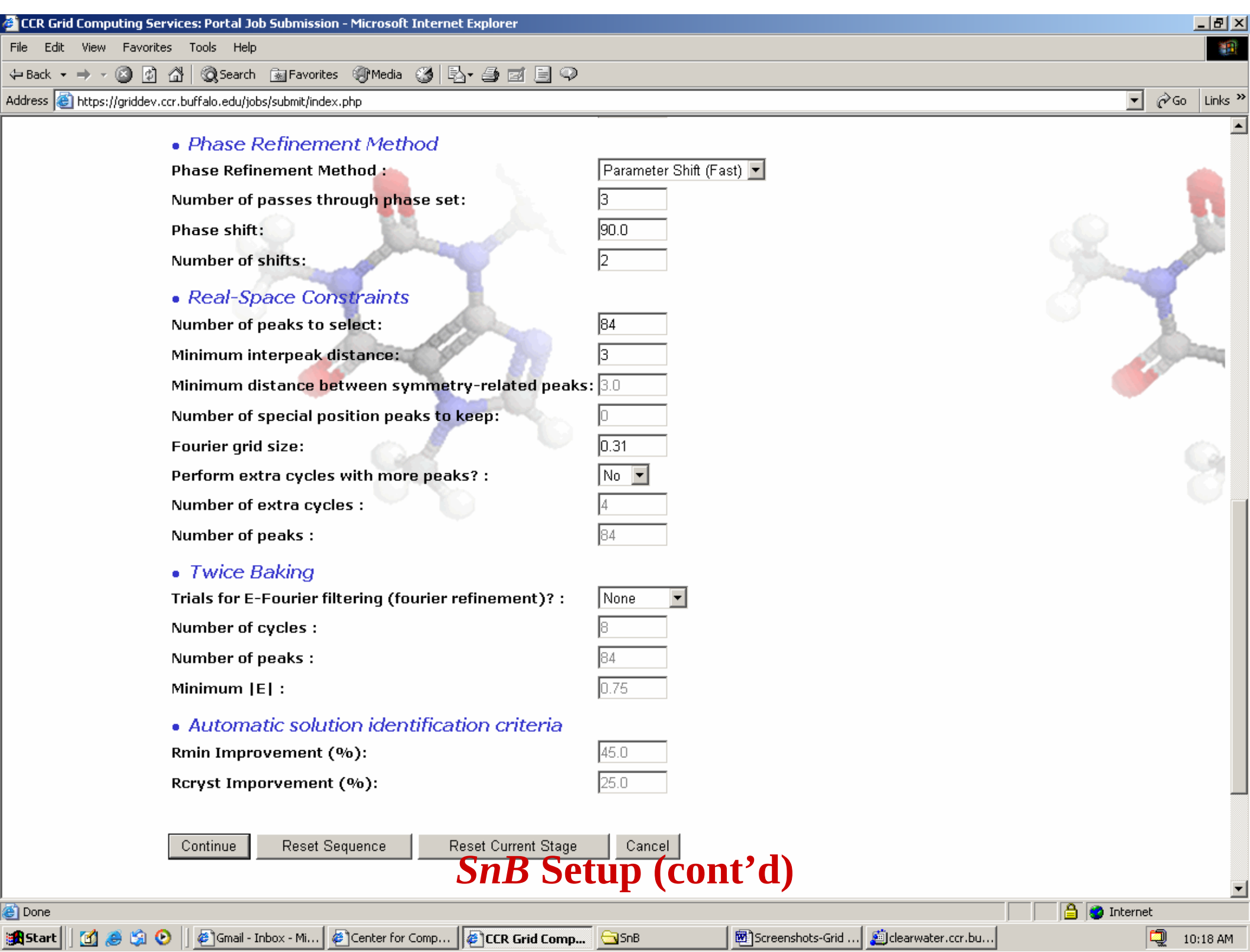
Staff Only
CCR HOME
Printer Friendly
SnB Setup
Grid Parameters
Preferred resource name: Grid Scheduler
Number of processors: 5
Wallclock time requested: (mins) 720
Job Prefix for results: job0
Queue: grid
SnB Run Parameters
• Invariants
Number of triplet invariants to use: 8400
• Trials To Process
Starting phases from: Random Atoms
Random seed (prime): 11909
Number of Trials: 1000
Starting Trial: 1
Input Phase File: none
Input Atom File: none
Keep complete (every trial) peak file? : Yes
• Cycles Information
Number of Shake-and-Bake cycles: 20
Keep complete (every cycle) trace file? : No
Terminate trials failing the R-Ratio test? : No
R-Ratio cutoff: 0.20
• Phase Refinement Method
SnB Setup
Done
Internet
Start
Gmail - Inbox - Mi...
Center for Comp...
CCR Grid Comp...
SnB
Screenshots-Grid ...
clearwater.ccr.bu...
10:17 AM



SnB Setup (cont'd)

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

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

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High Performance Grid Computing

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» Condor Flock Statistics

Data Grid

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Details for Grid Job 447 - iledhkl

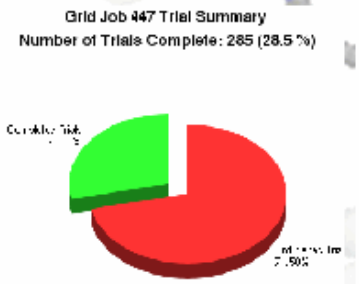
Job Detail Information

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

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

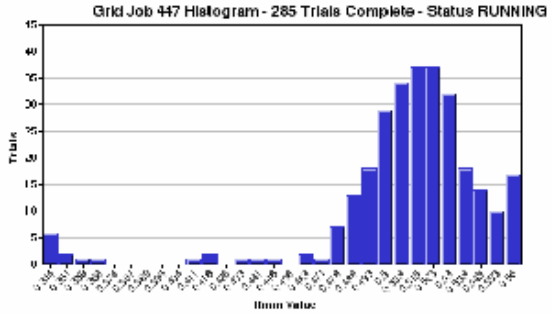
Best Trial Number: 34
Best Trial Rmin: 0.344
Processors: 5

Trial Summary



Walltime Summary

Grid Job Trial Histogram



Click on image for enlarged view.

Return to the Grid Job Menu

Graphical Representation of Intermediate Job Status

Advanced Center for Computational Research Data GRID

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

Internet

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

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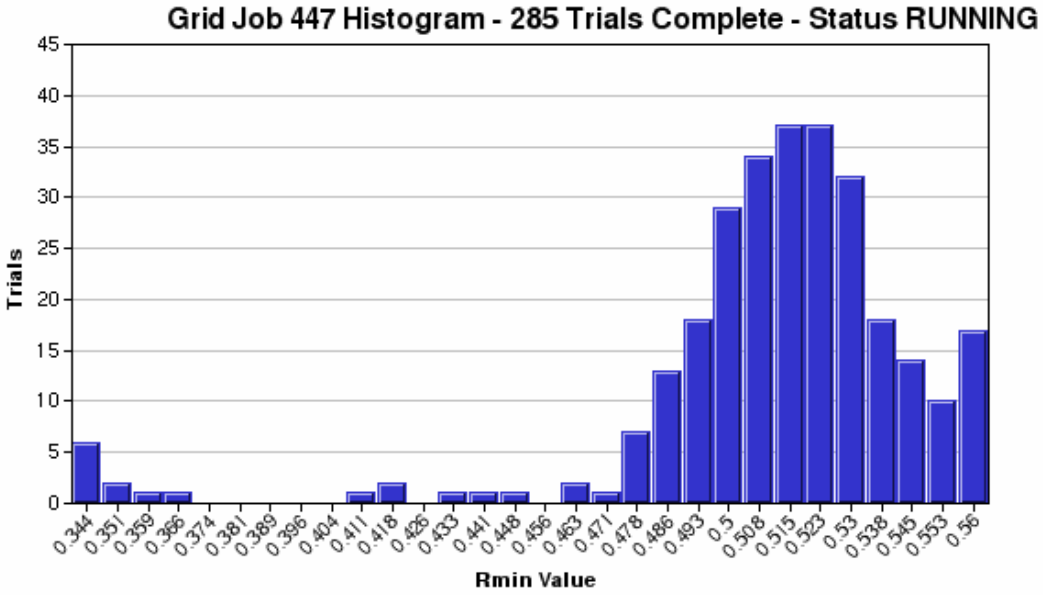

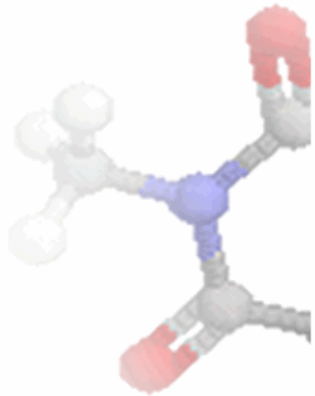

Return to Job Details

Return to the Grid Job Status List

Return to the Grid Job Menu

Histogram of Completed Trial Structures

Advanced Center for Computational Research

Done

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Grid Job Status
15-Mar-2005 10:23:49
Job Filter Criteria
Show GATs
BnP Auto Run
EADR
Ostrich
POM
Q-Chem
SnB
SnB DREAR
Job State
DEFINITION
STAGING
QUEUED
RUNNING
UPLOADING
COMPLETE
INCOMPLETE
Sort By
Job Id
Job Name
Resource
Num Procs
Status
Percent Complete
Last Update
Descending
Ascending
Filter Job List
SnB
Job Id | Job Name | Resource | Num Procs | Status | Percent Complete | Last Update | Cancel Job | Drilldown
447 iledhkl clearwater.ccr.buffalo.edu 5 RUNNING 28.5 15-Mar-2005 10:22:00
446 trilys clearwater.ccr.buffalo.edu 10 RUNNING 1 15-Mar-2005 10:22:00
444 64chkl nash.ccr.buffalo.edu 3 COMPLETE 100 14-Mar-2005 22:00:01
443 trilys clearwater.ccr.buffalo.edu 10 COMPLETE 100 10-Mar-2005 22:48:00
442 pr435hkl nash.ccr.buffalo.edu 5 COMPLETE 100 10-Mar-2005 17:26:01
441 vancohkl clearwater.ccr.buffalo.edu 10 COMPLETE 100 10-Mar-2005 18:08:01
434 16chkl clearwater.ccr.buffalo.edu 5 COMPLETE 100 10-Mar-2005 14:42:01
433 16chkl clearwater.ccr.buffalo.edu 5 COMPLETE 100 10-Mar-2005 14:38:01
Status of Jobs
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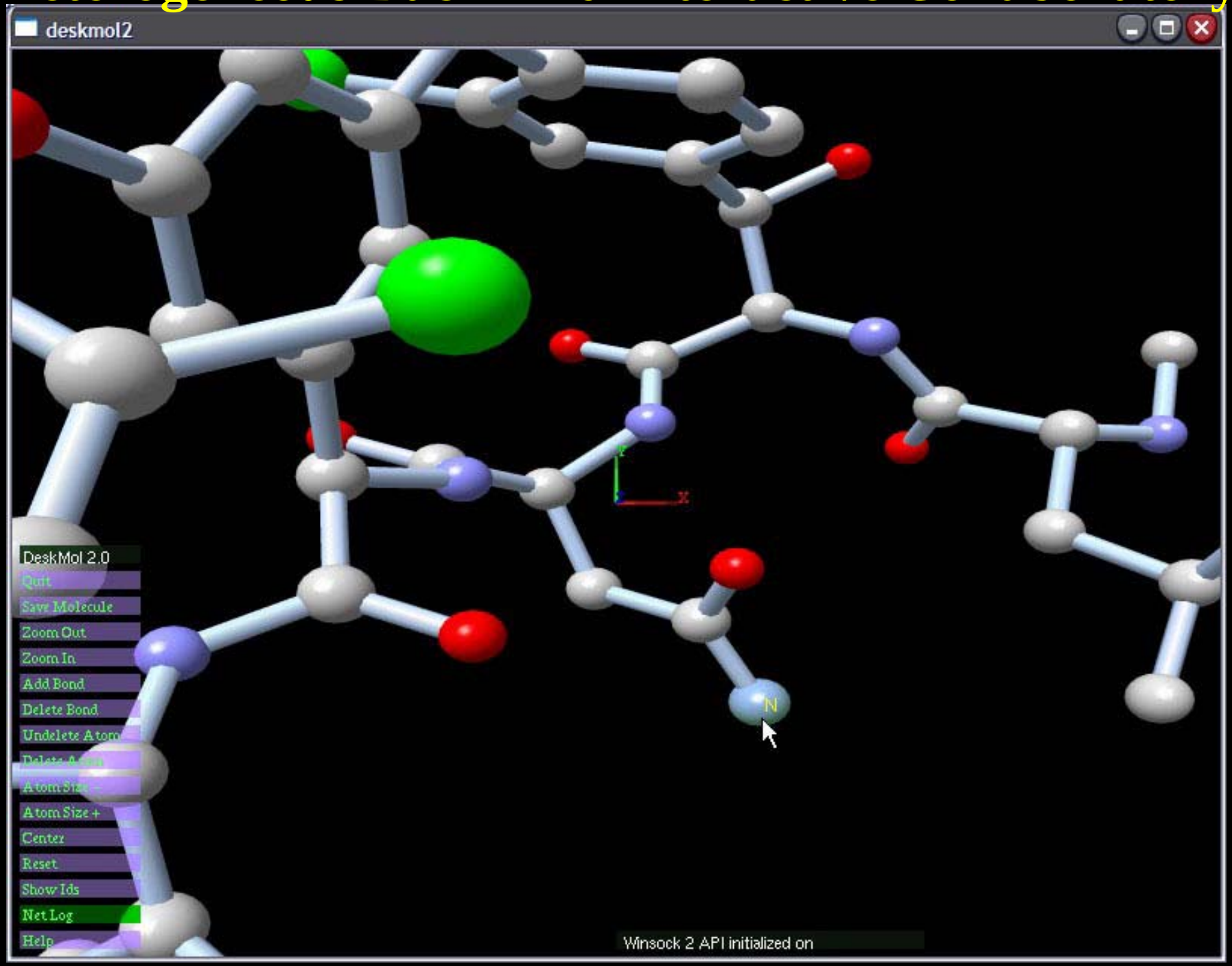
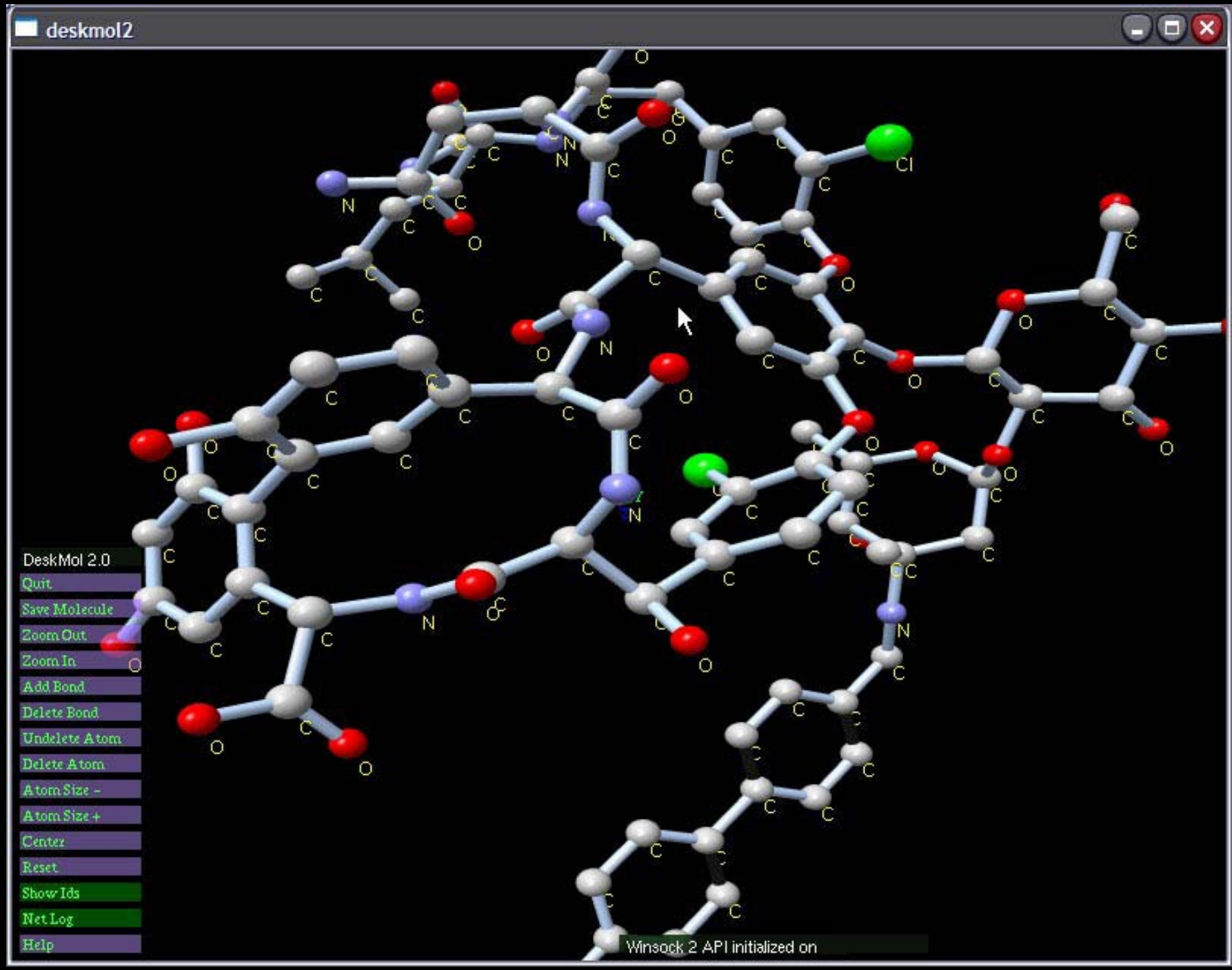
Internet
Start
Gmail - Inbox - Mi...
Center for Comp...
CCR Grid Comp...
SnB
Screenshots-Grid ...
clearwater.ccr.bu...
10:24 AM

Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Current Grid Efforts

- **Grass Roots NYS Grid**
  - SUNY-Buffalo
  - SUNY-Binghamton
  - SUNY-Albany
  - SUNY-Geneseo
  - Hauptman-Woodward Inst.
  - Columbia
  - Niagara University
  - Canisius College
- **Harden**
  - Dashboard
  - Predictive Scheduler
- **GRASE VO: Grid Resources for Advanced Science and Engineering Virtual Organization**
  - (Non-Physics Research)
  - Structural Biology
  - Groundwater Modeling
  - Earthquake Engineering
  - Computational Chemistry
  - GIS/BioHazards

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**

Acknowledgments

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- George DeTitta
- Herb Hauptman
- Charles Weeks
- Steve Potter
- Bruce Holm
- Janet Penksa
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