The Center for Computational Research

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Computers are used in Many Professions

- Science and Engineering
  - Physics, Chemistry, Biology
  - Aerospace, Mechanical, Civil, Environmental
- Architecture
  - Building and Bridge Design
- Computer Animation
  - Cartoons, Movies, Advertising
  - Games (Playstation, Nintendo, PC games, etc)
- Graphic Arts/Design
- Computer Programmers
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!
Beowulf Clusters

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

- **Operates as a Single System**

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

Thomas Sterling
Caltech
Supercomputers

- Fastest computers at any point in time
- Used to solve large and complex problems
- Machines 1000 times faster than a PC
- Machines 10 times slower than what you need to solve the most challenging problems

Cray1 - 1976

“Seymour Cray is the Thomas Edison of the supercomputing industry”
- Larry L. Smarr

Seymour Cray 1925-1996

University at Buffalo  The State University of New York  Center for Computational Research
# Fastest Computers

<table>
<thead>
<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>
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<tr>
<td>1986</td>
<td>Cray 2</td>
<td>4</td>
<td>2</td>
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<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>
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<tr>
<td>1992</td>
<td>TMC CM-5</td>
<td>1024</td>
<td>131</td>
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<tr>
<td>1993</td>
<td>Cray T3D</td>
<td>1024</td>
<td>152</td>
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<tr>
<td>1994</td>
<td>Fujitsu VPP</td>
<td>140</td>
<td>236</td>
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<tr>
<td>1996</td>
<td>Hitachi SR2</td>
<td>2048</td>
<td>368</td>
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<tr>
<td>1997</td>
<td>Intel ASCI-R</td>
<td>9152</td>
<td>1830</td>
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<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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A 1-year calc in 1980 = 5.4 sec today
A 1990 HPC = a laptop today
Growth of Peak Performance
Earth Simulator

- 40TFlops Peak
- Homogeneous, Centralized,

- Expensive!

- CFD-Weather, Climate, Earthquake
- 640 NEC SX/6 Nodes (5120 CPUs)
- Footprint = 4 tennis courts
- $6M/year in power
Center for Computational Research
1999-2003 Snapshot

- High-Performance Computing and High-End Visualization
  - 110 Research Groups in 27 Depts
  - 13 Local Companies
  - 10 Local Institutions

- External Funding
  - $111M External Funding
    - $13.5M as lead
    - $97.5M in support
  - $41.8M Vendor Donations

- Deliverables
  - 350+ Publications
  - Software, Media, Algorithms, Consulting, Training, CPU Cycles…
Major CCR Resources

- Dell Linux Cluster: #22 → #25 → #38
  - 600 P4 Processors (2.4 GHz)
  - 600 GB RAM; 40 TB Disk; Myrinet

- Dell Linux Cluster: #187 → #368 → off
  - 4036 Processors (PIII 1.2 GHz)
  - 2TB RAM; 160TB Disk; 16TB SN
  - Restricted Use (Skolnick)

- SGI Origin3800
  - 64 Processors (400 MHz)
  - 32 GB RAM; 400 GB Disk

- IBM RS/6000 SP
  - 78 Processors
  - 26 GB RAM; 640 GB Disk

- Sun Microsystems Cluster
  - 48 Sun Ultra 5s (333MHz)
  - 16 Dual Sunblades (750MHz)
  - 30 GB RAM, Myrinet

- SGI Intel Linux Cluster
  - 150 PIII Processors (1 GHz)
  - 75 GB RAM, 2.5 TB Disk Storage

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

- HP/Compaq SAN (4Q03)
  - 75 TB Disk; 200 TB Tape
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
Risk Mitigation

- Integrate information from several sources
  - Simulation results
  - Remote sensing
  - GIS data
- Develop realistic 3D models of geophysical mass flows
- Present information at user appropriate resolutions
Ability of proteins to perform biological function is attributed to their 3-D structure.

Protein folding problem refers to the challenge of predicting 3-D structure from amino-acid sequence.

Solving the protein folding problem will impact drug design.
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
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
StreetScenes® is a Virtual Reality (VR) software solution for 3D visualization of surface traffic.

- 3D model of proposed soccer stadium in Rochester
- Used StreetScenes® to import output file from Synchro traffic simulation.
Select WNY Synergies

- IBC Digital
  - Gov. Pataki Visit
  - Peace Bridge (Early & Current)
  - Buffalo-Niagara Medical Campus
  - Compute Cycles for Animation

- Bergmann Associates
  - Peace Bridge (Current)
  - NYS Thruway Toll Plaza

- Azar & More
  - Reenactment of 1901 Pan Am Exhibition
  - PHSCologram & Courses
  - Avid Digital Editing

- Niagara College
  - Start up
  - Peace Bridge (Current)

- Hauptman-Woodward Medical Research Institute
  - Computing
  - Collaboratory

- The Children’s Hospital of Buffalo
  - Medical Visualization

- Veridian
  - Battlespace Management
Contact Information

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