Center for Computational Research
All Hands Meeting - Tuesday, March 11, 2003

Russ Miller, Director
Tom Furlani, Associate Director

“Top 10 Worldwide Supercomputing Center”
- www.gapcon.com

University at Buffalo
The State University of New York
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<th>Time</th>
<th>Session</th>
<th>Presenter(s)</th>
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<tr>
<td>9:00</td>
<td>Introduction</td>
<td>Miller</td>
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<tr>
<td>9:15</td>
<td>CCR Overview</td>
<td>Miller</td>
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<td>Break</td>
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<td>Parallel Computing at CCR</td>
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<td>Overview of Joplin</td>
<td>Cornelius/Green</td>
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<td>Intro to Bioinformatics</td>
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Gordon E. Moore

- Co-Founder of Intel
- Predicted (1965/75) that transistor density would double every 12/18 months
- Processing speed doubling every 18 mos.
- Disk storage doubling every 12 mos.
- Aggregate bandwidth doubling every 9 mos.

A computation that took 1 year to run on a PC in 1985 would only take 5 mins to run on a PC today!

A computation that runs in 2 hours on a PC today would have taken 24 years to run on a PC in 1985!
What is a (Beowulf) Cluster?

- **Industry Standard Hardware and Software**
  - PC-Based Components (Intel or AMD)
  - Ethernet or Myrinet
  - Linux, PBS, MPI
  - “Commodity Off-The-Shelf” (COTS)
  - Introduced in 1995

- **Operates as a Single System**

- **Rivals Performance of Traditional Supercomputer at a Fraction of the Price**
## Fastest Computers

<table>
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<tr>
<th>Year</th>
<th>Mach</th>
<th>Procs</th>
<th>GFlops</th>
</tr>
</thead>
<tbody>
<tr>
<td>1976</td>
<td>Cray 1</td>
<td>1</td>
<td>0.1</td>
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<tr>
<td>1982</td>
<td>Cray X-MP</td>
<td>4</td>
<td>0.9</td>
</tr>
<tr>
<td>1986</td>
<td>Cray 2</td>
<td>4</td>
<td>2</td>
</tr>
<tr>
<td>1989</td>
<td>Cray Y-MP</td>
<td>8</td>
<td>2.7</td>
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<tr>
<td>1989</td>
<td>TMC CM-2</td>
<td>8192</td>
<td>28</td>
</tr>
<tr>
<td>1992</td>
<td>TMC CM-5</td>
<td>1024</td>
<td>131</td>
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<td>1993</td>
<td>Cray T3D</td>
<td>1024</td>
<td>152</td>
</tr>
<tr>
<td>1994</td>
<td>Fujitsu VPP</td>
<td>140</td>
<td>236</td>
</tr>
<tr>
<td>1996</td>
<td>Hitachi SR2</td>
<td>2048</td>
<td>368</td>
</tr>
<tr>
<td>1997</td>
<td>Intel ASCI-R</td>
<td>9152</td>
<td>1830</td>
</tr>
<tr>
<td>1999</td>
<td>SGI ASCI-BM</td>
<td>6144</td>
<td>3072</td>
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<tr>
<td>2000</td>
<td>IBM ASCI-W</td>
<td>8192</td>
<td>12,288</td>
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<tr>
<td>2002</td>
<td>NEC E.S.</td>
<td>5120</td>
<td>40,960</td>
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</table>

A 1-year calc in 1980 = 5.4 sec today  
A ~1990 HPC = a laptop today
Earth Simulator in Japan (NEC Vector Supercomputer)

40.9TF Peak
35.8TF Sustained

LANL Compaq
Current:
10.2TF Peak
7.7TF Sust
100TF in 2004
Earth Simulator

- 40TFlops Peak
- Homogeneous, Centralized, Proprietary, Vector
- Expensive!
- CFD-Weather, Climate, Earthquake
- 640 NEC SX/6 Nodes (5120 CPUs)
- Footprint = 4 tennis courts
- $6M/year in power
Center for Computational Research

- Facility Opened in May 1999
- Top Ten Worldwide Supercomputing Facility
  - 9 Teraflops Aggregate Capacity (PR)
  - 3+TF Generally Available (Top 40)
- Support Faculty-Based Research
- Foster High-Tech Research & Economic Development in WNY
  - High-Performance Computing
  - High-End Visualization
- Technology Transfer
  - Seminars, Workshops and Tutorials
General Information

- High-Performance Computing and High-End Visualization
  - 47 Active Research Groups in 27 Depts
- Leverage $300K NSF Grant ⇒
  - $41M Vendor Donations
  - $55M Grants & Contracts (non-bldg)
- Deliverables
  - 350 Publications & Pres., Hardware, Software, Algorithms
- Outreach (EOT)
  - Workshops, Training, Courses, Degree Programs
  - 25 Local Companies & Institutions
- Funding
  - NSF, NIH, NIMA, EPA, Keck, Sloan
  - NYS, SUNY, UB
  - IBM, SGI, Sun, DELL, HP (Compaq), Nortel, Myricom
Staff

■ **Director** – Dr. Russ Miller

■ **Associate Director** – Dr. Tom Furlani

■ **Computational Scientists**
  - Dr. Zihua Hu (Bioinformatics), Dr. Matt Jones (Physics), Dr. Jeff Tilson (Chemistry)

■ **Programmers**
  - Steve Gallo (Grid Computing), Quoc Nguyen (Bioinformatics)

■ **Visualization**
  - Adam Koniak (Urban Simulation), Martins Innus (Scientific Visualization)

■ **Systems Support**
  - Cynthia Cornelius, Jon Bednasz, Sam Guercio, Tony Kew, Deborah Loke, Dori Macchioni, Jason Rappleye

■ **Office Staff**
  - Brenda Sauka (Financial Manager), Sally Elder (Secretary), Penelope Krebs (Receptionist)
ExCom & AdvCom

Executive Committee
- Josephine Anstey, Media Study
- Corky Brunskill, SENS
- Philip Coppens, Chemistry
- David Kofke, Chemical Engineering
- Bruce Pitman, Math

Internal Advisory Committee
- Bruce Holm, Senior Vice Provost
- Voldemar Innus, CIO
- Mark Karwan, Dean School of Engineering
- Bruce McCombe, Assoc. Dean, CAS & Director, CAPEM
Space

- **1999**
  - Norton 9: 2800 sq ft + 1100 sq ft Machine Room

- **2002**
  - Norton 10 AGN, TDW: 600 sq ft
  - Norton 15 Machine Room: 1700 sq ft
  - Norton 118 Machine Room: 1700 sq ft
  - Norton 17 Office Area: 1600 sq ft

- **Jan., 2003 - Delayed**
  - Norton 5 & 7: 3000 sq ft
  - Provide Public Access to iDesk, AGN, Videoconferencing
  - Provide Appropriate Staff Office Space
  - Provide Visitor Office Space

- **UPS System – Delayed from 1/02 to 3/03**
Making CCR Easier to Use

- Website Update
  - New Look/Feel by end of month
  - User Info/Hotpage - Demonstration
- ccr-help@ccr.buffalo.edu (RT-Tracker)

- Grid Software on the Horizon
  - Grid: flexible, secure, coordinated resource sharing among dynamic collections of individuals, institutions, and resources
  - Grid Portal Under Development
    - HPC Machines, Condor Flocks, Storage, Visualization, Instruments
    - Domain-Specific Areas of Portal
- Computational Chemistry Portal (ECCE)
Machine Utilization

- Greater than 80% on most platforms

- Queuing Systems
  - Regularly adjusting queue structure to maximize throughput
  - 7 day queues discontinued
  - 3 day queue is now the longest
  - Throughput and utilization is significantly better
  - Feedback from users is welcome
  - Recent change under investigation: partition for parallel and sequential jobs on nash
Outreach

- Collaboration with local institutions
  - Buffalo Neuroimaging Analysis Center – MS MRI Visualization
  - Children’s Hospital – Medical Imaging
  - BuffLink – 3D Visualization of the Buffalo Niagara Medical Campus
  - Peace Bridge Authority
  - Bioinformatics in Buffalo (UB, Roswell Park, HWI)
  - H.S. Bioinformatics Clusters
  - Numerous Local Colleges

- H.S. Summer Workshop in Bioinformatics

- Tours
  - Faculty candidates, speakers, business leaders, politicians, funding agencies
Computational Resources

  - 64 Processors (400 MHz)
  - Shared memory
  - 32 GB RAM
  - 400 GB Fibre Channel Disk
- Full Maintenance for 2 years
- Primary Applications
  - Computational Fluid Dynamics
  - Quantum Chemistry (ADF/Jaguar/Q-Chem)
  - Computational Mechanics
  - Physics
Computational Resources

- **IBM RS/6000 SP (Stills): 1998+**
  - 78 Processors
  - 26 GB RAM
  - 640 GB Disk Storage

- **Primary Applications**
  - Computational Fluid Dynamics (CFX4)
  - Chemical Engineering (Molecular Dynamics, etc)
  - Quantum Chemistry (NWChem, ADF, Columbus, CHARMM, Q-Chem)
  - MAE (PETSC)

- **Off Maintenance Jan 2004**
  - Requires Exit Strategy
Computational Resources

- Sun Microsystems Cluster (Young): 1999+
  - 48 Sun Ultra 5s (333MHz)
  - 16 Dual Sunblades (750MHz)
  - 30 GB RAM, Myrinet
  - Sun Solaris OS
- Large Number of Sequential Jobs
- Primary Applications:
  - Quantum Chemistry (ADF)
  - Chemical Engineering
  - CHARMM
- Processors Showing Age
  - Redeploy when Opportunity Presents
Computational Resources

- SGI Intel Linux Cluster (Nash): 2000
  - 150 PIII Processors (1 GHz)
  - 75 GB RAM, 2.5 TB Disk Storage
  - Myrinet2000
- Primary Application Areas:
  - Chemical Engineering
  - Computational Fluid Dynamics
- Off Maintenance in 1.5 years
- Stability Issues due to Poor Hardware
- Consider Exit Strategy
Computational Resources

- New Dell Linux Cluster (Joplin): 2002
  - 600 P4 Processors (2.4GHz)
  - Myrinet2000
  - 600 GB RAM; 40 TB Disk
- 22nd Fastest Computer in the World
- Large Production Machine
- Highly Parallel Codes
- Primary Application Areas:
  - Chemical Engineering
  - Computational Mechanics
  - Computational Fluid Dynamics
  - Environmental Chemistry
  - Quantum Chemistry (ADF,NWChem)
Computational Resources

- **Sun Enterprise 6000 (Database): 1998**
  - 4 UltraSparc-II 336 MHz
  - 2 GB RAM
  - 38 GB disk + 2 × T3 Disk Arrays

- **Primary application areas:**
  - Large Oracle Database Application
  - Data Mining – Tops Friendly Markets
Computational Resources

- Apex Bioinformatics System: 2003
  - Sun V880 (3), 6800, 280R (2), PIIIs; Sun 3960: 7 TB Disk Storage

- BioACE (Bioinformatics Application Computing Environment)
  - Available Directly from CCR Website
  - Faculty/Staff/Students from UB, RPCI, HWI
  - Home to Many State-of-the-Art Bioinformatics Software Packages
    - DNA and Protein Sequence Analysis (on hold)
    - Database Search
    - Gene Expression Profiling
    - Data Visualization

- Missing Small Linux Cluster (DNA & Prot. Seq. Anal.)
- GCG Implementation Postponed
- Workshop Tomorrow on InforMax Packages
Visualization Displays

- **FakeSpace Sys ImmersaDesk**
  - Portable

- **3300W Visualization Display**
  - 2 Channel Superwide Display – Dual Barco 808 Projectors

- **Tiled Display Wall**
  - 2D
  - 11.5’ x 6.5’ image
  - Myrinet Interconnect
  - 20 projectors/Dell 530’s
  - Resolution: 5105 x 3072 pixels (15M Pixels)
Visualization Computing

- **SGI Onyx 300 – 10 Processors**
  - Infinite Reality 4 Graphics Pipes (1GB Texture memory)
  - Used to drive the iDesk and the 3300W simultaneously

- **SGI Onyx2 – 6 Processors**
  - Infinite Reality 2 Graphics Pipes (64MB Texture memory)
Access Grid Node (AGN)

- Facilitates group to group collaboration
Personnel: $1.2M/yr by UB

Discretionary Operating: ≤ $100K/yr by UB
- Travel, training, equipment, software, maintenance, memberships, repairs, tapes, supplies, phones, installs, shipping, promotional material, networking, furniture, etc

Equipment Acquisitions: Ad Hoc
- Approx. $6.5M to date (4 year period)

Comparison

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<th>Staff</th>
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<tr>
<td>CCR</td>
<td>$1.3M</td>
<td>18</td>
</tr>
<tr>
<td>NCSC</td>
<td>$7.6M</td>
<td>23</td>
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<tr>
<td>OSC</td>
<td>$6.6M</td>
<td>48</td>
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<tr>
<td>U Minn</td>
<td>$7.0M</td>
<td>24</td>
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CCR-Leveraged Grants & Contracts

- CCR Grants & Contracts: $12M
- Vendor Donations (in-kind): $41M
- External Research Funding: $43M
  ($290M incl corporate, construction funds, foundation support, etc.)

User Support

- Critical that CCR is included in routing sheet for proposals that will use facilities
- Direct costs for CCR are very important in these financial times

Student Support from Operating, Workstudy, or External Grants (including REUs)
Charge-Back Scheme

- Schemes for Cost-Recovery Under Consideration
- Basic Rates Have Been Determined
  - SGI Linux: $0.4 per processor per hour
  - SGI Origin: $0.6 per processor per hour
  - IBM SP: $1.0 per processor per hour
  - iDesk: $69.0 per hour
- What Does This Mean for Users?
  - $1,000 - $22,000 per month
- Status of Charge-Back Scheme Unknown
Visualization Review

- External Panel Convened to Review Visualization Efforts on Campus
- Site Visit on Dec 19th, 2002
- Committee did not read Documents
- No Debriefing with Committee
- Brief Conversation with Provost in Feb.
- Positive Feedback on CCR
- Central Funding Should be Provided
- Charge-Back Model is Not an Option
- Formation of Provost Advisory Panel for CCR
Consolidation & Upgrade Plan

- **Retain**
  - Dell Linux P4 Cluster

- **Acquire**
  - 1TF SMP System (Regatta, Alpha, Itanium)
  - 0.5TF General Purpose PC farm
  - Storage Area Network (SAN)

- **Evaluate**
  - Sun6000 Database System

- **Retire/Redeploy**
  - IBM SP
  - Sun Cluster
  - SGI Linux Cluster

- **Derailed with Cancellation of $6.5M HP EV7 & Intel Systems (PC Farm & BioCCR System)**
Future Plans

- Finances Restrict Planning
- Needs Assessment
  - Stable and Reasonable Operating Budget
    - Level Similar to NCSC, U Minn, OSC
    - Will Allow for Strategic Planning
  - Constant Refresh of Equipment
  - Travel, Training, Workstations, Supplies
  - Software, Tapes, Cables
- ???Administrative Discussion???
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