

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

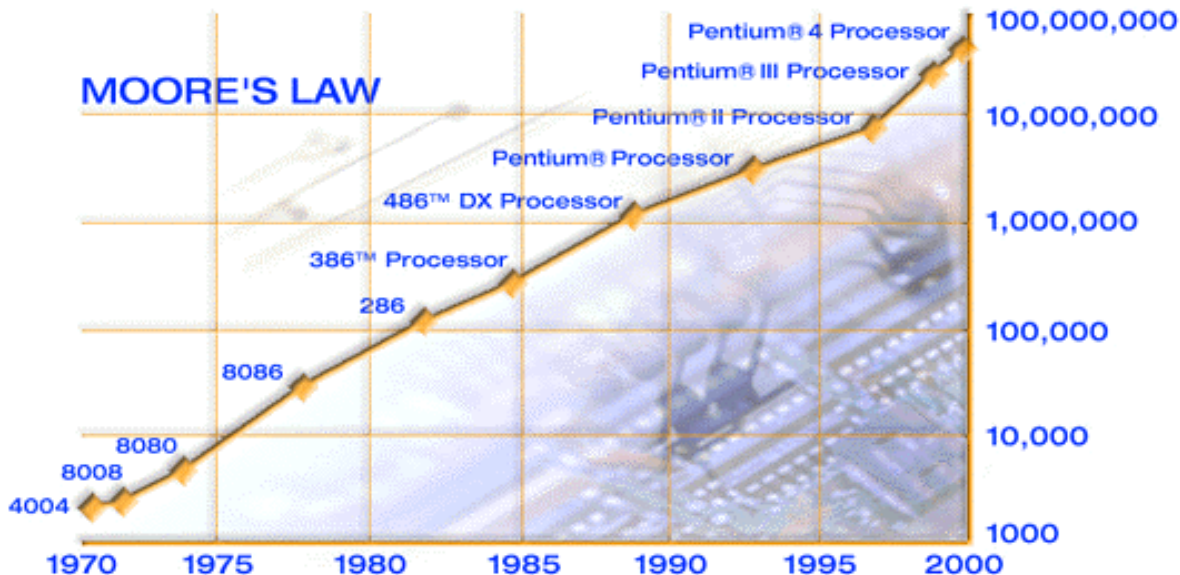


Gordon E. Moore

- 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.



Gordon E. Moore



- 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

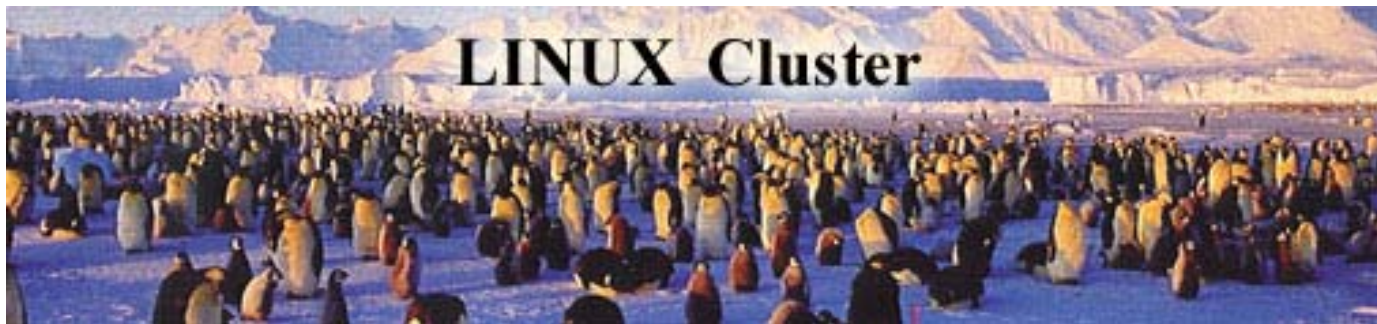
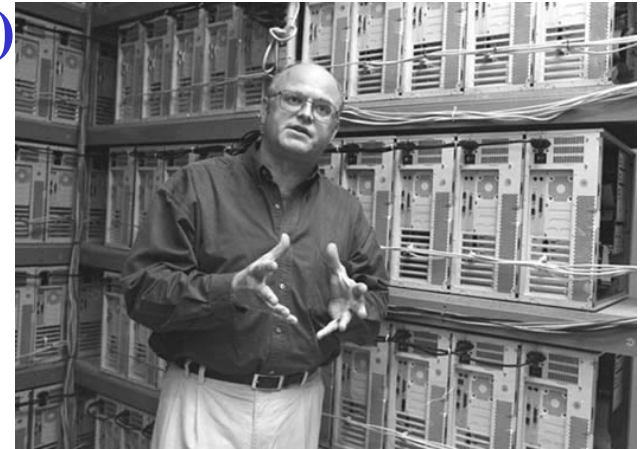
■ Industry Standard Hardware and Software

Thomas Sterling
Caltech

- ❑ PC-Based Components (Intel or AMD)
- ❑ Ethernet or Myrinet
- ❑ Linux, PBS, MPI
- ❑ “Commodity Off-The-Shelf” (COTS)

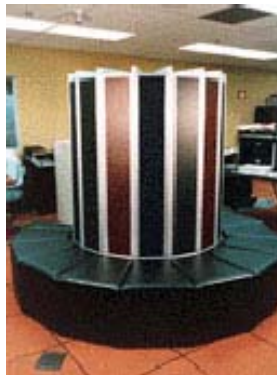
■ Operates as a Single System

■ Rivals Performance of Traditional Supercomputer at a Fraction of the Price

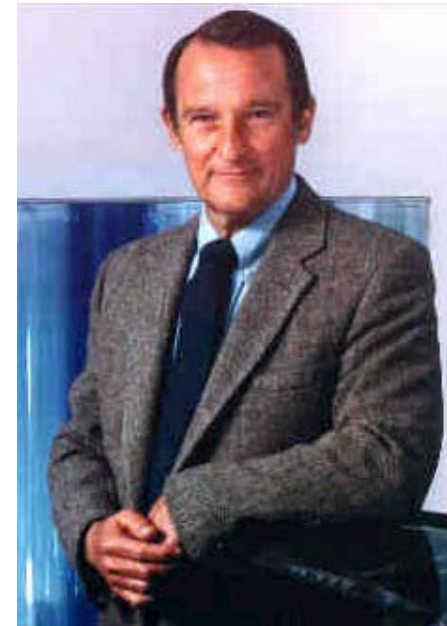


Supercomputers

- 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

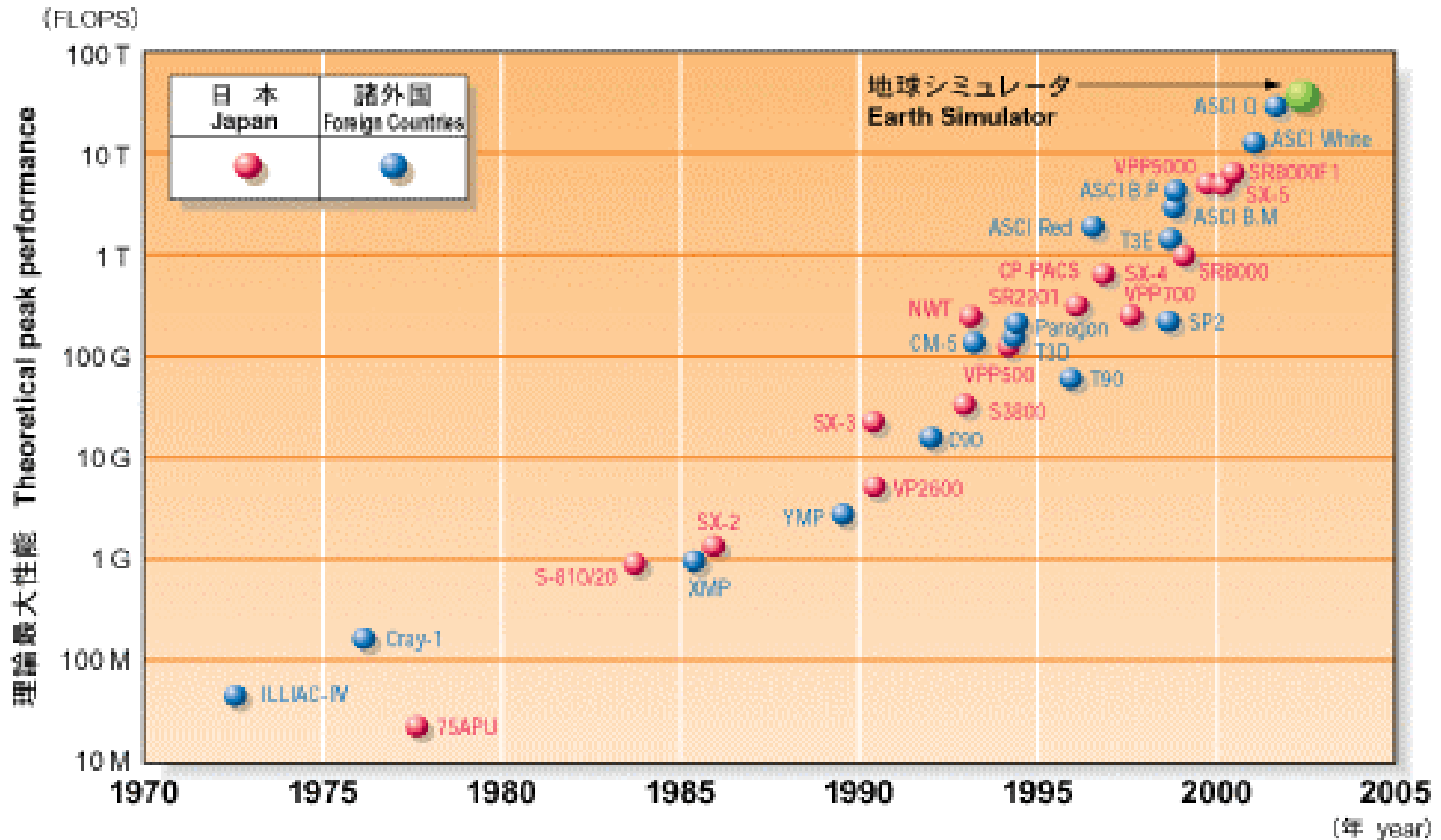


“Seymour Cray is the Thomas Edison of the supercomputing industry” Seymour Cray
- Larry L. Smarr 1925-1996

Fastest Computers

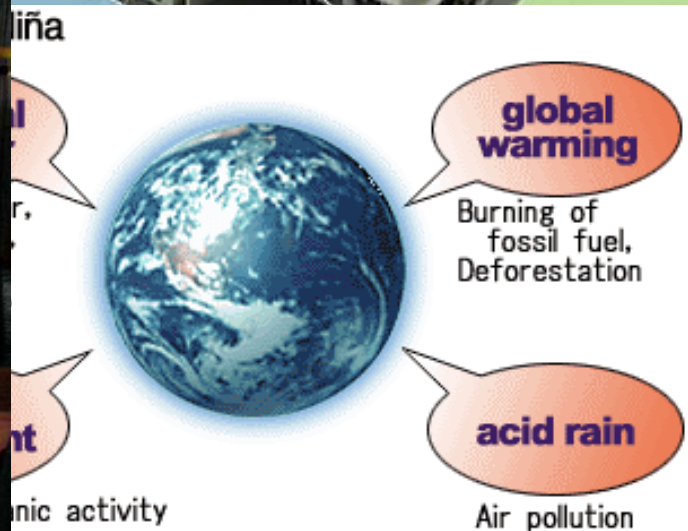
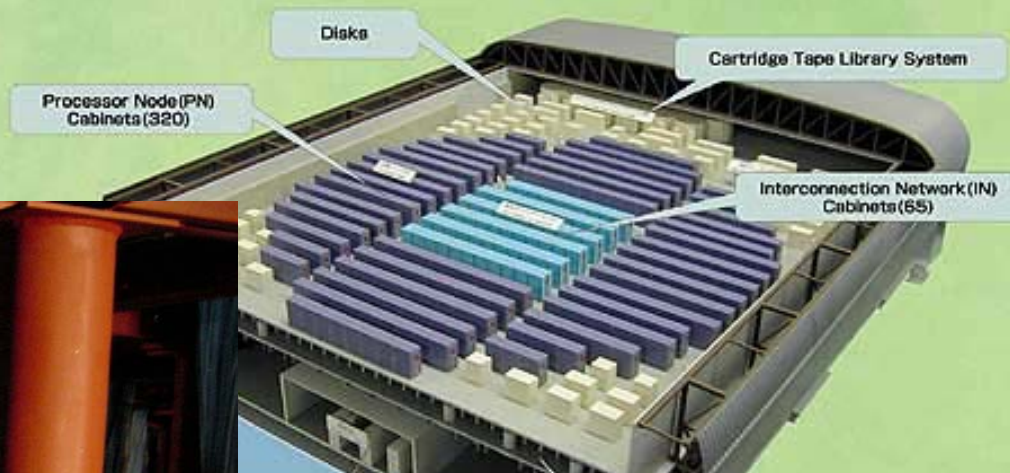
Year	Mach	Procs	GFlops		Year	Mach	Procs	GFlops
1976	Cray 1	1	0.1		1993	Cray T3D	1024	152
1982	Cray X-MP	4	0.9		1994	Fujitsu VPP	140	236
1986	Cray 2	4	2		1996	Hitachi SR2	2048	368
1989	Cray Y-MP	8	2.7		1997	Intel ASCI-R	9152	1830
1989	TMC CM-2	8192	28		1999	SGI ASCI-BM	6144	3072
1992	TMC CM-5	1024	131		2000	IBM ASCI-W	8192	12,288
<p>A 1-year calc in 1980 = 5.4 sec today A 1990 HPC = a laptop today</p>					2002	NEC E.S.	5120	40,960

Growth of Peak Performance



Earth Simulator

- 40TFlops Peak
- Homogeneous, Centralized,



Center for Computational Research 1999-2003 Snapshot

■ High-Performance Computing and High-End Visualization

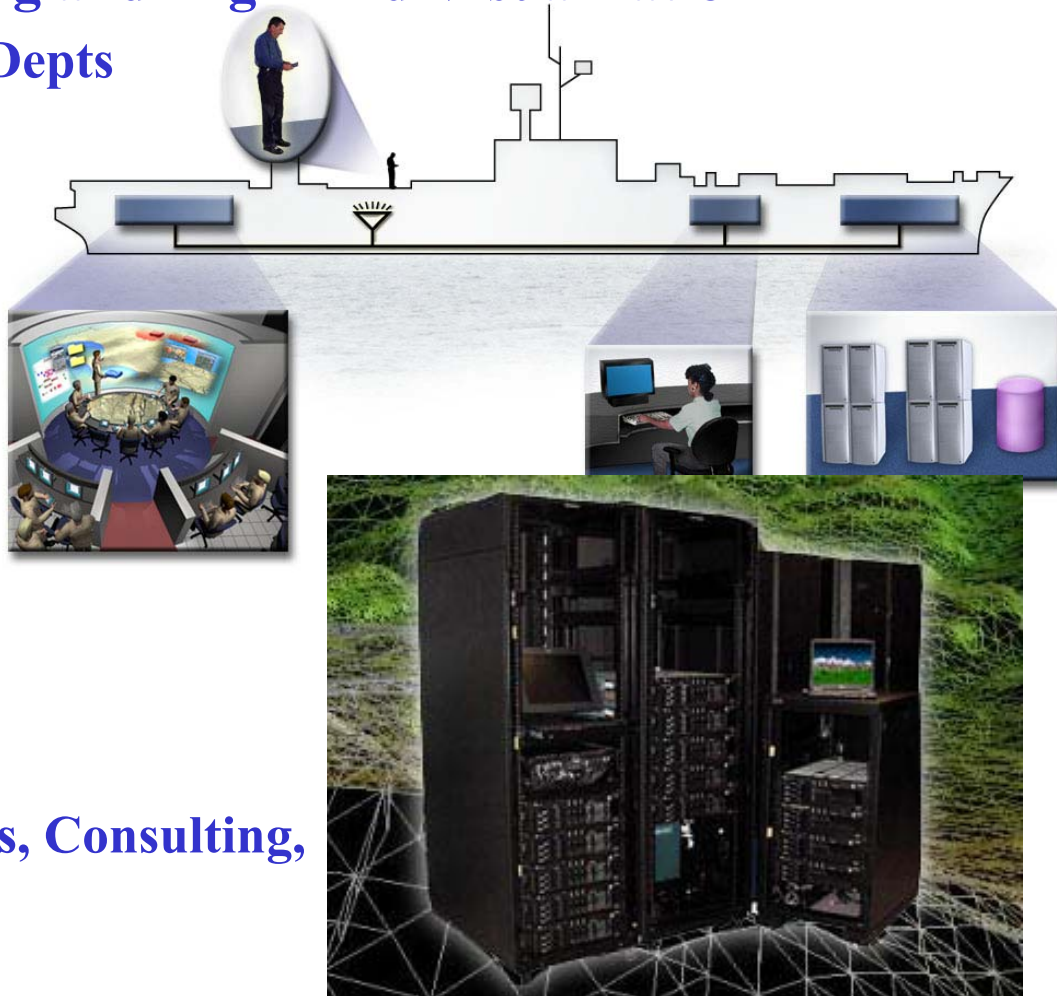
- ❑ 110 Research Groups in 27 Depts
- ❑ 13 Local Companies
- ❑ 10 Local Institutions

■ 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

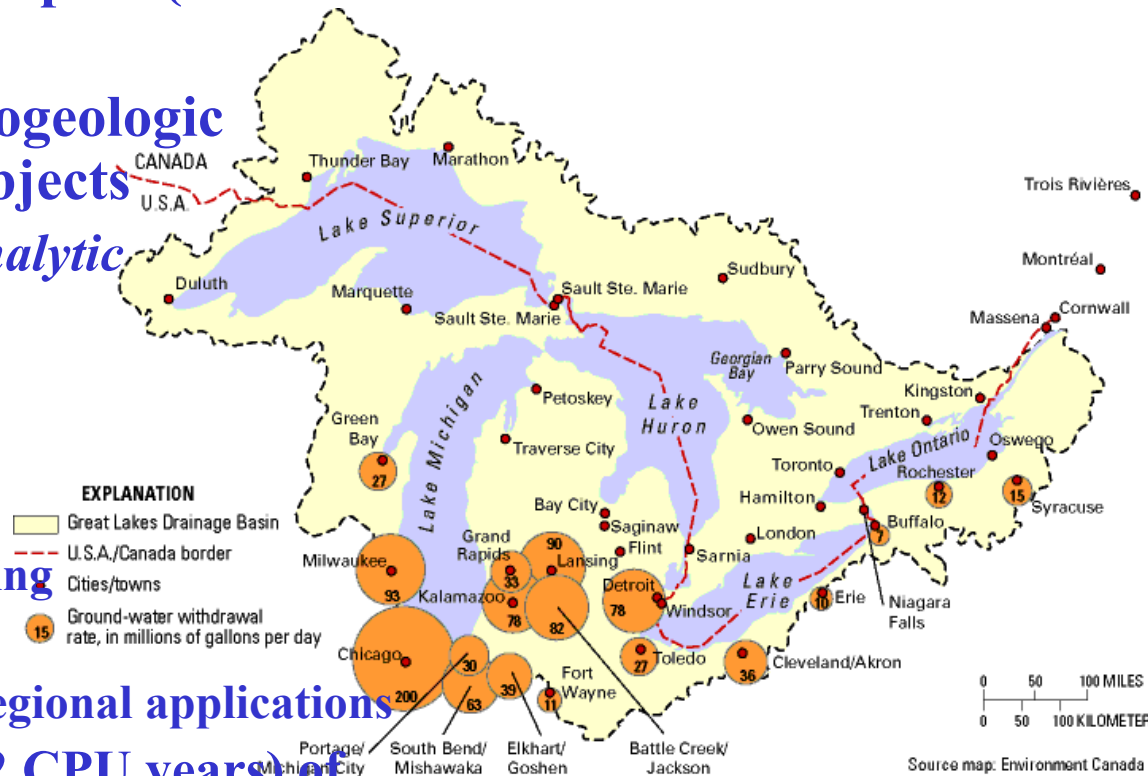


■ HP/Compaq SAN (4Q03)

- ❑ 75 TB Disk; 200 TB Tape

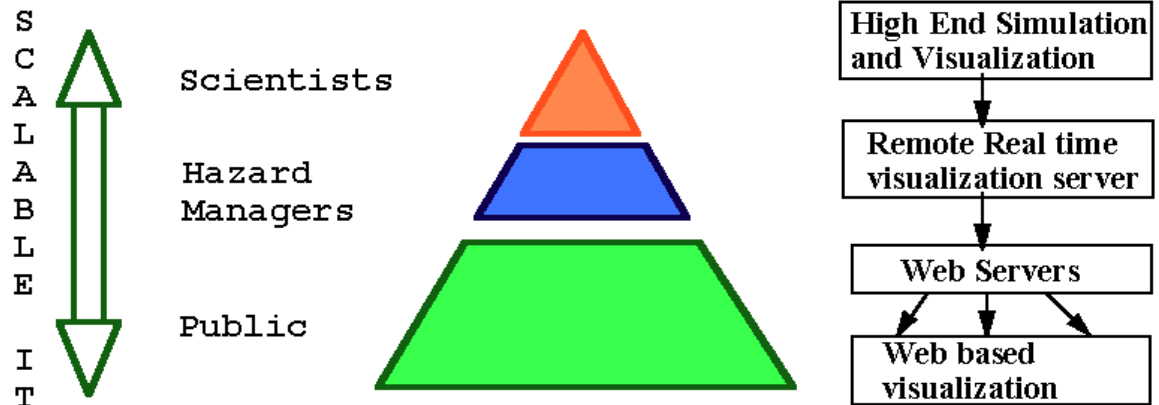
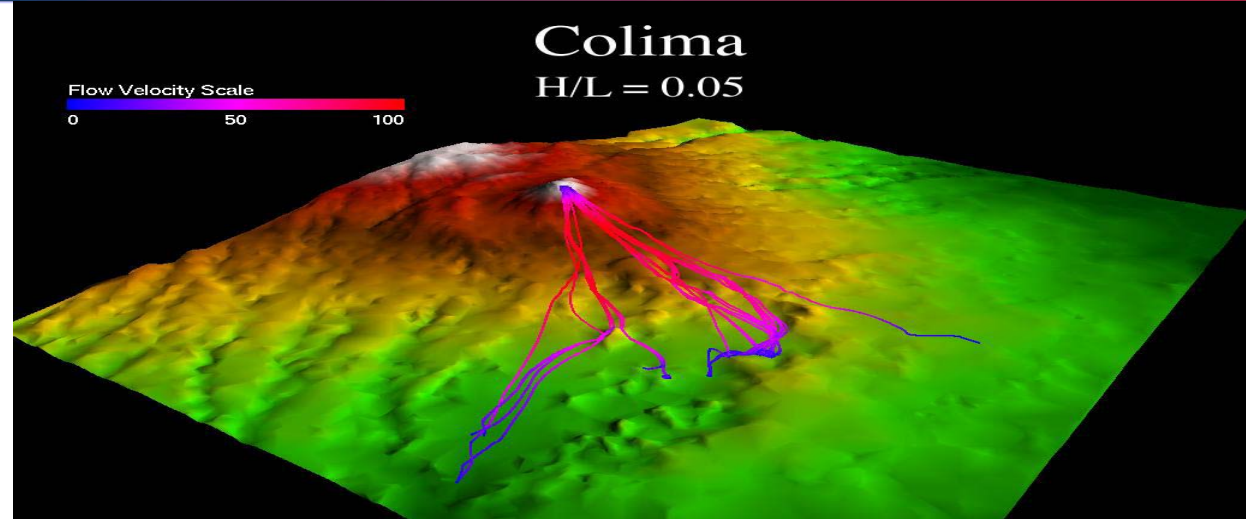
Groundwater Flow Modeling

- 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



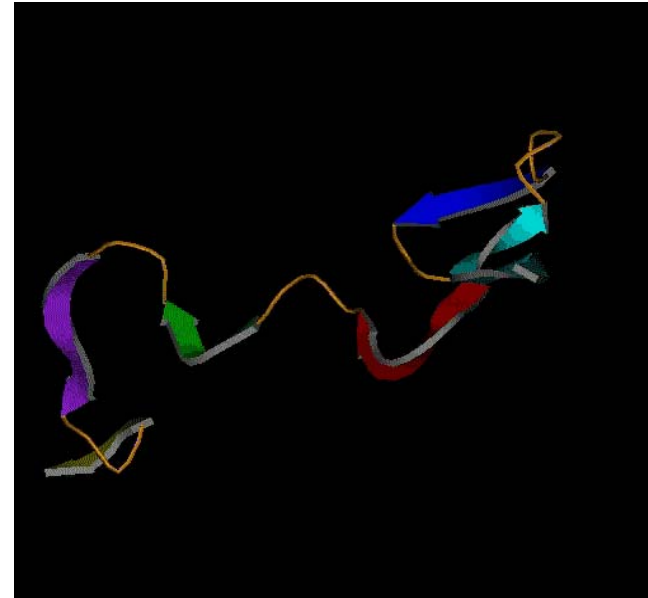
Risk Mitigation

- 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



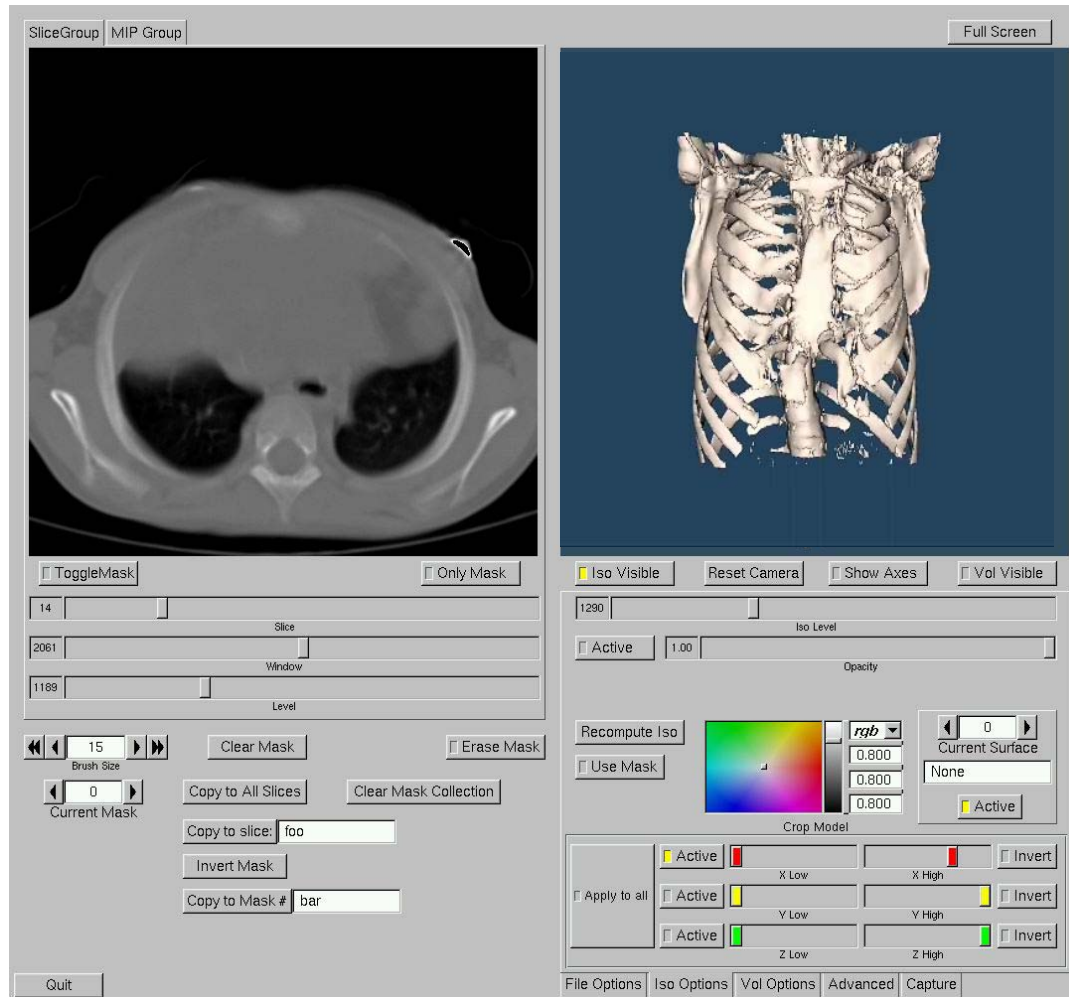
Protein Folding

- 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

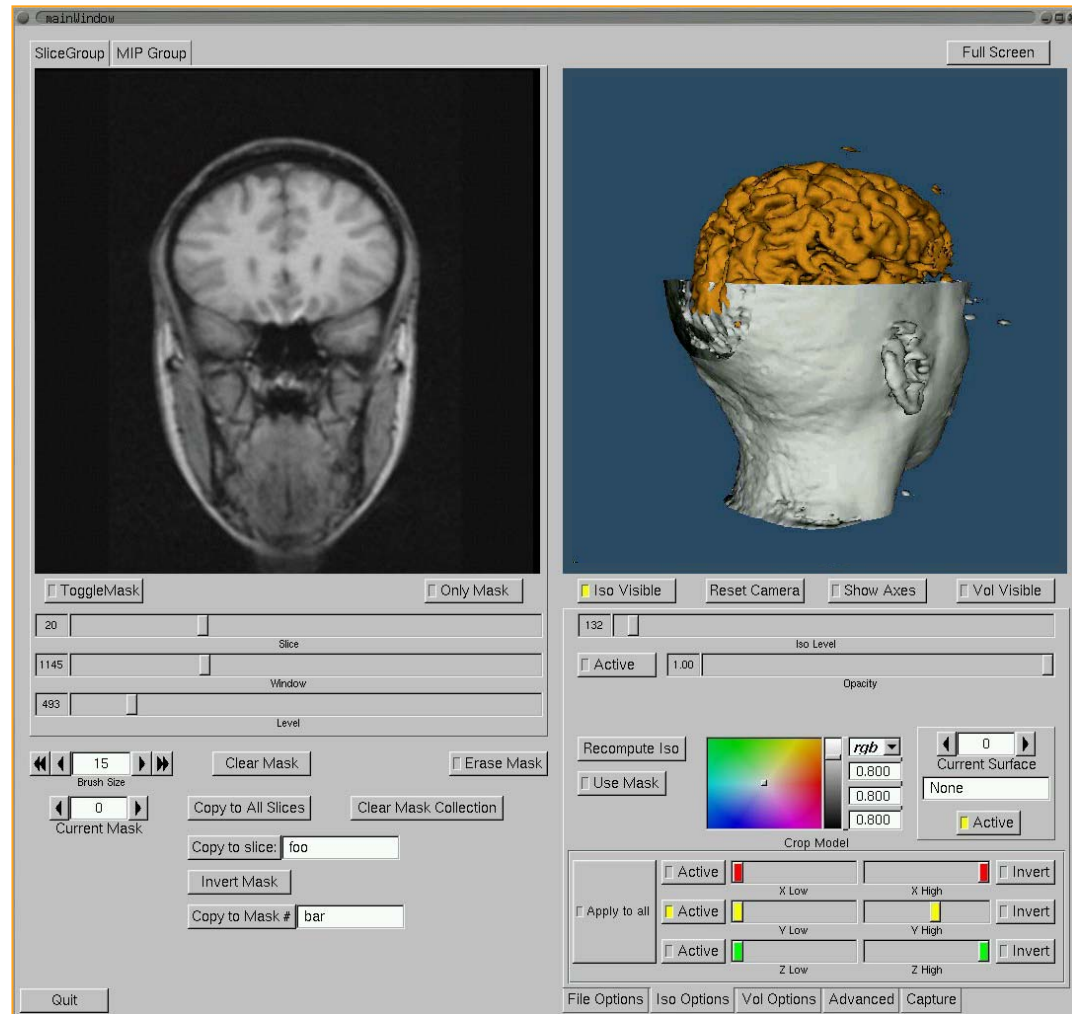


Multiple Sclerosis Project

- 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® Demo

- *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



University of
Business of

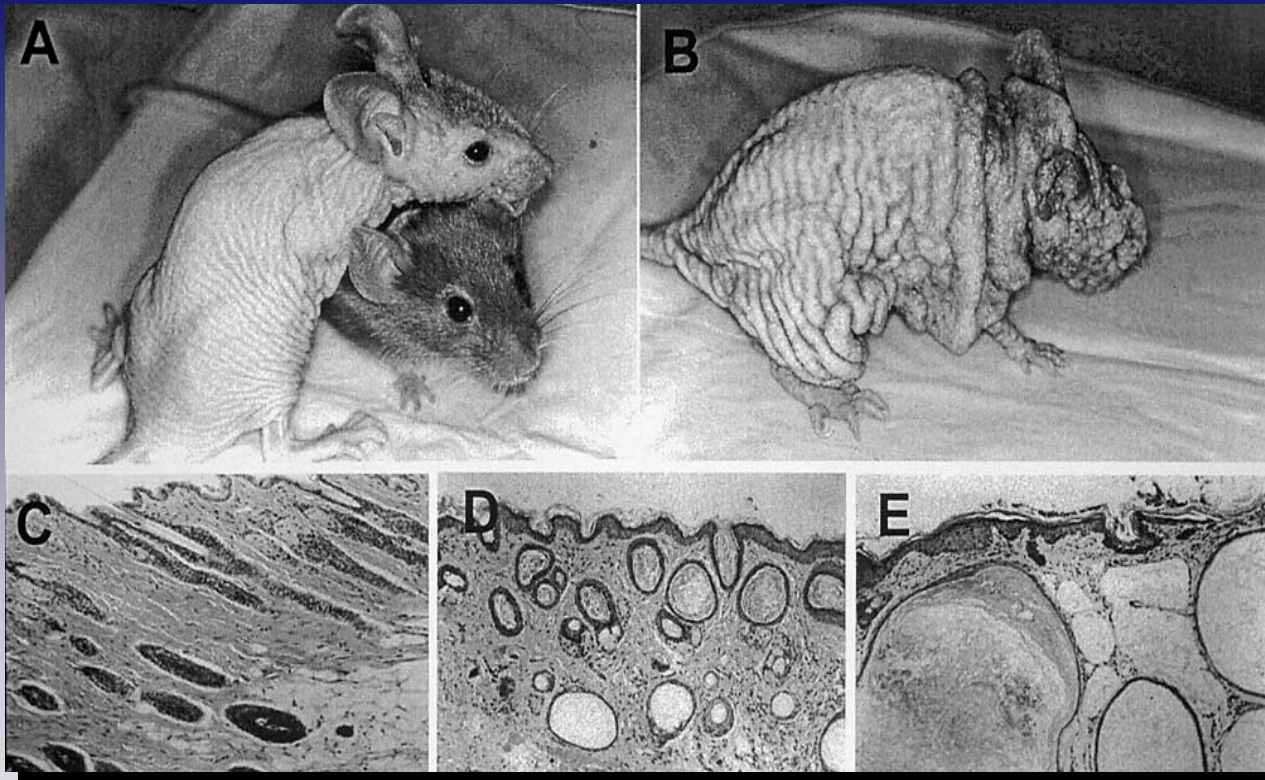
Outreach

CCR

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