The Center for Computational Research

Russ Miller

Director, Center for Computational Research

UB Distinguished Professor, Computer Science & Engineering

Senior Research Scientist, Hauptman-Woodward Medical Inst

University at Buffalo

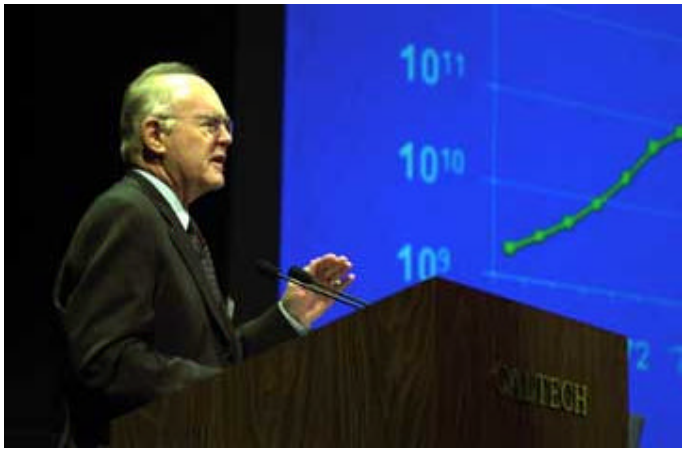
The State University of New York

Computers are used in Many Professions

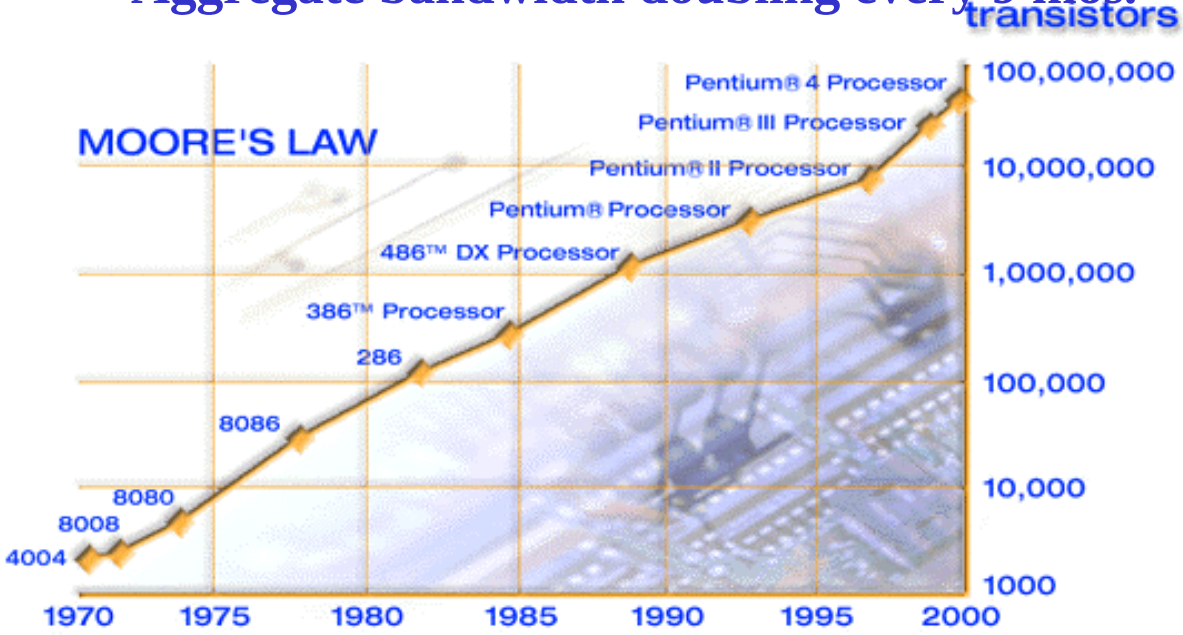
- Science and Engineering
  - Physics, Chemistry, Biology
  - Aerospace, Mechanical, Civil, Environmental
- Architecture
  - Building and Bridge Design
- Computer Animation
  - Cartoons, Movies, Advertising
  - Games (Playstation, Nintendo, PC games, etc)
- Graphic Arts/Design
- Computer Programmers

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

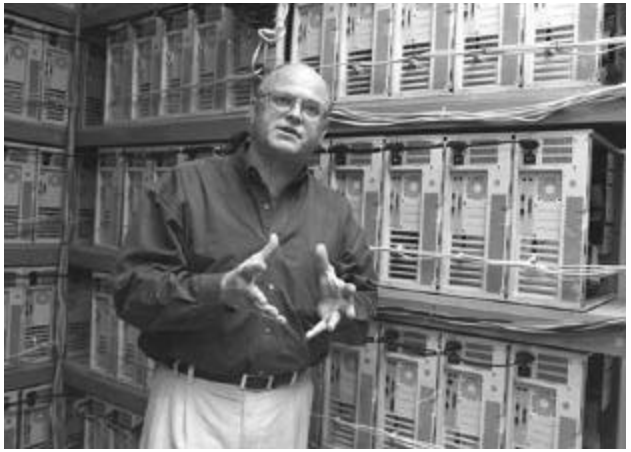


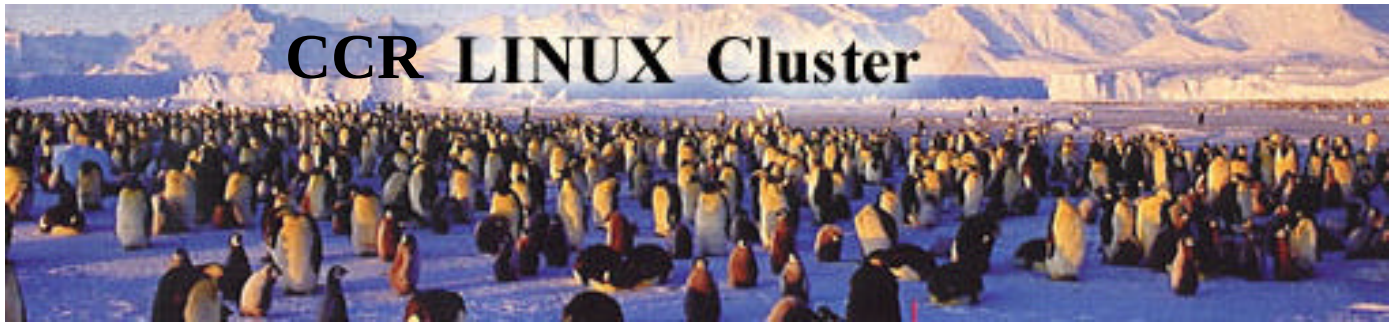
- A computation that took 1 year to run on a PC in 1985 would only take 5 mins to run on a PC today!
- A computation that runs in 2 hours on a PC today would have taken 24 years to run on a PC in 1985!

Beowulf Clusters

- **Industry Standard Hardware and Software**
  - **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**

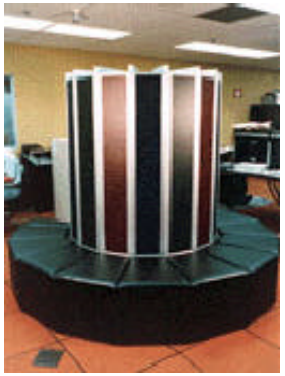
Thomas Sterling
Caltech



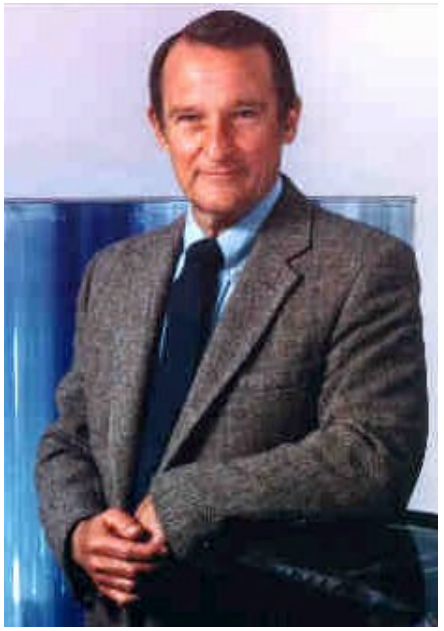


Supercomputers

- **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**



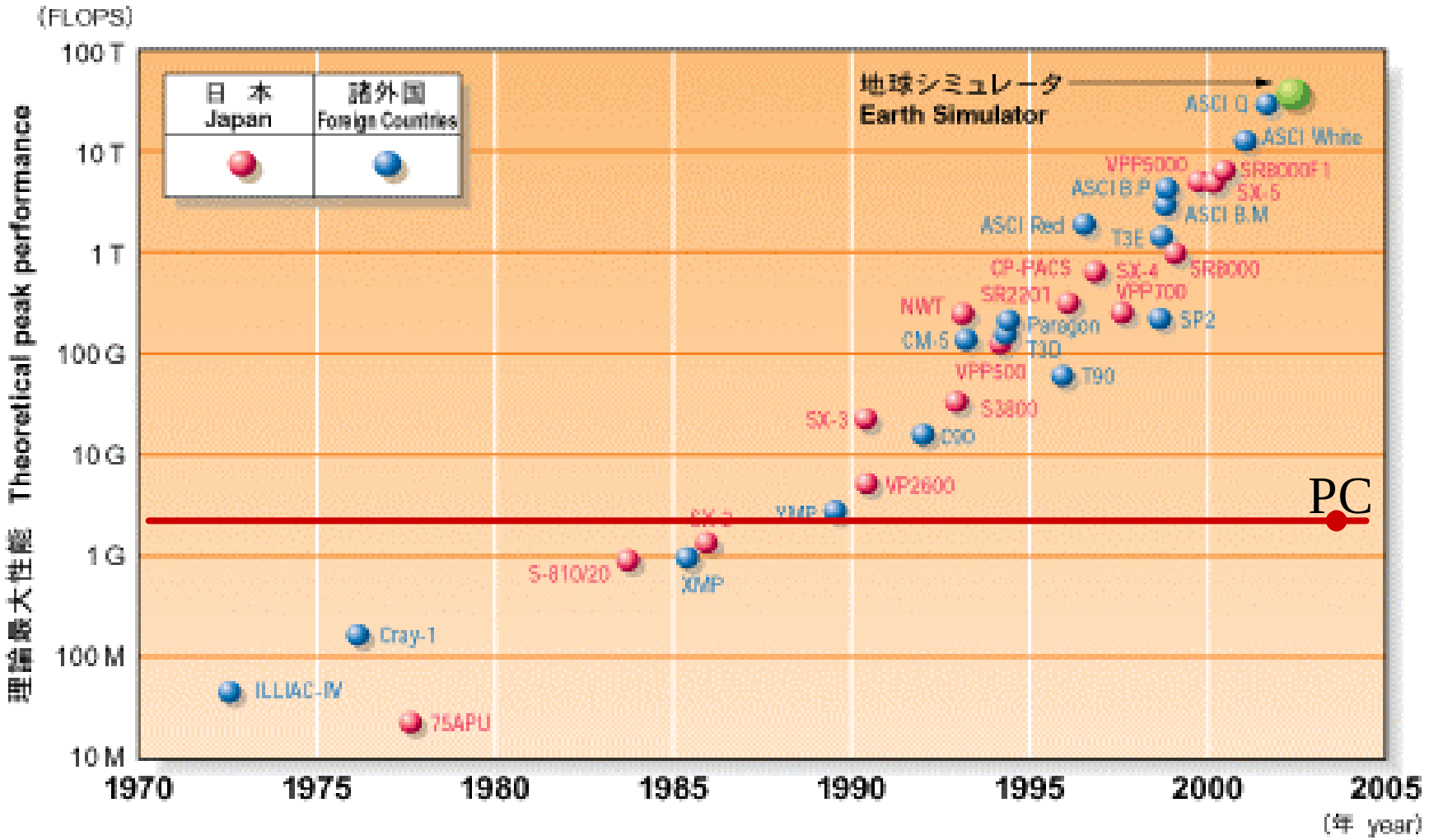
Cray1 - 1976



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

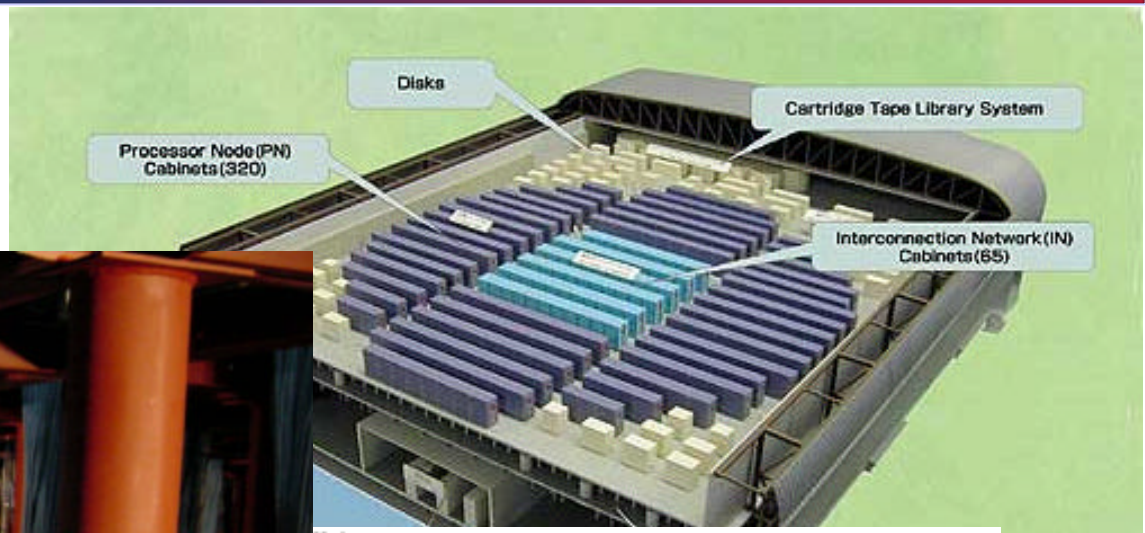
Seymour Cray
1925-1996

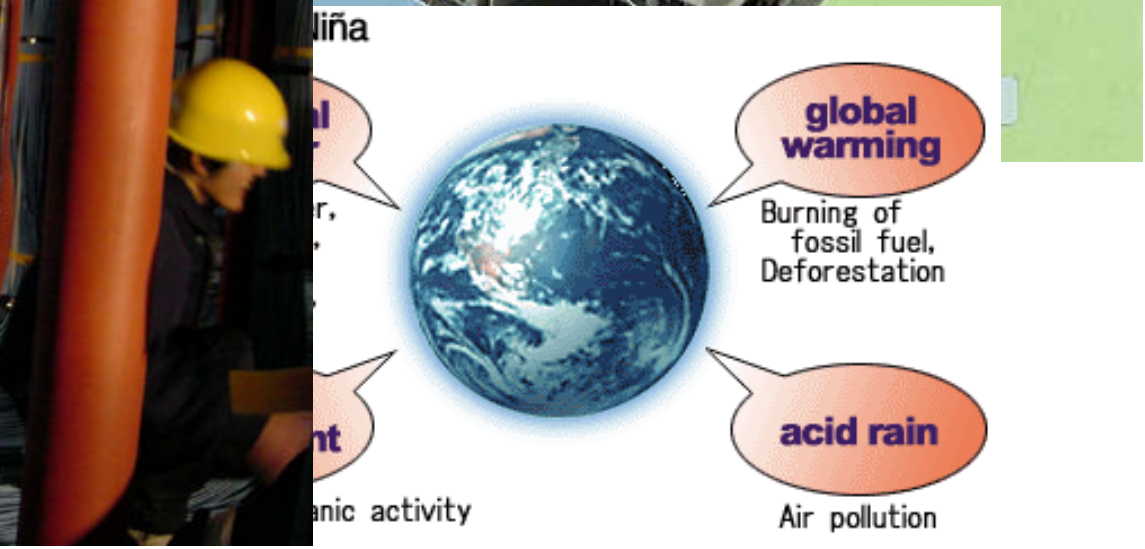
Growth of Peak Performance



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

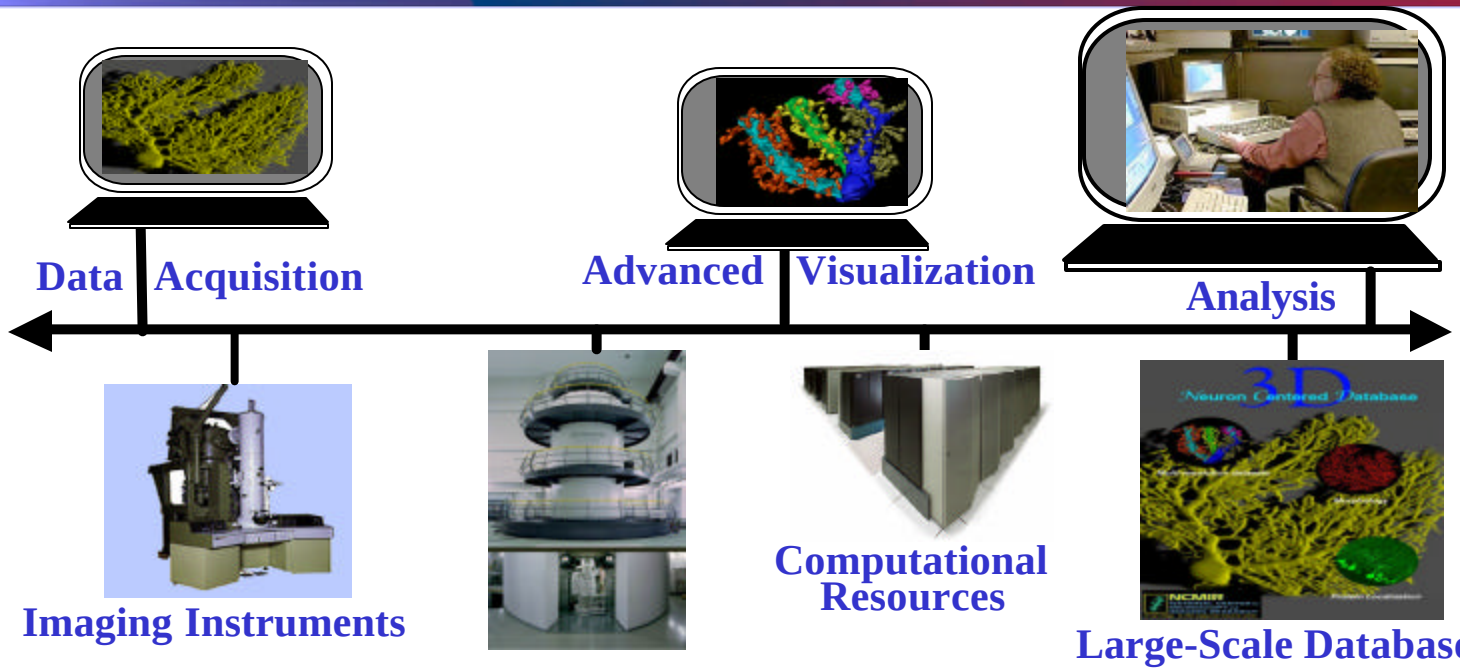
- Dell Linux Cluster: #22 ® #25 ® #38
  - 600 P4 Processors (2.4 GHz)
  - 600 GB RAM; 40 TB Disk; Myrinet
- Dell Linux Cluster: #187 ® #368 ® off
  - 4036 Processors (PIII 1.2 GHz)
  - 2TB RAM; 160TB Disk; 16TB SN
  - Restricted Use (Skolnick)

- SGI Origin3800
  - 64 Processors (400 MHz)
  - 32 GB RAM; 400 GB Disk
- Apex Bioinformatics System
  - Sun V880 (3), 6800, 280R (2), PIIIs
  - Sun 3960: 7 TB Disk Storage
- HP/Compaq SAN
  - 75 TB Disk; 190 TB Tape

Exit Strategy Required for Following

- IBM RS/6000 SP
  - 78 Heterogeneous Processors
- Sun Microsystems Cluster
  - 80 Heterogeneous Processors
  - Myrinet
- SGI Intel Linux Cluster
  - 150 PIII Processors (1 GHz)
  - Myrinet

Grid Computing Overview



Thanks to Mark Ellisman

- 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

Advanced CCR Data Center (ACDC) Computational Grid Overview

Nash: Compute Cluster

75 Dual Processor
1 GHz Pentium III
RedHat Linux 7.3
1.8 TB Scratch Space

Joplin: Compute Cluster

300 Dual Processor
2.4 GHz Intel Xeon
RedHat Linux 7.3
38.7 TB Scratch Space

Mama: Compute Cluster

9 Dual Processor
1 GHz Pentium III
RedHat Linux 7.3
315 GB Scratch Space

ACDC: Grid Portal

4 Processor Dell 6650
1.6 GHz Intel Xeon
RedHat Linux 9.0
66 GB Scratch Space

Young: Compute Cluster

16 Dual Sun Blades
47 Sun Ultra5
Solaris 8
770 GB Scratch Space

Crosby: Compute Cluster

SGI Origin 3800
64 - 400 MHz IP35
IRIX 6.5.14m
360 GB Scratch Space

Fogerty: Condor Flock Master

1 Dual Processor
250 MHz IP30
IRIX 6.5

Expanding

RedHat, IRIX, Solaris, WINNT, etc

CCR

19 IRIX, RedHat, & WINNT Processors

T1 Connection

Computer Science & Engineering

25 Single Processor Sun Ultra5s

School of Dental Medicine

9 Single Processor Dell P4 Desktops

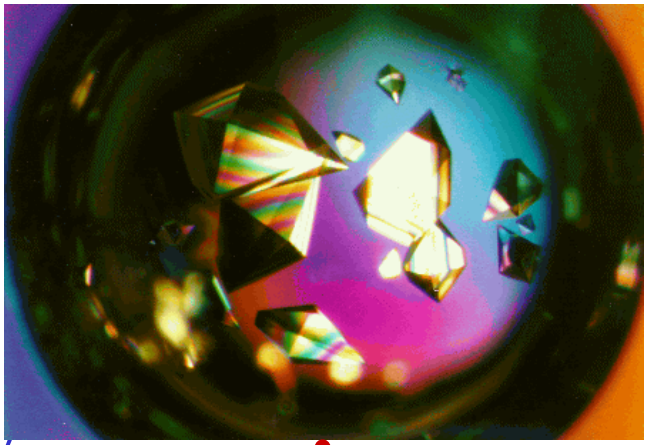
Hauptman-Woodward Institute

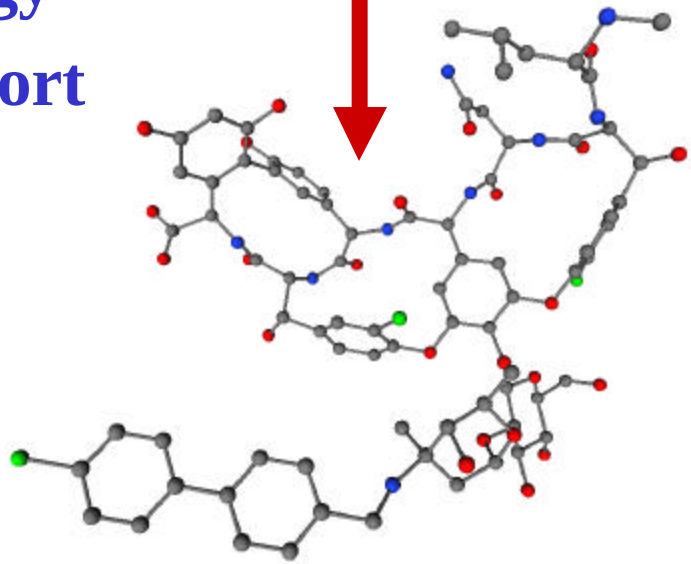
13 Various SGI IRIX Processors

Note: Network connections are 100 Mbps unless otherwise noted.

Molecular Structure Determination via *Shake-and-Bake*

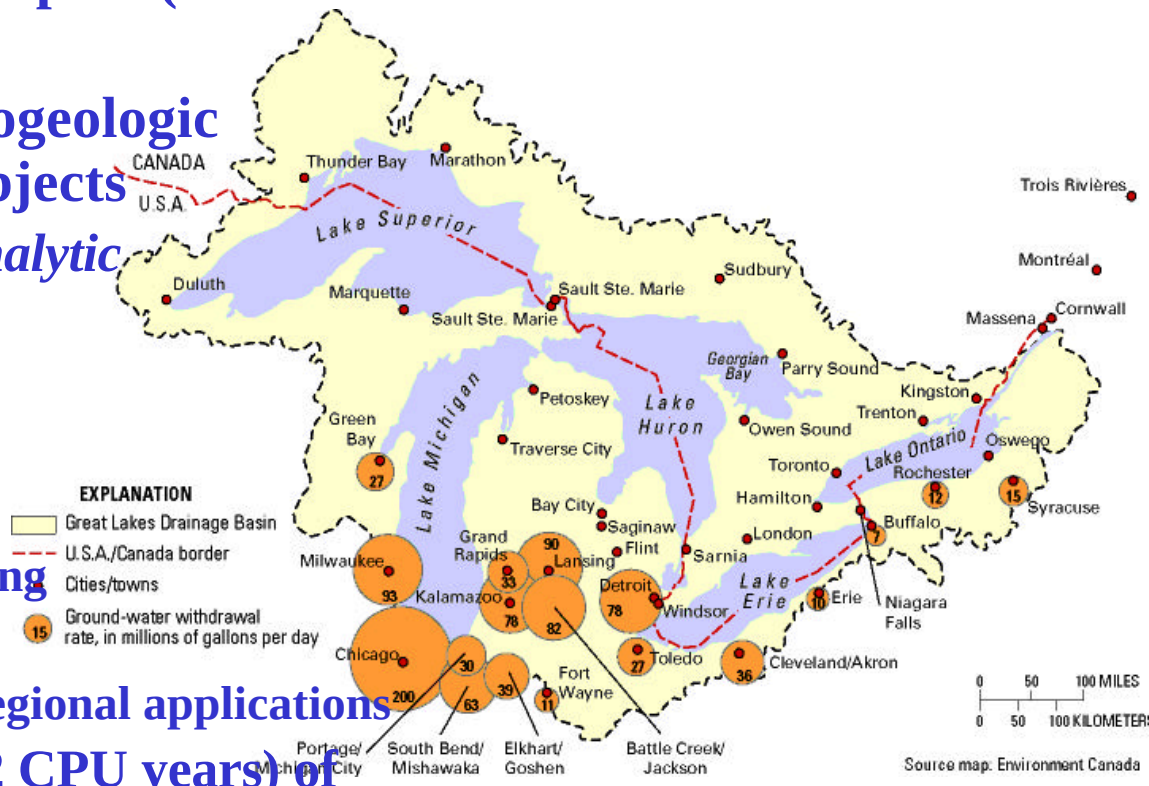
- ***SnB* Software by UB/HWI**
  - **"Top Algorithms of the Century"**
- **Worldwide Utilization**
- **Critical to Rational Drug Design**
- **Important Link in Structural Biology**
- **Vancomycin: Antibiotic of Last Resort**
- **Current Effort**
  - **Grid**
  - **Collaboratory**
  - **Intelligent Learning**





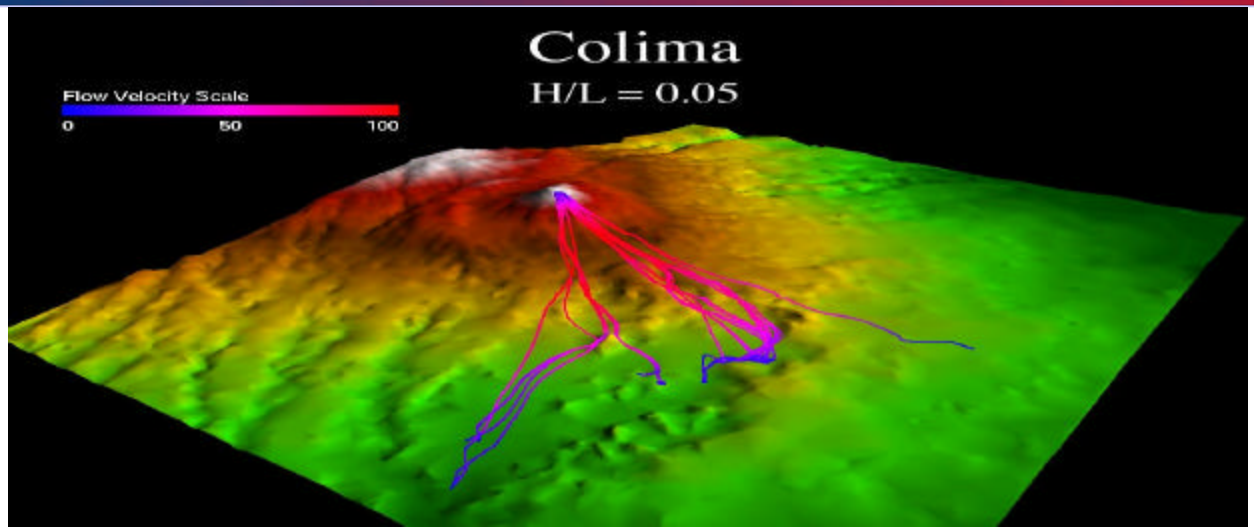
Groundwater Flow Modeling

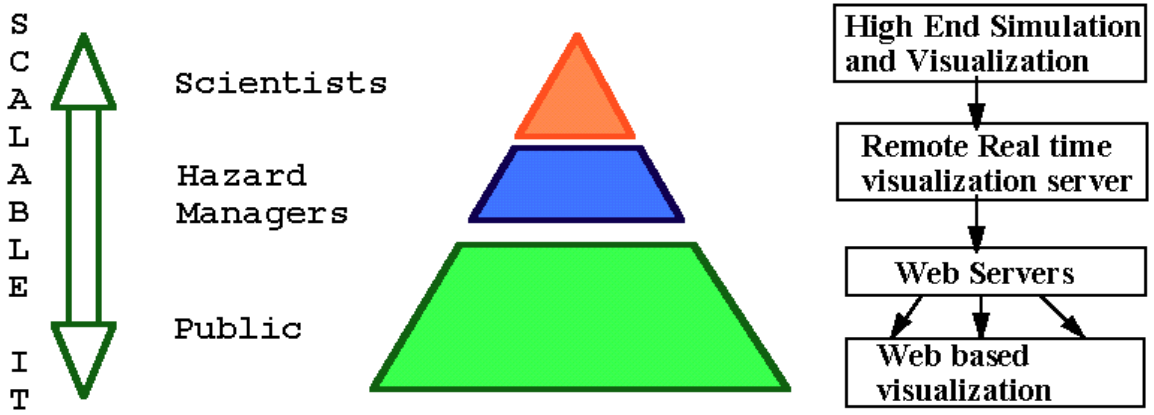
- **Regional-scale modeling of groundwater flow and contaminant transport (Great Lakes Region)**
- **Ability to include all hydrogeologic features as independent objects**
- **Current work is based on *Analytic Element Method***
- **Key features:**
  - **High precision**
  - **Highly parallel**
  - **Object-oriented 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

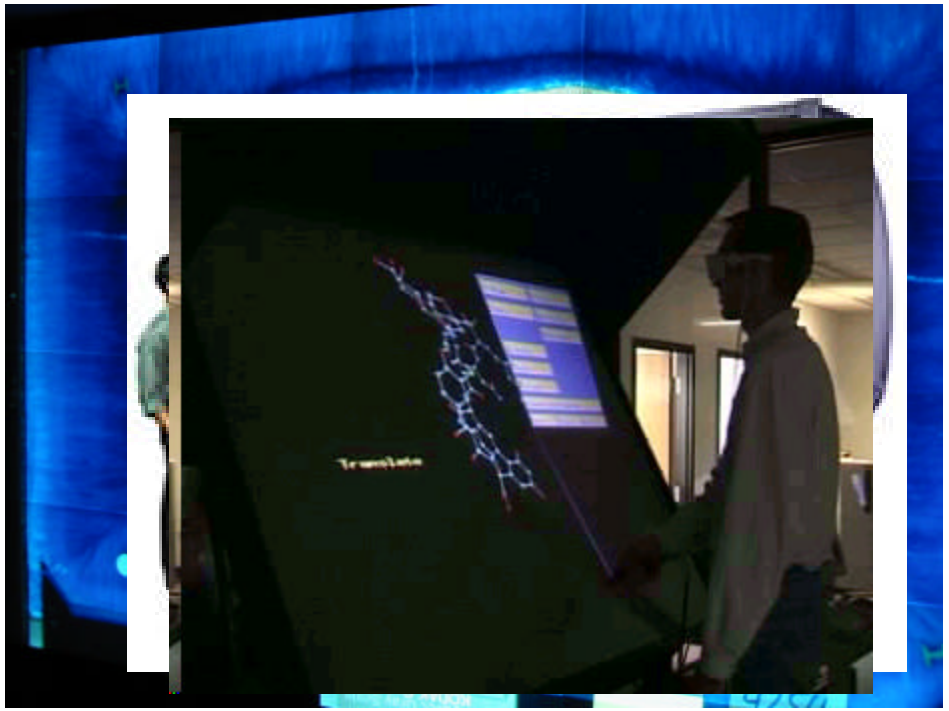
- Integrate information from several sources
  - Simulation results
  - Remote sensing
  - GIS data
- Develop realistic 3D models of geophysical mass flows
- Present information at user appropriate resolutions





CCR Visualization Resources

- **Fakespace ImmersaDesk R2**
  - Portable 3D Device
- **Tiled-Display Wall**
  - 20 NEC projectors: 15.7M pixels
  - Screen is 11’ ´ 7’
  - Dell PCs with Myrinet2000
- **Access Grid Node**
  - Group-to-Group Communication
  - Commodity components
- **SGI Reality Center 3300W**
  - Dual Barco’s on 8’ ´ 4’ screen
- **VREX VR-4200 Stereo Imaging Projector**
  - Portable projector works with PC



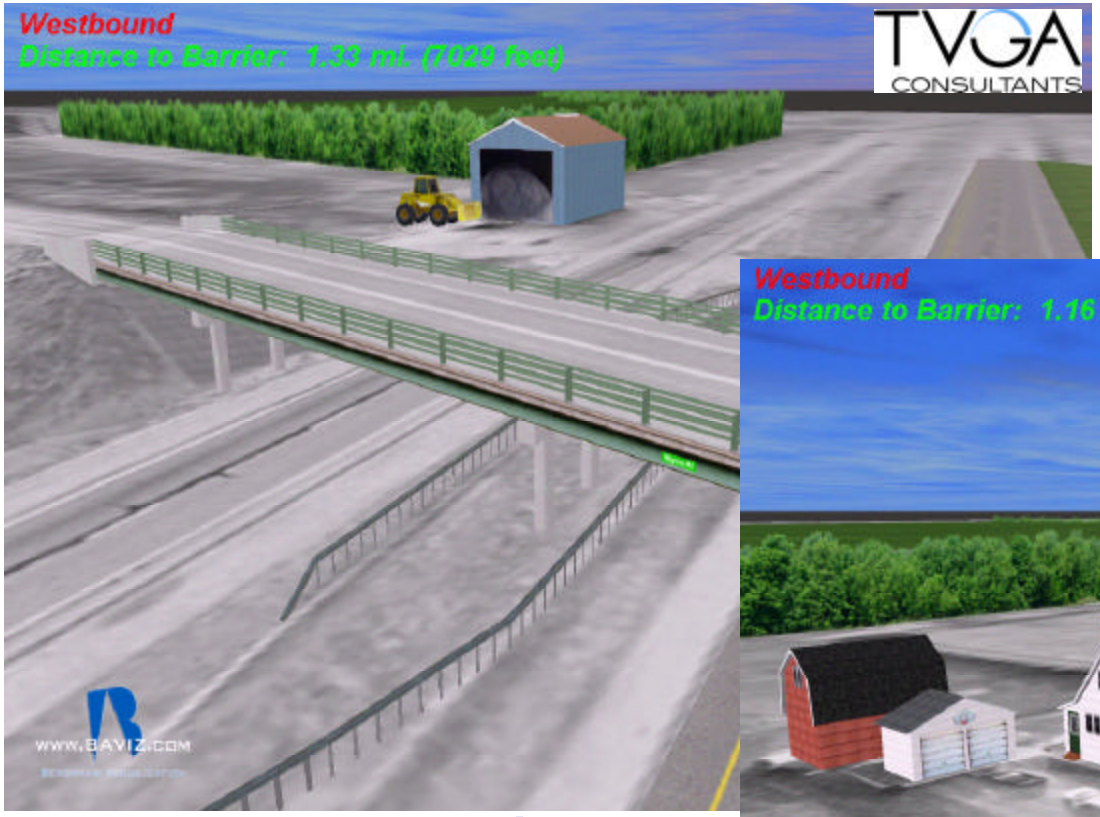
Visualization in Planning Studies

Bergmann Associates: Indian Street Bridge - Florida

Williamsville Toll Barrier Improvement Project

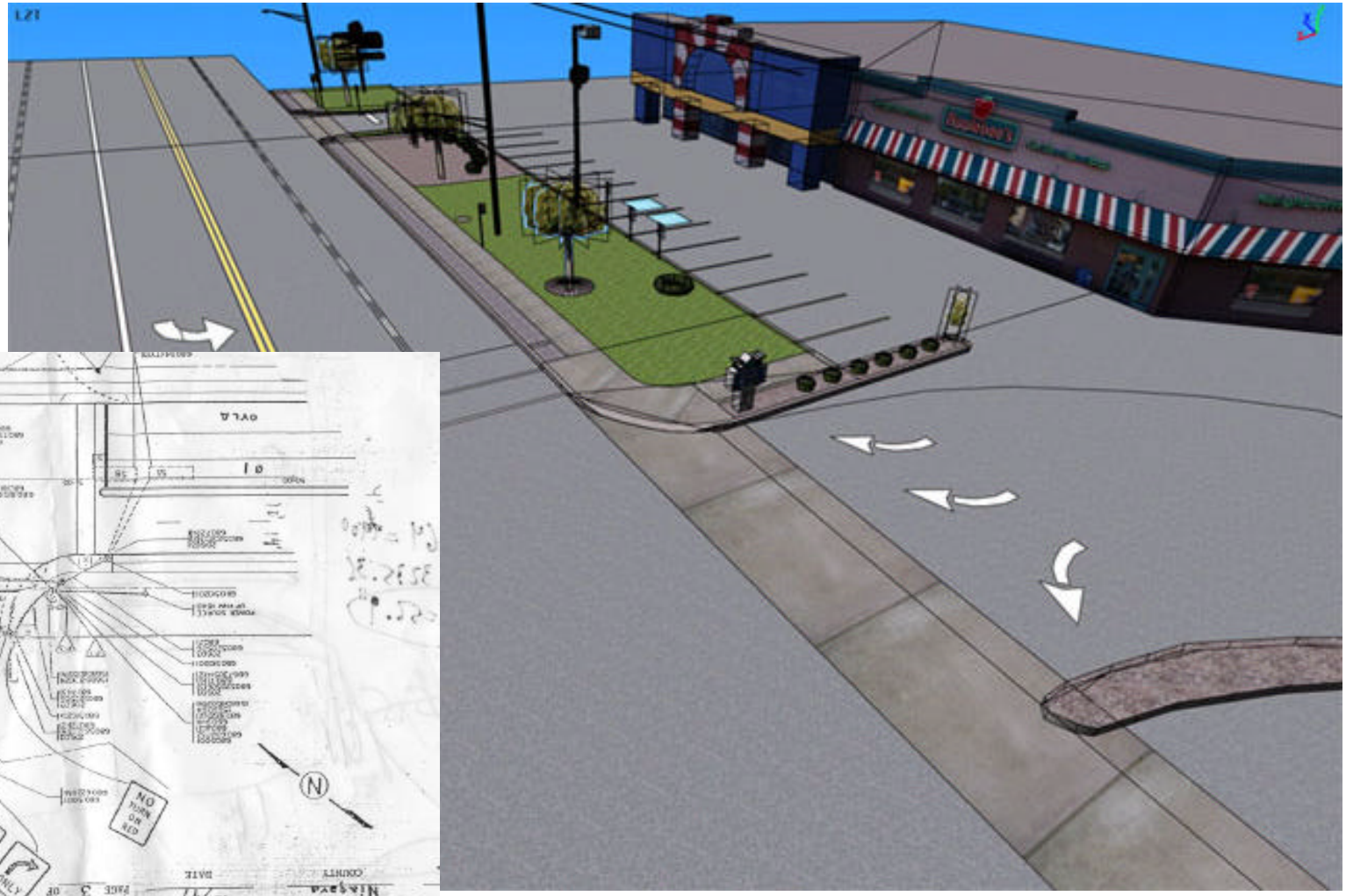
Initial Photo Match incorporating real and computer-generated components

Real-time Simulation

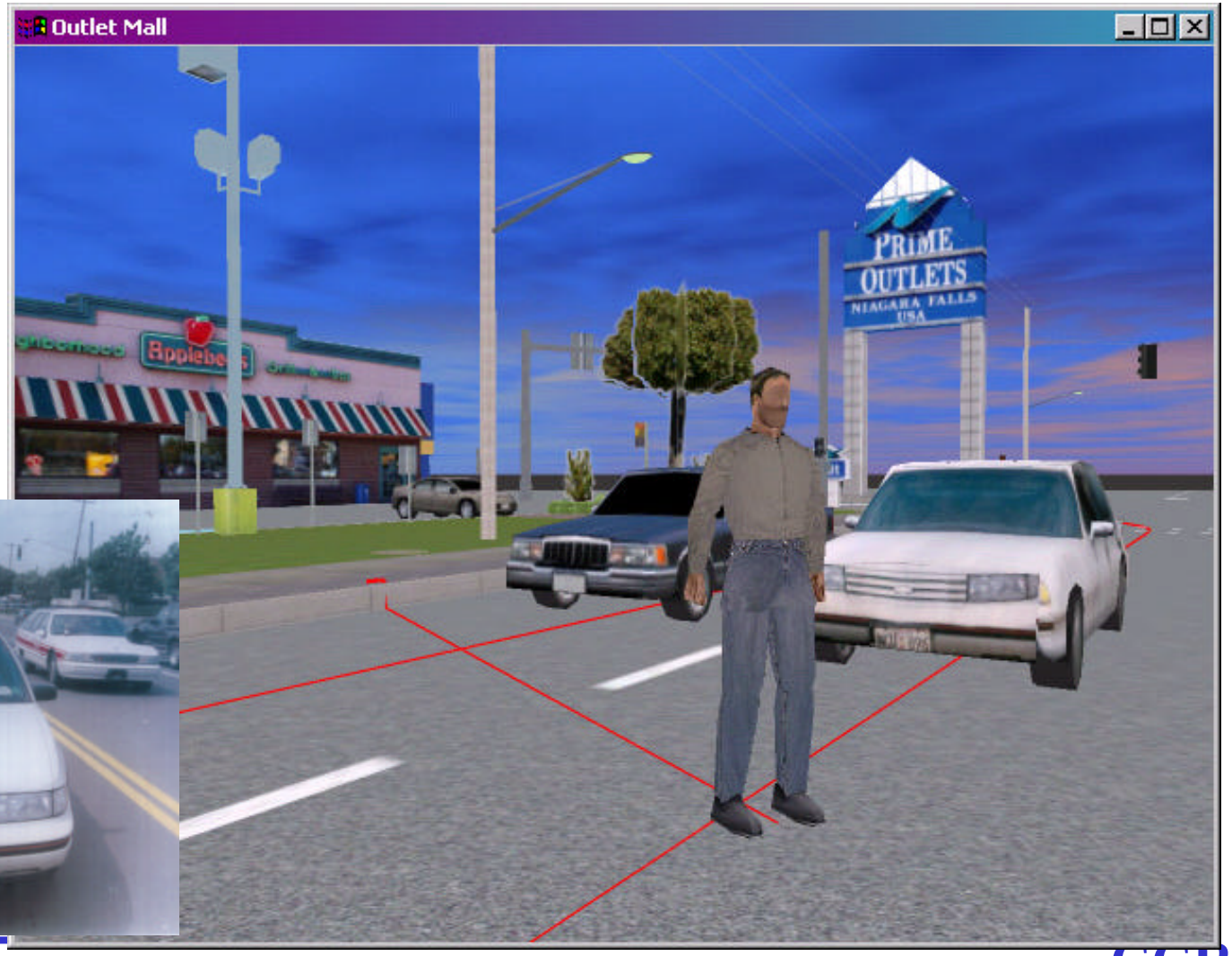


- Key Receptor Sites
- Multiple Viewpoints
- Fully Interactive
- Aerial Photography

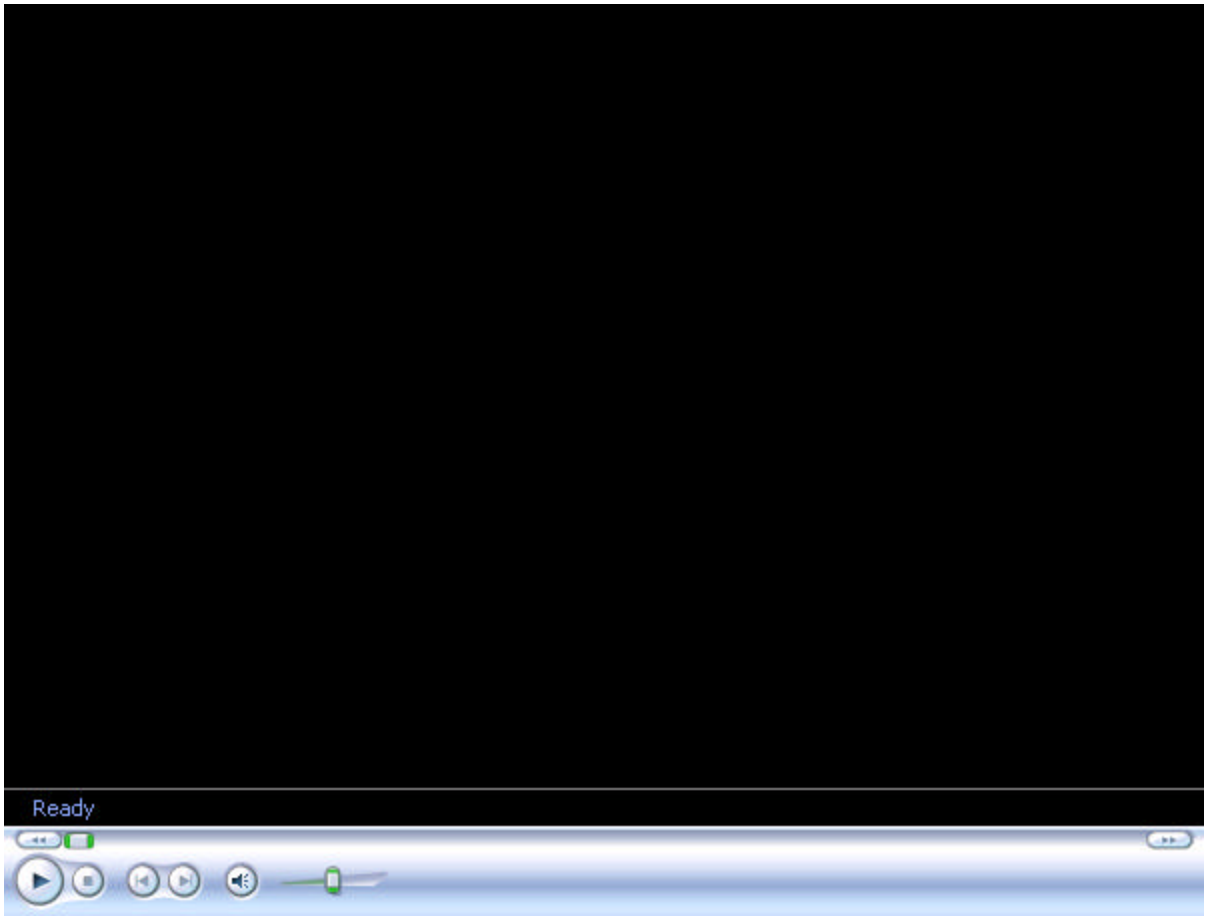
Accident Reconstruction



The Accident

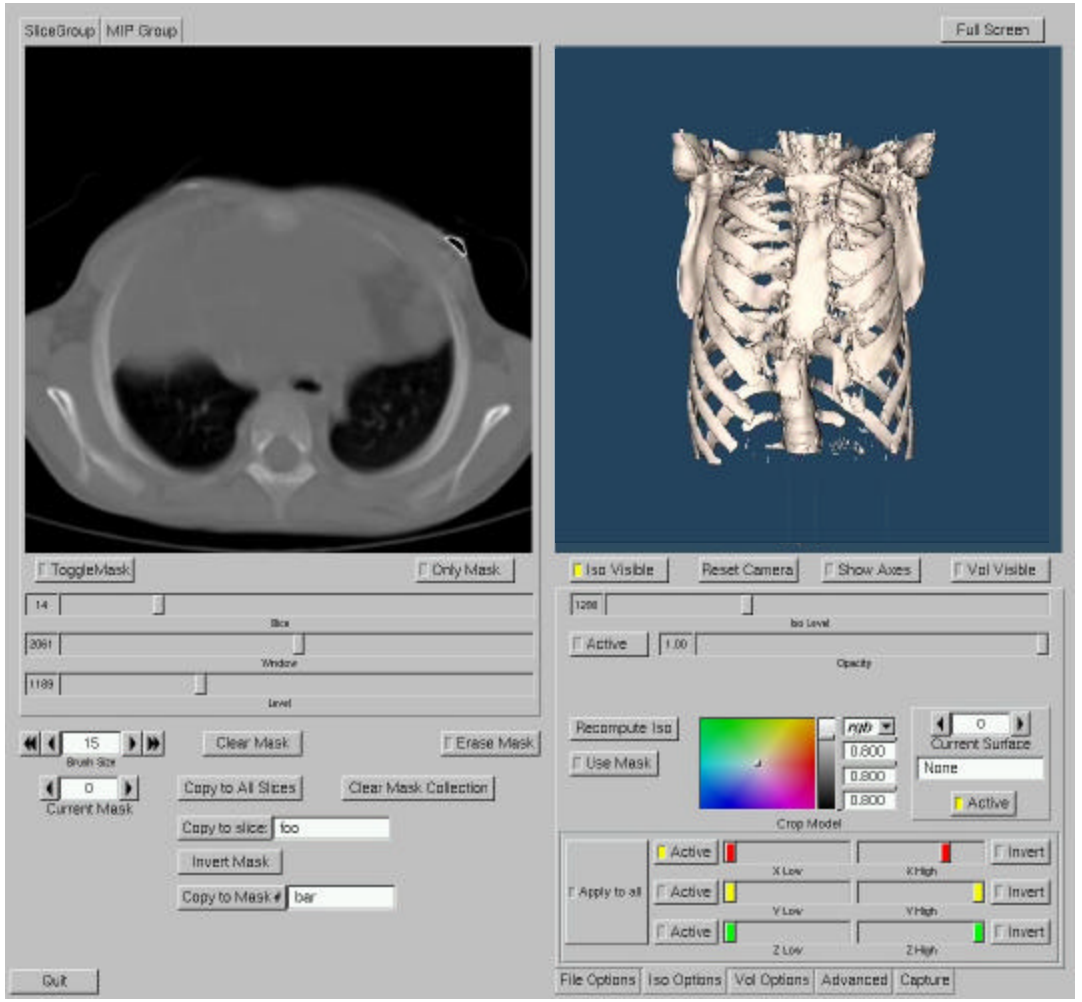


Accident Animation (Driver's View)



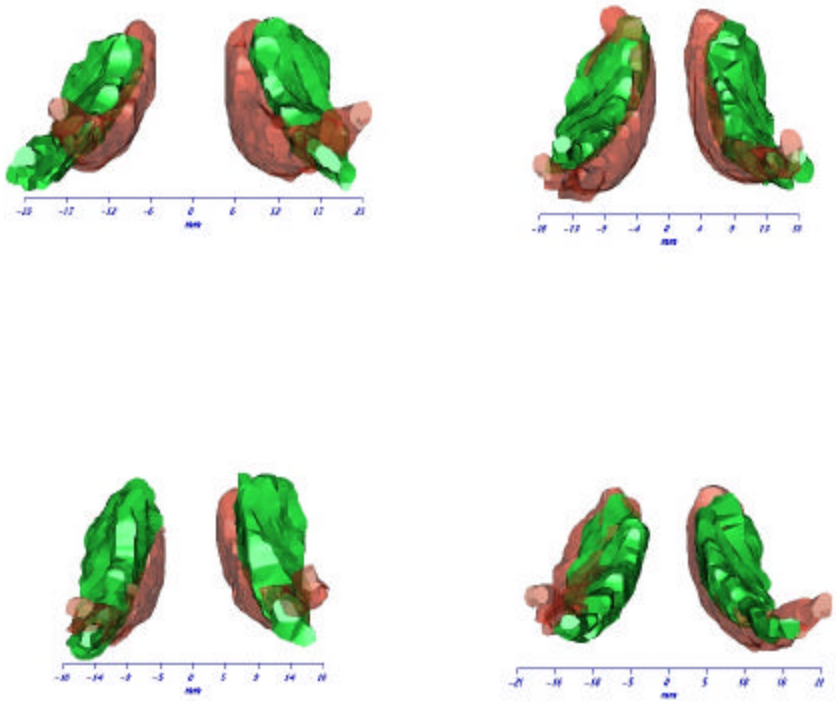
3D Medical Visualization App

- 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

- Compare caudate nuclei between MS patients and healthy controls
- Looking for size as well as structure changes
  - Localized deformities
  - Spacing between halves
- Able to see correlation between disease progression and physical structure changes



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

Outreach

- **HS Summer Workshops in Computational Science**
  - **Chemistry, Bioinformatics, Visualization**
  - **10-14 HS Students Participate Each Summer for 2 weeks**
  - **Project-Based Program**

Outreach

- **Pilot HS Program in Computational Science**
  - **Year long extracurricular activity at Mount St. Mary's, City Honors, and Orchard Park HS**
  - **Produce next generation scientists and engineers**
  - **Students learn Perl, SQL, Bioinformatics**
  - **$50,000 startup funding from Verizon, PC's from HP**

Media Coverage

BUFFALO
Business First
Western New York's Business Newspaper

HMOs cut Medicare premiums

Patio home development proposed for Town of Aurora

Grammy: Designs on Buffalo

Ani DiFranco, art director up for award

UB brings bioinformatics to a younger generation

THE BUFFALO NEWS

EDUCATION

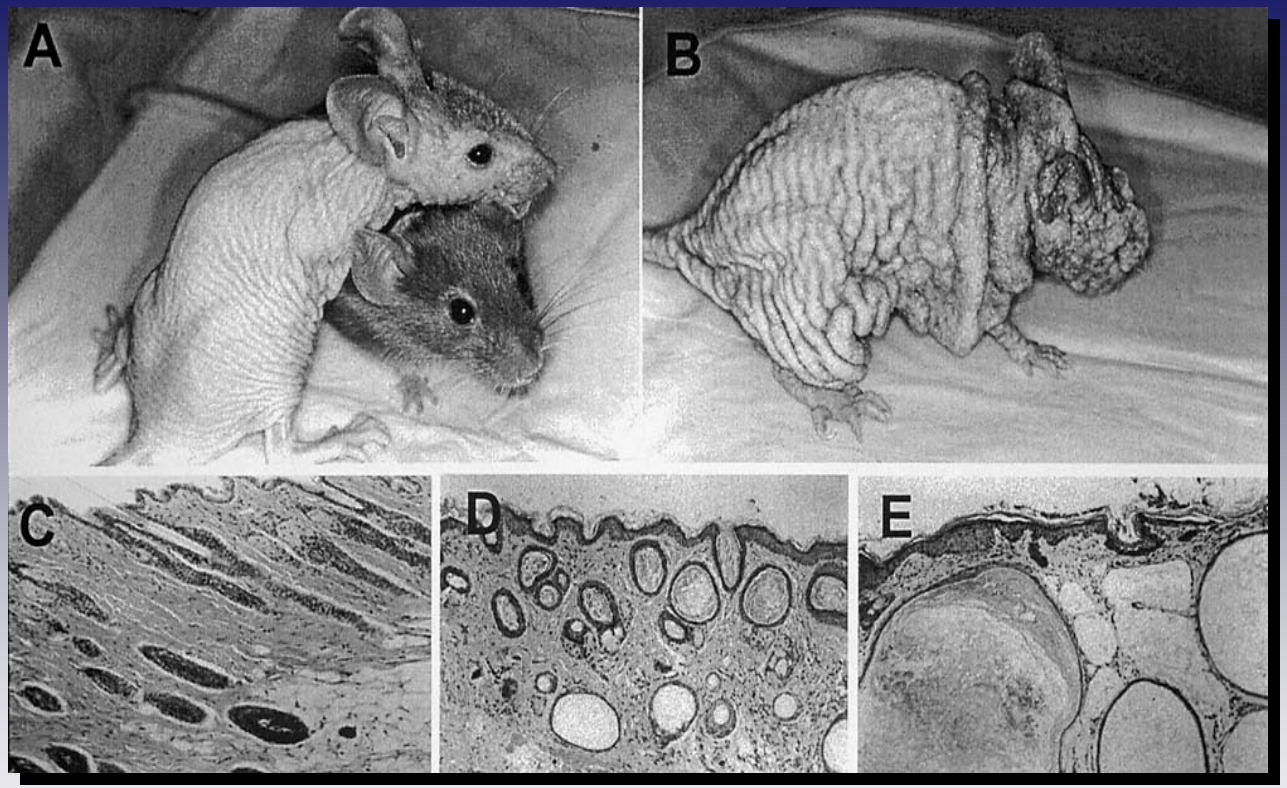
University at Buffalo undergraduate David Walla works with Jaclyn Shaw, right, to demonstrate the "Next Generation Scientists" program. At left is Shannon D'Arcy.

An early look at bioinformatics

By EMMA D. SAPONG
News Northtowns Bureau


Outreach
CCR

Contact Information



miller@buffalo.edu
www.ccr.buffalo.edu