The Cyberinfrastructure Laboratory: Middleware Overview

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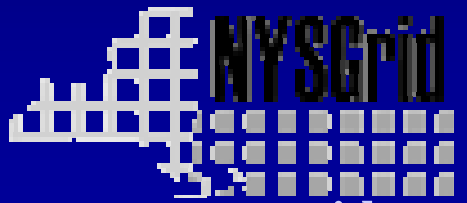
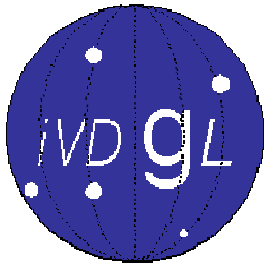
NSF, NIH, DOE, NIMA, NYS, HP

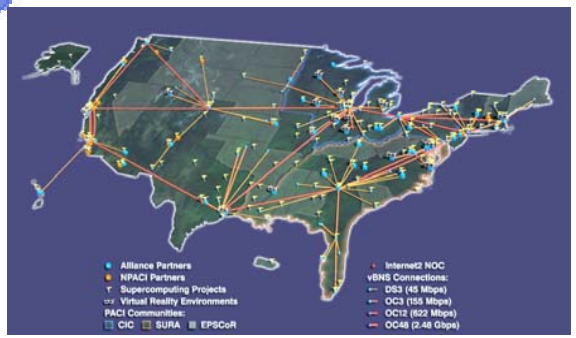
www.cse.buffalo.edu/faculty/miller/CI/

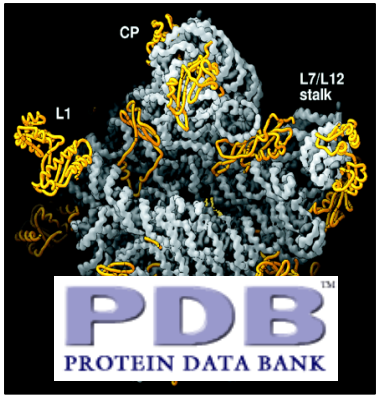


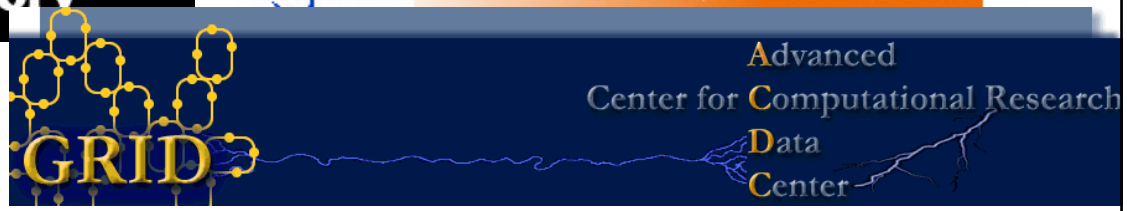
www.nysgrid.org

Grid Computing

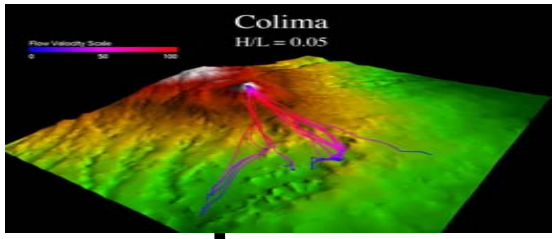




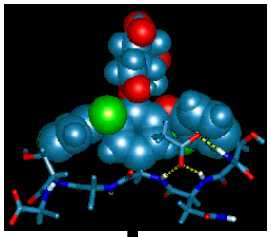




Grid Computing Overview



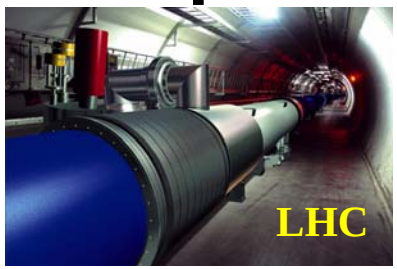
Data Acquisition

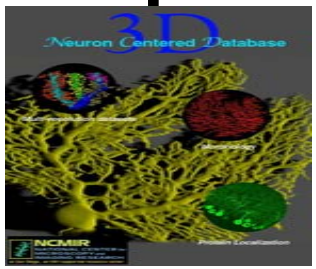


Advanced Visualization

Analysis

Imaging Instruments



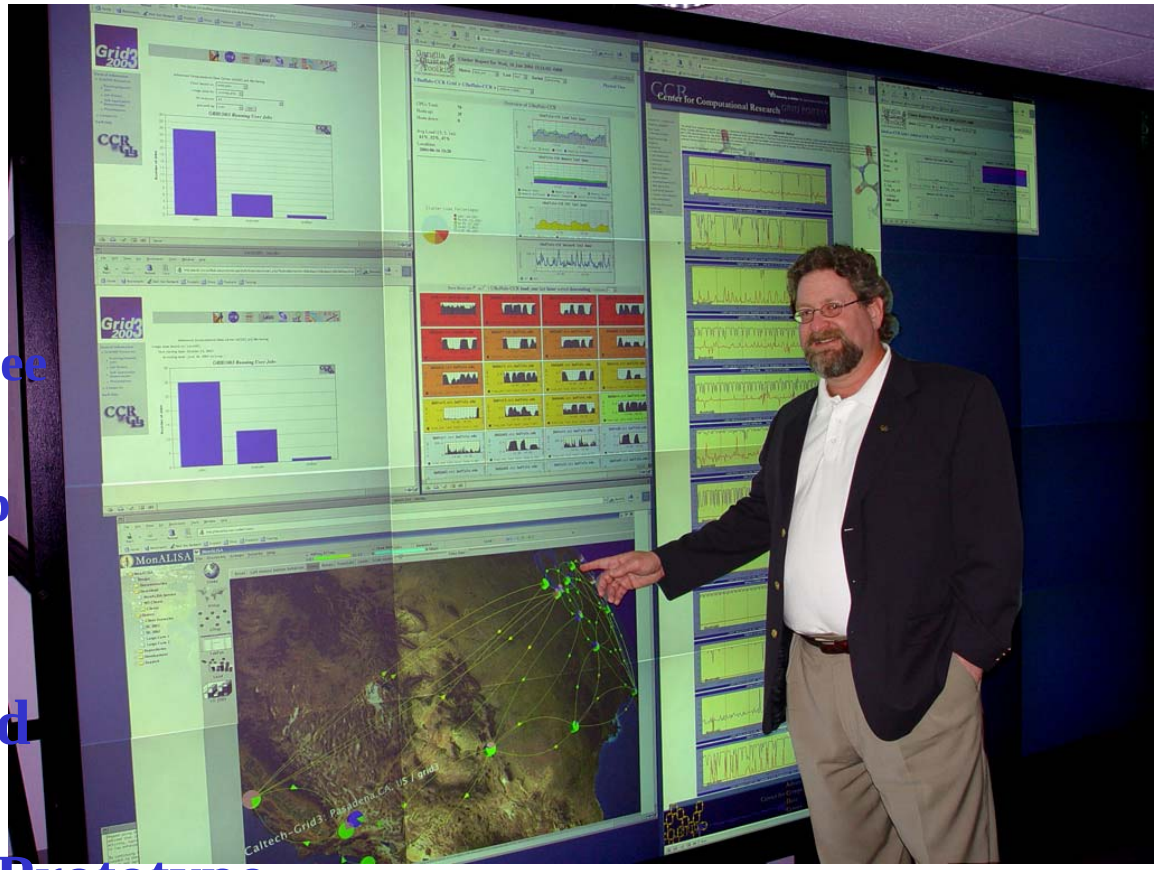


Large-Scale Databases

- 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 I

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



ACDC-Grid Collaborations II

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

"Middleware"

- Intermediate Software Layer between Application Codes and Grid Resources
- Required for applications, users, and resource providers to operate effectively in a manner transparent to the user
- Security; Resource Management; Data Access; Policies; Accounting;
- Globus; Condor
- Checks availability of Resources
  - CPUs; Storage; Networking; Render Farms; etc.
- Scheduling / Workload Management System
- Resource Broker
  - Evaluates Job and Breaks Up/Submits

NSF Middleware Initiative (NMI)

- **Develop, improve, and deploy a suite of reusable software components for use in national-scale "cyberinfrastructure".**
- **APST, Condor, CPM, DataCutter, DataCutter STORM, Globus Toolkit, GPT, Gridconfig, GridPort, GridSolve, GSI OpenSSH, Inca, KX.509/KCA, Look, MPICH-G2, MyProxy, Network Weather Service, OpenSAML, PERMIS, PyGlobus, Shibboleth, SRB Client, UberFTP, and WebISO (Web Initial Sign-on).**

Grid Issues

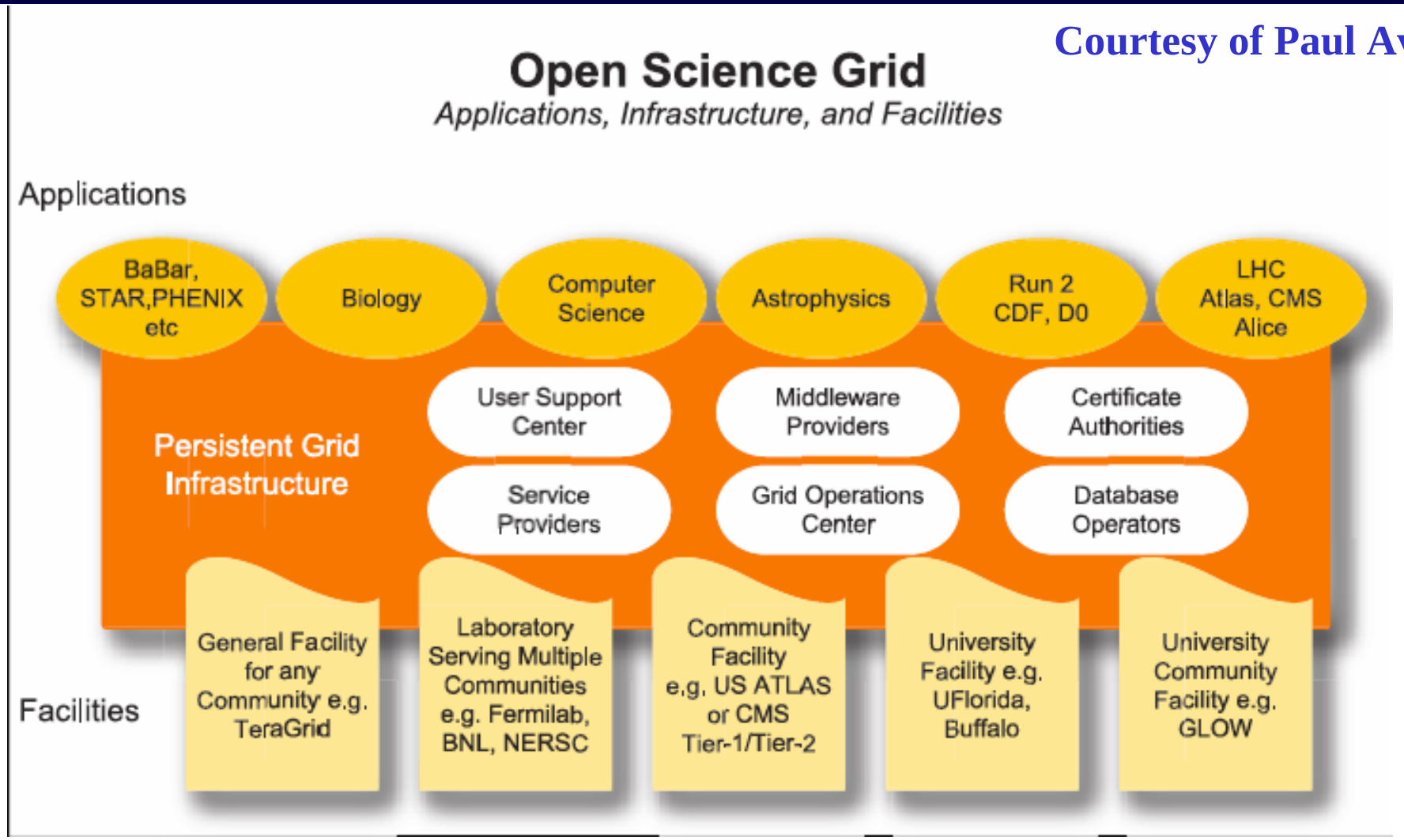
- High-Throughput Computing
- Transparent Integration of Data, Computing, Sensors/Devices, Networking
- Heterogeneous Resources
- Standards (Grid, Data)
- Major User Communities
  - High-Energy Physics and Astrophysics
  - Medicine and Biological Sciences
  - Earth Sciences
- Public Funding Still Critical
- Grids are in their Infancy

Major Grid Initiatives

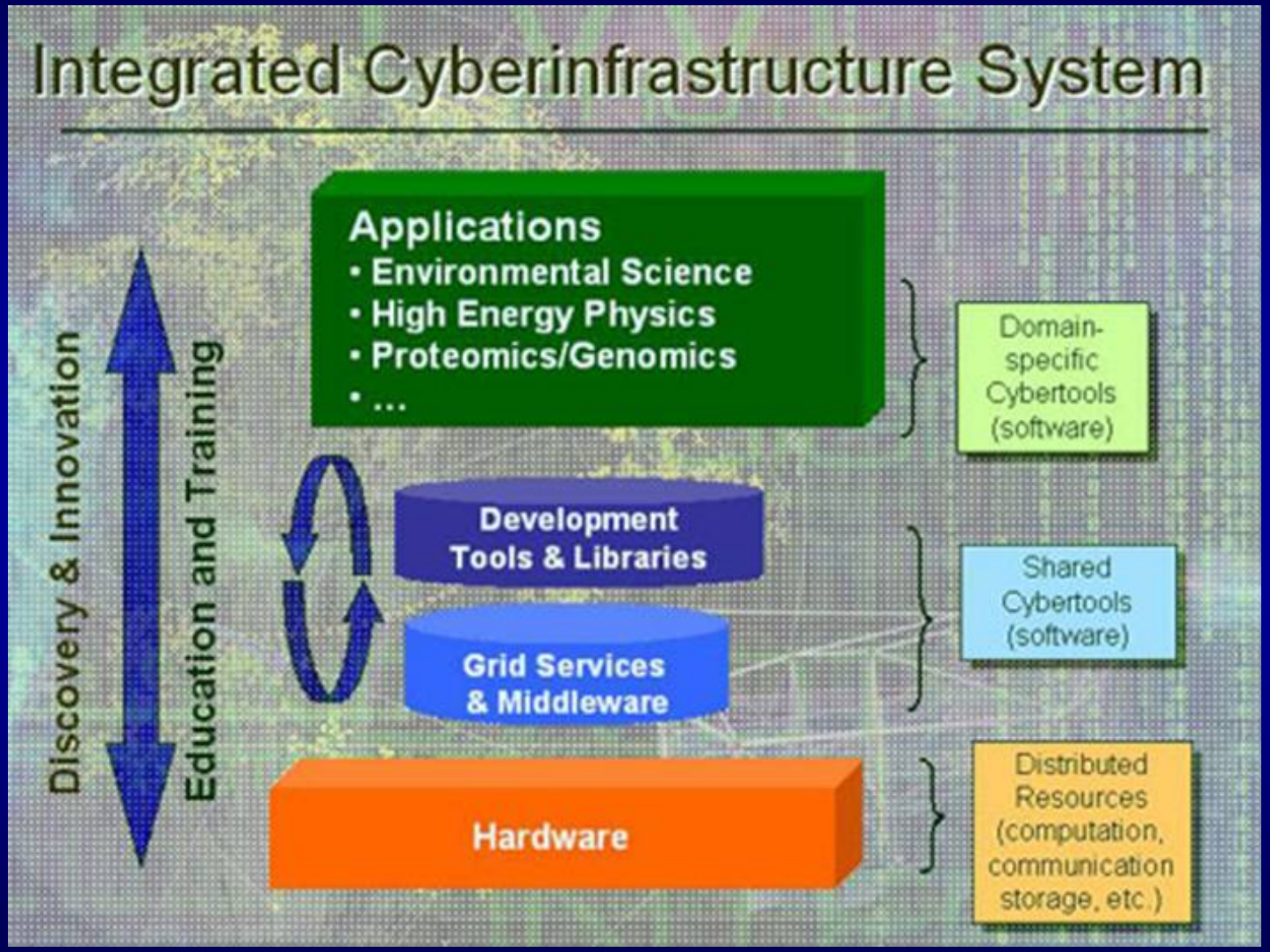
- EGEE: Enabling Grids for E-SciencE (European Commision)
  - Initial Focus on CERN (5PB of Data/Year)
    - High-Energy Physics and Life Sciences
  - Expanded Focus Includes Virtually All Scientific Domains
  - 200 Institutions; 40 Countries
  - 20K+ CPUs; 5PB; 25,000 jobs per day!
- OSG (DOE, NSF)
  - High-Throughput Distributed Facility
  - Open & Heterogeneous
  - Biology, Computer Science, Astrophysics, LHC
  - 57 Compute Sites; 11 Storage Sites;
  - 10K CPUS; 6PB
- TeraGrid (NSF)
  - Integrates High-End Resources
  - High-Performance (Dedicated) Networks
  - 9 Sites; 100TF & 15PB
  - 100+ Databases Available

Open Science Grid

Courtesy of Paul Avery



NSF Integrated Cyberinfrastructure

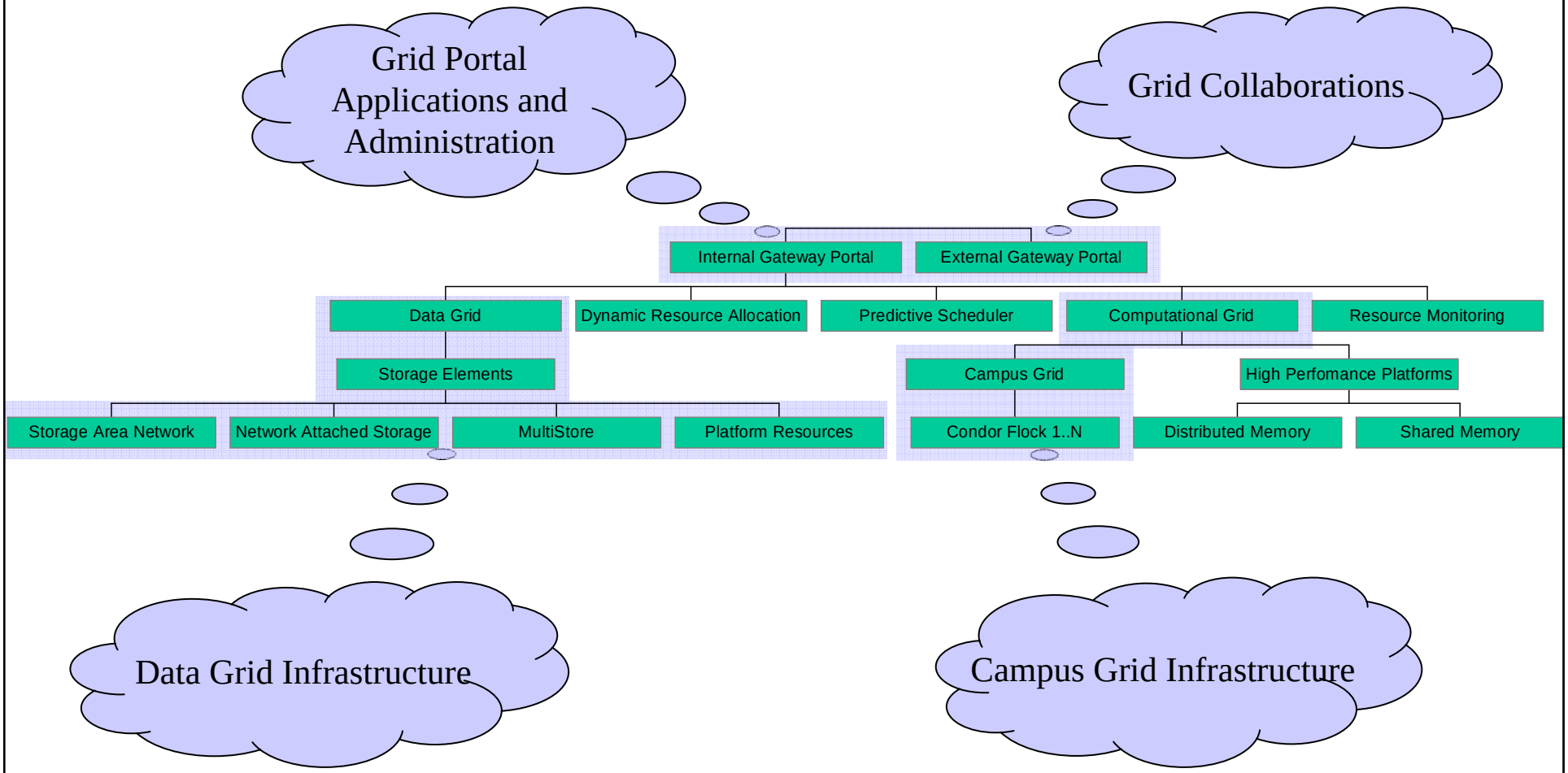


NSF Director Arden L. Bement: "leadership in cyberinfrastructure may determine America's continued ability to innovate – and thus our ability to compete successfully in the global arena."

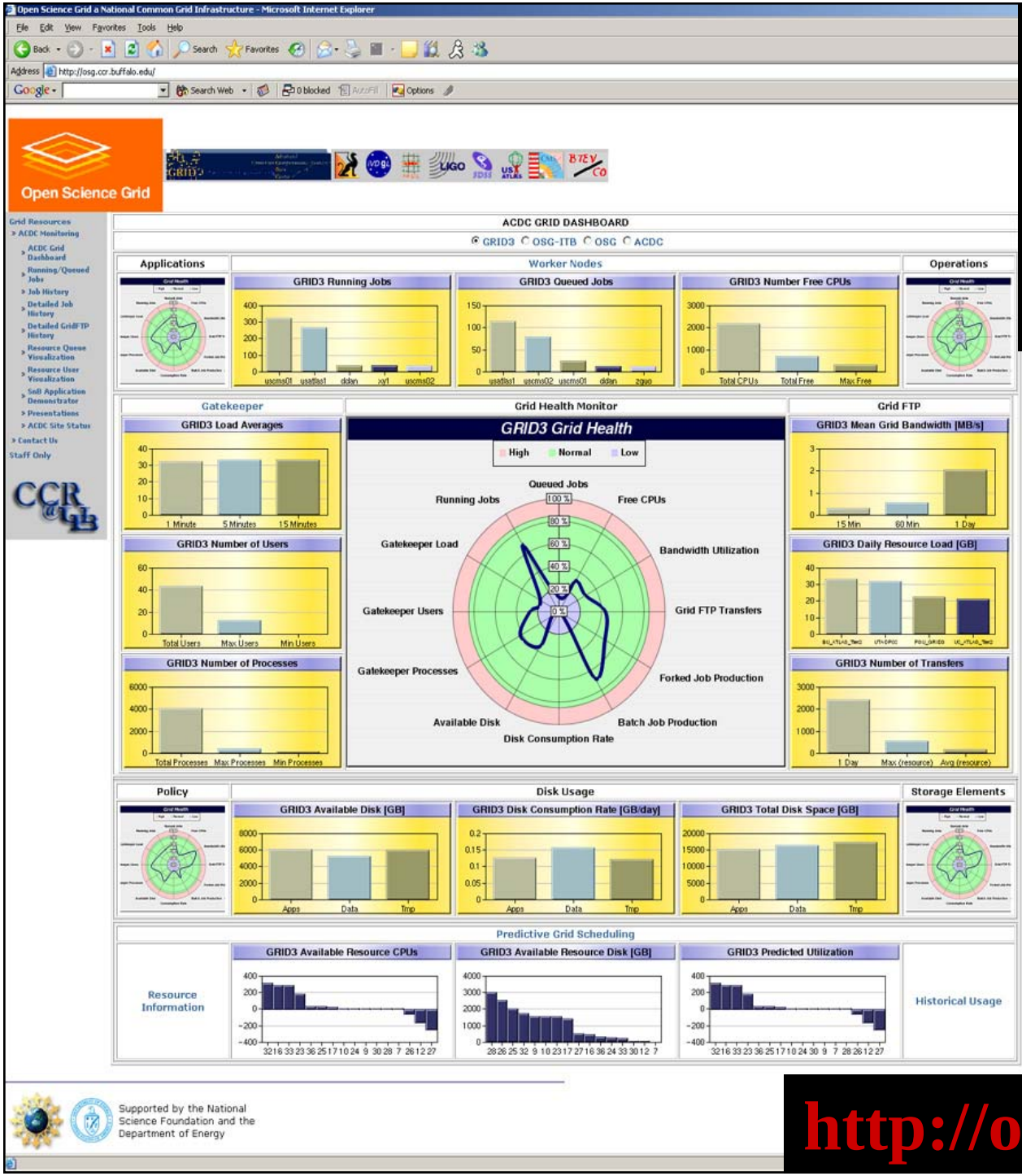
ACDC-Grid Cyberinfrastructure

- **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.**
- **Integrated Data Grid**
  - **Automated Data File Migration based on profiling users.**
- **Grid Portal**

ACDC-Grid System Architecture



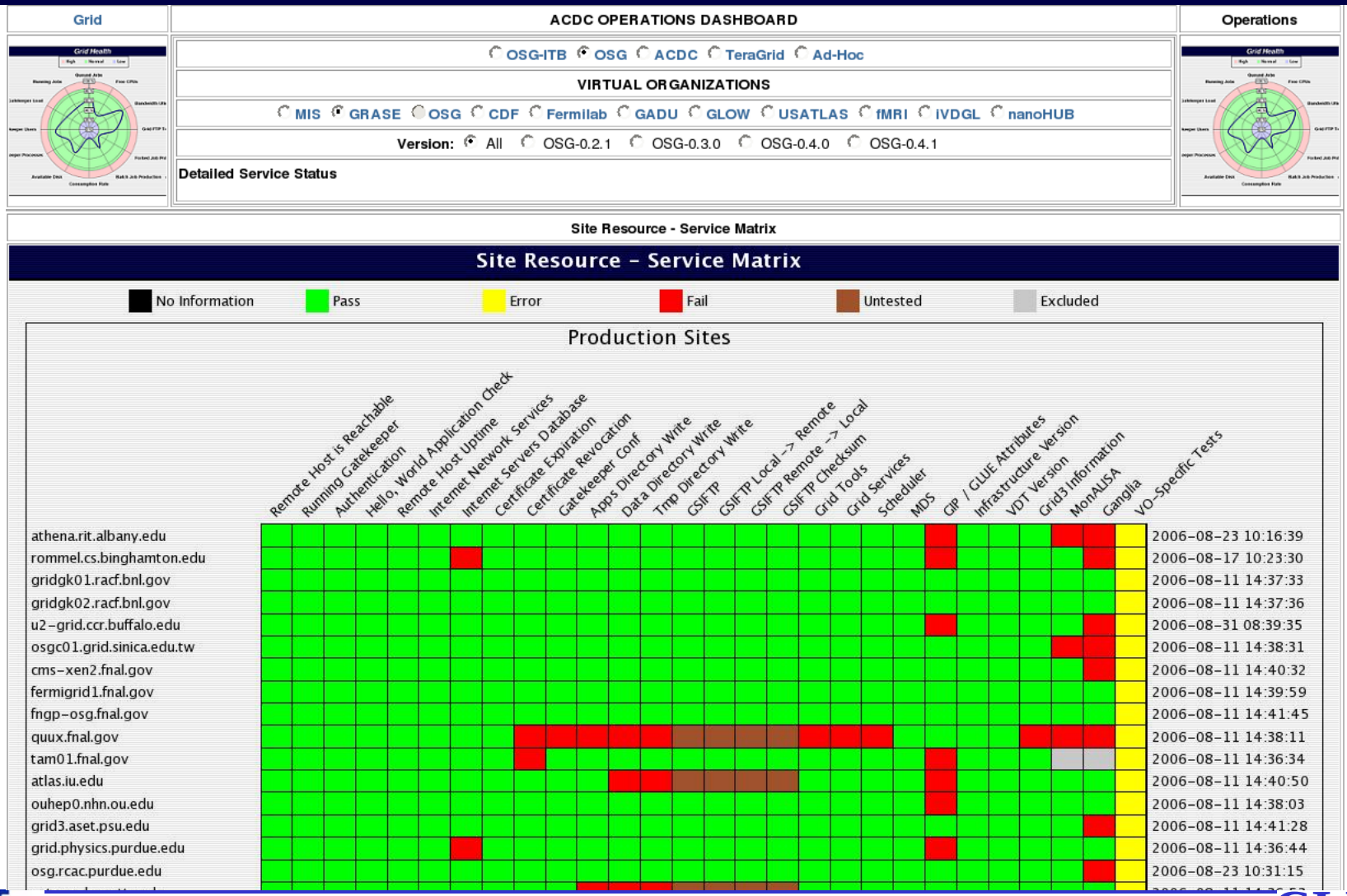
ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD



http://osg.ccr.buffalo.edu

ACDC Monitor

http://osg.ccr.buffalo.edu/operations-dashboard.php?grids=3&vos=10



Predictive Scheduler

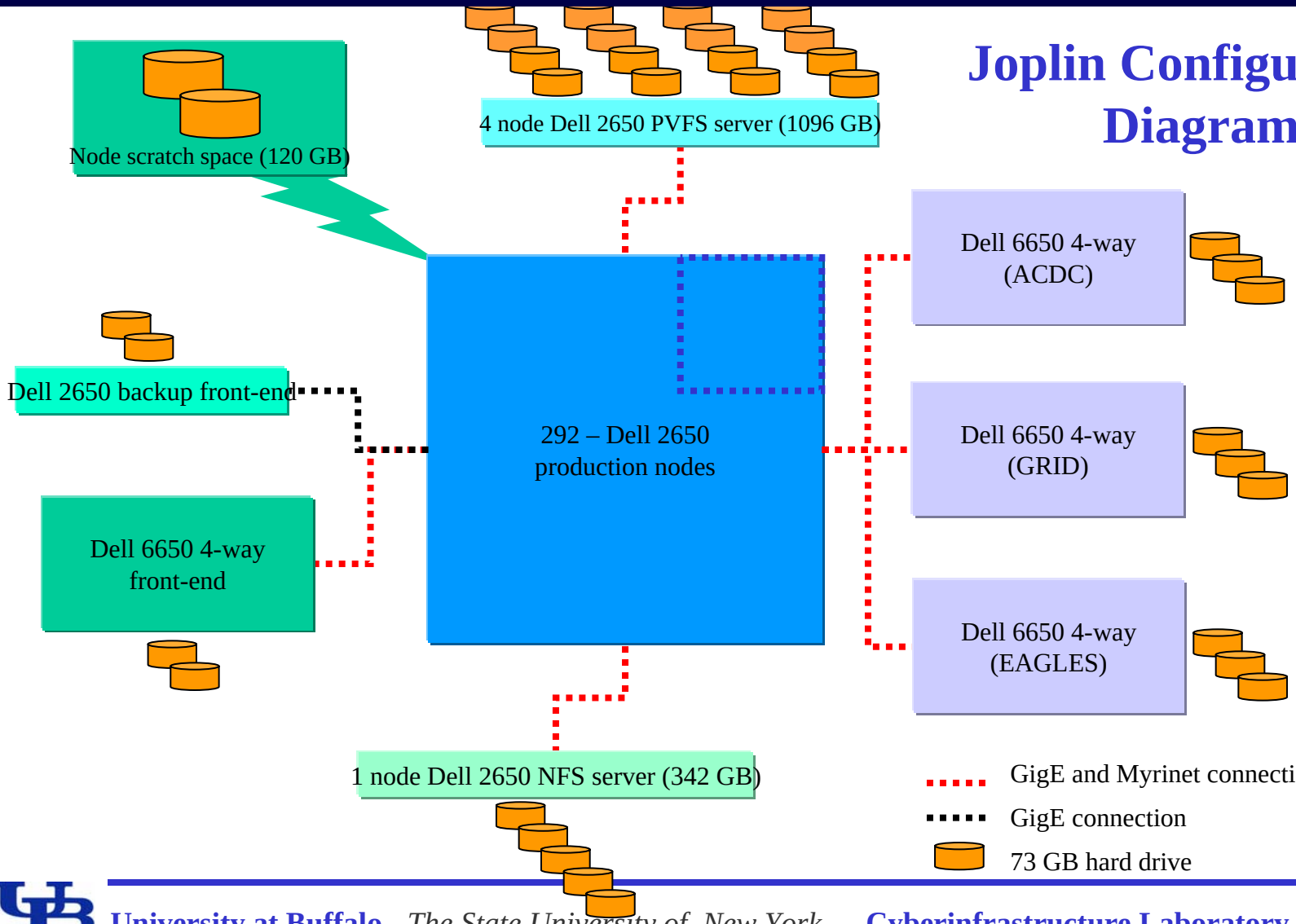
- **Build profiles based on statistical analysis of logs of past jobs**
  - **Per User/Group**
  - **Per Resource**
- **Use these profiles to predict runtimes of new jobs**
- **Make use of these predictions to determine**
  - **Resources to be utilized**
  - **Availability of Backfill**

ACDC-Grid Dynamic Resource Allocation at SC03 with Grid3

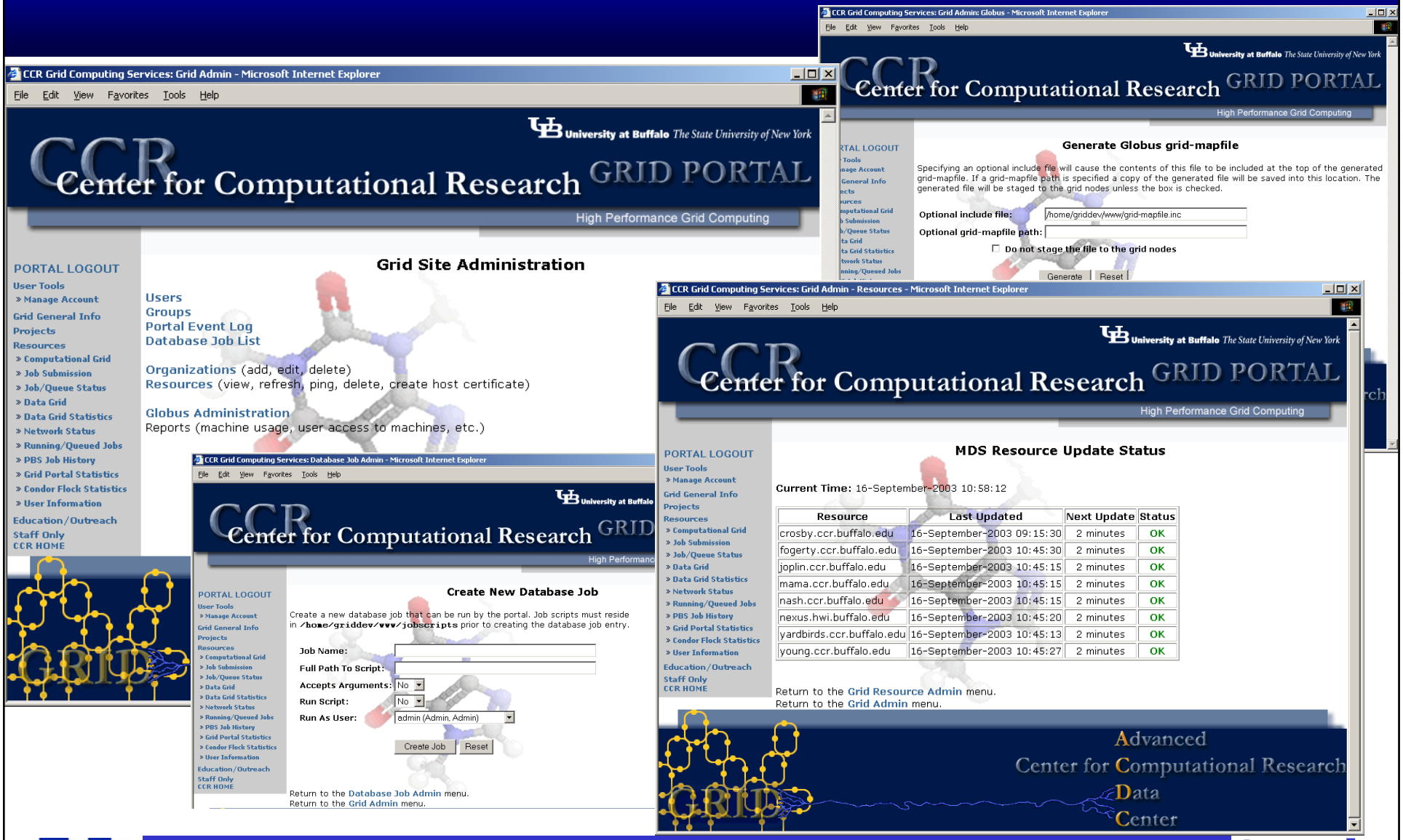
- **Small number (40) of CPUs were dedicated at night**
- **An additional 400 CPUs were dynamically allocated during the day**
- **No human intervention was required**
- **Grid applications were able to utilize the resources and surpassed the Grid3 goals**

ACDC-Grid Dynamic Resource Allocation

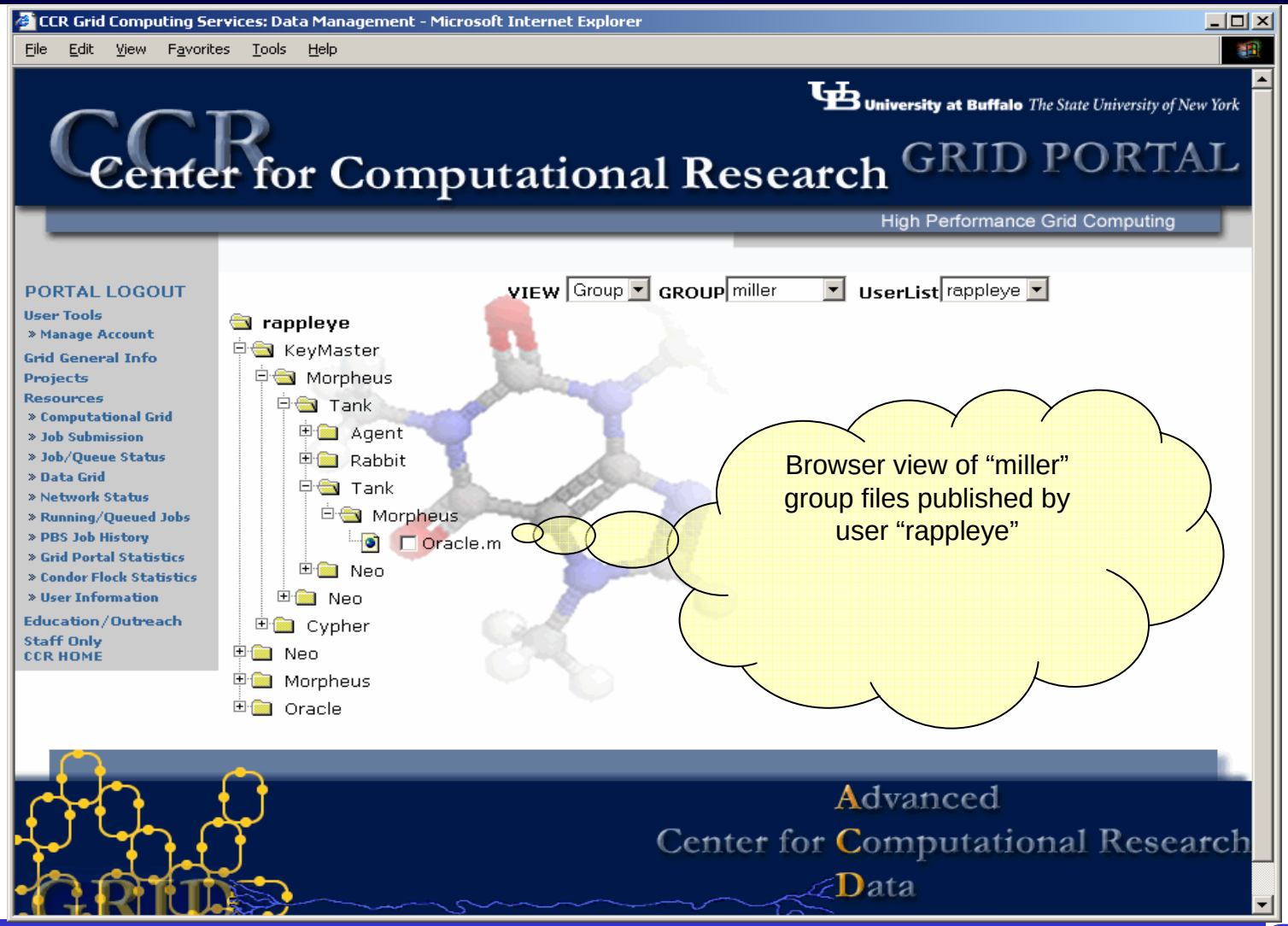
Joplin Configuration Diagram



ACDC-Grid Administration



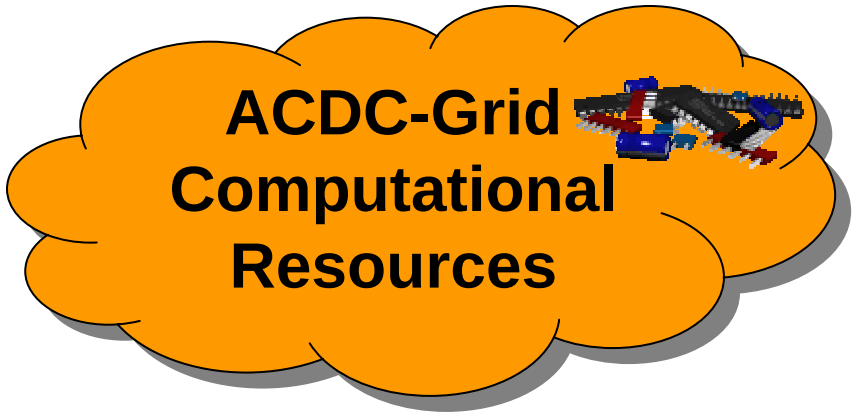
ACDC-Grid Data Grid

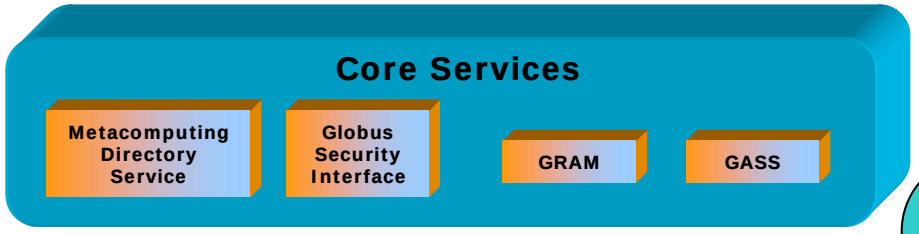


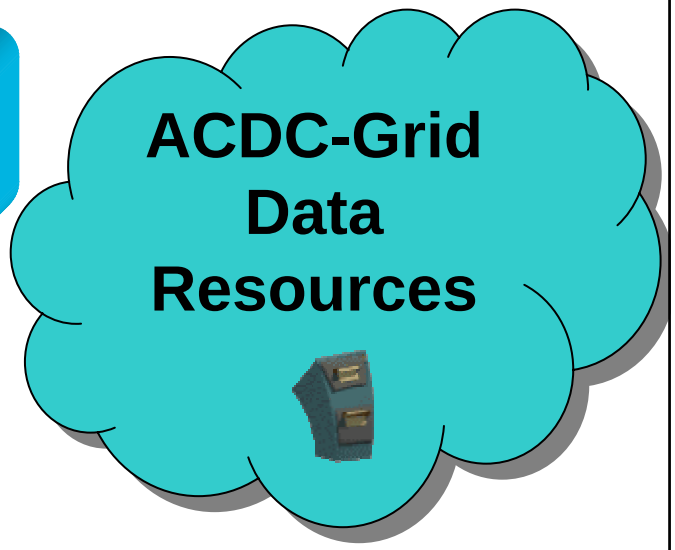
ACDC-Grid Data Grid Functionality

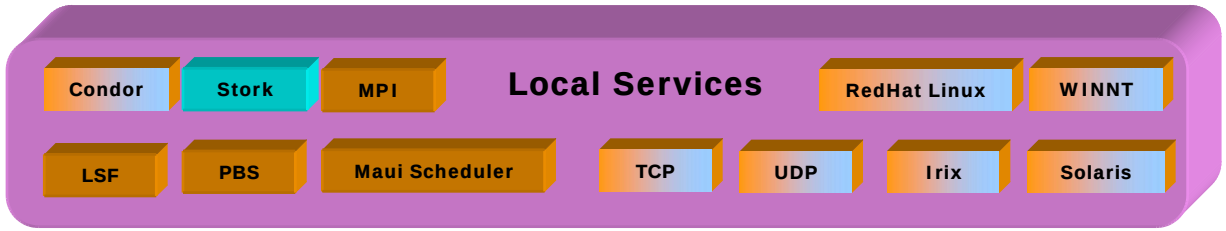
- **Basic file management functions are accessible via a platform-independent web interface.**
- **User-friendly menus/interface.**
- **File Upload/Download to/from the Data Grid Portal.**
- **Simple Web-based file editor.**
- **Efficient search utility.**
- **Logical display of files (user/ group/ public).**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

Grid Services and Applications









Adapted from Ian Foster and Carl Kesselman

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**

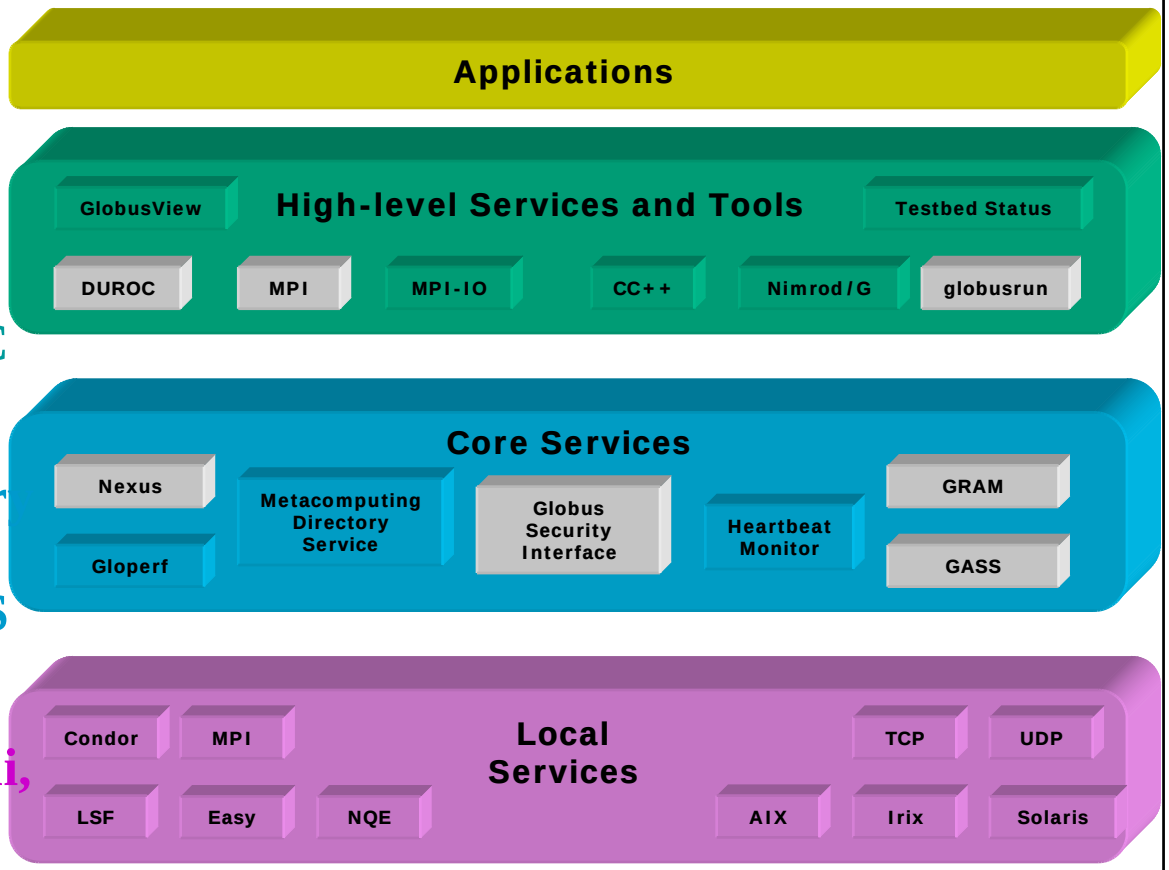
Grid Enabled *SnB*

- **Required Layered Grid Services**
  - **Grid-enabled Application Layer**
    - ***Shake – and – Bake* application**
    - **Apache web server**
    - **MySQL database**
  - **High-level Service Layer**
    - **Globus, NWS, PHP, Fortran, and C**
  - **Core Service Layer**
    - **Metacomputing Directory Service, Globus Security Interface, GRAM, GASS**
  - **Local Service Layer**
    - **Condor, MPI, PBS, Maui, WINNT, IRIX, Solaris, RedHat Linux**

Required Grid Services

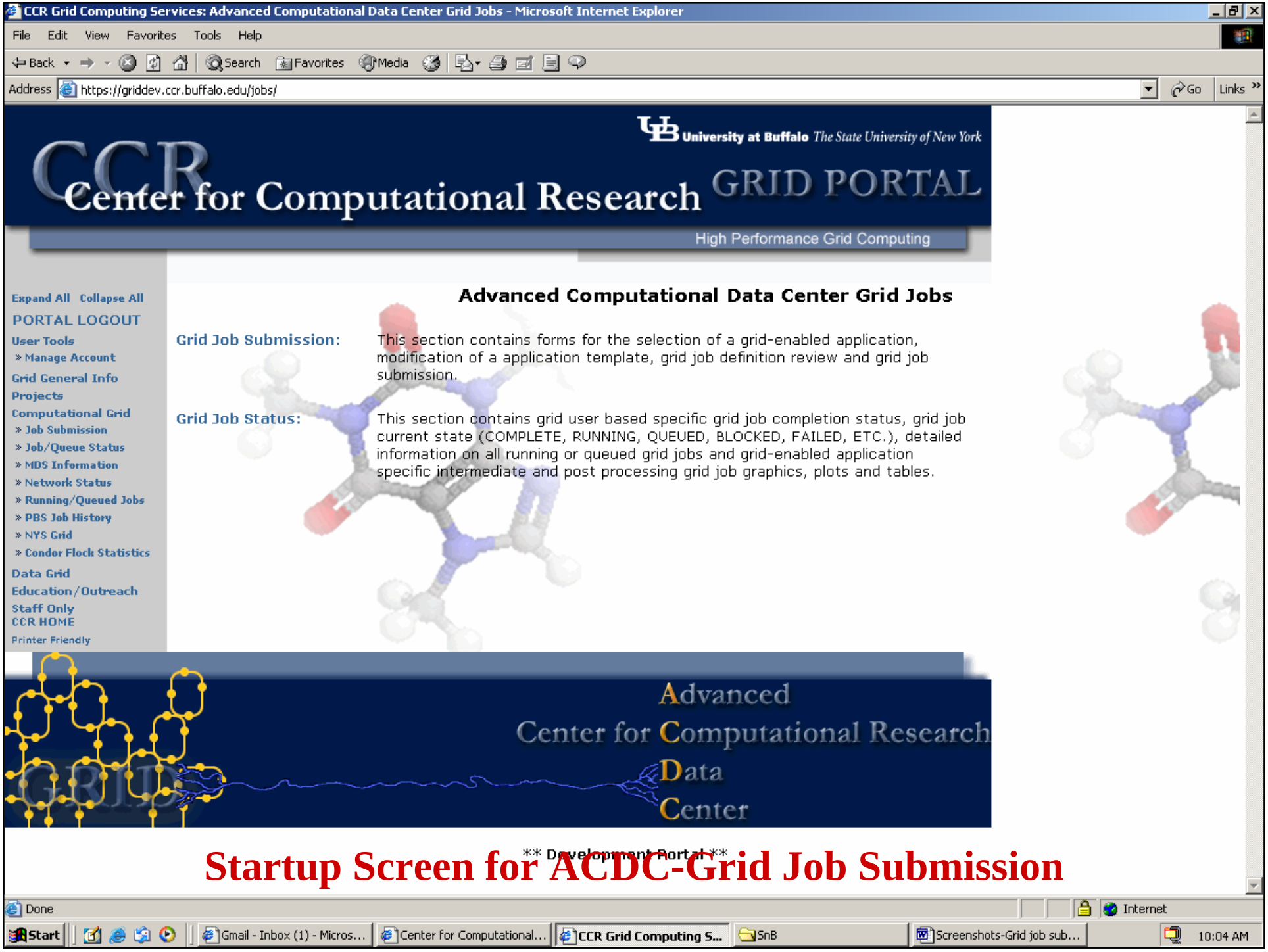
- **Application Layer**
  - *Shake-and-Bake*
  - Apache web server
  - MySQL database
- **High-level Services**
  - Globus, PHP, Fortran, C
- **Core Services**
  - Metacomputing Director Service, Globus Security Interface, GRAM, GASS
- **Local Services**
  - Condor, MPI, PBS, Maui, WINNT, IRIX, Solaris, RedHat Linux

Grid Implementation as a Layered Set of Services

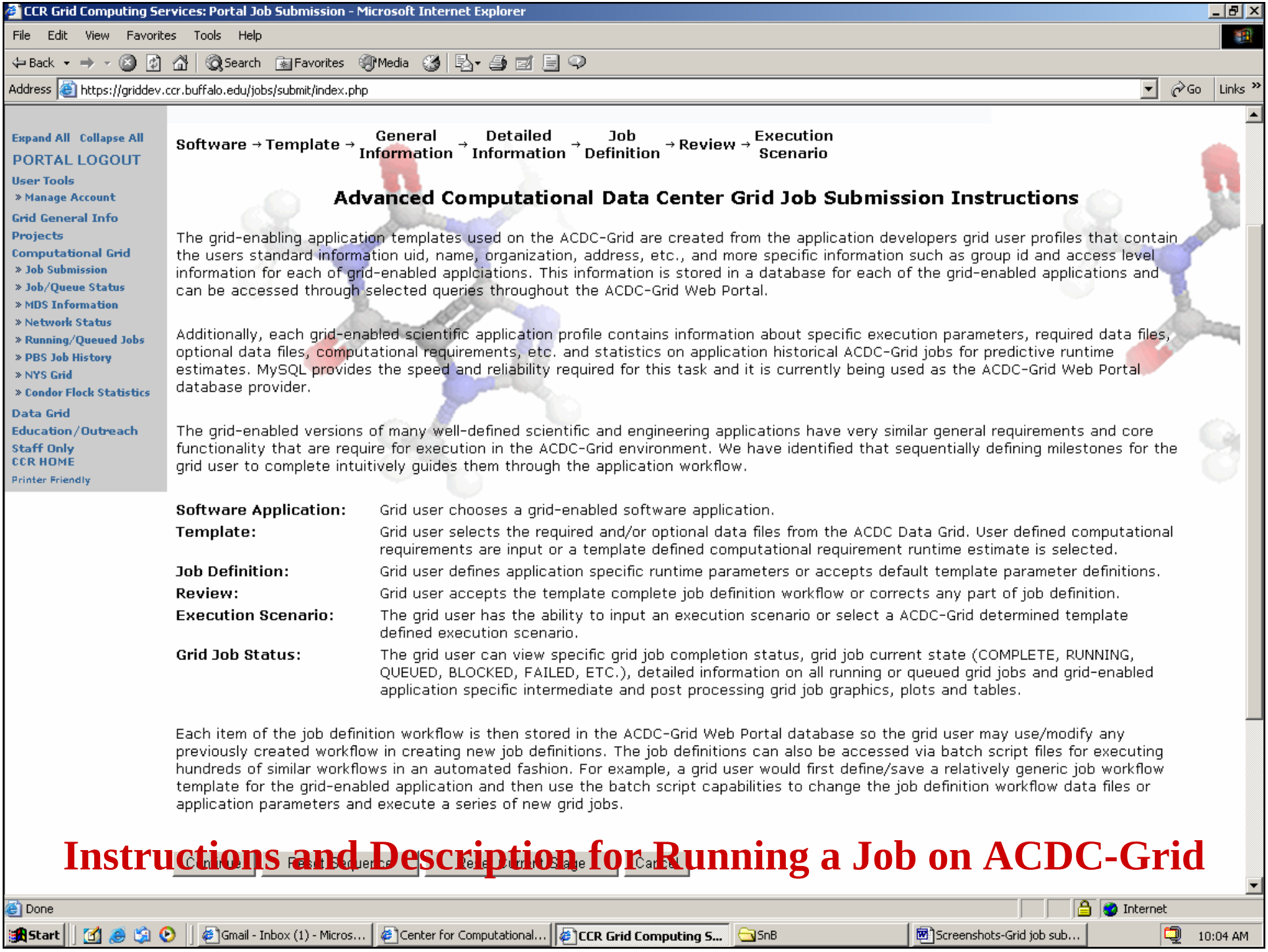


Grid Enabled *SnB* Execution

- **User**
  - **defines Grid-enabled *SnB* job using Grid Portal or *SnB***
  - **supplies location of data files from Data Grid**
  - **supplies *SnB* mode of operation**
- **Grid Portal**
  - **assembles required *SnB* data and supporting files, execution scripts, database tables.**
  - **determines available ACDC-Grid resources.**
- **ACDC-Grid job management includes:**
  - **automatic determination of appropriate execution times, number of trials, and number/location of processors,**
  - **logging/status of concurrently executing resource jobs, &**
  - **automatic incorporation of *SnB* trial results into the molecular structure database.**



Startup Screen for ACDC-Grid Job Submission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Data Grid
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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
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Start
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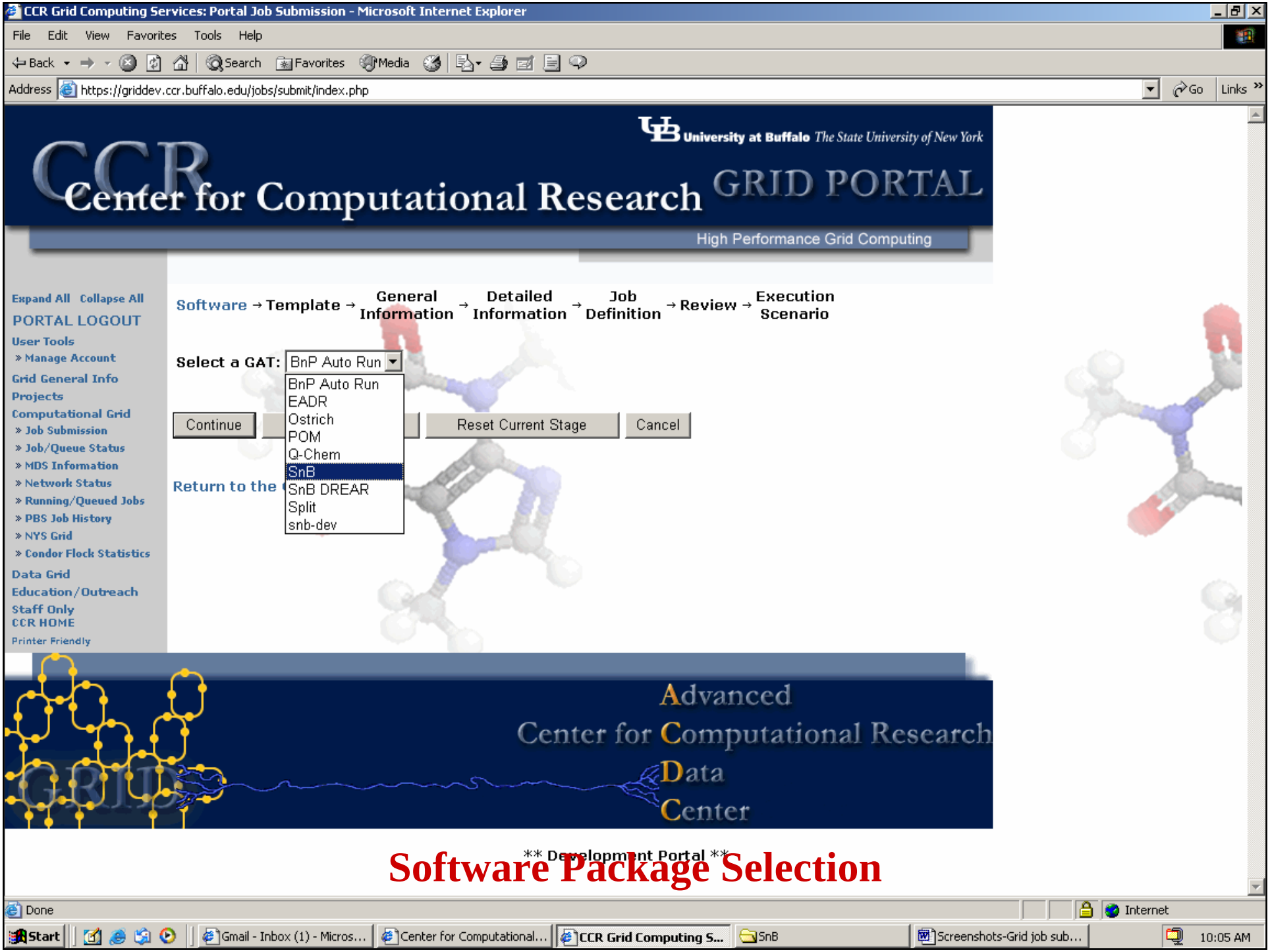
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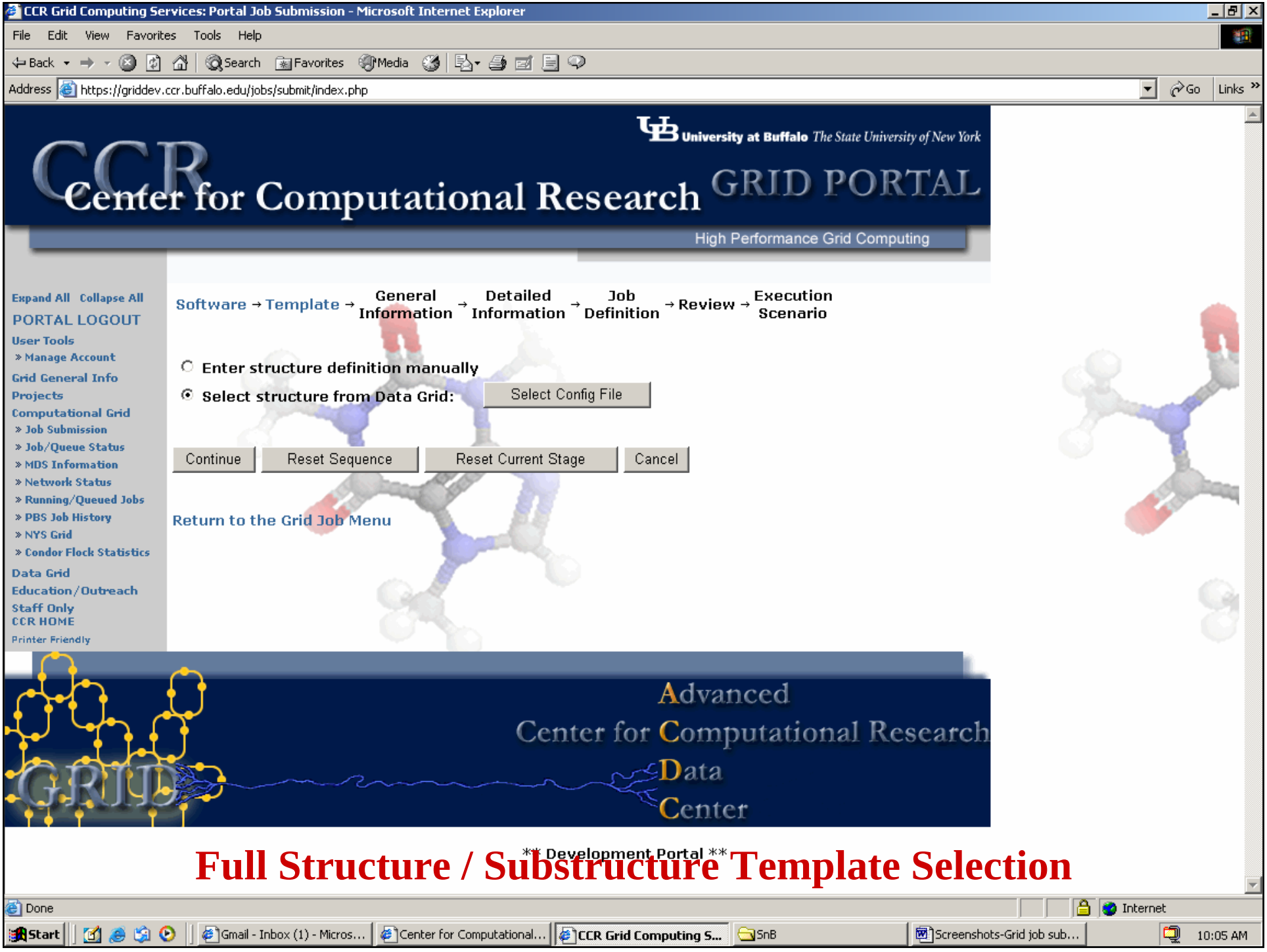
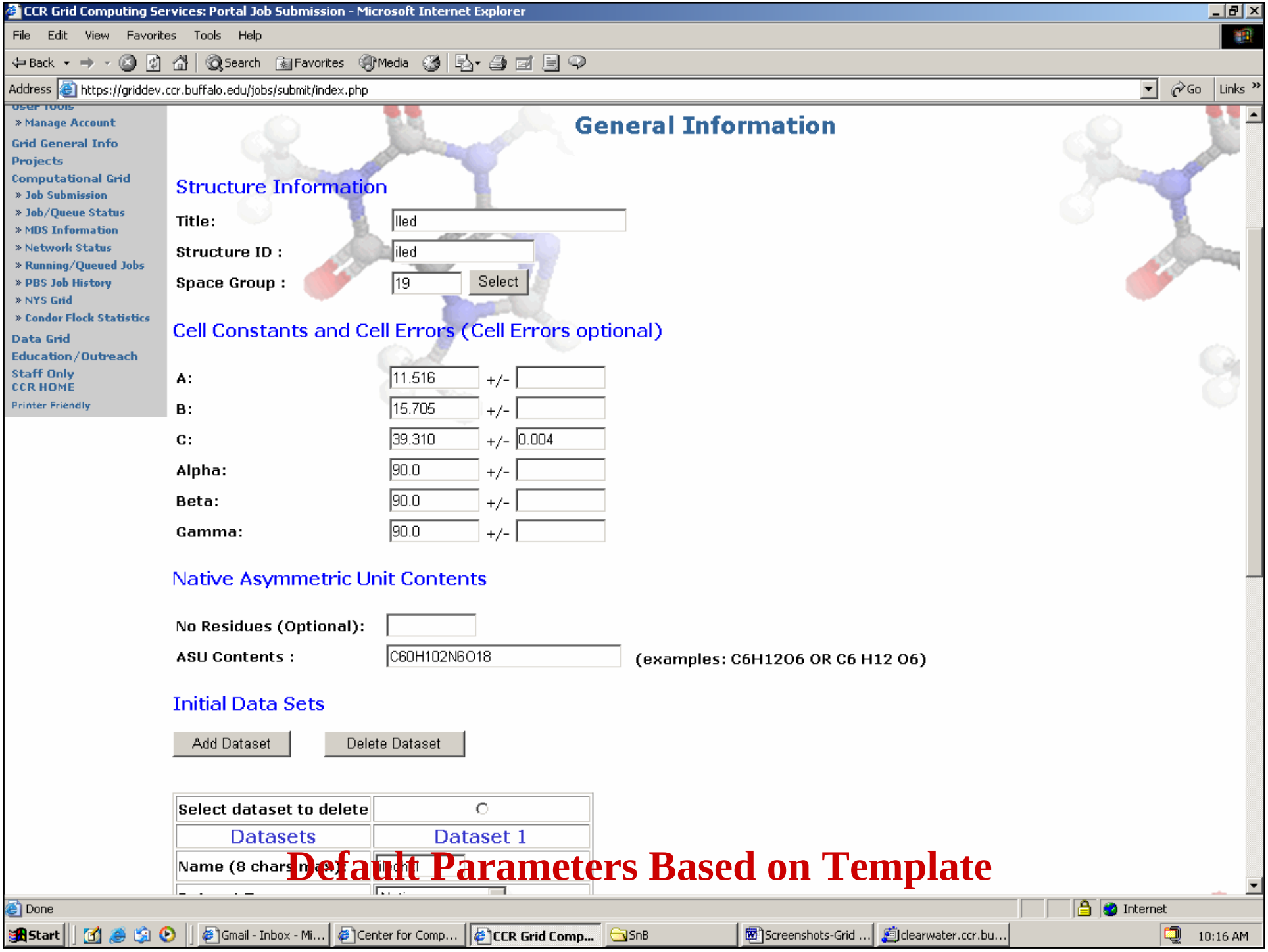


Full Structure / Substructure Template Selection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General Information
Structure Information
Title: lled
Structure ID : iled
Space Group : 19 Select
Cell Constants and Cell Errors (Cell Errors optional)
A: 11.516 +/-
B: 15.705 +/-
C: 39.310 +/- 0.004
Alpha: 90.0 +/-
Beta: 90.0 +/-
Gamma: 90.0 +/-
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No Residues (Optional):
ASU Contents : C60H102N6O18 (examples: C6H12O6 OR C6 H12 O6)
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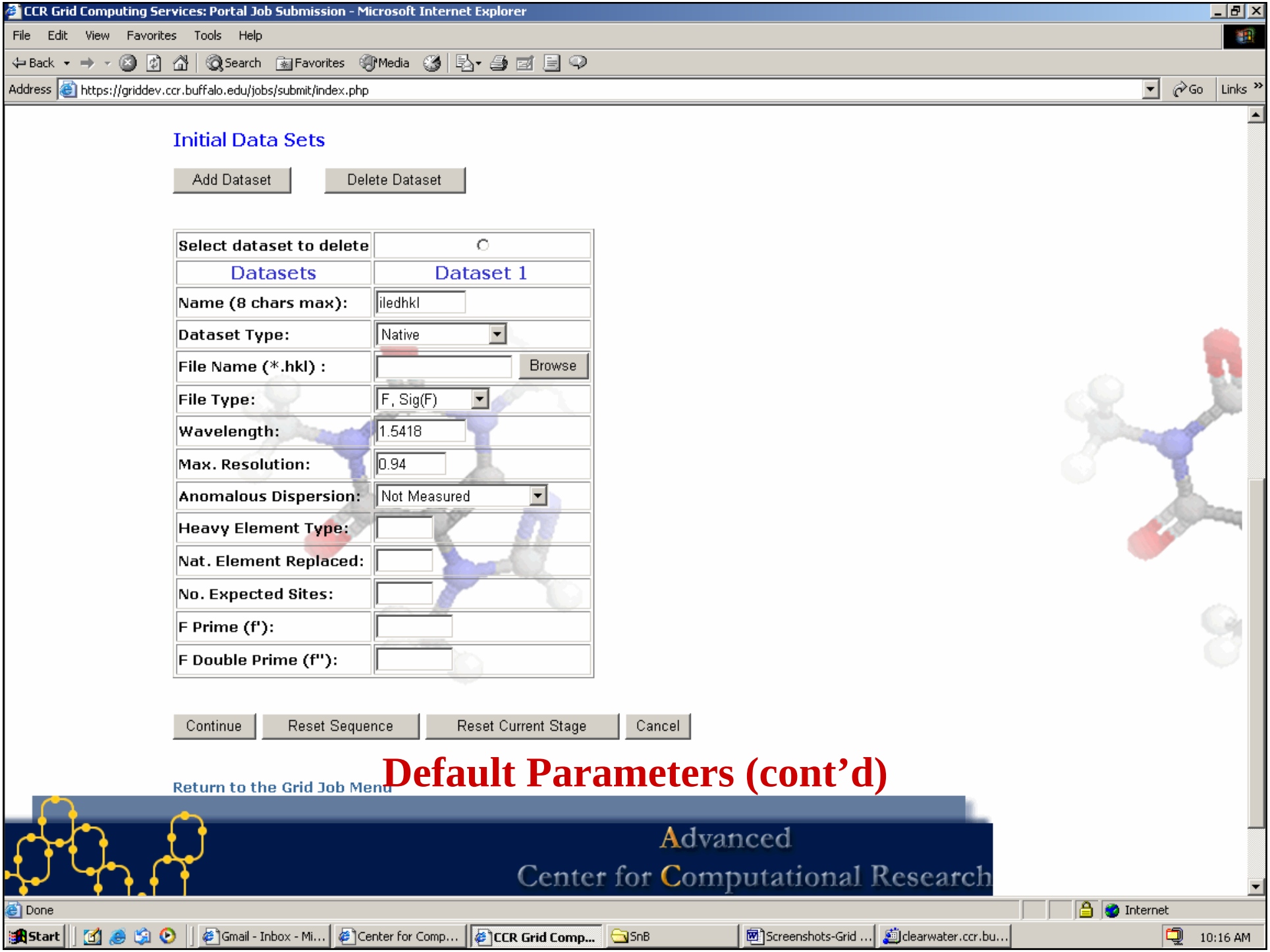

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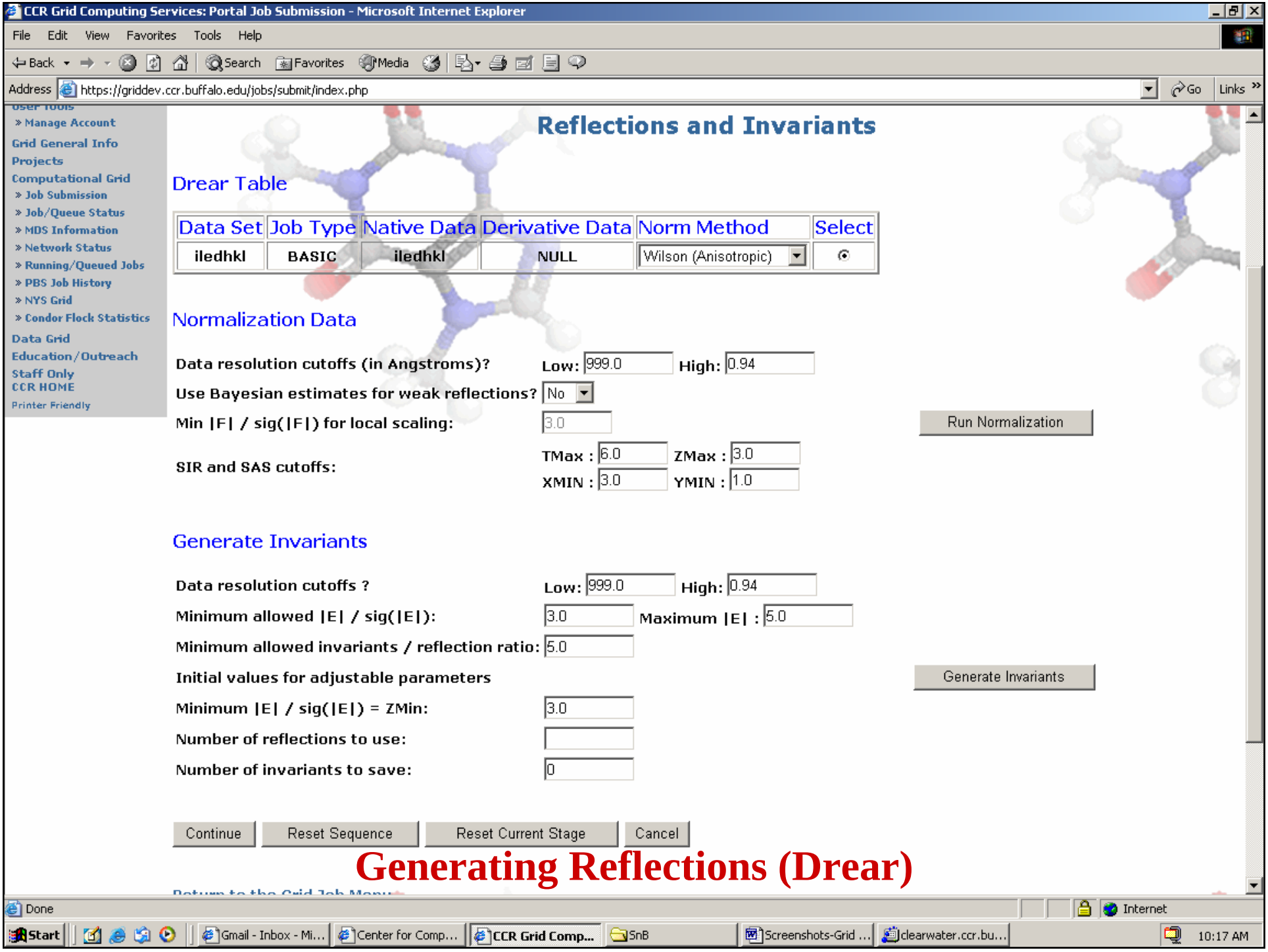
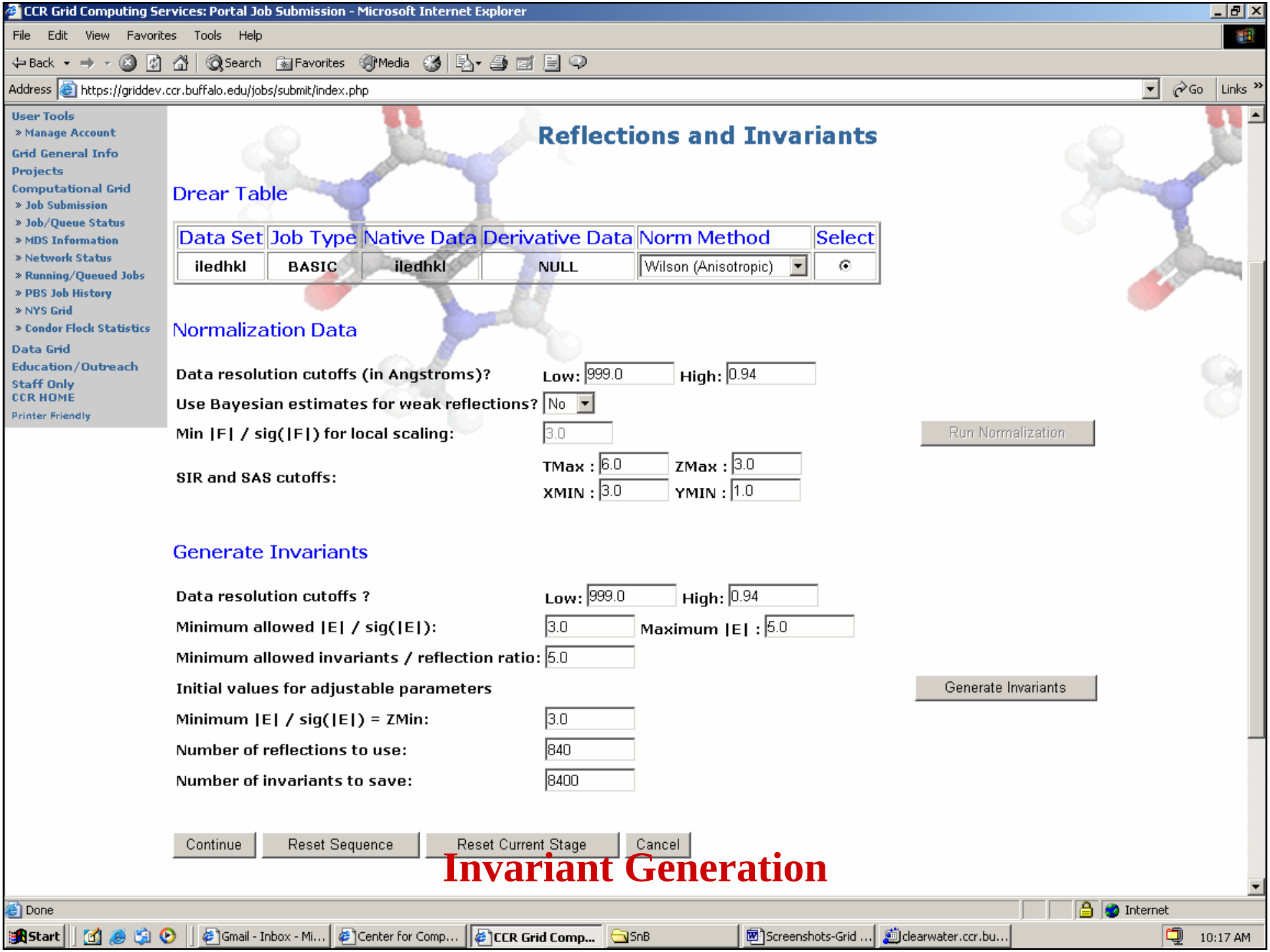


Generating Reflections (Drear)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iledhkl
BASIC
iledhkl
NULL
Wilson (Anisotropic)
Normalization Data
Data resolution cutoffs (in Angstroms)?
Low: 999.0
High: 0.94
Use Bayesian estimates for weak reflections?
No
Min |F| / sig(|F|) for local scaling:
3.0
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
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CCR Grid Comp...
SnB
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clearwater.ccr.bu...
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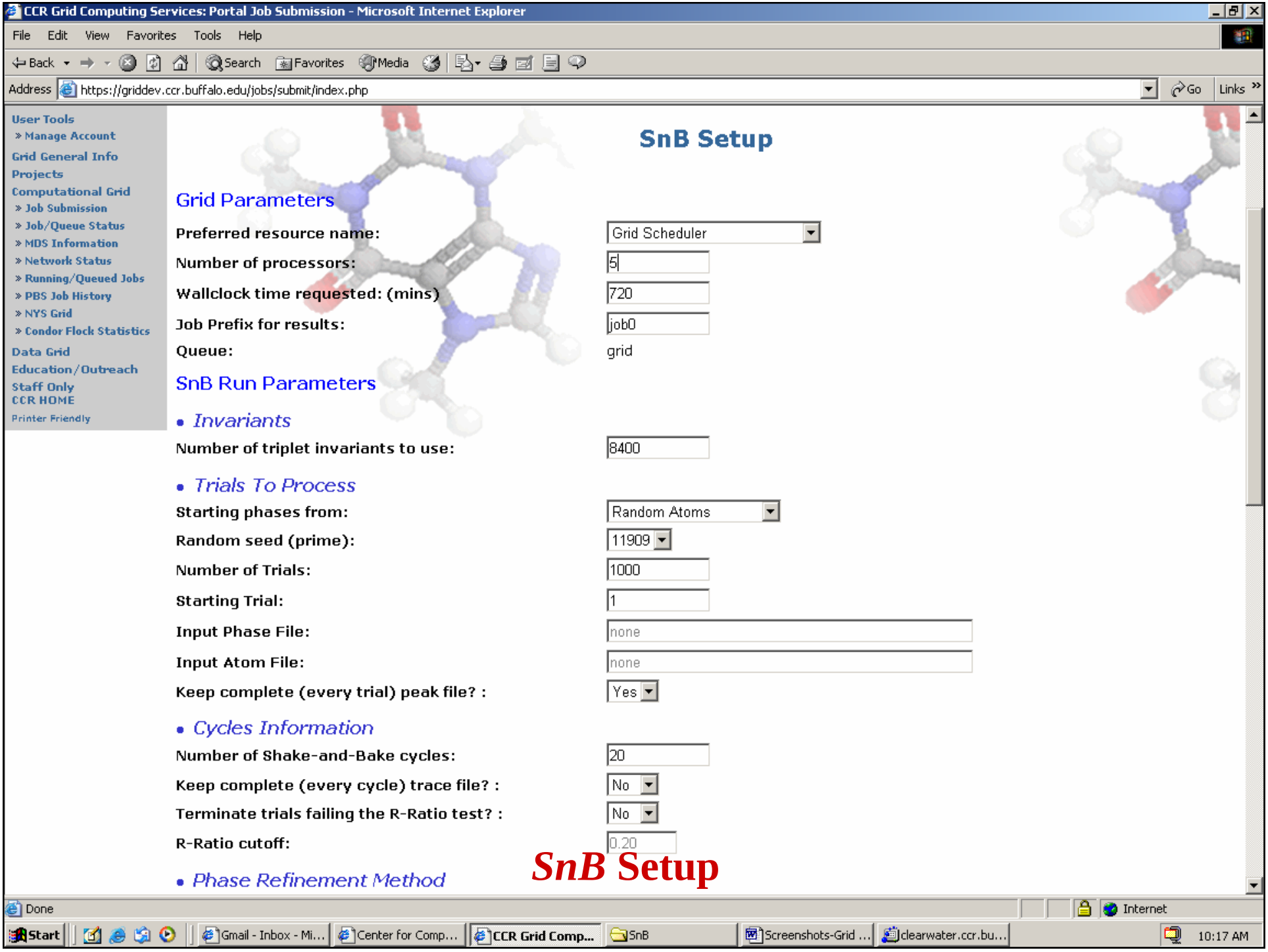
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» Condor Flock Statistics
Data Grid
Education/Outreach
Staff Only
CCR HOME
Printer Friendly
SnB Setup
Grid Parameters
Preferred resource name: Grid Scheduler
Number of processors: 5
Wallclock time requested: (mins) 720
Job Prefix for results: job0
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
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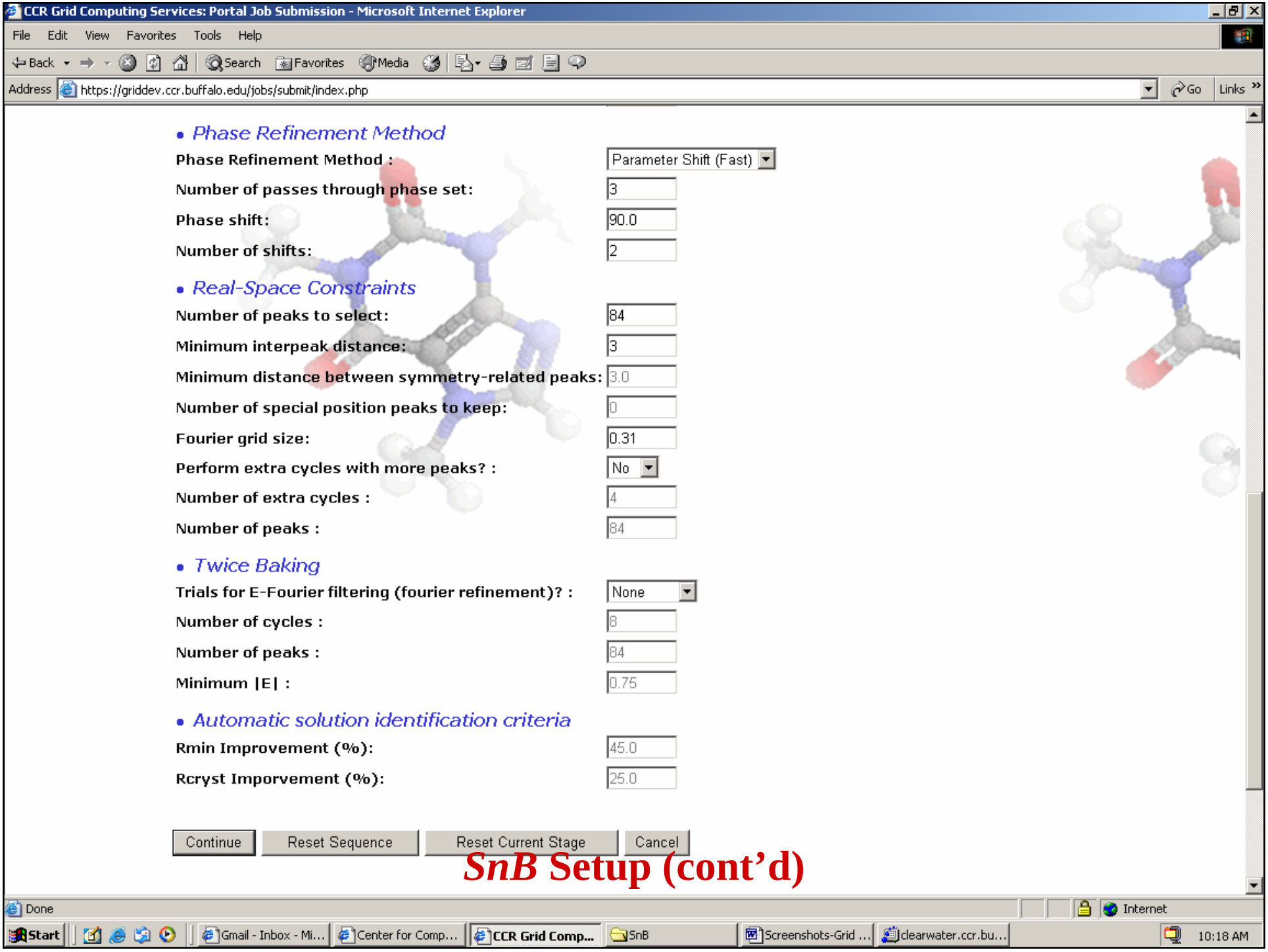
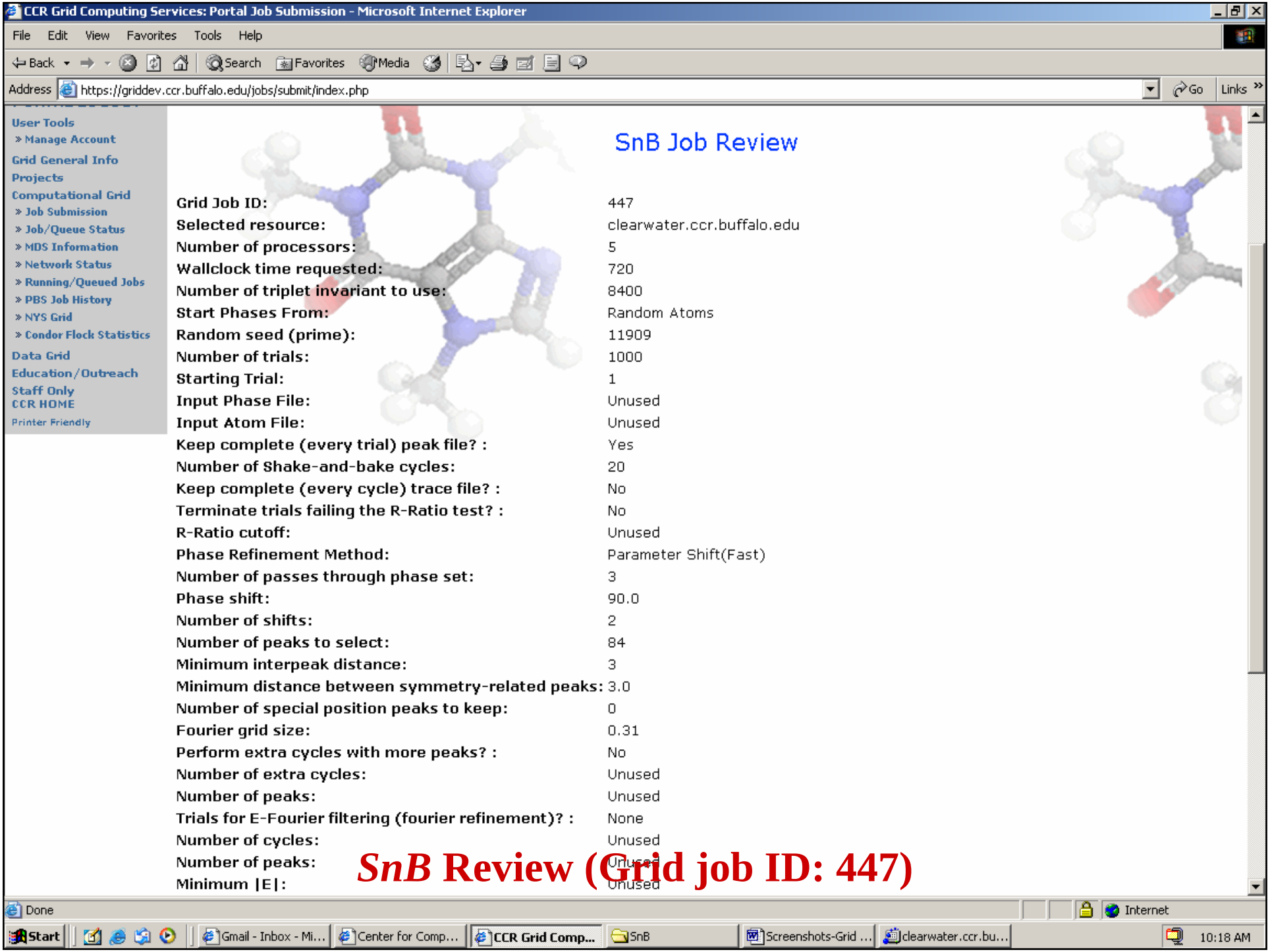


SnB Setup (cont'd)



***SnB* Review (Grid job ID: 447)**

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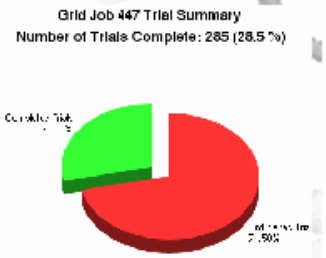
Details for Grid Job 447 - iledhkl

Job Detail Information

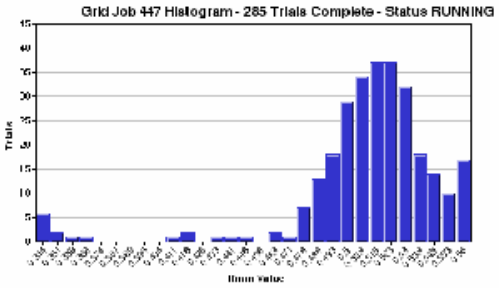
Status: RUNNING
Total Trials: 1000
Best Trial Number: 34
Rmin Min: 0.344 **Rmin Max:** 0.56
Complete Trials: 285
Best Trial Rmin: 0.344
Last Updated: 15-Mar-2005 10:22:00
Resource: clearwater.ccr.buffalo.edu **Processors:** 5

Trial Summary



Walltime Summary

Grid Job Trial Histogram



Click on image for enlarged view.

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Graphical Representation of Intermediate Job Status

Advanced Center for Computational Research Data

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

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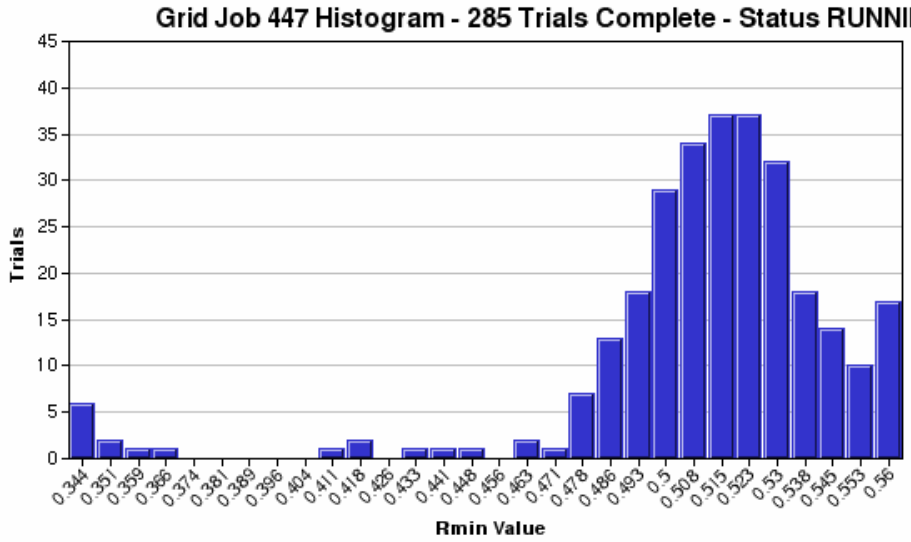

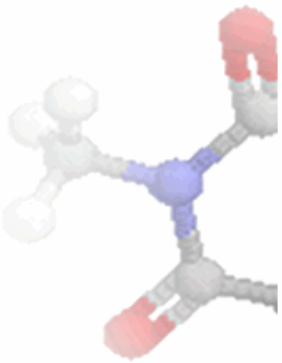

Return to Job Details

Return to the Grid Job Status Page

Return to the Grid Job Menu

Histogram of Completed Trial Structures

Advanced Center for Computational Research

Done

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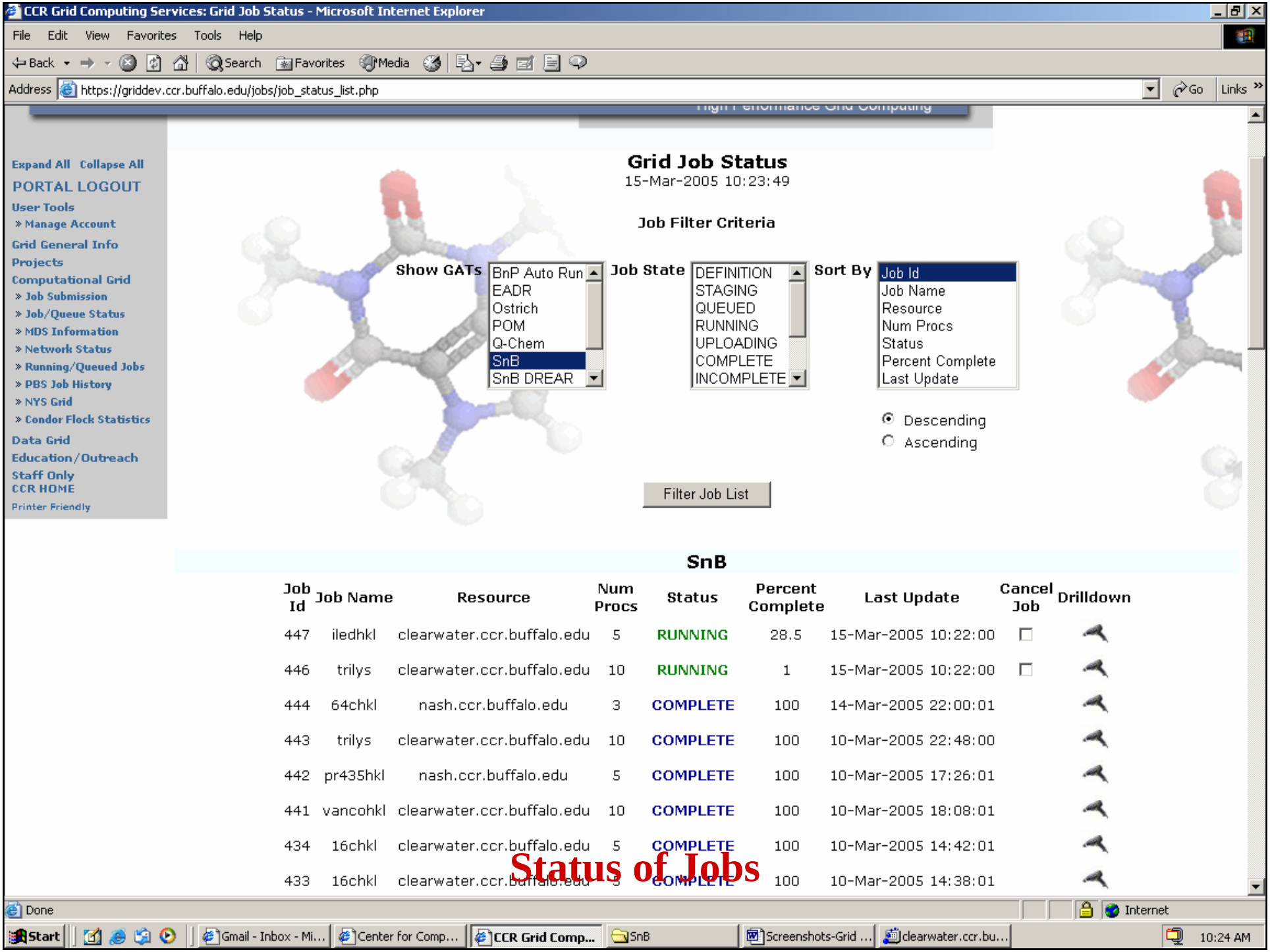
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Grid Job Status
15-Mar-2005 10:23:49
Job Filter Criteria
Show GATs
BnP Auto Run
EADR
Ostrich
POM
Q-Chem
SnB
SnB DREAR
Job State
DEFINITION
STAGING
QUEUED
RUNNING
UPLOADING
COMPLETE
INCOMPLETE
Sort By
Job Id
Job Name
Resource
Num Procs
Status
Percent 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
Done
Internet
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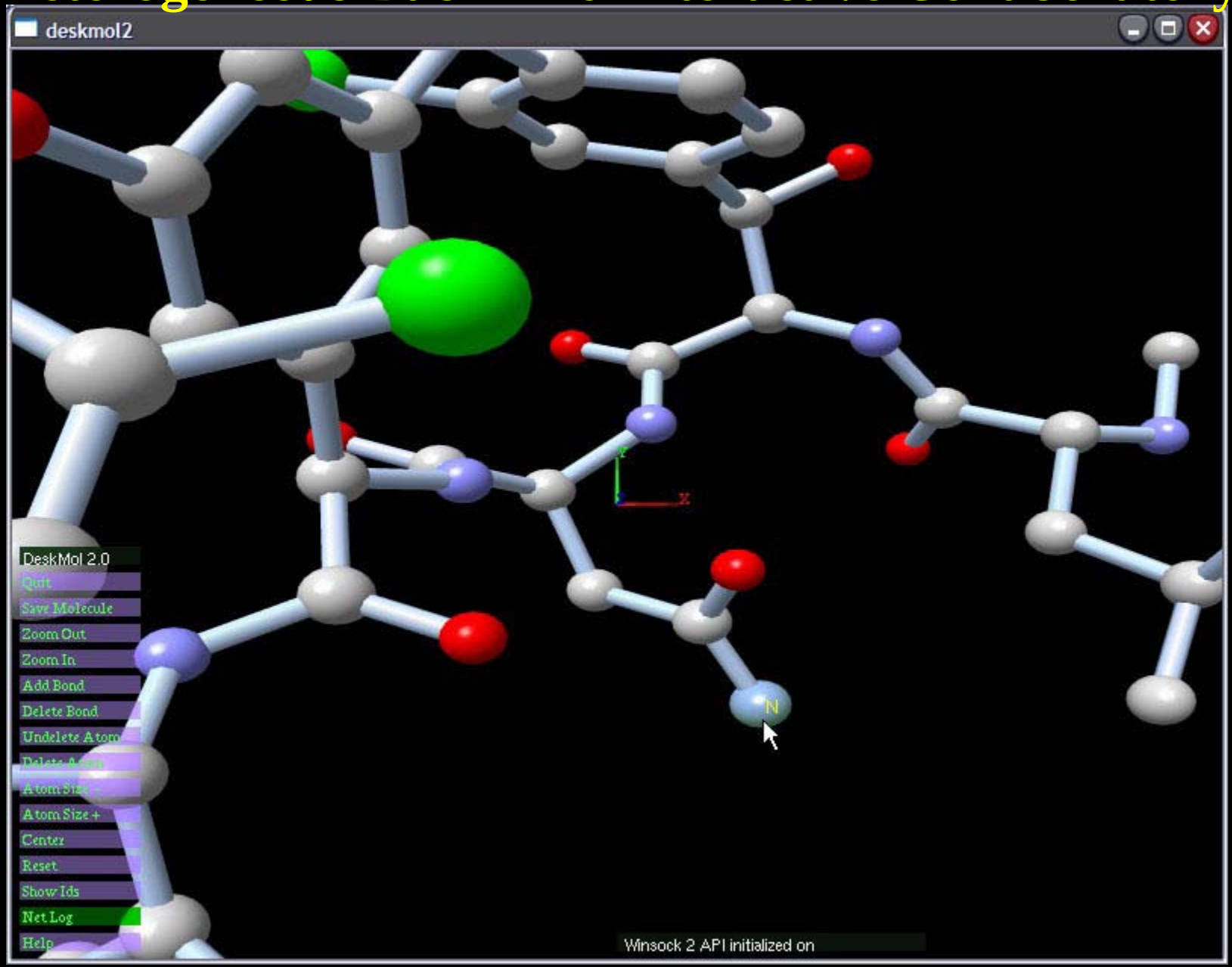
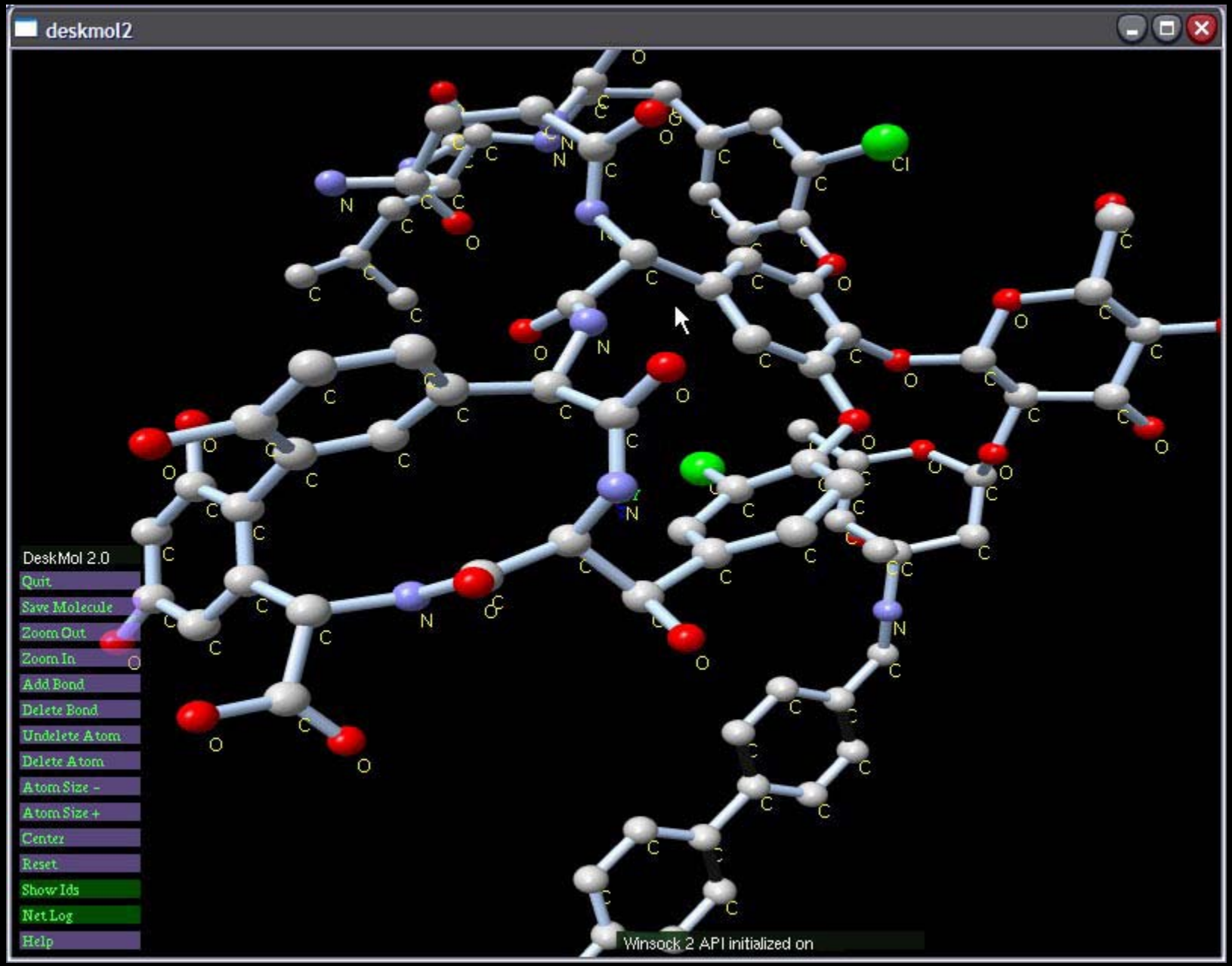
Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Acknowledgments

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