High-End Computing in New York State

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



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
 - **OHead Nodes: Dell 1950 (Intel)**
 - OWorkers: Intel 8×2×4 & AMD 8×2×2
 - \square Virtual Memory Machines (2 × Intel 4×4)
 - **□** Dell GigE Managed Switches
 - ☐ InfiniBand
 - **□ 22 TB Dell Storage (2)**
 - □ Condor Flock (35 Intel/AMD)
- **Acquisition in Progress (30-50TF)**
- **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}



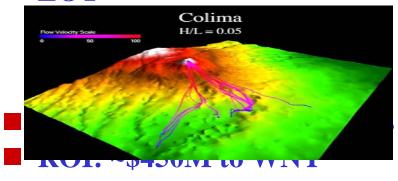
NYS Grid Resources

- 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



Center for Computational Research (CCR)

- **Founding Director (1998-2006)**
- **Facts & Figures**
 - **☐** Top Academic HPC Center in World
 - □ ~25 TF of HPC
 - □ ~600 TB of High-End Storage
 - **☐** Significant Visualization
 - **☐** Special-Purpose Systems
 - □ ~30 FTEs Staff
 - **□** 140 Projects Annually
- **EOT**







CCR Highlights (1998-2006)

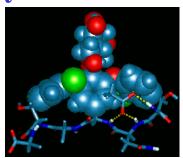
- Provide HE-Comp
- Provide HE-Vis + AGN
- **Special Purpose Systems**
 - ☐ Bioinformatics
 - □ Data Warehouse / Mining
- **Support Local/National Efforts Industry + Acad**
- **Create jobs in WNY**
- **Certificate Program**
- **Workshops** + **Tours**
 - □ Campus, Industry
 - ☐ High-School

- **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









SUNY-Buffalo 2008 (13TF; 75TB)

- **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
- **HP/Compaq SAN**
 - **□75** TB Disk; 190 TB Tape
 - □ 64 Alpha Processors (400 MHz)
 - **□32 GB RAM**; 400 **GB Disk**



RPI (110 TF)

- Partnership with NYS and IBM (\$100M total including in-kind contributions)
- Computational Center for Nanotechnology **Innovations (CCNI)**
- Power-Based AIX Cluster
- AMD Cluster (2168 processors; 10 TF)
- IBM BlueGene/L (32K processors; 92 TF)
 - □ Rank #12 on 11/2007 Top 500
- Some availability outside of RPI



Brookhaven National Laboratory (103 TF)

- Partnership (BNL/Stony Brook University) with NYS and IBM (\$100M total including in-kind contributions)
- New York Center for Computational Sciences (NYCCS)
- Blue Gene/L (36864 Processors)
- 100 TF; Rank #10 on 11/2007 Top 500
- Applications include wide range of Science and Engineering
- Potential availability outside of BNL/SBU



Rochester Institute of Technology (75TF; 67 TB)

- **Campus Computational Grid**
- **Condor Flock with 1000 Cores**
 - **□**Windows, Macintosh, Solaris, Linux
 - **□**Eight (8) Departments Participating
- 1.5 TB of Memory
- 67 TB of Disk
- 75 TF of Computing



Cornell University

- Cornell University Center for Advanced Computing (new name for "The Theory Center")
- **Store several large Databases**
- Part of TeraGrid
- **EOT**



