Molecular Structure Determination, Grid Computing, and the Center for Computational Research

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NSF, NIH, DOE
NIMA, NYS, HP
Center for Computational Research
1998-2006 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
Major Compute/Storage Resources
(22TF Peak; 600TB Storage)

- 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; 160 TB Disk; 16 TB SAN

- IBM BladeCenter Cluster (3TF peak)
  - 532 P4 Processors (2.8 GHz)
  - 5 TB SAN

- SGI Altix3700 (0.4TF peak)
  - 64 Processors (1.3GHz ITF2)
  - 256 GB RAM
  - 2.5 TB Disk

- CCR Biinformatics 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 circa 3/2006
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
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
Initial Photo Match incorporating real and computer-generated components
Peace Bridge Visualization:
Animation & Simulation

The Problem

- 75 year old bridge
- 3 lanes – poor capacity
- Existing US plaza: small and poor design

Proposed Options

- Relocate US plaza
- Build a 3-lane companion span & rehab existing bridge
- Build a six lane signature span
Song: I’m OK (I Promise)
Band: Chemical Romance
Gaming Environment: Death Jr.
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 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
Science & Engineering
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

Colima
H/L = 0.05

Flow Velocity Scale

0  50  100

High End Simulation and Visualization

Remote Real time visualization server

Web Servers

Web based visualization

UCB
University at Buffalo  The State University of New York  Center for Computational Research
Shake-and-Bake

Molecular Structure Determination from X-Ray Crystallographic Data
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.

Reciprocal or “Phase” Space

Real Space

X-Ray Data

Molecular Structure

FFT

FFT⁻¹
Conventional Direct Methods

Trial Phases → Phase Refinement

Tangent Formula → FFT → Density Modification (Peak Picking)

Reciprocal Space → Real Space

Solutions → ?
Shake-and-Bake Method: Dual-Space Refinement

**Reciprocal Space**

- **“Shake”**
  - Phase Refinement
  - Parameter Shift
  - Tangent Formula

**Real Space**

- **“Bake”**
  - Density Modification (Peak Picking) (LDE)
  - FFT
  - FFT⁻¹

Trial Structures

Structure Factors

Trial

Phases

Solutions

"Shake-and-Bake"
A Direct Methods Flowchart

Start

Normalize data

Generate invariants

Generate trial

Refine phases

Another cycle? yes

Another trial? yes

FFT

Modify density

Solution found? yes

Automated stop

Compute FOMs

FFT^-1

Stop? yes

Stop?
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 \( |E_H| \approx |F_H| \) normalized in resolution shells

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

Weights: \( W_{HK} = A_{HK} = 2N^{-1/2} |E_H E_K E_{-H-K}| \)
Phasing and Structure Size

- Se-Met with *Shake-and-Bake*
- Se-Met
- Multiple Isomorphous Replacement
- *Shake-and-Bake*

- Conventional Direct Methods
- Vancomycin

567 kDa (160 Se)

Number of Atoms in Structure

0  100  1,000  10,000  100,000
Grid Computing
Grid Computing

University at Buffalo, The State University of New York
CCRCenter for Computational Research
Data Intensive Science

SDSC/UCSD • NCSA/UIUC • Caltech • ANL

NSF PACI

PDB
PROTEIN DATA BANK

EuroGRID
Asia-Pacific Advanced Network

Advanced Center for Computational Research
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

LHC

Computational Resources

Large-Scale Databases
ACDC-Grid Collaborations

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

- Dell 2650 backup front-end
- Dell 6650 4-way front-end
- 292 – Dell 2650 production nodes
- 4 node Dell 2650 PVFS server (1096 GB)
- 1 node Dell 2650 NFS server (342 GB)
- Node scratch space (120 GB)
- Dell 6650 4-way (ACDC)
- Dell 6650 4-way (GRID)
- Dell 6650 4-way (EAGLES)

GigE and Myrinet connection
GigE connection
73 GB hard drive
ACDC-Grid Monitoring: The ACDC-Grid DASHBOARD

http://osg.ccr.buffalo.edu
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
Advanced Computational Data Center Grid Job Submission Instructions

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

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

The grid-enabled versions of many well-defined scientific and engineering applications have very similar general requirements and core functionality that are 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 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.
Full Structure / Substructure Template Selection
General Information

Structure Information

Title:  
Structure ID:  
Space Group:  

Cell Constants and Cell Errors (Cell Errors optional)

A: 11.516 +/- 
B: 16.705 +/- 
C: 39.310 +/- 0.004 
Alpha: 
Beta: 
Gamma: 

Native Asymmetric Unit Contents

No Residues (Optional):  
ASU Contents: C6H12O6  (examples: C6H12O6 OR C6H12O6)  

Initial Data Sets

Add Dataset  Delete Dataset
### Initial Data Sets

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<thead>
<tr>
<th>Datasets</th>
<th>Dataset 1</th>
</tr>
</thead>
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<td>I001.hkl</td>
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<tr>
<td>Dataset Type:</td>
<td>Native</td>
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<tr>
<td>File Name (*.hkl):</td>
<td></td>
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<tr>
<td>File Type:</td>
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<td>Nat. Element Replaced:</td>
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<tr>
<td>No. Expected Sites:</td>
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<tr>
<td>F Prime (F):</td>
<td></td>
</tr>
<tr>
<td>F Double Prime (F''):</td>
<td></td>
</tr>
</tbody>
</table>

**Default Parameters (cont’d)**
Reflections and Invariants

Drear Table

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Job Type</th>
<th>Native Data</th>
<th>Derivative Data</th>
<th>Norm Method</th>
<th>Select</th>
</tr>
</thead>
<tbody>
<tr>
<td>iledhkl</td>
<td>BASIC</td>
<td>NULL</td>
<td>NULL</td>
<td>Wilson (Anisotropic)</td>
<td></td>
</tr>
</tbody>
</table>

Normalization Data

- Data resolution cutoffs (in Angstroms)?
  - Low: 3.0, High: 0.94
- Use Bayesian estimates for weak reflections?
  - No
- Min |E| / \text{sig}(|E|) for local scaling:
  - 1.0
- SIR and SAS cutoffs:
  - TMax: 6.0, ZMax: 3.0
  - XMin: 3.0, YMin: 1.0

Generate Invariants

- Data resolution cutoffs?
  - Low: 3.0, High: 0.94
- Minimum allowed |E| / \text{sig}(|E|): 3.0
- Minimum allowed invariants / reflection ratio: 5.0
- Initial values for adjustable parameters
  - Minimum |E| / \text{sig}(|E|) = ZMin:
    - 3.0
  - Number of reflections to use:
    - 0
  - Number of invariants to save:
    - 0

Generating Reflections (Drear)
# Reflections and Invariants

## Drear Table

<table>
<thead>
<tr>
<th>Data Set</th>
<th>Job Type</th>
<th>Native Data</th>
<th>Derivative Data</th>
<th>Norm Method</th>
<th>Select</th>
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</thead>
<tbody>
<tr>
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<td>BASIC</td>
<td>iedhkl</td>
<td>NULL</td>
<td>Wilson (Anisotropic)</td>
<td></td>
</tr>
</tbody>
</table>

## Normalization Data

- Data resolution cutoffs (in Angstroms)?
  - Low: 3.986
  - High: 0.94

- Use Bayesian estimates for weak reflections?
  - No

- Min $|F| / \sigma(|F|)$ for local scaling:
  - 3.0

- SIR and SAS cutoffs:
  - $T_{\text{Max}}: 6.0$
  - $Z_{\text{Max}}: 3.0$
  - $X_{\text{MIN}}: 3.0$
  - $Y_{\text{MIN}}: 1.0$

## Generate Invariants

- Data resolution cutoffs?
  - Low: 3.986
  - High: 0.94

- Minimum allowed $|F| / \sigma(|F|)$:
  - 3.0

- Minimum allowed Invariants / reflection ratio:
  - 5.0

- Initial values for adjustable parameters
  - Minimum $|F| / \sigma(|F|) = Z_{\text{Min}}$: 3.0
  - Number of reflections to use: 840
  - Number of invariants to save: 8400

---

**Invariant Generation**
SnB Setup

Grid Parameters

Preferred resource name: Grid Scheduler
Number of processors: 8
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): 113017
  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: 0.30

• Phase Refinement Method

SnB Setup
• **Phase Refinement Method**

  Phase Refinement Method: Parameter Shift (Fast)

  Number of passes through phase set: 3

  Phase shift: 0.0

  Number of shifts: 2

• **Real-Space Constraints**

  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: 4

  Number of peaks: 84

• **Twice Baking**

  Trials for E-Fourier filtering (fourier refinement)?: None

  Number of cycles: 3

  Number of peaks: 84

  Minimum |E|: 0.75

• **Automatic solution identification criteria**

  Rmin Improvement (%): 45.0

  Rcryst Improvement (%): 25.0
SnB Job Review

Grid Job ID: 447
Selected resource: clearwater.ccr.buffalo.edu
Number of processors: 5
Wallclock time requested: 7200
Number of triplet invariant to use: 8400
Start Phases From:
Random seed (prime):
Number of trials: 11909
Number of trials:
Starting Trial:
Input Phase File:
Input Atom File:
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:
Phase Refinement Method: Parameter Shift (Fast)
Number of passes through phase set: 3
Phase shift:
Number of shifts: 90.0
Number of peaks to select: 0
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:
Number of peaks:
Trials for E-Fourier filtering (fourier refinement)?:
Number of cycles:
Number of peaks:
Minimum $|E|$: Unused
Unused
Unused
Histogram of Completed Trial Structures
## Grid Job Status


### Job Filter Criteria

- **Sort By**:
  - Job Id
  - Job Name
  - Resource
  - Num Proc
  - Status
  - Percent Complete
  - Last Update

### SnB

<table>
<thead>
<tr>
<th>Job Id</th>
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</table>

### Status of Jobs
User starts up – default image of structure.
Molecule scaled, rotated, and labeled.
Acknowledgments

- Mark Green
- Cathy Ruby
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- Igor Janckovic
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- Abani Patra
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- TVGA
- Bergmann Associates
- Peace Bridge Authority
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- Janet Penksa
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www.ccr.buffalo.edu