Miller’s Cyberinfrastructure Laboratory (MCIL)

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NSF, NIH, DOE, NIMA, NYS, HP
www.cse.buffalo.edu/faculty/miller/CI/
Cyberinfrastructure

- Foster & Kesselman: “a domain-independent computational infrastructure designed to support science.”
- NSF: “comprehensive phenomenon that involves creation, dissemination, preservation, and application of knowledge”
- Generic: transparent and ubiquitous application of technologies central to contemporary engineering and science
- NSF Cyberinfrastructure (OCI)
  - HPC Hardware and Software
  - Data Collections
  - Science Gateways/Virtual Organizations
  - Support of Next Generation Observing Systems
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.”
Grid Computing Overview

- 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

Imaging Instruments

Data Acquisition Advanced Visualization Analysis

LHC Computational Resources

Large-Scale Databases
Cyberinfrastructure Laboratory
Ubiquitous High-End Computing, Data, Networking, & Visualization

Dr. Russ Miller
UB Distinguished Professor

Introduction

In the 21st century, leading academic institutions will embrace our digital data-driven society and empower students to compete in this knowledge-based economy. In order to support research, scholarship, education, and community outreach, the Cyberinfrastructure Laboratory (CI Lab) is dedicated to the integration of research in disciplinary domains, including science, engineering, and biomedicine, with research in enabling technologies and interfaces. The goal is to allow students and scientists to transparently collect, manage, organize, analyze, and visualize data without having to worry about details such as where the data is stored, where the data is processed, where the data is rendered, and so forth. This ease of use and high availability of data and information processing tools will allow for revolutionary advances in all areas of science, engineering, and beyond.

Cyberinfrastructure sits at the core of modern simulation and modelling, which allows for entirely new methods of investigation that allow scholars to address previously unsolvable problems. Specifically, the development of necessary software, algorithms, portals, and interfaces that will enable research and scholarship by freeing end-users from dealing with the complexity of various computing environments is critical to extending the reach of high-end computing, storage, networking, and visualization to the general user community.

Projects in the CI Lab are currently supported by an NSF ITR award, an NSF CRI award, and the Center for Computational...
Miller’s Cyberinfrastructure Lab

- **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

- Experimental Equipment (1.25 TF; 140 Cores; 22TB)
  - Clusters
    - Head Nodes: Dell 1950 (Intel)
    - Workers: Intel 8×2 ×4 & AMD 8×2×2
  - Virtual Memory Machines (2 × Intel 4×4)
  - Dell GigE Managed Switches
  - InfiniBand
  - 22 TB Dell Storage (2)
  - Condor Flock (35 Intel/AMD)
  - In process: 40-50TF system

- Production Equipment
  - Dell Workstations; Dell 15 TB Storage
  - Access to CCR equipment (13TF Dell/Intel clusters)
Evolution of CI 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}
NYS Grid Resources

- Albany: 8 Dual-Processor Xeon Nodes
- Binghamton: 15 Dual-Processor Xeon Nodes
- Buffalo: 1050 Dual-Processor Xeon Nodes
- Cornell: 30 Dual-Processor Xeon Nodes
- Geneseo State: Sun/AMD with 128 Compute Cores
- Hauptman-Woodward Institute: 50 Dual-Core G5 Nodes
- Marist: 9 P4 Nodes
- Niagara University: 64 Dual-Processor Xeon Nodes
- NYU: 58 Dual-Processor PowerPC Nodes
- RIT: 4 Dual-Processor Xeon Nodes
- Syracuse: 8 Dual-Processor Xeon Nodes
CI 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
CI 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
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

SQL Database

Resource 1

Resource 2

Resource n

Predictive Scheduler

User 1

User 2

... User m

Maintain Profiles and Predict
• running time
• backfill on resources
• grid load and utilization
### ACDC-Grid Dynamic Resource Allocation

**Dell 2650 backup front-end**

**Dell 6650 4-way front-end**

**Node scratch space (120 GB)**

**4 node Dell 2650 PVFS server (1096 GB)**

**1 node Dell 2650 NFS server (342 GB)**

**292 – Dell 2650 production nodes**

**Dell 6650 4-way (ACDC)**

**Dell 6650 4-way (GRID)**

**Dell 6650 4-way (EAGLES)**

<table>
<thead>
<tr>
<th>Node scratch space (120 GB)</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Dell 2650 backup front-end</th>
</tr>
</thead>
</table>

| Dell 6650 4-way (ACDC)       |

| Dell 6650 4-way (GRID)       |

| Dell 6650 4-way (EAGLES)     |

**Diagram**

- GigE and Myrinet connection
- GigE connection
- 73 GB hard drive

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**University at Buffalo**

**The State University of New York**

**Cyberinfrastructure Laboratory**

**CI Lab**
Grid Administration

Grid Site Administration

Generate Globus Grid-mapfile

Optional Include Dir:

Optional Grid-mapfile path:

Create New Database Job

Current Time: 16-Sep-2003 10:58:12

MDS Resource Update Status

Resource | Last Updated | Next Update Status
---------|--------------|---------------------
Cory@ccr.buffalo.edu | 16-Sep-2003 10:45:15 | 2 minutes | OK
fogerty.ccr.buffalo.edu | 16-Sep-2003 10:45:16 | 2 minutes | OK
jsep.ccr.buffalo.edu | 16-Sep-2003 10:45:15 | 2 minutes | OK
mama.ccr.buffalo.edu | 16-Sep-2003 10:45:15 | 2 minutes | OK
rash.ccr.buffalo.edu | 16-Sep-2003 10:45:15 | 2 minutes | OK
renus.has.buffalo.edu | 16-Sep-2003 10:45:15 | 2 minutes | OK
yardbirds.ccr.buffalo.edu | 16-Sep-2003 10:45:19 | 2 minutes | OK
young.ccr.buffalo.edu | 16-Sep-2003 10:45:27 | 2 minutes | OK

Return to the Grid Resource Admin menu.
Return to the Grid Admin menu.
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

Browser view of “miller” group files published by user “rappleye”
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-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
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 diffraction data.
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.

X-Ray Data & Corresponding Molecular Structure
Shake-and-Bake Method: Dual-Space Refinement

Trial Structures → Structure Factors → Trial Phases

Phase Refinement

Tangent Formula

Parameter Shift

FFT → FFT⁻¹

Density Modification (Peak Picking) (LDE)

Solutions

Reciprocal Space “Shake”

Real Space “Bake”
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 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.
NYS Grid Portal
Welcome to the Cyberinfrastructure Laboratory Grid Portal

The Cyberinfrastructure Laboratory, in conjunction with the Center for Computational Research, has created an Integrated Data and Computational Grid. This site is devoted to a Grid Portal that provides access to applications that can be run on a variety of grids. A related site contains a Grid Monitoring System designed by the Cyberinfrastructure Laboratory.

Applications may be run on the Cyberinfrastructure Laboratory's ACDC Grid, Western New York Grid, and New York State Grid, which includes computational and data storage systems from dozens of institutions throughout the State of New York.

The applications available to the users cover a variety of disciplines, including Bioinformatics, Computational Chemistry, Crystallography and Medical Imaging, to name a few.

The grids developed by the CI Lab support teaching and research activities, as well as providing infrastructure that includes high-end data, computing, imaging, grid-enabled software, all of which relies on the New York State Research Network (NYSERNET).

This work is funded by the National Science Foundation (ITR, MRI, CRI), three program projects from The National Institutes of Health, and the Department of Energy.
Instructions and Description for Running a Job on ACDC-Grid

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 such as name, organization, address, etc., and more specific information such as group id and access level information for each of grid-enabled applications. This information is stored in a database for each of the grid-enabled applications and can be accessed through selected queries throughout the ACDC-Grid Web Portal.

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

The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are required 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 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.
Software Package Selection

Full Structure / Substructure Template Selection
General Information

Structure Information

Title: Iled
Structure ID: Iled
Space Group: 19

Cell Constants and Cell Errors (Cell Errors optional)

A: 11.516 +/- 
B: 15.705 +/- 
C: 19.310 +/- 0.004
Alpha: 90.0 +/- 
Beta: 90.0 +/- 
Gamma: 90.0 +/- 

Native Asymmetric Unit Contents

No Residues (Optional): 
ASU Contents: C60H12O6 (examples: C6H12O6 OR C6 H12 O6)

Initial Data Sets

Default Parameters Based on Template
Initial Data Sets

Add Dataset  Delete Dataset

Select dataset to delete

Datasets
Name (8 chars max): Etdlkl
Dataset Type: Native
File Name (*.hkl): 
File Type: F, Sig(F)
Wavelength: 1.5418
Max. Resolution: 0.94
Anomalous Dispersion: Not Measured
Heavy Element Types:
Nat. Element Replaced: 
No. Expected Sites: 
F Prime (F): 
F Double Prime (F''): 

Continue  Reset Sequence  Reset Current Stage  Cancel

Default Parameters (cont’d)
### SnB Job Review (Grid job ID: 447)

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Grid Job ID</td>
<td>447</td>
</tr>
<tr>
<td>Selected resource</td>
<td>clearwater.ccr.buffalo.edu</td>
</tr>
<tr>
<td>Number of processors</td>
<td>5</td>
</tr>
<tr>
<td>Wallclock time requested</td>
<td>720</td>
</tr>
<tr>
<td>Number of triplet invariant to use</td>
<td>8400</td>
</tr>
<tr>
<td>Start Phases From</td>
<td>Random Atoms</td>
</tr>
<tr>
<td>Random seed (prime)</td>
<td>11909</td>
</tr>
<tr>
<td>Number of trials</td>
<td>1000</td>
</tr>
<tr>
<td>Starting Trial</td>
<td>1</td>
</tr>
<tr>
<td>Input Phase File</td>
<td>Unused</td>
</tr>
<tr>
<td>Input Atom File</td>
<td>Unused</td>
</tr>
<tr>
<td>Keep complete (every trial) peak file?</td>
<td>Yes</td>
</tr>
<tr>
<td>Number of Shake-and-bake cycles</td>
<td>20</td>
</tr>
<tr>
<td>Keep complete (every cycle) trace file?</td>
<td>No</td>
</tr>
<tr>
<td>Terminate trials failing the R-Ratio test?</td>
<td>No</td>
</tr>
<tr>
<td>R-Ratio cutoff</td>
<td>Unused</td>
</tr>
<tr>
<td>Phase Refinement Method</td>
<td>Parameter Shift(Fast)</td>
</tr>
<tr>
<td>Number of passes through phase set</td>
<td>3</td>
</tr>
<tr>
<td>Phase shift</td>
<td>90.0</td>
</tr>
<tr>
<td>Number of shifts</td>
<td>2</td>
</tr>
<tr>
<td>Number of peaks to select</td>
<td>04</td>
</tr>
<tr>
<td>Minimum interpeak distance</td>
<td>3</td>
</tr>
<tr>
<td>Minimum distance between symmetry-related peaks</td>
<td>3.0</td>
</tr>
<tr>
<td>Number of special position peaks to keep</td>
<td>0</td>
</tr>
<tr>
<td>Fourier grid size</td>
<td>0.31</td>
</tr>
<tr>
<td>Perform extra cycles with more peaks?</td>
<td>No</td>
</tr>
<tr>
<td>Number of extra cycles</td>
<td>Unused</td>
</tr>
<tr>
<td>Number of peaks</td>
<td>Unused</td>
</tr>
<tr>
<td>Trials for E-Fourier filtering (fourier refinement)?</td>
<td>None</td>
</tr>
<tr>
<td>Number of cycles</td>
<td>Unused</td>
</tr>
<tr>
<td>Number of peaks</td>
<td>Unused</td>
</tr>
<tr>
<td>Minimum</td>
<td>E</td>
</tr>
</tbody>
</table>
Graphical Representation of Intermediate Job Status

Histogram of Completed Trial Structures
Grid Job Status

Job Filter Criteria

Job State
- DEFINITION
- STAGING
- QUEUED
- RUNNING
- UPLOADING
- COMPLETE
- INCOMPLETE

Sort By

Job Id
- Job Name
- Resource
- Num Proc
- Status
- Percent Complete
- Last Update

Filter Job List

SnB

<table>
<thead>
<tr>
<th>Job Id</th>
<th>Job Name</th>
<th>Resource</th>
<th>Num Proc</th>
<th>Status</th>
<th>Percent Complete</th>
<th>Last Update</th>
<th>Cancel Job</th>
<th>Drilldown</th>
</tr>
</thead>
<tbody>
<tr>
<td>447</td>
<td>ilodhlk</td>
<td>clearwater.ccr.buffalo.edu</td>
<td>5</td>
<td>RUNNING</td>
<td>28.5</td>
<td>15-Mar-2005 10:22:00</td>
<td></td>
<td></td>
</tr>
<tr>
<td>446</td>
<td>triyys</td>
<td>clearwater.ccr.buffalo.edu</td>
<td>10</td>
<td>RUNNING</td>
<td>1</td>
<td>15-Mar-2005 10:22:00</td>
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</tr>
<tr>
<td>444</td>
<td>64chkl</td>
<td>nash.ccr.buffalo.edu</td>
<td>3</td>
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<td>100</td>
<td>14-Mar-2005 22:00:01</td>
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<td></td>
</tr>
<tr>
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<td>10-Mar-2005 22:48:00</td>
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<td></td>
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<tr>
<td>442</td>
<td>pr433hkl</td>
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<td>5</td>
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</tr>
<tr>
<td>441</td>
<td>vanochkl</td>
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<td>10</td>
<td>COMPLETE</td>
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<td>10-Mar-2005 18:00:01</td>
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<td></td>
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<tr>
<td>434</td>
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<td>clearwater.ccr.buffalo.edu</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>433</td>
<td>16chkl</td>
<td>clearwater.ccr.buffalo.edu</td>
<td>5</td>
<td>COMPLETE</td>
<td>100</td>
<td>10-Mar-2005 14:38:01</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Status of Jobs
Heterogeneous Back-End Interactive Collaboratory

User starts up – default image of structure.
Molecule scaled, rotated, and labeled.
New York State Grass Roots Cyberinfrastructure Initiative

- Miller’s NYS Grid used as fundamental infrastructure.
- Currently an initiative of NYSERNet.
- Open to academic and research institutions.
- Mission Statement: To create and advance collaborative technological infrastructure that supports and enhances the research and educational missions of institutions in NYS.
- Enable Research, Scholarship, and Economic Development in NYS.
- Currently, no significant utilization.
TRUN: Transborder Research University Network

- Ontario: York, Toronto, Western Ontario, McMaster, Queen’s, Waterloo, Guelph
- NYS: Buffalo, Rochester, Syracuse, Cornell, Albany, RIT

Mission Statement: Expand and support cooperation among research universities in the border region of Province of Ontario and NYS:
- Collaborative/consortial research
- Joint applications for external funding
- Cooperative academic programs
- Faculty and student exchanges
- Shared facilities
- Joint conferences, symposia, workshops

www.trun.ca
TRUN: Transborder Research University Network

- Current Focus
  - Great Lakes Sustainable Energy
  - IT-Supported Disciplinary Research
  - High Performance Computing
  - Canada-U.S. Policy and Standardization of Binational Data

- General Issues
  - Public Policy Issues, Regional Governance
  - Border Security and Mobility
  - Economic and Workforce Development
  - University Partnerships with Government and Industry
  - Health Care and Policy
  - Basic Research and Technology Transfer

www.trun.ca
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- NSF MRI
- NYS
- CCR