High-Performance Computing ⇒ Discovery & Innovation

Russ Miller
Cyberinfrastructure Lab, SUNY-Buffalo Hauptman-Woodward Med Res Inst

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

Societal Challenges (Knowledge & Discovery)
- Disaster Management
- Health Care
- Environmental Modeling

Computational Sci & Eng
- Multiprocessor Computing
- Data/Computer Security
- Data Mining & Fusion
- Graphics, Haptics, Speech

Human-Computer Interaction
- Ontology & Reasoning
- Learning & Recognition

Departments, Colleges, Centers, Institutes, & User Support Staff: HPC, Viz, Networking, Storage, Interfaces
- High-Performance Systems, Networks, Storage, Visualization

CYBERINFRASTRUCTURE

Modeling Physical Multi-Systems & Phenomena ("Simulation-Based Eng Sci")
- Interactive Systems
- Ubiquitous Computing Environments
- Computational Digital Art

Strategy for Excellence (International Prominence)
- Parallel, Cluster, and Grid Computing
- Multiprocessor Computing
- Data/Computer Security
- Data Mining & Fusion
- Multiscale Modeling
- Ontology & Reasoning
- Learning & Recognition
- Graphics, Haptics, Speech
- Interactive Systems
- Ubiquitous Computing Environments
- Computational Digital Art

CI Lab
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 at 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

Sen. Clinton
Sen. Schumer
Rep. Reynolds
Gov. Pataki
M. Capellas
Michael Dell
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
  - Build a six lane signature span
Public Forum
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

University at Buffalo  The State University of New York  Cyberinfrastructure Laboratory
**VR-Fact!**

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

- Direct Methods Structure Determination
  - Listed on “Top Ten Algorithms of the 20th 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

- 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

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

Flow models of Colima volcano
In Mexico – courtesy Rupp et. al.’06
Cosmological Parameter Estimation

- Wealth of new precision cosmological data
- WMAP Cosmic Microwave Background 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)

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:
  - 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
Nanomedicine Program

World class Research Program Melding Nanotechnology with Biomedical Sciences

Bionanocompatibility/Distribution

Multi-Modal Imaging

Cellular Imaging

In Vivo Imaging

Drug Delivery

Gene Delivery

Targeted Therapy

Therapeutic Payload

Optical Probe

Silica Shell

Targeting agent

In Vivo Sensing

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

“Leading the Way to Technology through Innovation”

P. Prasad

www.biophotonics.buffalo.edu

University at Buffalo The State University of New York

Cyberinfrastructure Laboratory

CI Lab
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 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.
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

Reciprocal Space  Real Space

Trial Phases

Phase Refinement

Tangent Formula

FFT

Density Modification (Peak Picking)

Solutions

Conventional Direct Methods

Reciprocal Space  Real Space

Trial Phases

Phase Refinement

Tangent Formula

FFT

Density Modification (Peak Picking)

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

Shake-and-Bake

- Trial Structures
- Structure Factors
- Trial Phases

Phase Refinement
- Tangent Formula
- Parameter Shift

FFT

Density Modification (Peak Picking) (LDE)

FFT⁻¹

Reciprocal Space
“Shake”

Real Space
“Bake”

Solutions

Method:
- Dual-Space Refinement
Ph8755: SnB Histogram

Atoms: 74
Space Group: P1

Phases: 740
Triples: 7,400

Trials: 100
Cycles: 40

Rmin range: 0.243 - 0.429
Phasing and Structure Size

0              100           1,000        10,000       100,000

Conventional Direct Methods

Se-Met

Multiple Isomorphous Replacement

567 kDa (160 Se)

Shake-and-Bake

Se-Met with *Shake-and-Bake*

Vancomycin

Number of Atoms in Structure
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
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

- 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}
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)**
  - Define quality of service estimates of job completion, by better estimating job runtimes by profiling users.

- **Predictive Scheduler**
  - Develop automated procedures for dynamic computational resource allocation.

- **Dynamic Resource Allocation**
  - Develop automated procedures for dynamic data repository creation and deletion.

- **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**
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**
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
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.

Software: BnP
Field: Protein crystal structure determination
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.
General Information

Structure Information
Title: Hlad
Structure ID: Hlad
Space Group: 19

Cell Constants and Cell Errors (Cell Errors optional)

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<th>Value</th>
<th>Error</th>
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<tr>
<td>Gamma</td>
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Native Asymmetric Unit Contents

| No Residues (Optional): | |
| ASU Contents: | C60H1206 |

(Examples: C6H12O6 OR C6 H12 O6)

Initial Data Sets

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Select dataset to delete: 0

Datasets
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<th>Dataset 1</th>
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Name (8 chars max): Hladkl
### 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  
**Number of trials:** 11909  
**Starting Trial:** 1000  
**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:** 04  
**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 I/E?** Unused
Graphical Representation of Intermediate Job Status

Histogram of Completed Trial Structures
## Status of Jobs

### Grid Job Status

### Job Filter Criteria
- **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

### SnB

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</table>
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
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- Martins Innus
- Cynthia Cornelius

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

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

CI Lab

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