High-Performance Computing ⇒ Discovery & Innovation

Russ Miller

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NSF, NIH, DOE, NIMA, NYS, Dell

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

Academia in the 21st Century: Goals

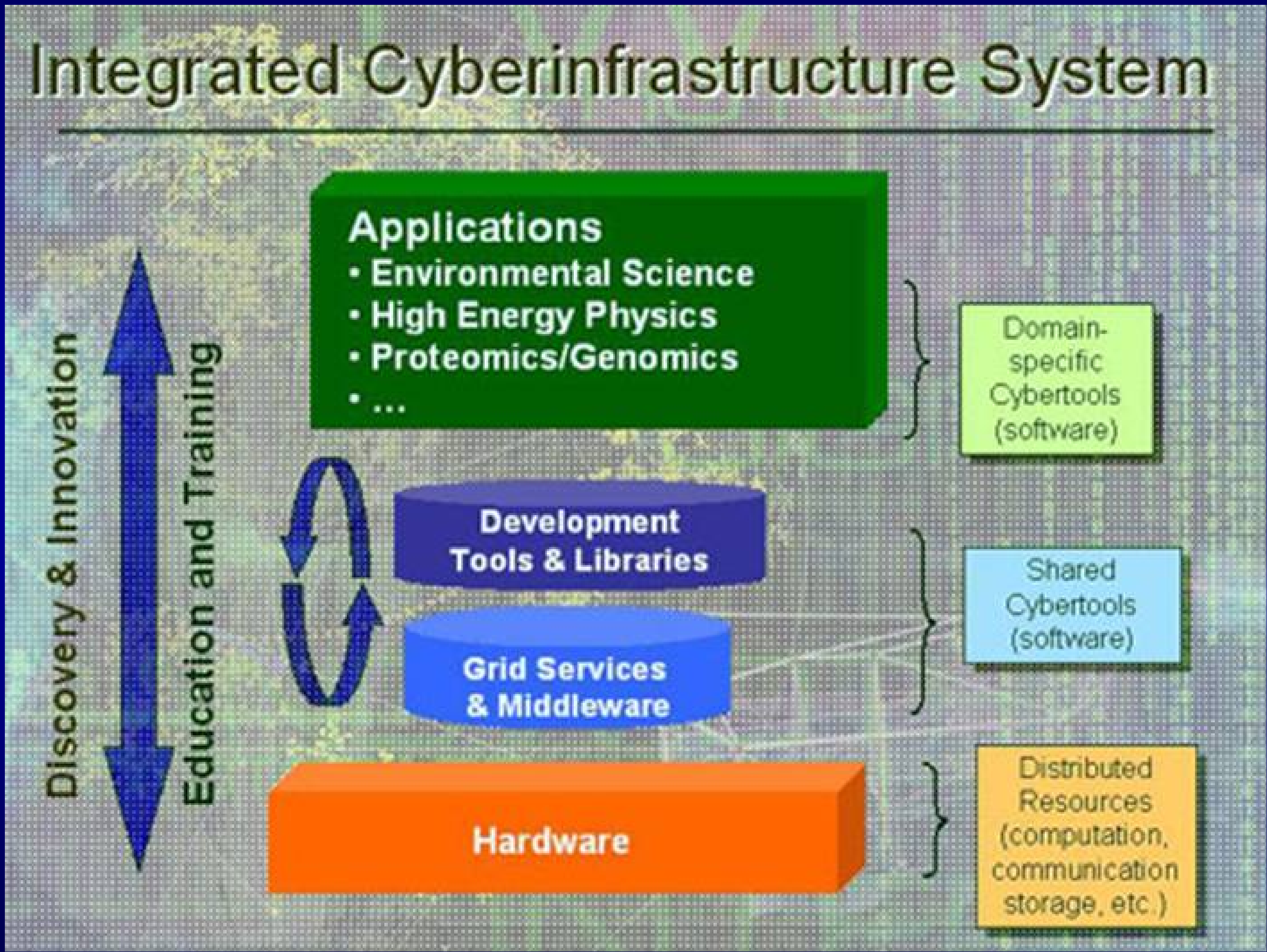
- **Empower students to compete in knowledge-based economy**
- **Embrace digital data-driven society**
- **Accelerate discovery and comprehension**
- **Enhance virtual organizations**
- **Provide increased education, outreach, and training**
- **Enhance and expand relationships between academia and the corporate world**

Academia in the 21st Century: Implementation

- Support HPC infrastructure, research, and applications.
- Enable the efficient, transparent, and ubiquitous
  - Collection of data
  - Management/Organization of data
  - Distribution of data
  - Analysis of data
  - Visualization of data
- Create links between enabling technologists and disciplinary users.
- Improve efficiency of knowledge-driven applications in myriad disciplines.
  - New Techniques
  - New Algorithms
  - New Interactions (people & systems)

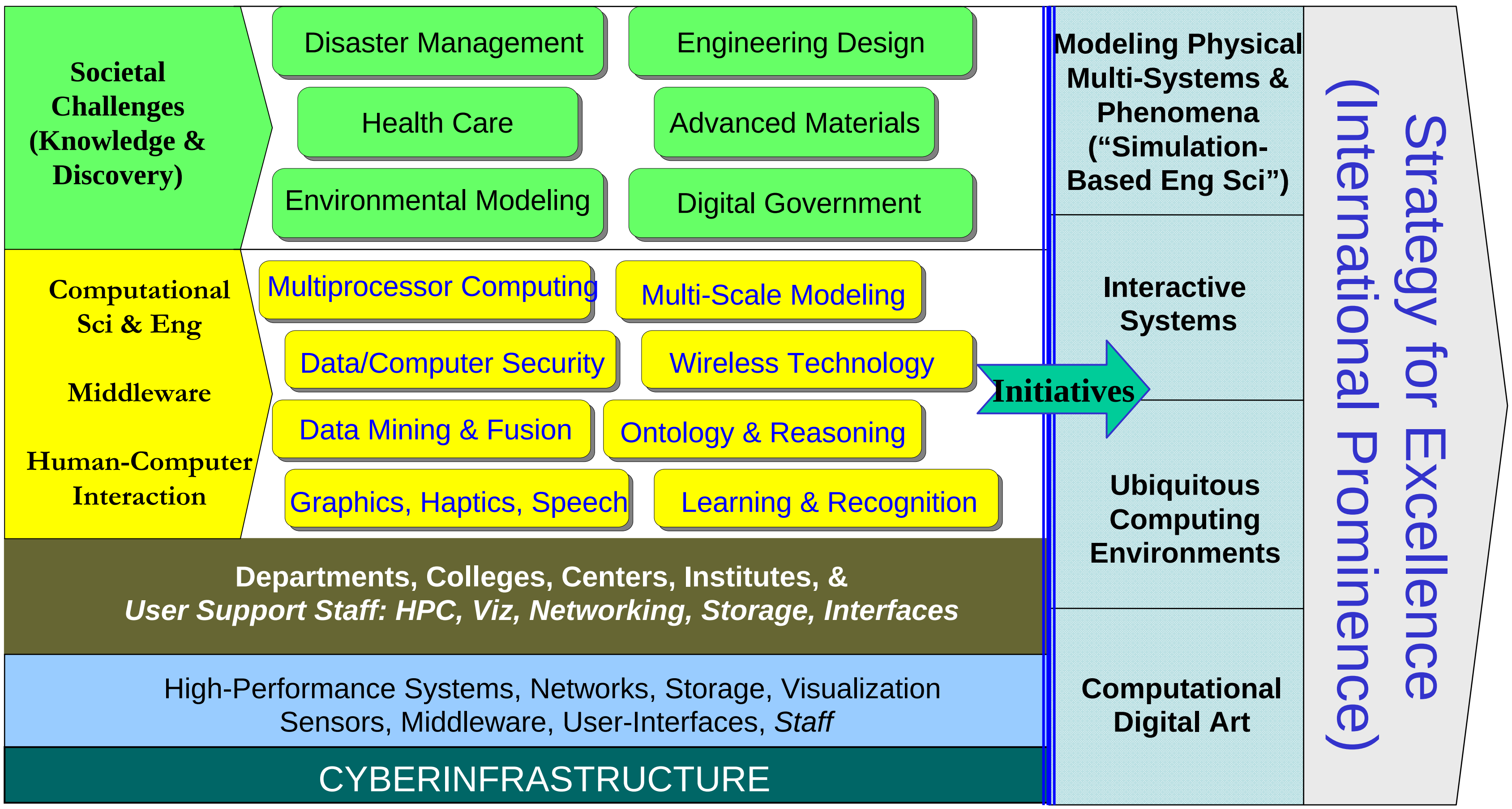
Cyberinfrastructure:

transparent and ubiquitous application of technologies central to contemporary engineering and science



Former *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."*

Academic Computing Initiative: A Sample Inverted Umbrella

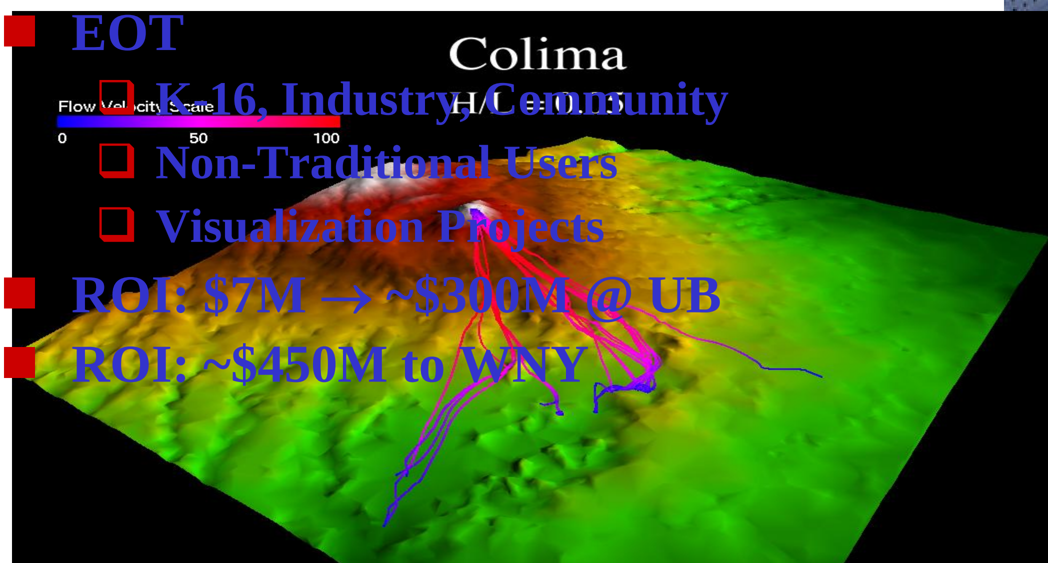


Academic HPC Initiative

- Pervasive Across the Entire University
- Removes Barriers
- Interactions
  - Research Groups
  - Support Staff
  - Students
  - Departments
  - Colleges
- Issues
  - Tenure & Promotion
  - University vs Colleges vs Departments vs Faculty vs Centers/Institutes vs Degrees vs Courses
- Details are University Dependent

Center for Computational Research (CCR): 1998-2006

- **Founding Director**
- **Facts & Figures**
  - **Top Academic HPC Center World-Wide for a period of time**
  - **Significant Visualization**
  - **Special-Purpose Systems**
  - **~30 FTEs Staff**
  - **140 PI-Sponsored Projects Annually**
- **EOT**
  - **K-16, Industry, Community**
  - **Non-Traditional Users**
  - **Visualization Projects**
- **ROI: $7M → ~$300M @ UB**
- **ROI: ~$450M to WNY**

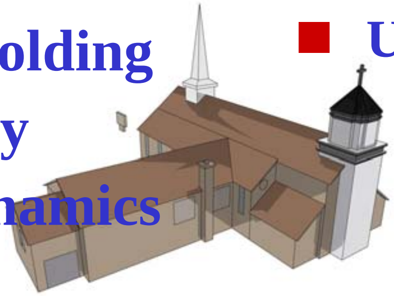


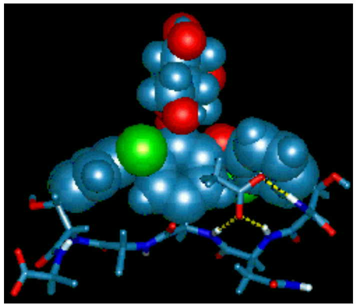
CCR Highlights (1998-2006)

- Provide HE-Comp
- Provide HE-Vis + AGN
- Special Purpose Systems
  - Bioinformatics
  - Data Warehouse / Mining
- Support Local/National Efforts – Industry + Acad
- Create jobs in WNY
- Certificate Program
- Workshops + Tours
  - Campus, Industry
  - High-School
- Urban Planning & Design
- MTV Videos
- Peace Bridge, Med Campus
- Olmsted Parks, Thruway
- NYS Agencies
- Elected Officials
- Magnet on Campus
- Significant Funds
- Numerous Awards
- Significant Publicity

CCR Research & Projects

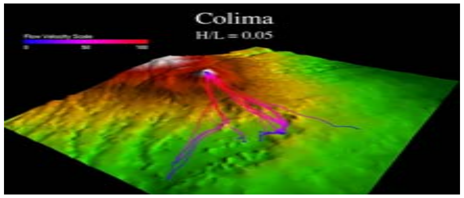
- Archaeology
- Bioinformatics/Protein Folding
- Computational Chemistry
- Computational Fluid Dynamics
- Data Mining/Database
- Earthquake Engineering
- Environ Modeling & Simulation
- Grid Computing
- Molecular Structure Determination
- Physics

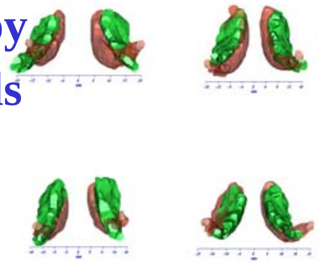




- Videos: MTV
- Urban Simulation and Viz
  - StreetScenes
  - I-90 Toll Barrier
  - Medical Campus
  - Peace Bridge

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





CCR Funding (1998-2006)

- **CCR-Enabled to SUNY-Buffalo**
  - **$170M External Funds**
  - **$140M In-Kind Contributions**
- **CCR-Enabled to WNY**
  - **$200M External Funds**
- **Federal Appropriations**
- **New York State Appropriations**
- **Local WNY Foundations**
- **In-Kind Contributions (Dell, SGI, Sun, etc.)**
- **Grants (NSF, NIH, DOE, etc.)**
- **Projects with Local Companies**
- **Government Projects**
- **SUNY-Buffalo: staff and space**

Real-Time Visualization

StreetScenes: Real-Time 3D Traffic Simulation

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

Animation & Simulation

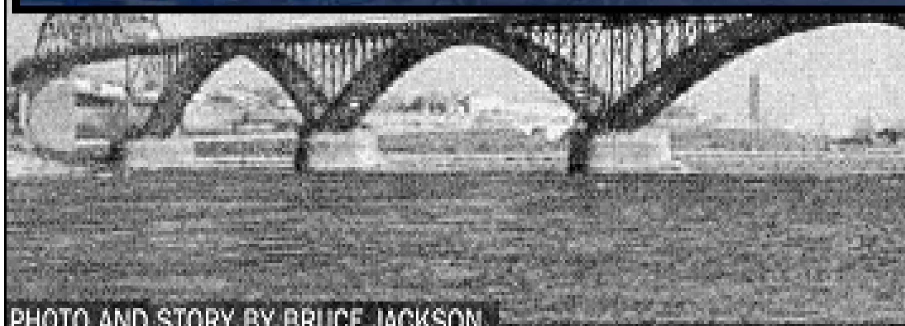
Rendered Scenes

Williamsville Toll Barrier Improvement Project

Initial Photo Match incorporating real and computer-generated components

Peace Bridge Visualization: Animation & Simulation

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



Public Forum

MTV

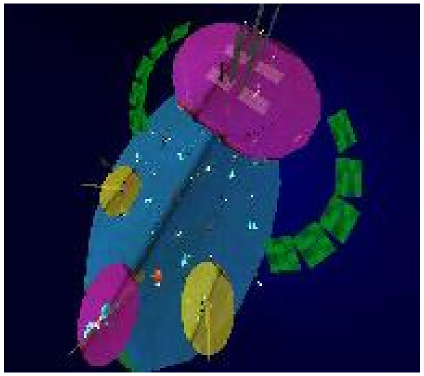
IBC Digital & CCR

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

Virtual Reality

Alive on the Grid: PAAPAB

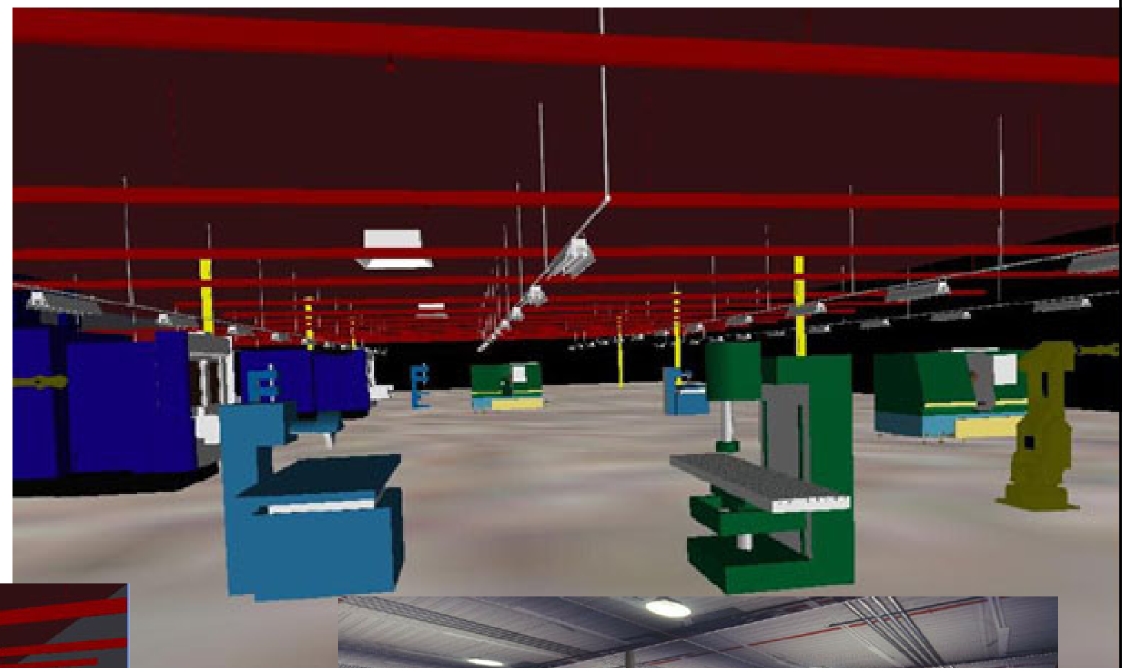
- Networked art application for CAVE
  - Users from around the world
  - First performance 2001
- Dance-floor environment
  - Inhabited by life-size puppets
  - Dance with each other
  - Synchro
- Recording Booth
  - User enters booth
  - User dances
  - System records dance from tracking on head and hands
  - Dance mapped to Avatar

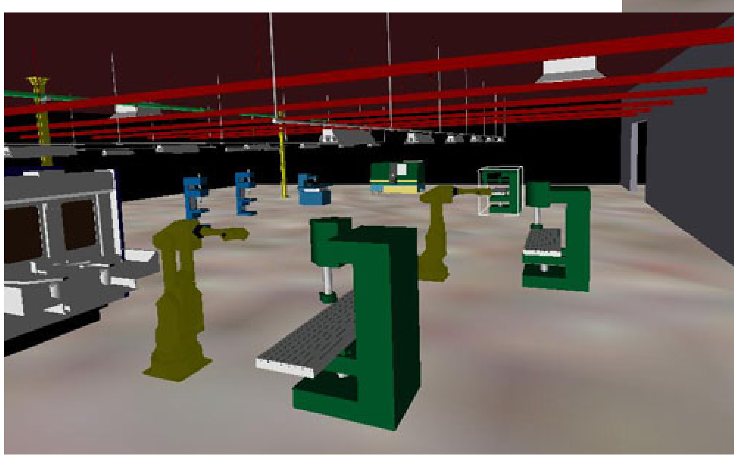


J. Anstey

VR-Fact!

- Interactive virtual factory
- Creates digital mock-up of factory
- Drag & place modular machines
- Mathematical algorithms for consistency checks





Kesh

Western New York

Some Facts

Buffalo, New York

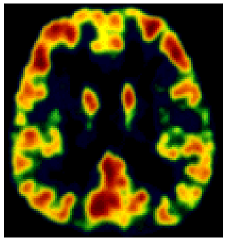
- **The Queen City: 2nd Largest City in NYS**
- **City of Lights**
  - **First U.S. city to have electric street lights**
  - **Pan American Exposition (1901)**
    - **Pres. McKinley Shot**

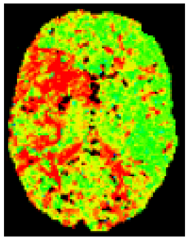
- **Architecture**
  - **Frederick Law Olmsted**
  - **Frank Lloyd Wright**
- **Underground Railroad**
  - **Slaves escaped to freedom in Canada**
- **Four straight Super Bowl appearances**

- **Culinary Delights**
  - **Beef on Weck, Pizza, Fish Fries**
  - **(Buffalo) Wings: Anchor Bar, 1964**
- **Health Problems**
  - **Heart Disease/Stroke**
  - **Multiple Sclerosis**

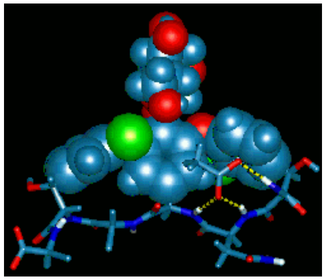
Recent Biomedical Advances (Buffalo, NY)

- 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 20^{th} Century"

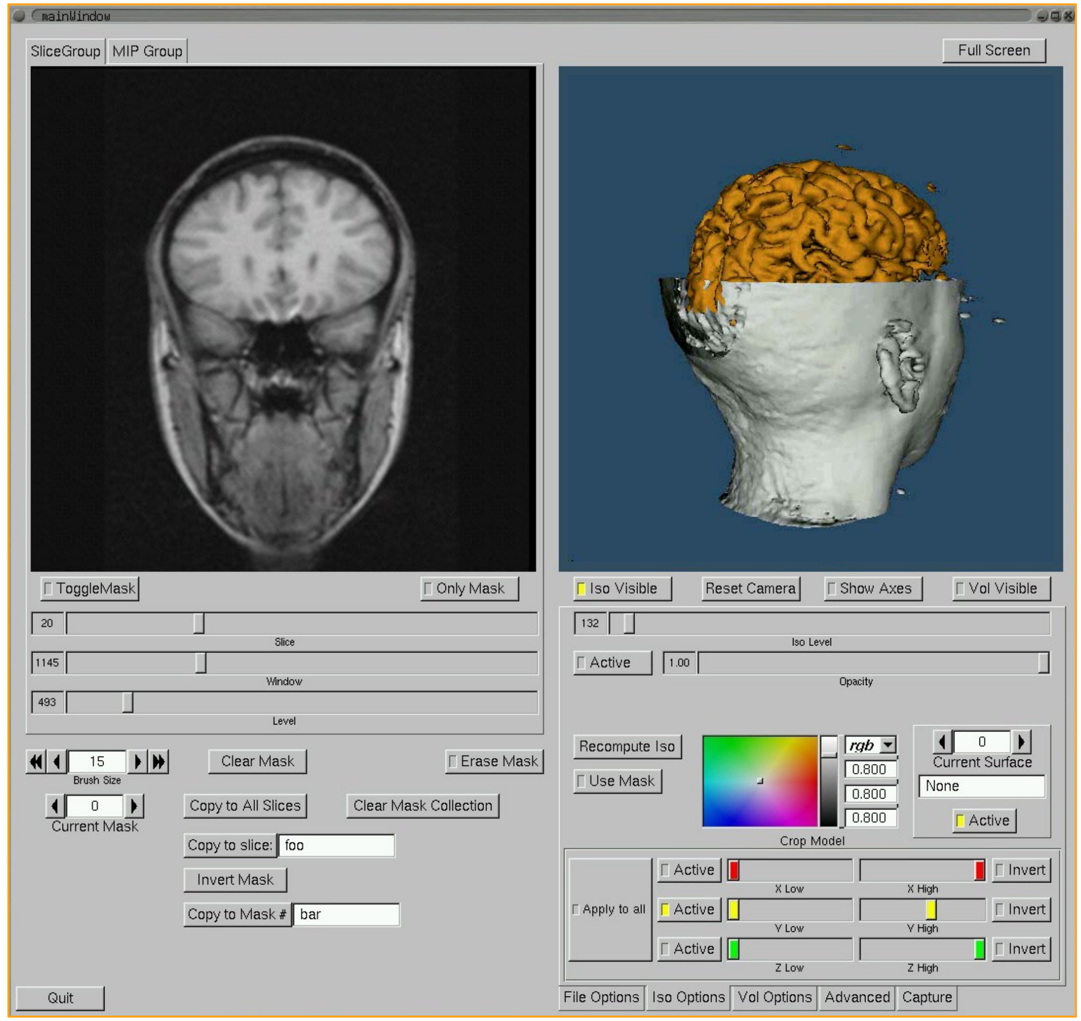


- Vancomycin
- Gramacidin A
- High Throughput Crystallization Method: Patented
- NIH National Genomics Center: Northeast Consortium
- Howard Hughes Medical Institute: Center for Genomics & Proteomics

Scientific Visualization

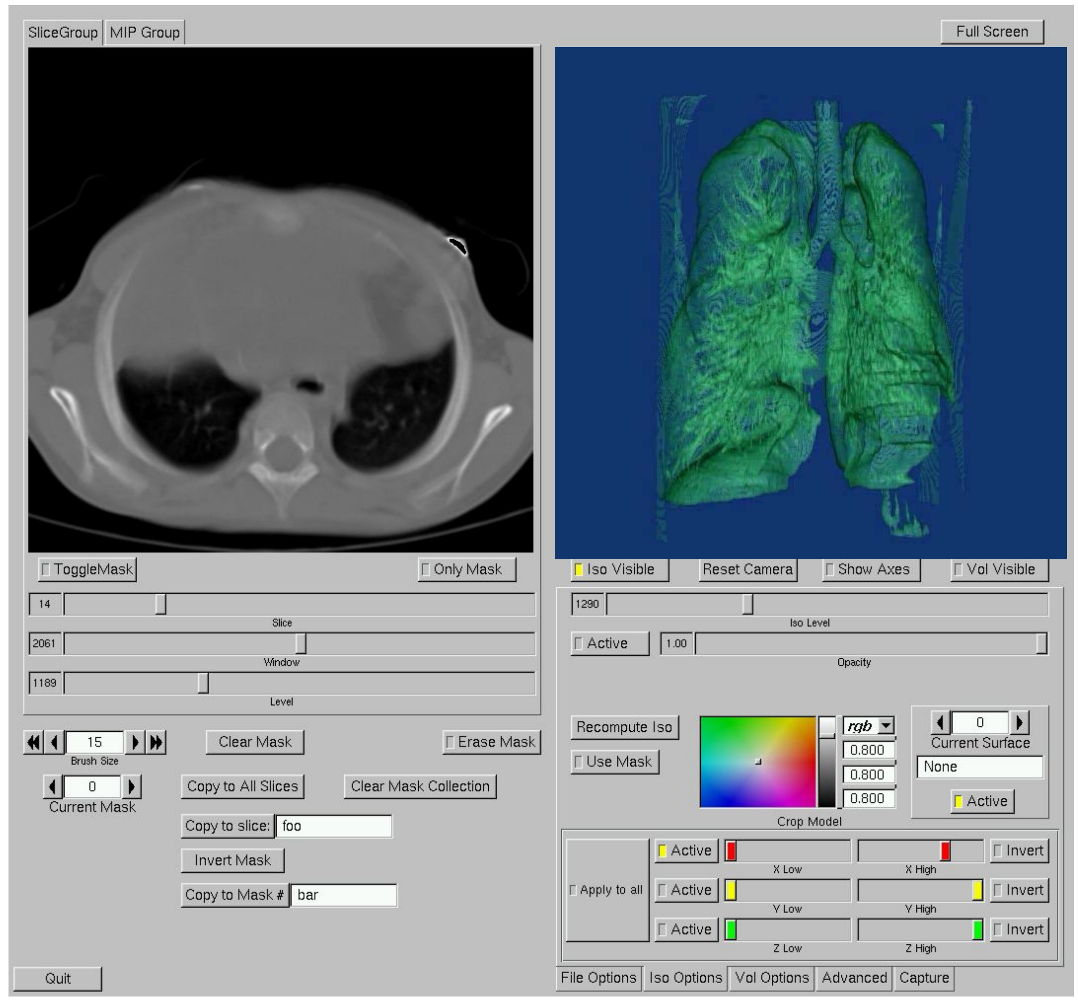
Multiple Sclerosis Project

- **Collaboration with Buffalo Neuroimaging Analysis Center (BNAC)**
  - **Developers of Avonex, drug of choice for treatment of MS**
- **MS Project examines patients and compares scans to healthy volunteers**



3D Medical Visualization

- Reads data output from a CT or MRI Scan
- Collaboration with Children's Hospital
- Visualize multiple surfaces and volumes
- Export images, movies or CAD file
- Pre-surgical planning
- Runs on a PC



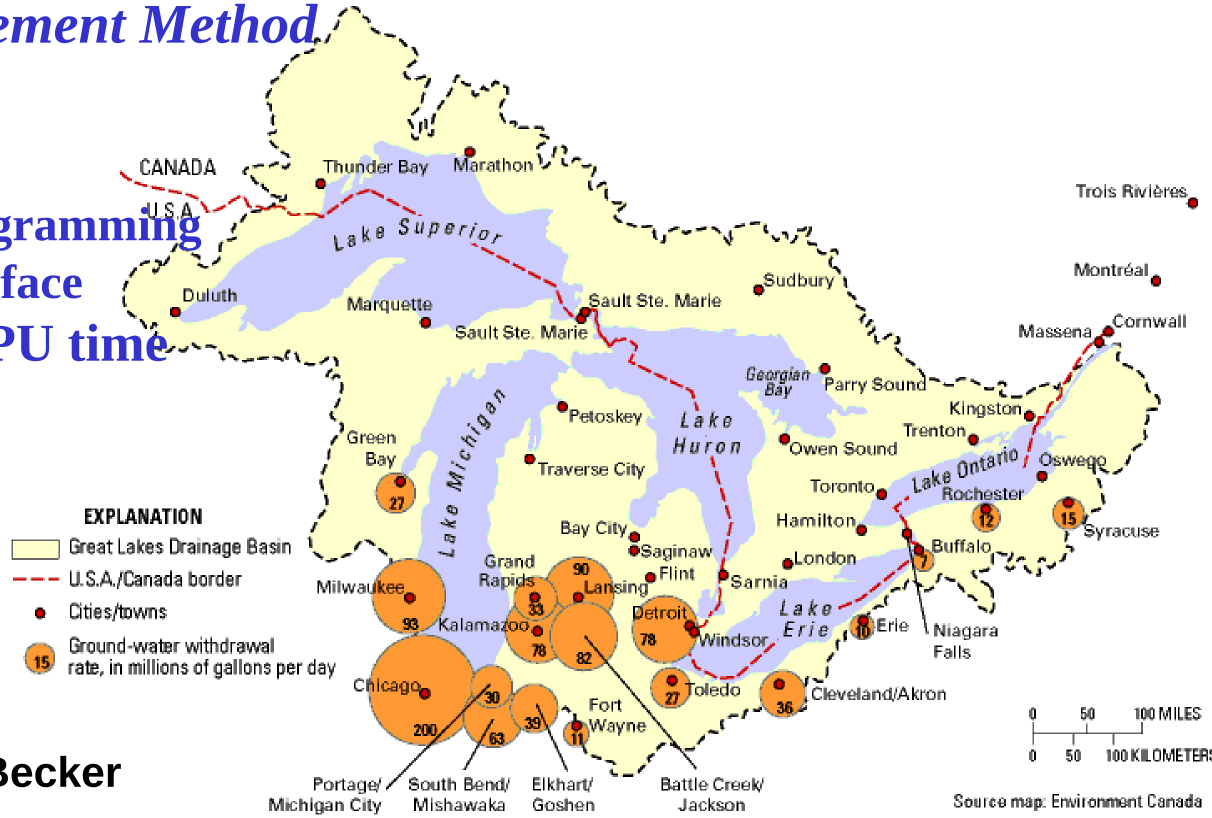
M. Innus

Science & Engineering

Small Subset of Projects

Groundwater Flow Modeling

- **Regional scale modeling of groundwater flow and contaminant transport (Great Lakes)**
- **Ability to include all hydrogeologic features as independent objects**
- **Based on *Analytic Element Method***
- **Key features:**
  - **Highly parallel**
  - **Object-oriented programming**
  - **Intelligent user interface**
- **Utilized 42 years of CPU time on CCR computers in 1 calendar year**

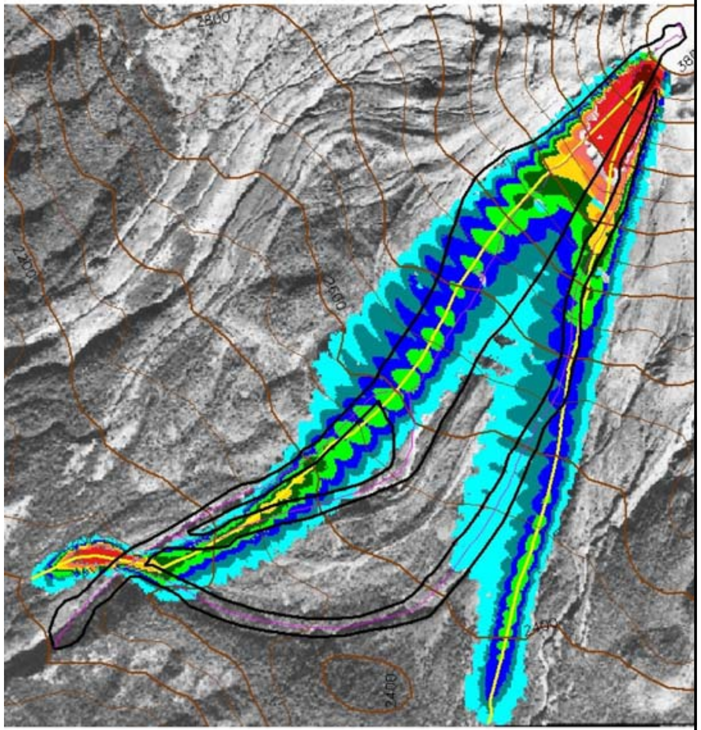


A. Rabideau, I. Jankovic, M. Becker

Avalanches, Volcanic and Mud Flows

Geology, Engineering

- **Modeling of Volcanic Flows, Mud flows (flash flooding), and avalanches**
- **Integrate information from several sources**
  - **Simulation results**
  - **Remote sensing**
  - **GIS data**
- **Present information to decision makers using custom visualization tools local & remote**
- **GRID enabled for remote access**
- **Key Features**
  - **Parallel Adaptive Computation**
  - **Integrated with GIS System for flows on natural terrain**

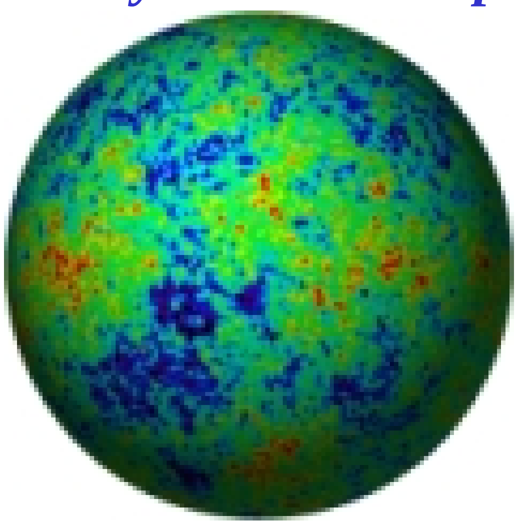


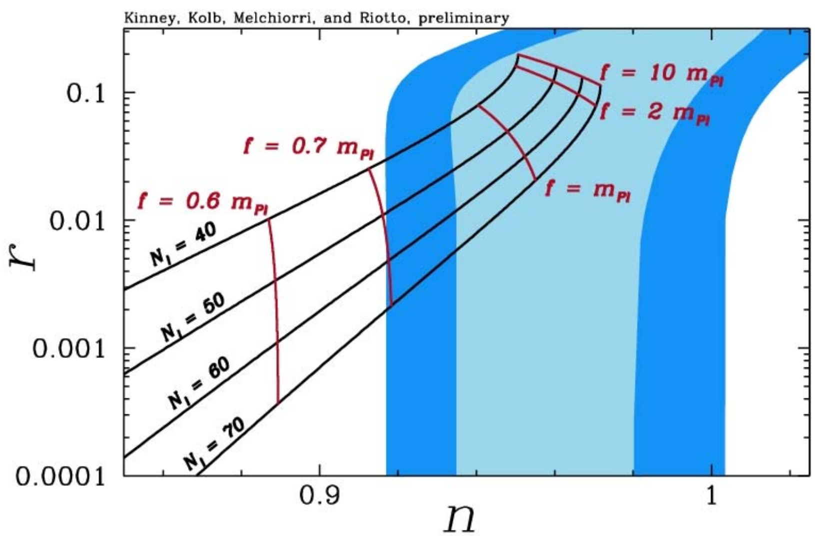
Flow models of Colima volcano
In Mexico – courtesy Rupp et. al.'06

A. Patra, B. Pitman, M. Sheridan, M. Jones

Cosmological Parameter Estimation

- **Wealth of new precision cosmological data**
- **WMAP Cosmic Microwave Background Measurement**
- **Sloan Digital Sky Survey: 3-D map of a million galaxies**
- **Interpret implications of data for models of the first trillionth of a second of the universe: *inflation***
- ***Monte Carlo Markov Chain data analysis: stochastic exploration of many-dimensional parameter spaces***



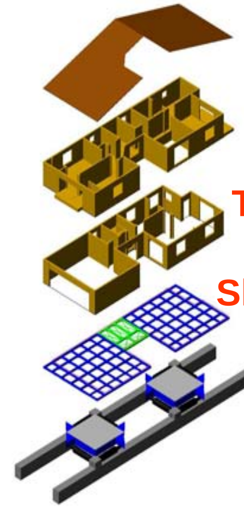


W. Kinney

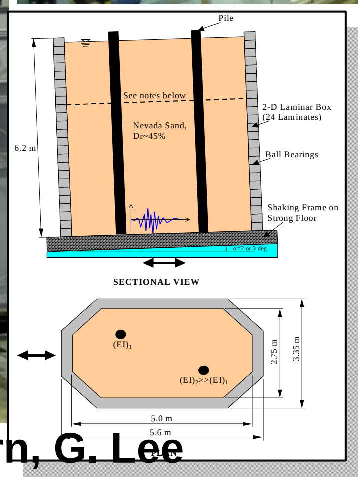
UB's Structural Engineering and Earthquake Simulation Laboratory (SEESL)

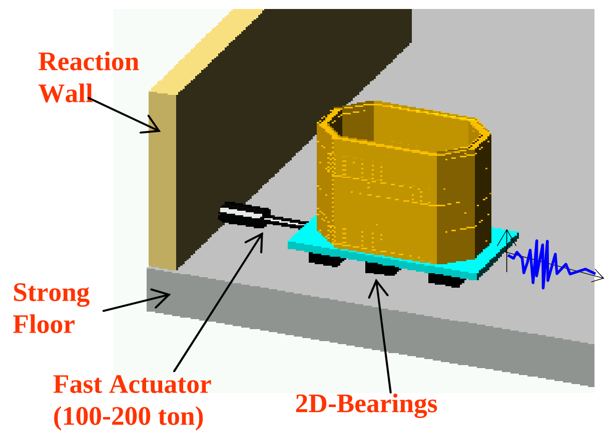
Structural Engineering

NEESWood: Development of a Performance-Based Seismic Design for Woodframe Construction:



Two-story Townhouse on Twin Shake Tables



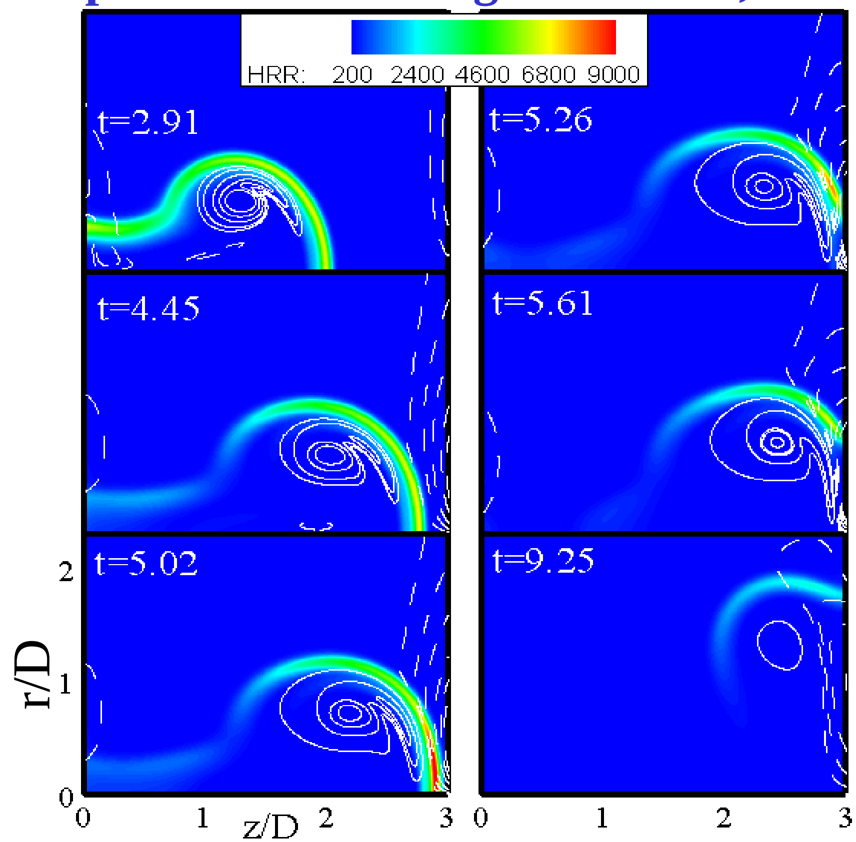


2-D Geotechnical Laminar Box Tests of Pile Foundations Subjected to Soil Liquefaction

M. Bruneau, A. Reinhorn, G. Lee

Understanding Combustion

- Flame-wall interaction modeling for a non-premixed flame propelled by a vortex ring.
- In this figure different time instants are shown during the interaction. White line contours and color contours represent vortex ring and flame, respectively.
- Key Features:
  - Modeling of Detailed GRI3. Mechanism for Methane Combustion
  - Parallel algorithm using mpi
  - 85-90% Parallel efficiency for up to 64 processors
- FWI study is important to determine
  - Engine Design
  - Quenching Distances
  - Flame Structure
  - Unburned hydrocarbon
  - Maximum Wall heat fluxes

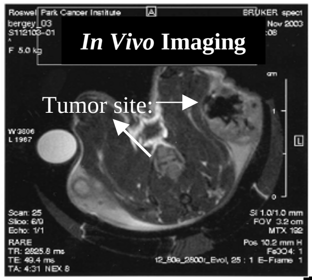


C. Madnia

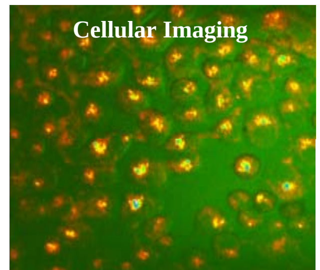
Institute for Lasers, Photonics, and Biophotonics

Nanomedicine Program

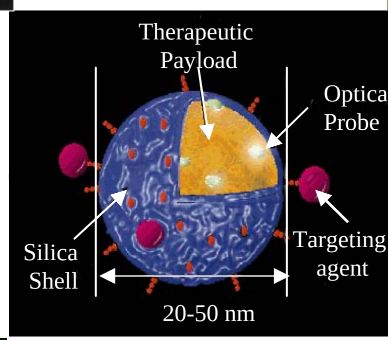
World class Research Program Melding Nanotechnology with Biomedical Sciences



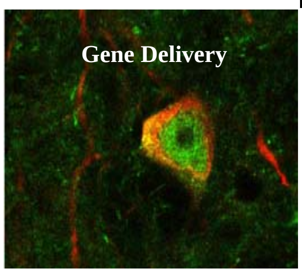
Multi-Modal Imaging



BioCompatibility/ Distribution



***In Vivo* Sensing**



Targeted Therapy

Building from the Bottom Up

State of the Art Molecular Imaging and Nanocharacterization Facilities

- Multiphoton Laser Scanning System
- Confocal Imaging including FRET, FLIM & FRAP analysis
- Coherent Anti-Stokes Raman Imaging
- Optical Trapping/Dissection
- Advanced Laser Systems

P. Prasad *www.biophotonics.buffalo.edu*

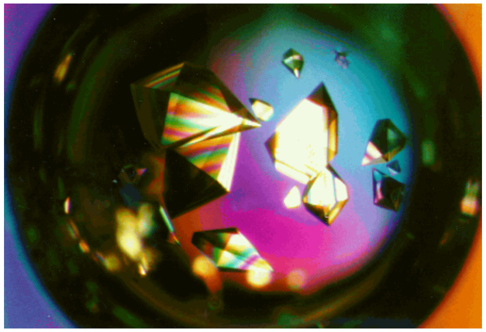
"Leading the Way to Technology through Innovation"

Shake-and-Bake

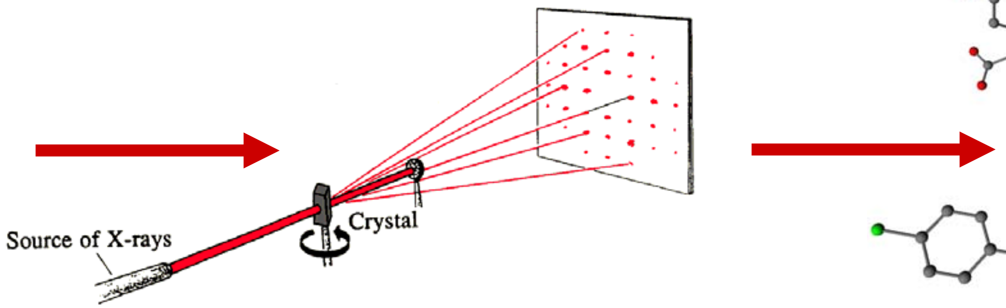
Molecular Structure Determination from X-Ray Crystallographic Data

Molecular Structure Determination via *Shake-and-Bake*

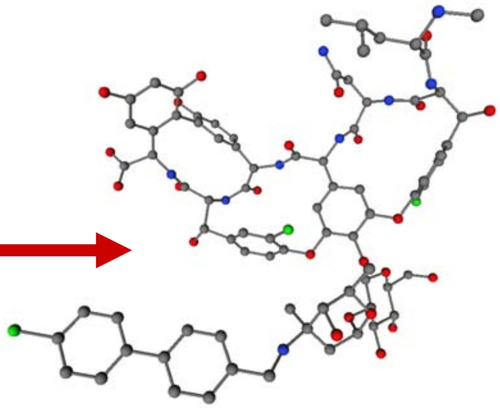
- ***SnB* Software by UB/HWI**
  - **"Top Algorithms of the Century"**
- **Worldwide Utilization**
- **Critical Step**
  - **Rational Drug Design**
  - **Structural Biology**
  - **Systems Biology**
- **Vancomycin**
  - **"Antibiotic of Last Resort"**
- **Current Efforts**
  - **Grid**
  - **Collaboratory**
  - **Intelligent Learning**



1. Isolate a single crystal



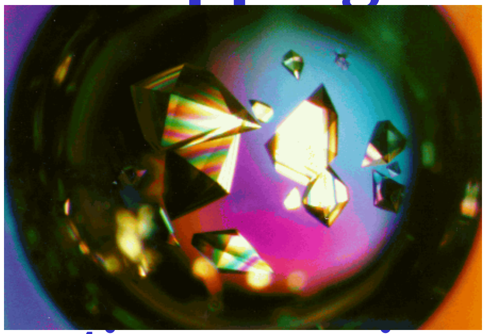
2. Perform the X-Ray diffraction experiment



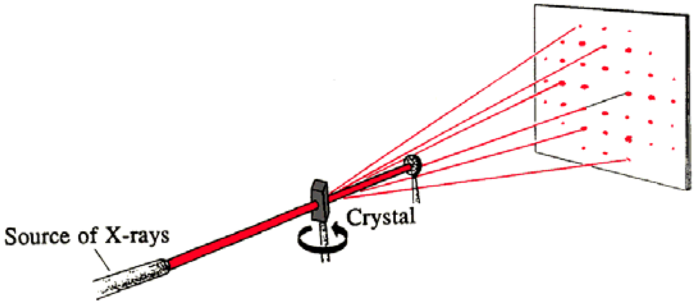
3. Determine the crystal structure

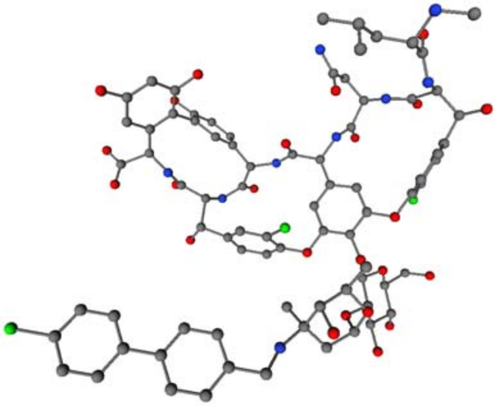
X-Ray Crystallography

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



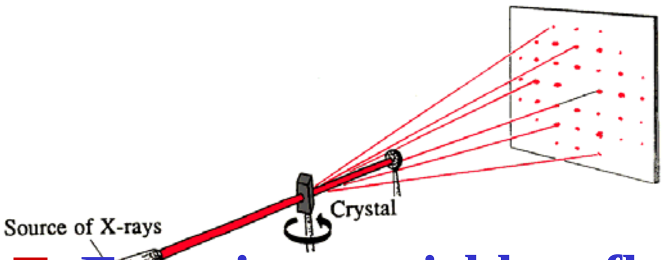
1. **Isolate a single crystal.**
2. **Perform the X-Ray diffraction experiment.**



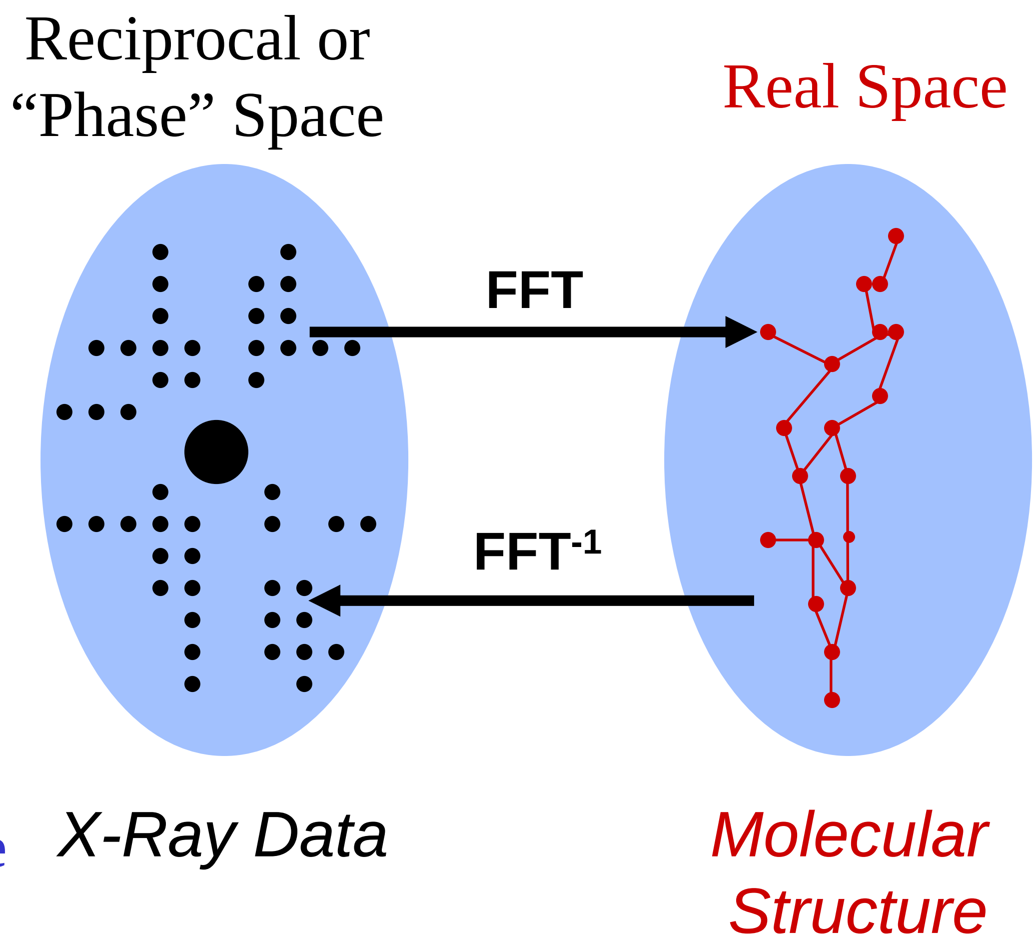


3. **Determine molecular structure that agrees with diffration data.**

X-Ray Data & Corresponding Molecular Structure



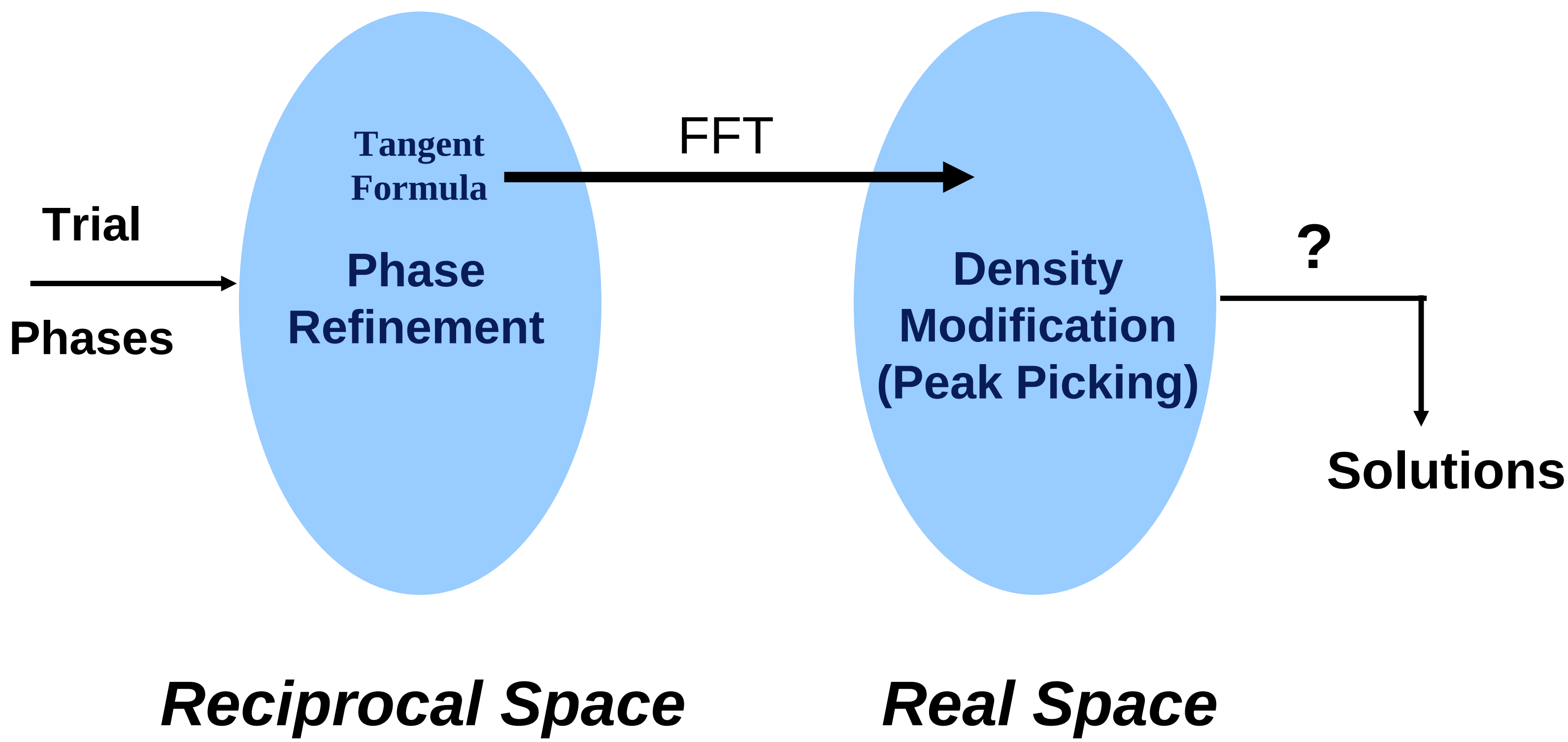
- **Experiment yields reflections and associated intensities.**
- **Underlying atomic arrangement is related to the reflections by a 3-D Fourier transform.**
- ***Phase angles are lost in experiment.***
- ***Phase Problem*: Determine the set of phases corresponding to the reflections.**



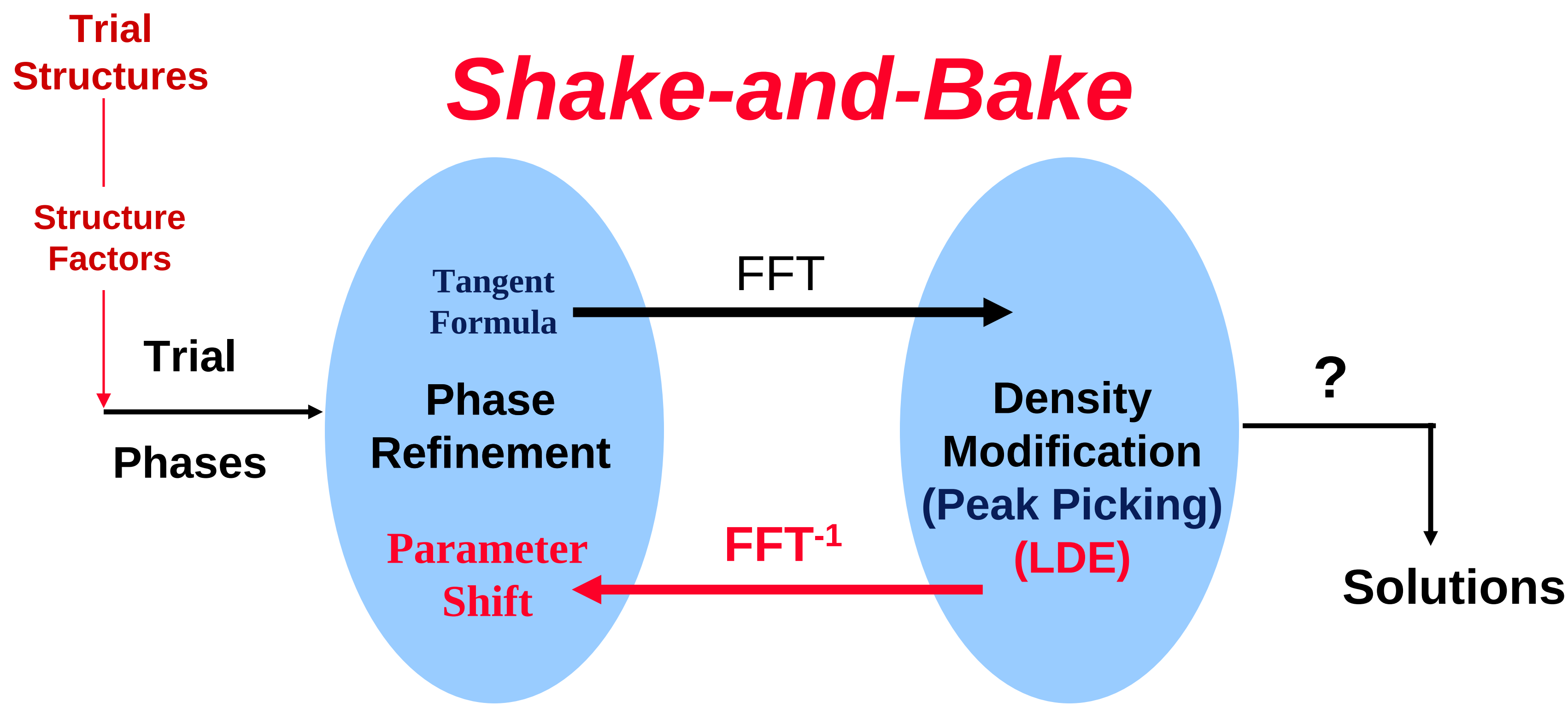
The Phase Problem

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

Conventional Direct Methods



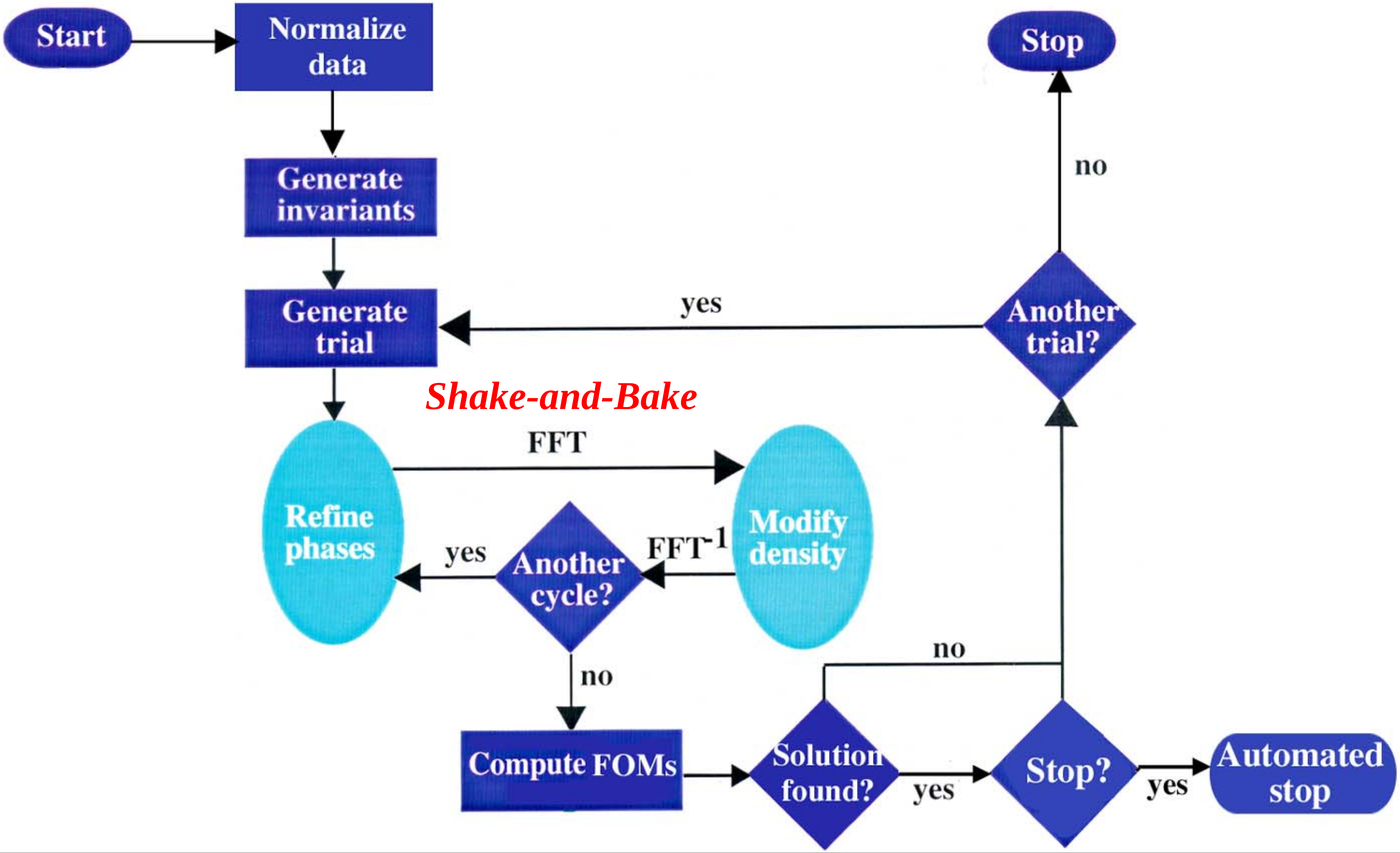
Shake-and-Bake Method: Dual-Space Refinement



Reciprocal Space **"Shake"**

Real Space **"Bake"**

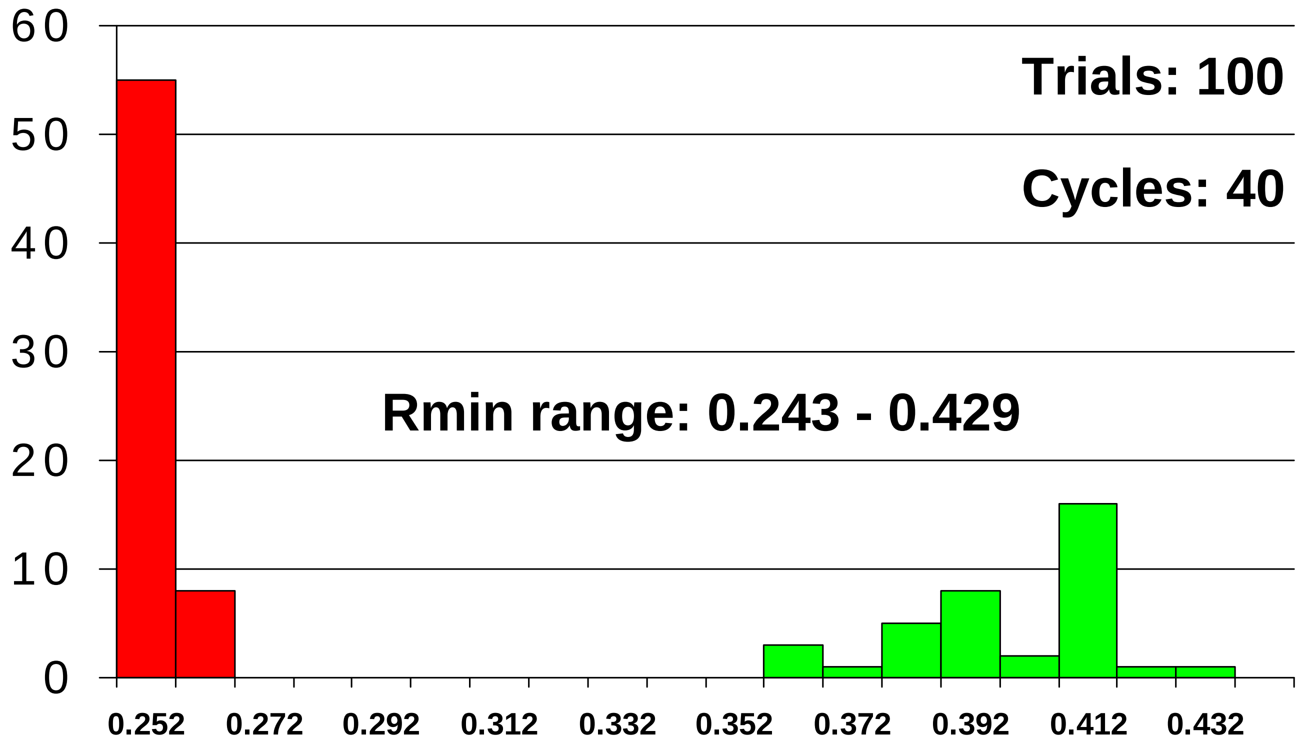
A Direct Methods Flowchart



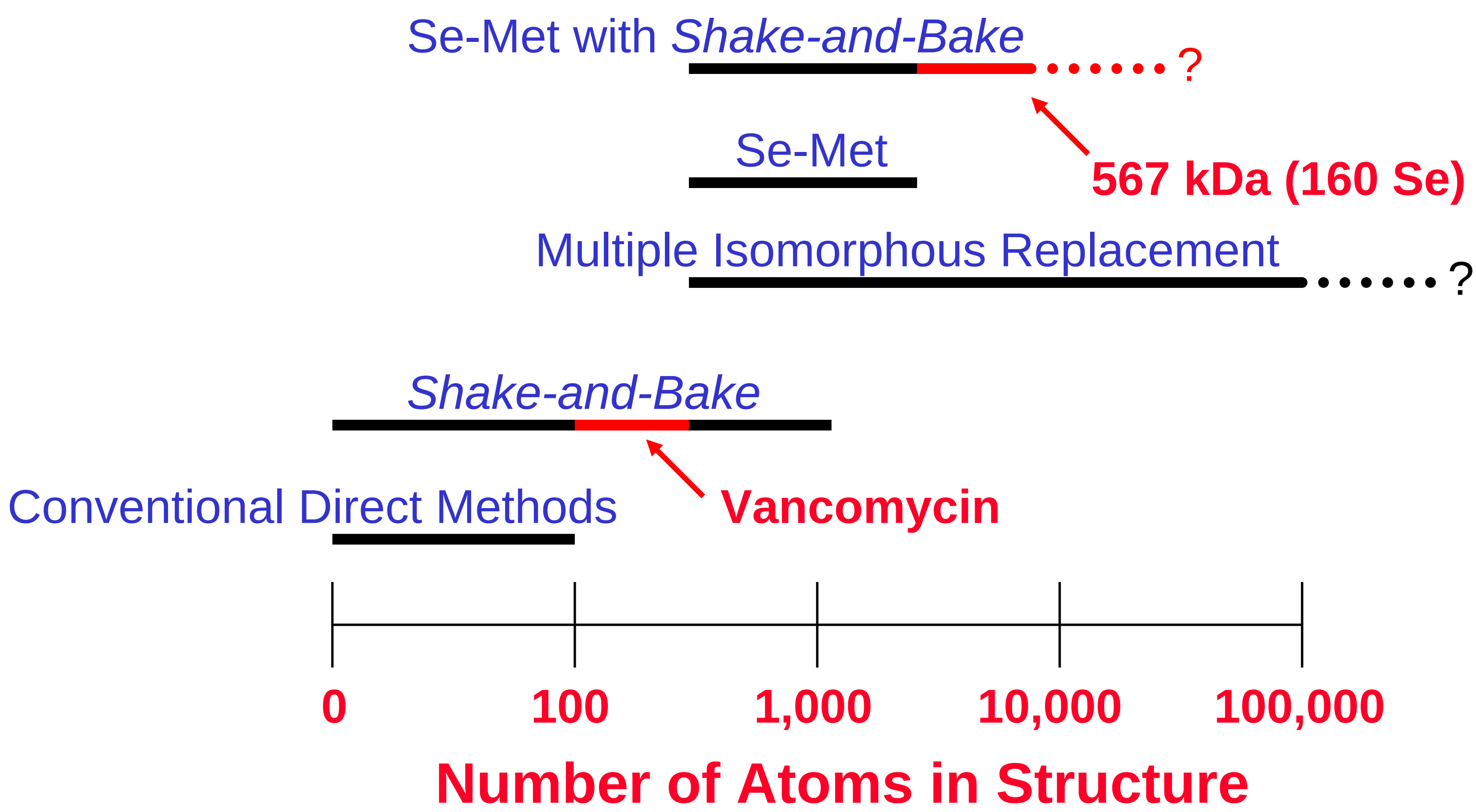
Ph8755: *SnB* Histogram

Atoms: 74
Space Group: P1

Phases: 740
Triples: 7,400

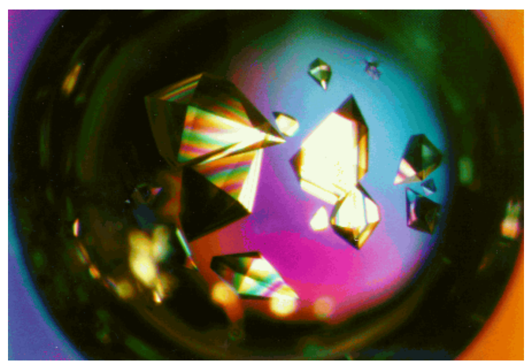


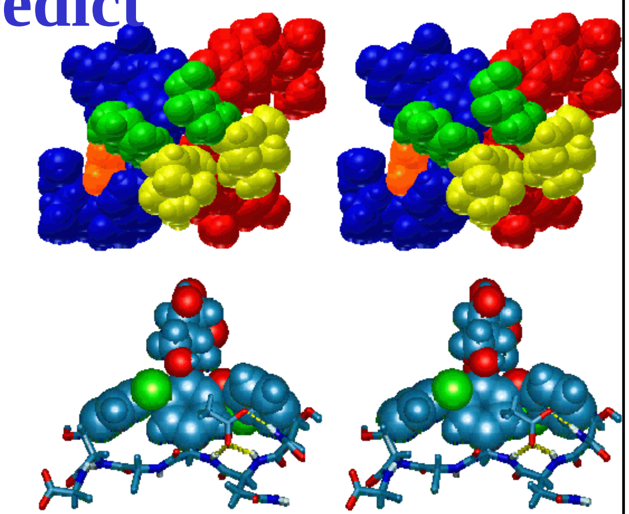
Phasing and Structure Size



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





Miller's Cyberinfrastructure Laboratory (MCIL)

MCIL Overview

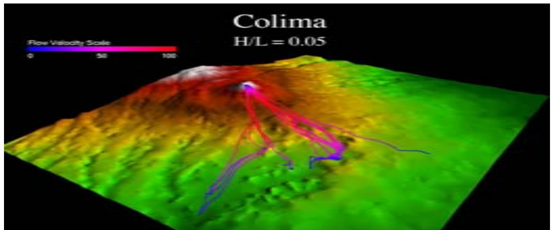
- **Working Philosophy**
  - **CI sits at core of modern simulation & modeling**
  - **CI allows for new methods of investigation to address previously unsolvable problems**
- **Focus of MCIL is on development of *algorithms*, *portals*, *interfaces*, *middleware***
- **Goal of MCIL is to free end-users to do disciplinary work**
- **Funding (2001-pres)**
  - **NSF: ITR, CRI, MRI**
  - **NYS appropriations**
  - **Federal appropriations**

MCIL Equipment (50+ TF)

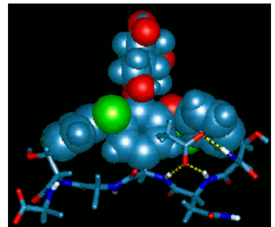
- Experimental Equipment (57.5 TF; 22TB; 156 Traditional Cores; 15 nVidia Tesla GPGPUs)
  - Clusters
    - Head Nodes: Dell 1950 (Intel)
    - Workers: Intel 8×2 ×4, Intel 8×1 ×2, & AMD 8×2×2
    - 13 nVidia S1070s & 2 nVidia S870s
  - Virtual Memory Machines (2 × Intel 4×4)
  - Dell GigE Managed Switches
  - InfiniBand
  - 22 TB Dell Storage (2)
  - Condor Flock (35 Intel/AMD)

- Production Equipment
  - Dell Workstations; Dell 15 TB Storage
  - Access to CCR equipment (13TF Dell/Intel clusters)

Grid Computing Tutorial



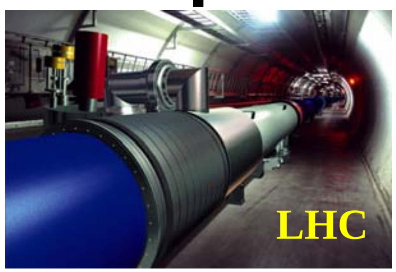
Data Acquisition

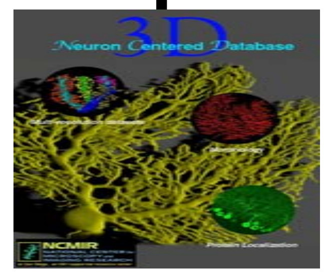


Advanced Visualization

Analysis

Imaging Instruments





Large-Scale Databases

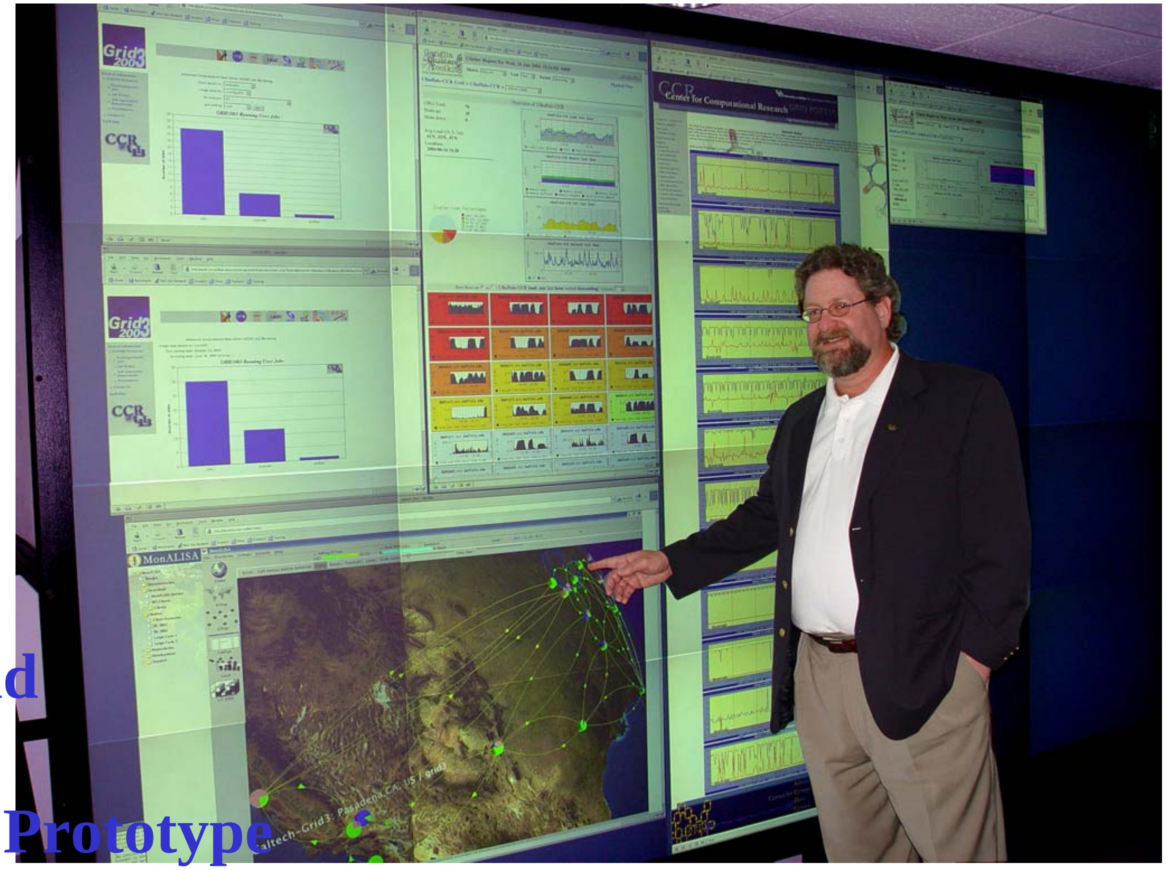
- Coordinate Computing Resources, People, Instruments in Dynamic Geographically-Distributed Multi-Institutional Environment
- Treat Computing Resources like Commodities
  - Compute cycles, data storage, instruments
  - Human communication environments
- No Central Control; No Trust
- Examples: TeraGrid,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

Evolution of MCIL Lab Projects

- **Buffalo-Based Grid**
  - **Experimental Grid: Globus & Condor**
  - **Integrate Data & Compute, Monitor, Portal, Node Swapping, Predictive Scheduling/Resource Management**
  - **GRASE VO: Structural Biology, Groundwater Modeling, Earthquake Eng, Comp Chemistry, GIS/BioHazards**
  - **Buffalo, Buffalo State, Canisius, Hauptman-Woodward**
- **Western New York Grid**
  - **Heterogeneous System: Hardware, Networking, Utilization**
  - **Buffalo, Geneseo, Hauptman-Woodward, Niagara**
- **New York State Grid**
  - **Extension to Hardened Production-Level System State-Wide**
  - **Albany, Binghamton, Buffalo, Geneseo, Canisius, Columbia, HWI, Niagara, [Cornell, NYU, RIT, Rochester, Syracuse, Marist], {Stony Brook, RPI, Iona}**

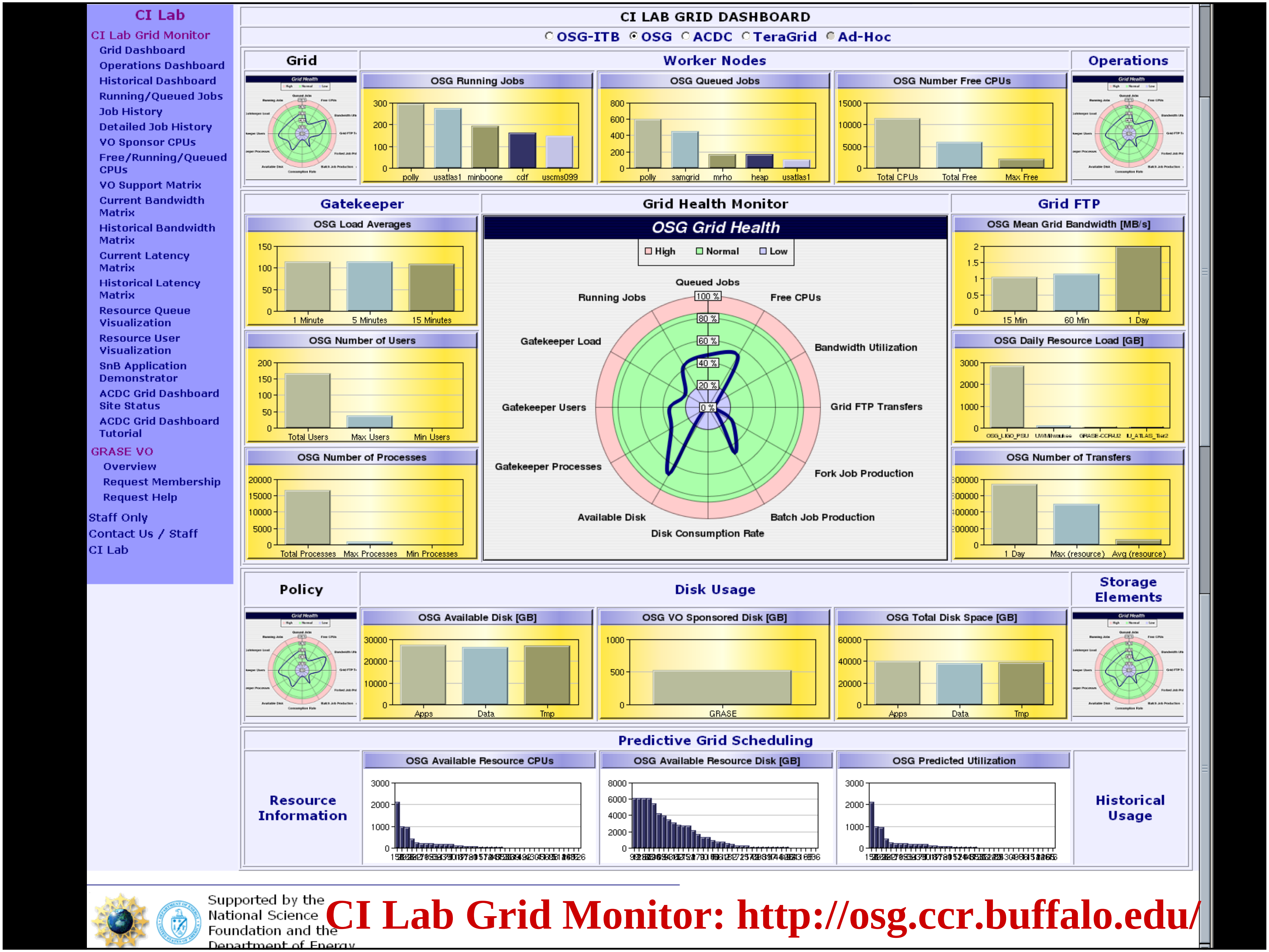
MCIL Lab Collaborations

- High-Performance Networking Infrastructure
- Grid3+ Collaboration
- iVDGL Member
  - Only External Member
- Open Science Grid
  - GRASE VO
- NYS CI Initiative
  - Executive Director
  - Various WGs
- Grid-Lite: Campus Grid
  - HP Labs Collaboration
- Innovative Laboratory Prototype
  - Dell Collaboration

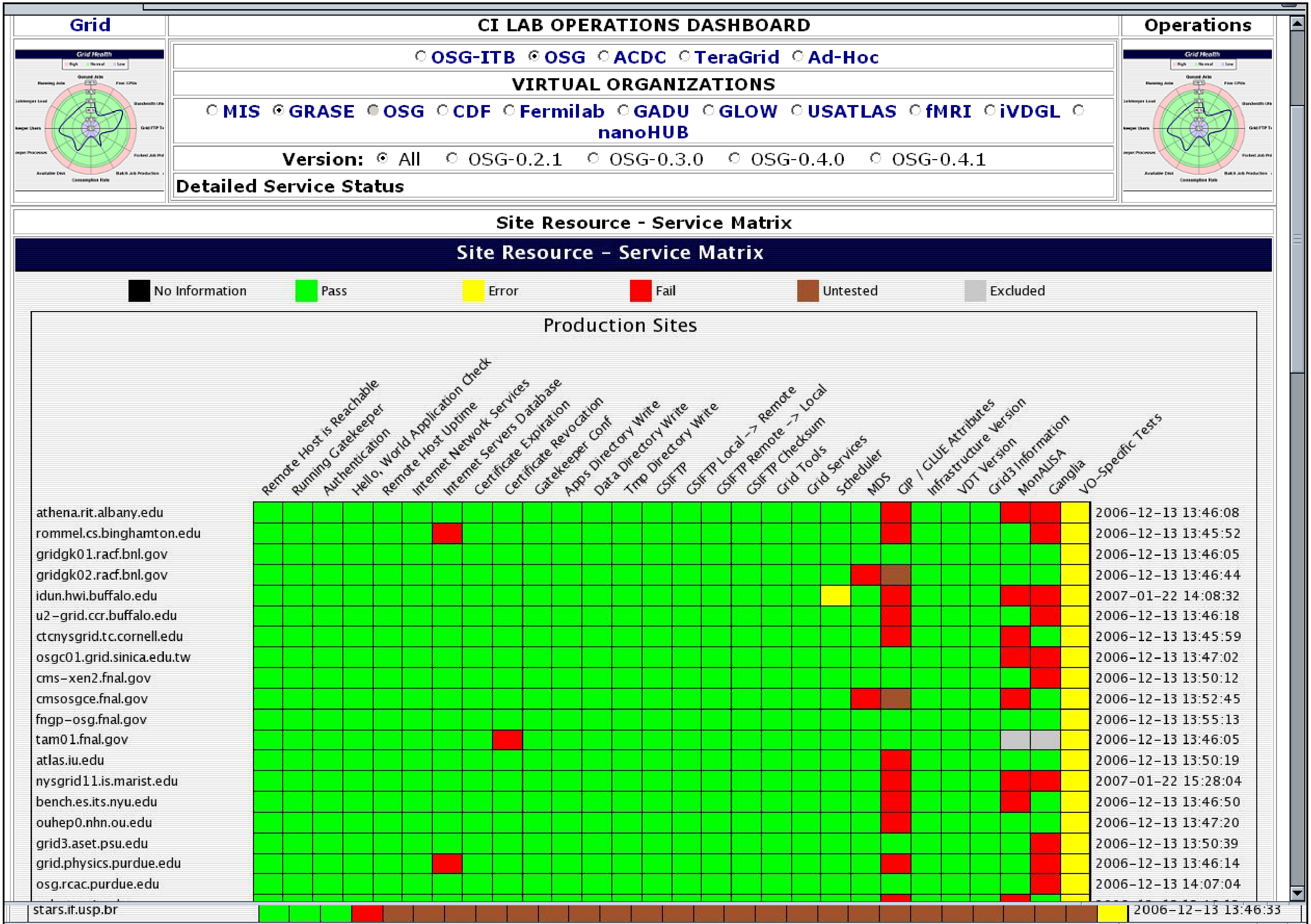


MCIL Lab Projects

- 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



CI Lab Grid Monitor: http://osg.ccr.buffalo.edu/



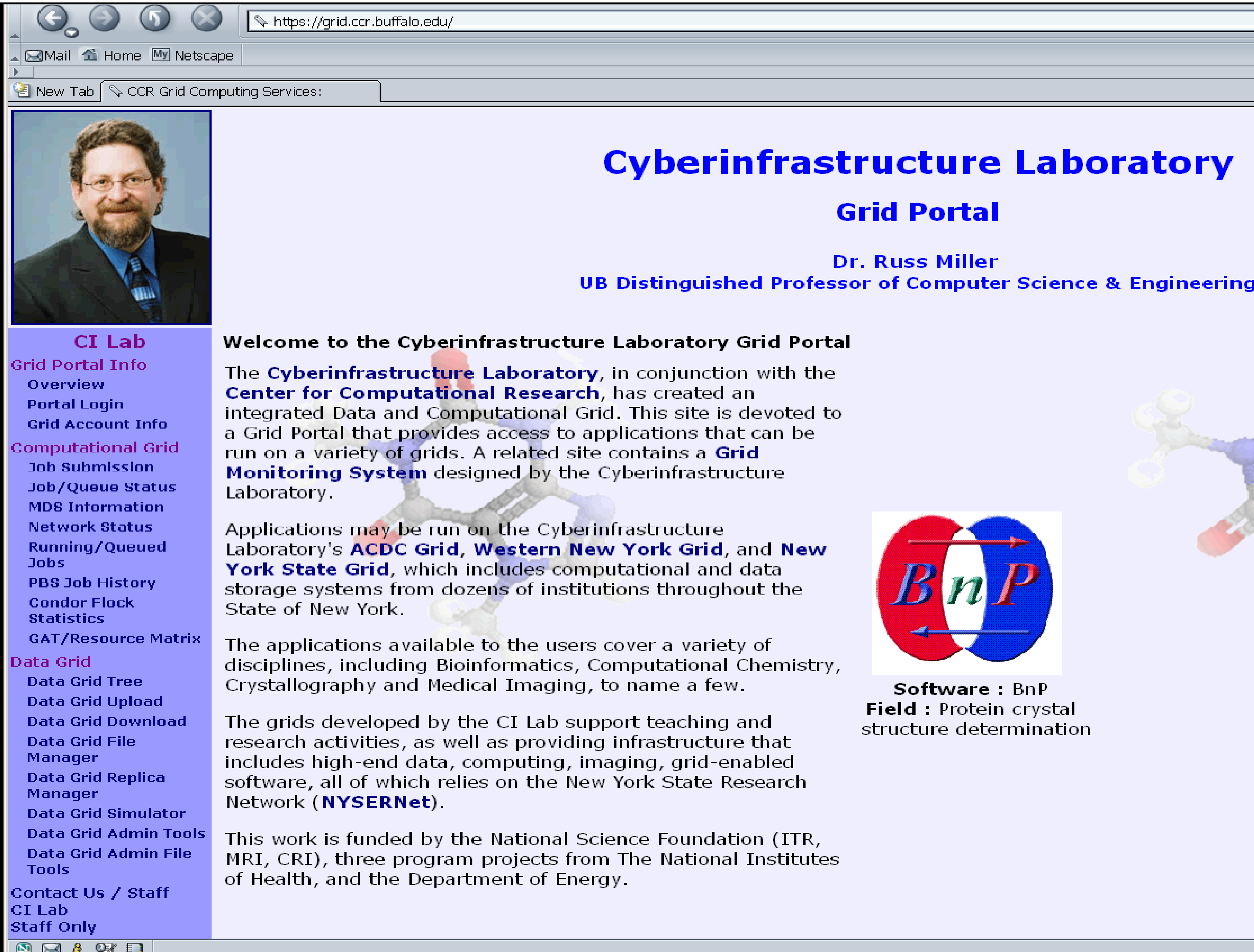
CI Lab Operations Dashboard

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



Startup Screen for CI Lab 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 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.

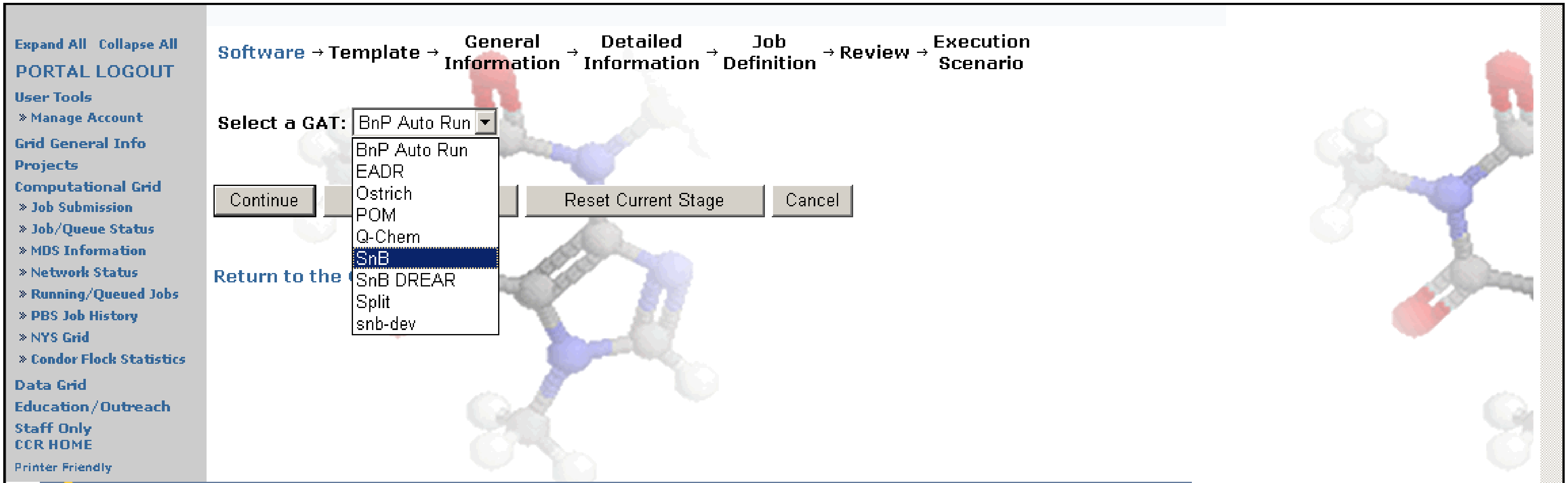
The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are require for execution in the ACDC-Grid environment. We have identified that sequentially defining milestones for the grid user to complete intuitively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

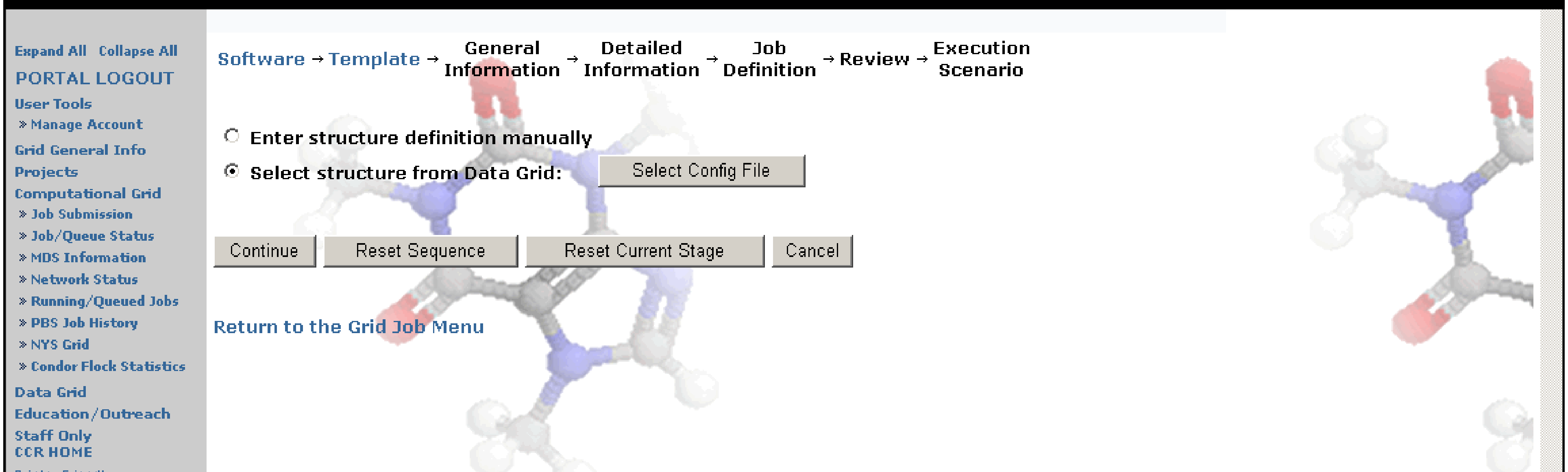
Each item of the job definition workflow is then stored in the ACDC-Grid Web Portal database so the grid user may use/modify any previously created workflow in creating new job definitions. The job definitions can also be accessed via batch script files for executing hundreds of similar workflows in 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.

Continue | Reset Sequence | Reset Current Stage | Cancel

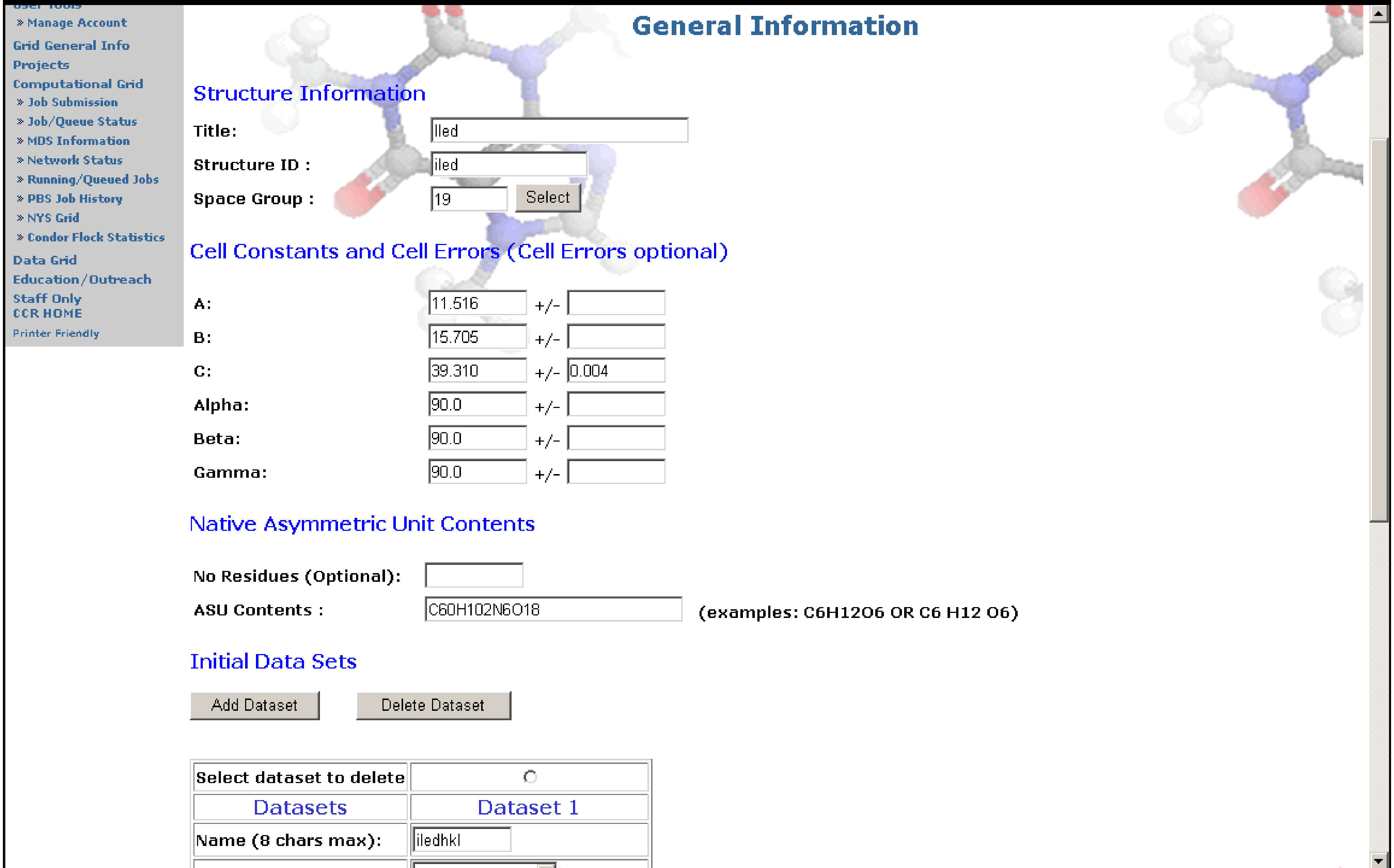
Instructions and Description for Running a Job on ACDC-Grid



Software Package Selection



Full Structure / Substructure Template Selection

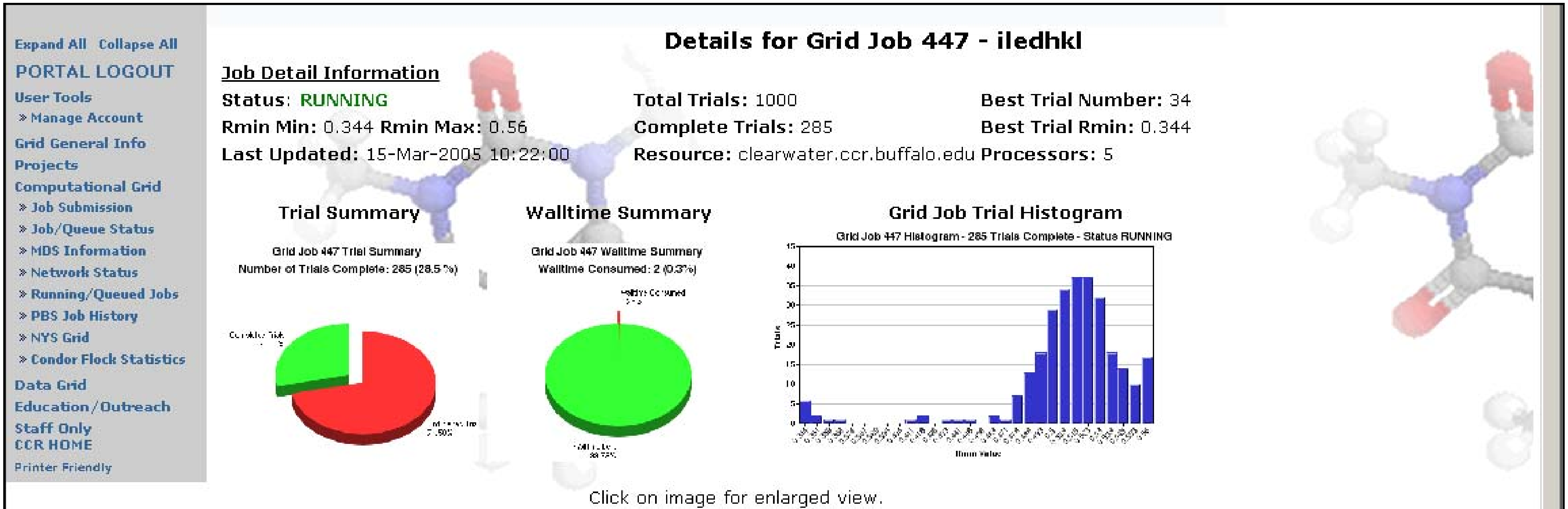


Default Parameters Based on Template

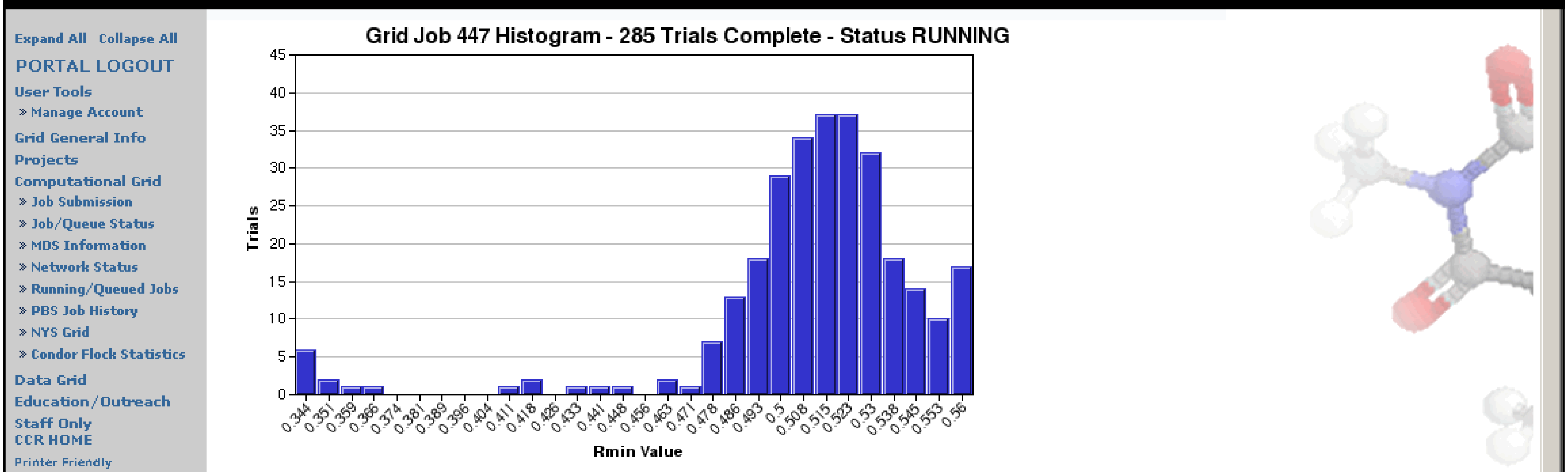
SnB Job Review

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

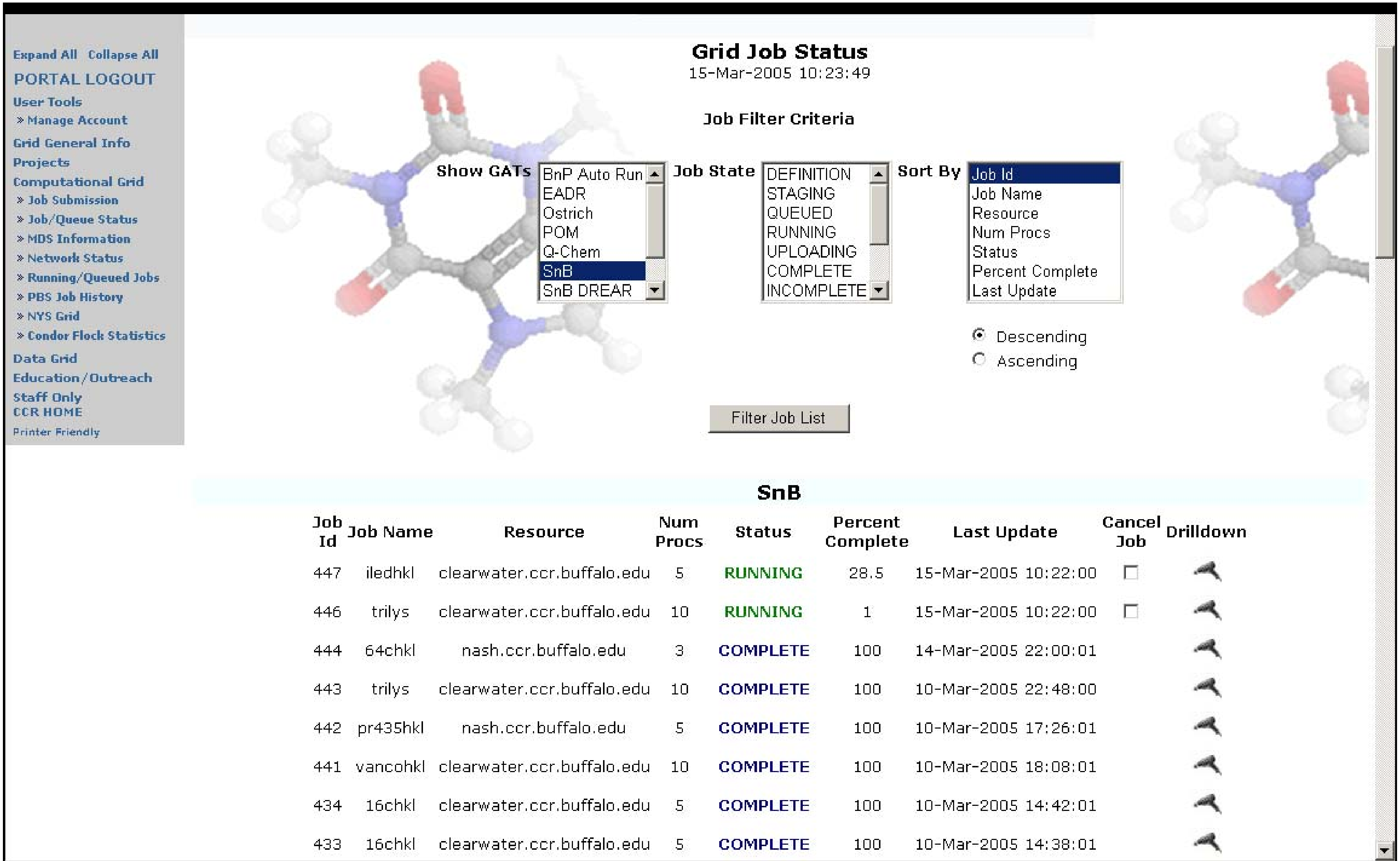
SnB Review (Grid job ID: 447)



Graphical Representation of Intermediate Job Status



Histogram of Completed Trial Structures



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

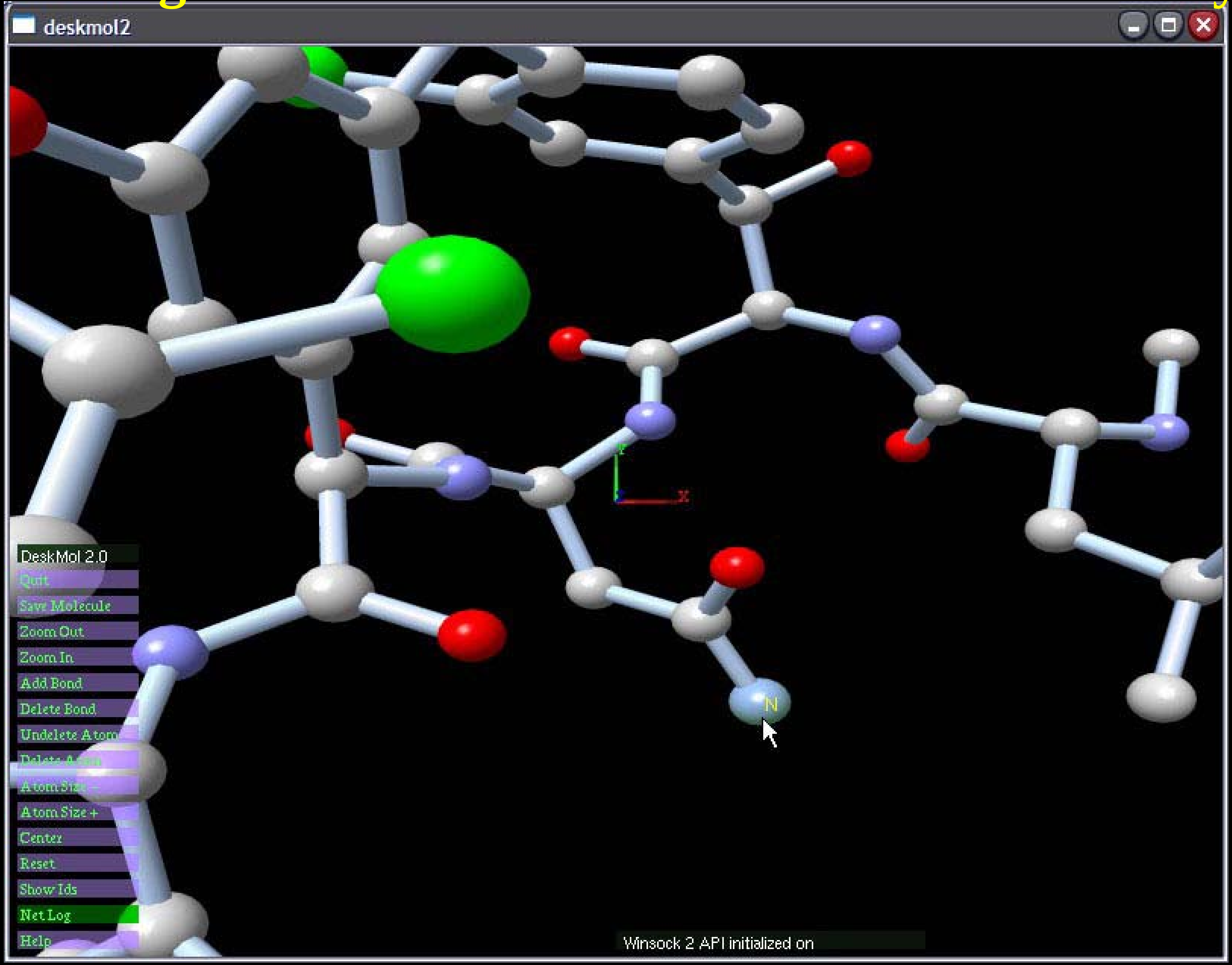
Filter Job List

SnB

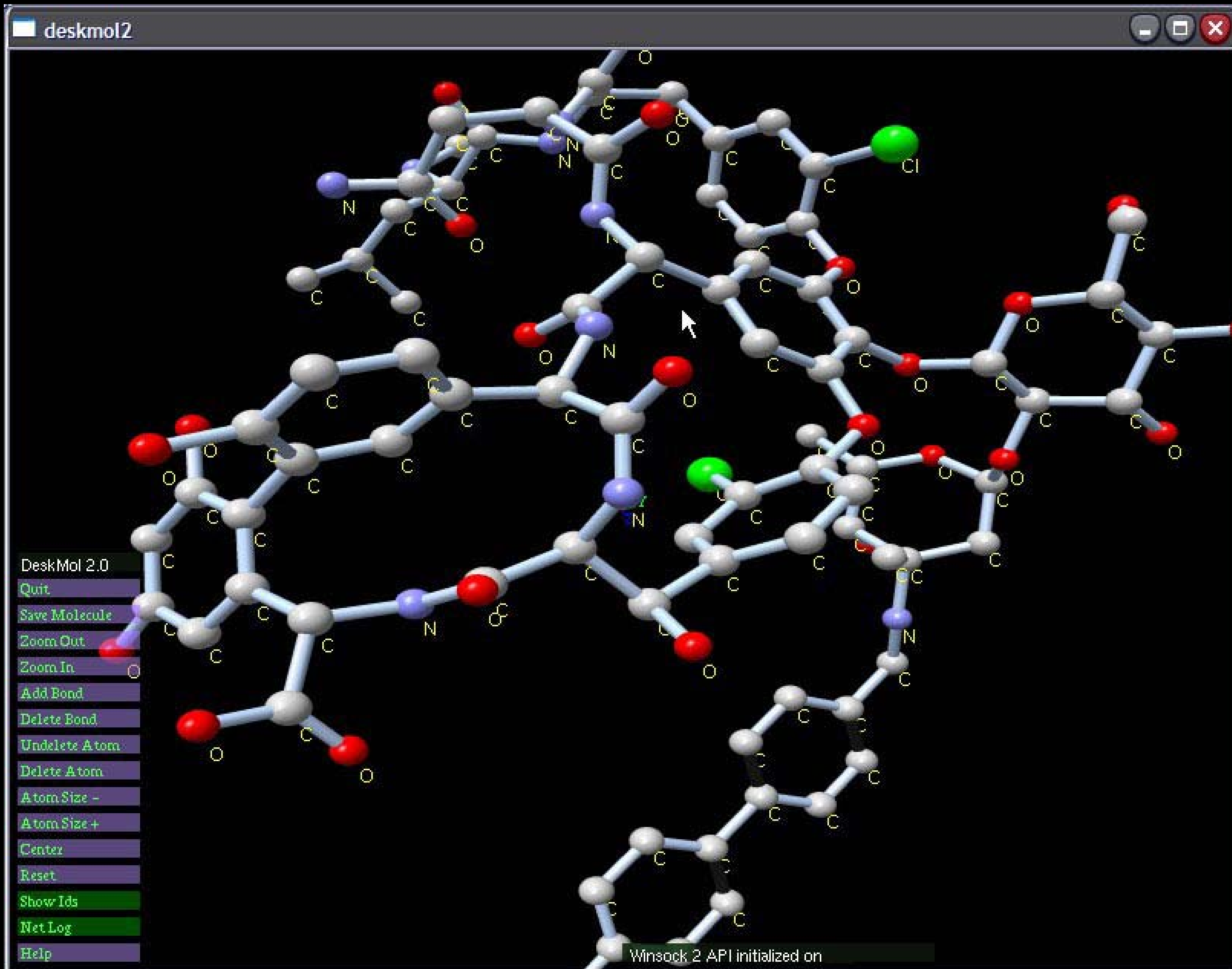
Job Id	Job Name	Resource	Num Procs	Status	Percent Complete	Last Update	Cancel Job	Drilldown
447	iledhkl	clearwater.ccr.buffalo.edu	5	RUNNING	28.5	15-Mar-2005 10:22:00	☐	
446	trilys	clearwater.ccr.buffalo.edu	10	RUNNING	1	15-Mar-2005 10:22:00	☐	
444	64chkl	nash.ccr.buffalo.edu	3	COMPLETE	100	14-Mar-2005 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

Heterogeneous Back-End Interactive Collaboratory



User starts up – default image of structure.



Molecule scaled, rotated, and labeled.

Acknowledgments

- Mark Green
- Cathy Ruby
- Amin Ghadersohi
- Naimesh Shah
- Steve Gallo
- Jason Rappleye
- Jon Bednasz
- Sam Guercio
- Martins Innus
- Cynthia Cornelius

- George DeTitta
- Herb Hauptman
- Charles Weeks
- Steve Potter

- Alan Rabideau
- Igor Janckovic
- Michael Sheridan
- Abani Patra
- Matt Jones

- NSF ITR
- NSF CRI
- NSF MRI
- NYS
- CCR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