

# 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*

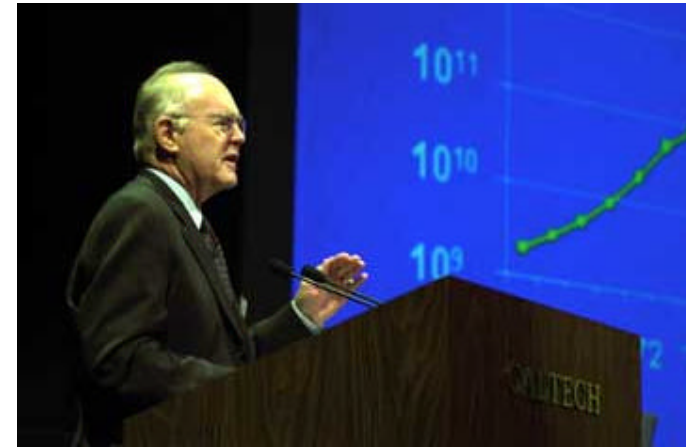
# Computers are used in Many Professions

- 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

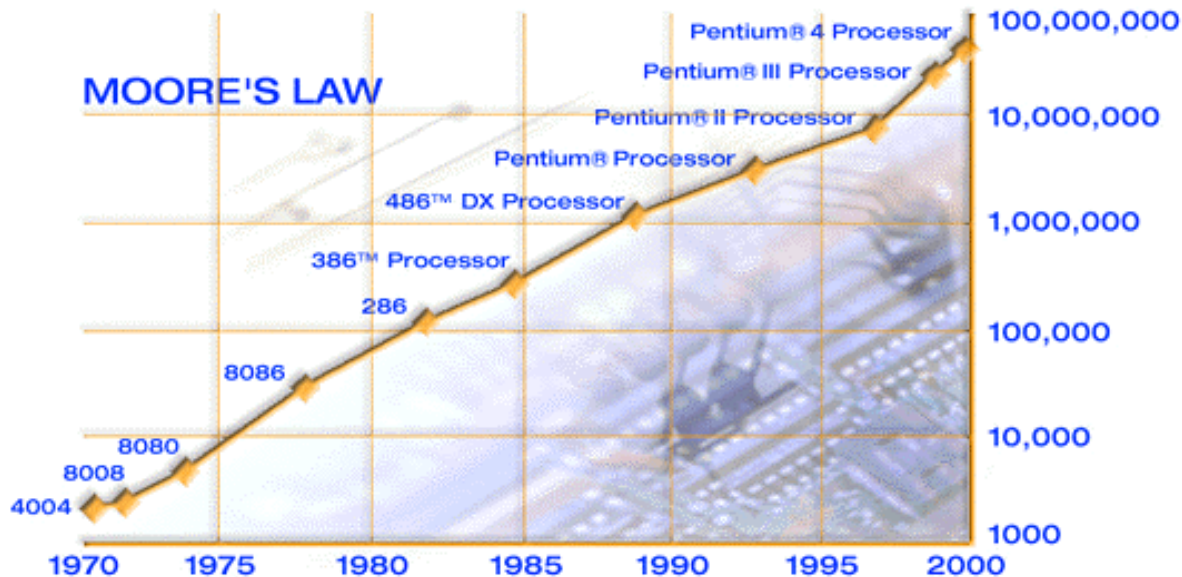


# Gordon E. Moore

- 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

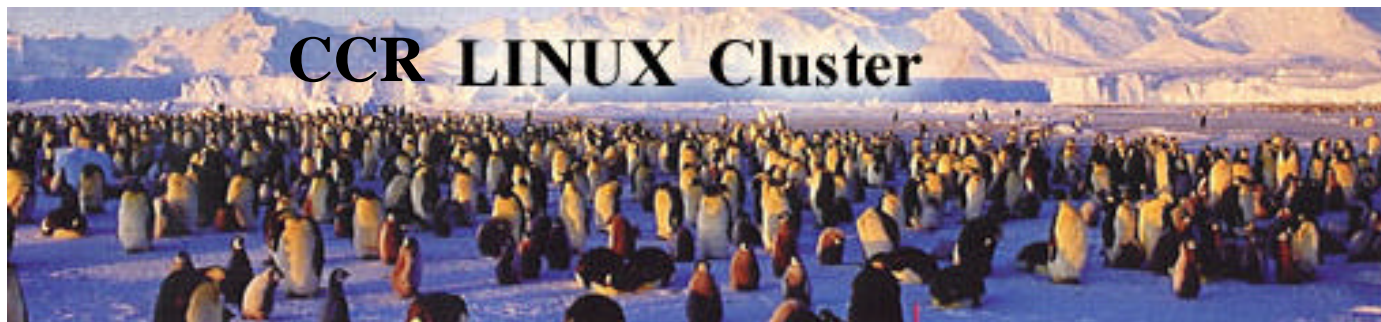
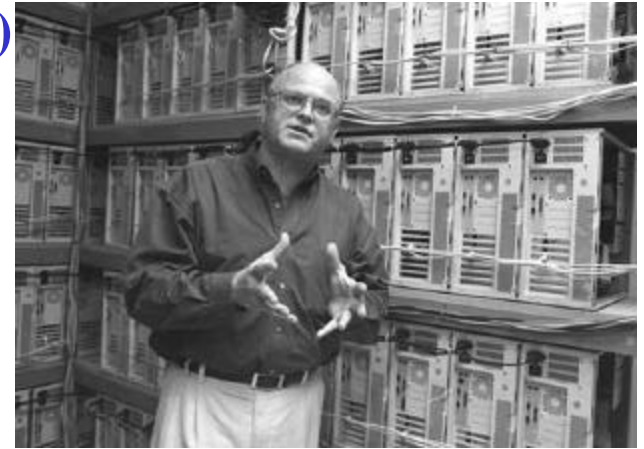
## ■ Industry Standard Hardware and Software

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”**

**- Larry L. Smarr**

**Seymour Cray**  
1925-1996

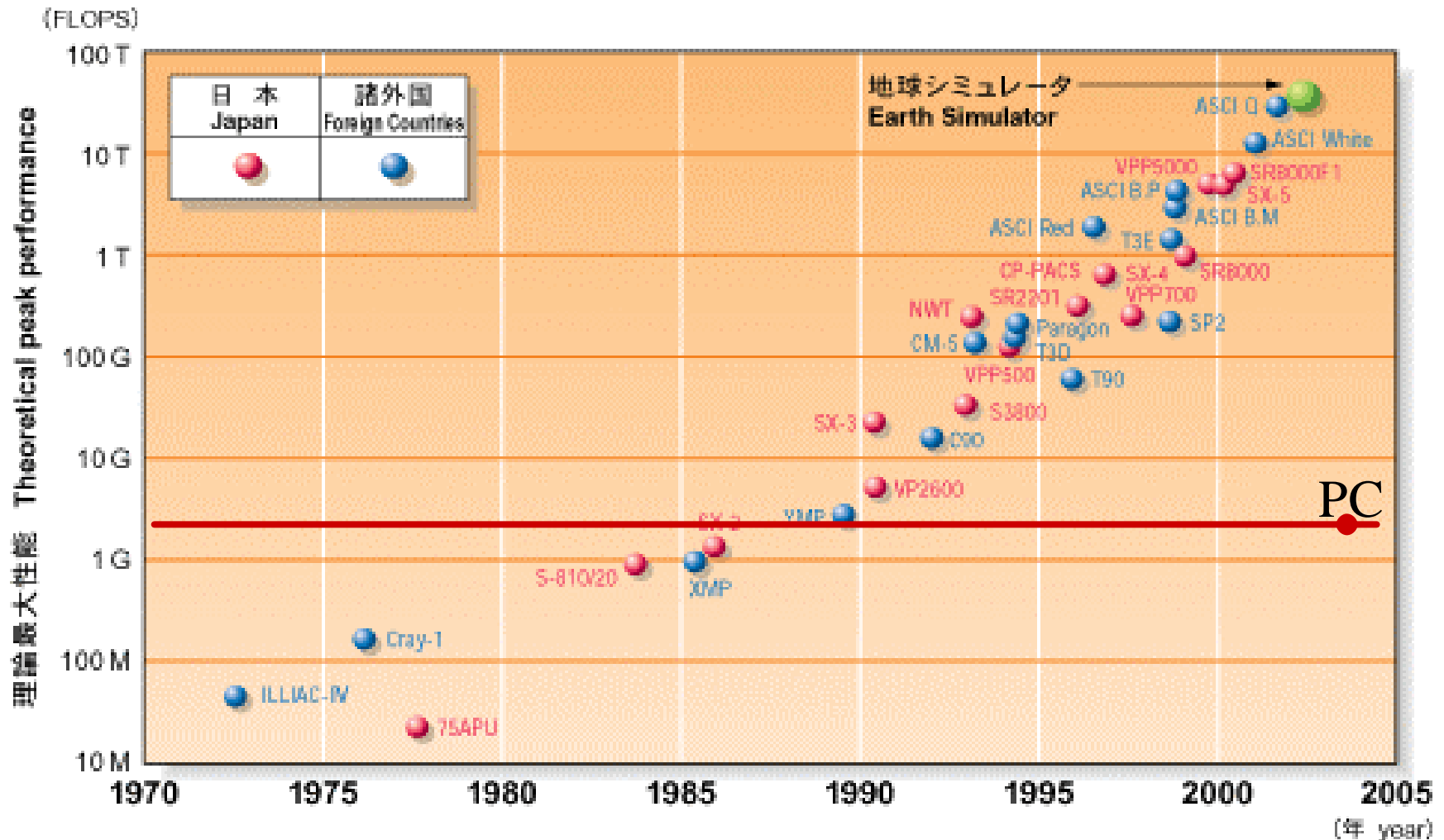


University at Buffalo *The State University of New York*

Center for Computational Research

**CCR**

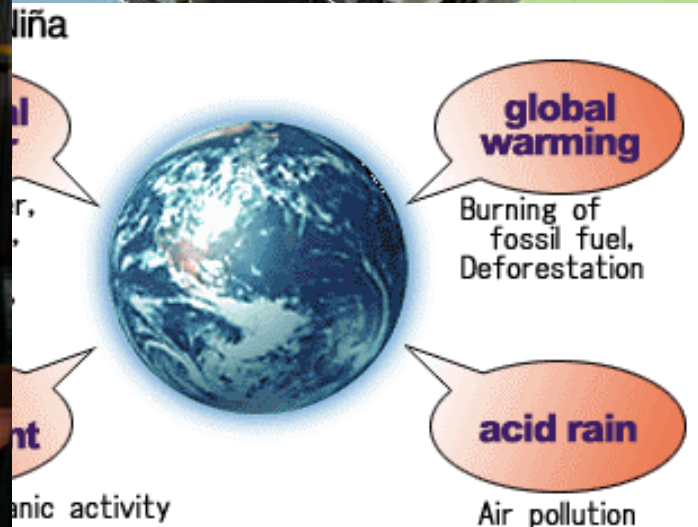
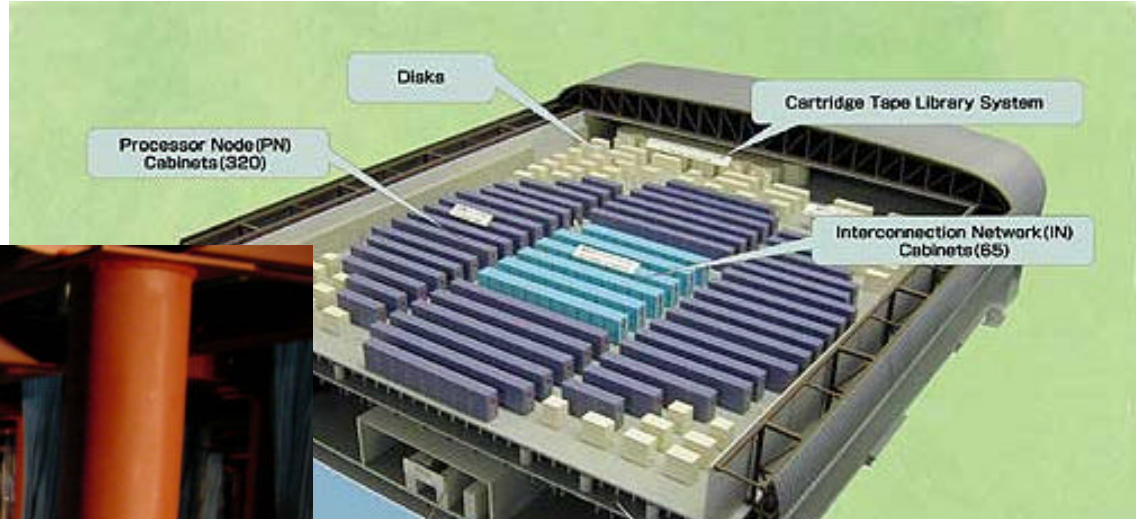
# Growth of Peak Performance





# 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



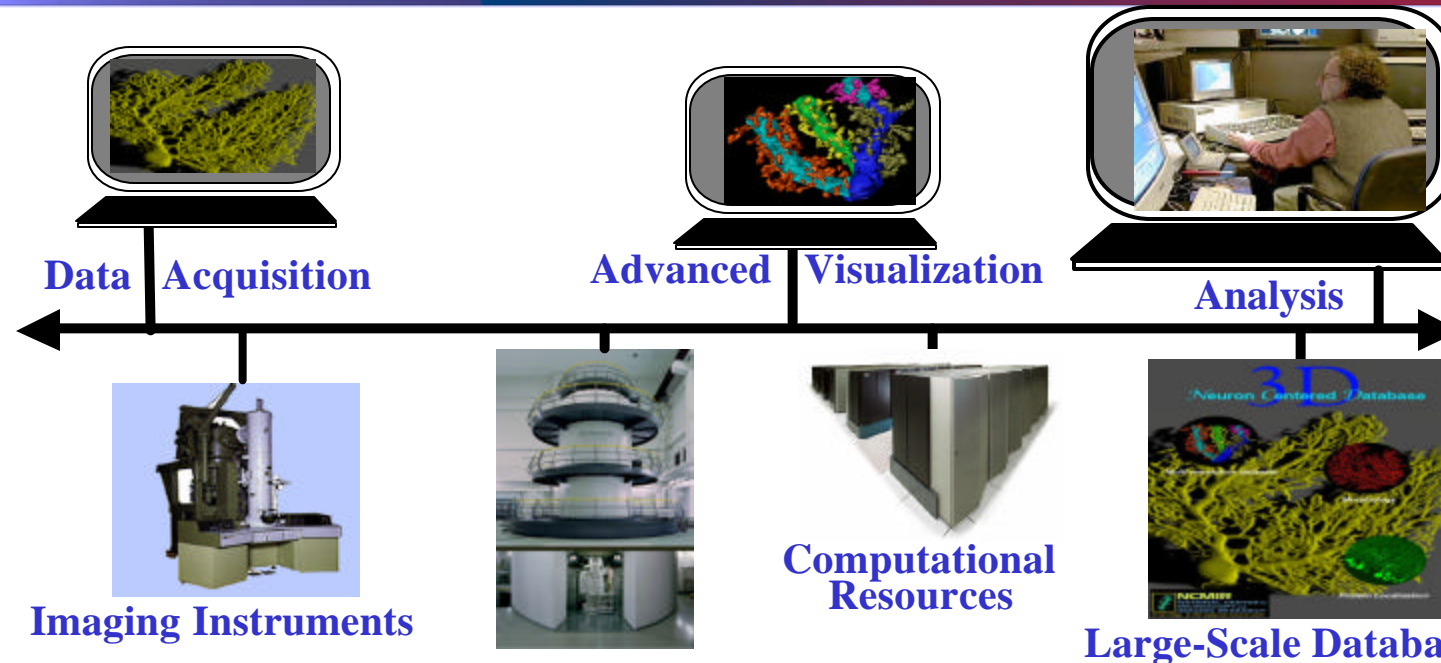
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## Exit Strategy Required for Following

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- **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

## Joplin: Compute Cluster

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



## Nash: Compute Cluster



75 Dual Processor  
1 GHz Pentium III  
RedHat Linux 7.3  
1.8 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



## Expanding

RedHat, IRIX, Solaris,  
WINNT, etc

## Fogerty: Condor Flock Master

1 Dual Processor  
250 MHz IP30  
IRIX 6.5



## CCR

19 IRIX, RedHat, &  
WINNT Processors

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

T1 Connection

Note: Network connections are 100 Mbps unless otherwise noted.



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The State University of New York

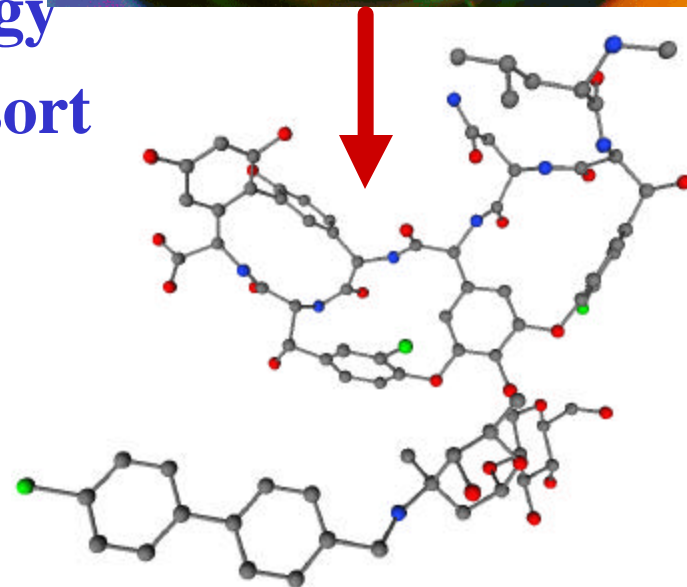
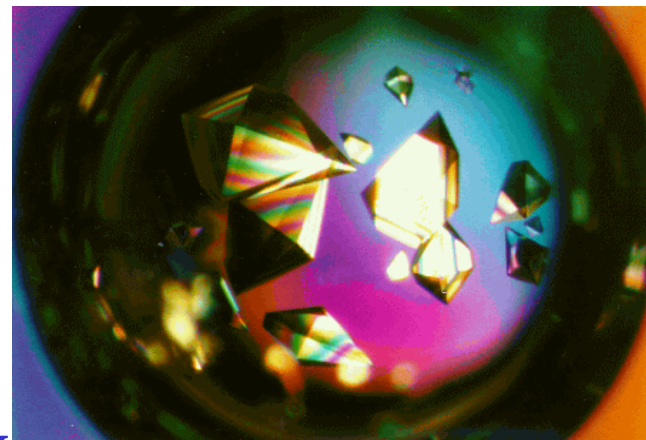
Center for Computational Research

CCR



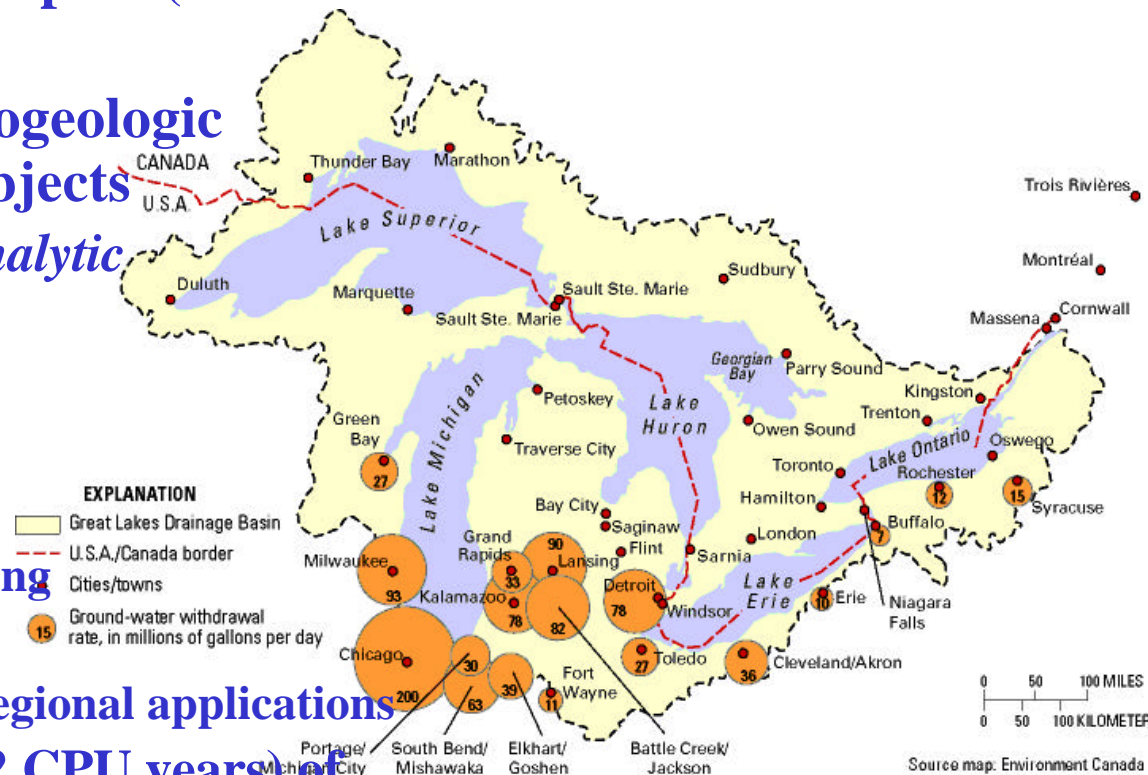
# Molecular Structure Determination via *Shake-and-Bake*

- *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



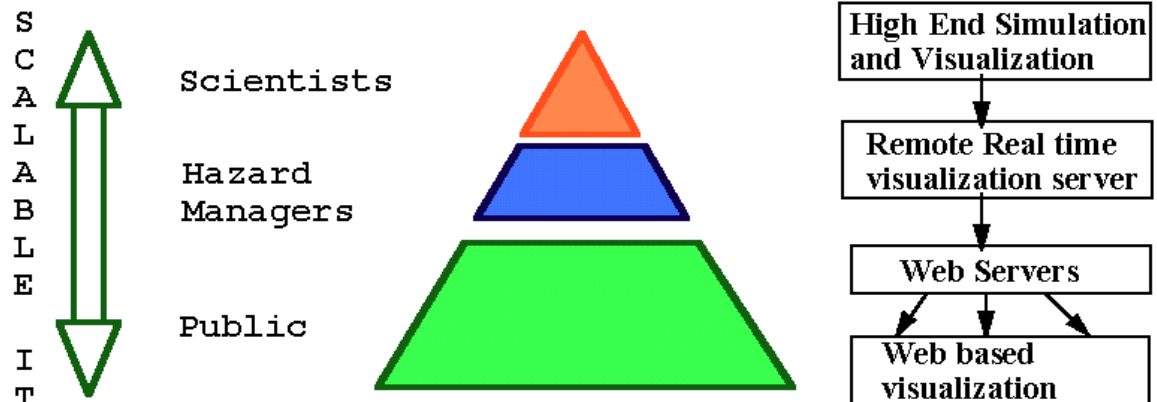
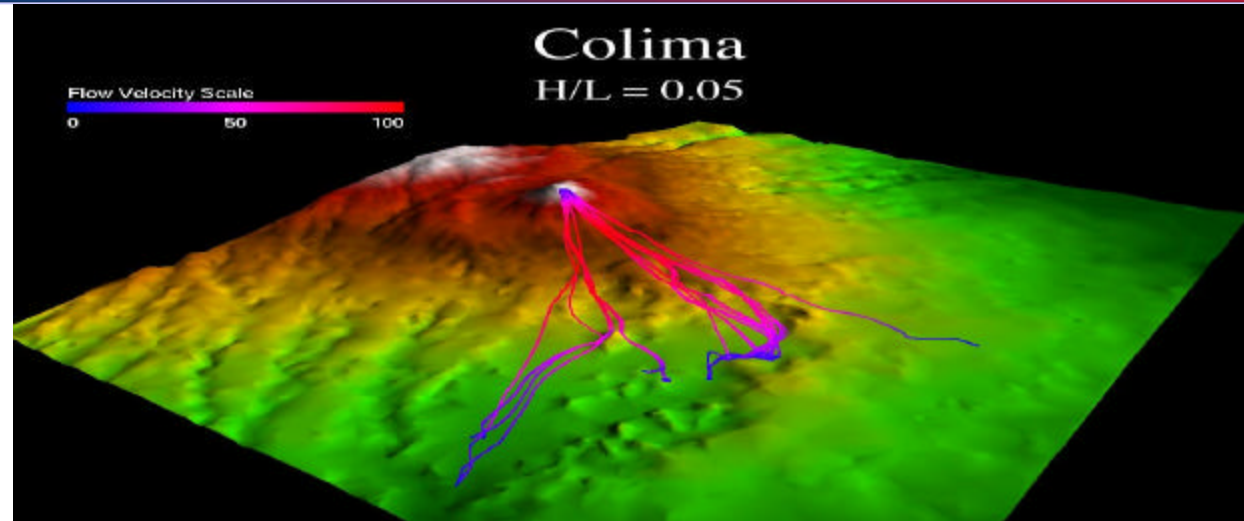
# Groundwater Flow Modeling

- 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

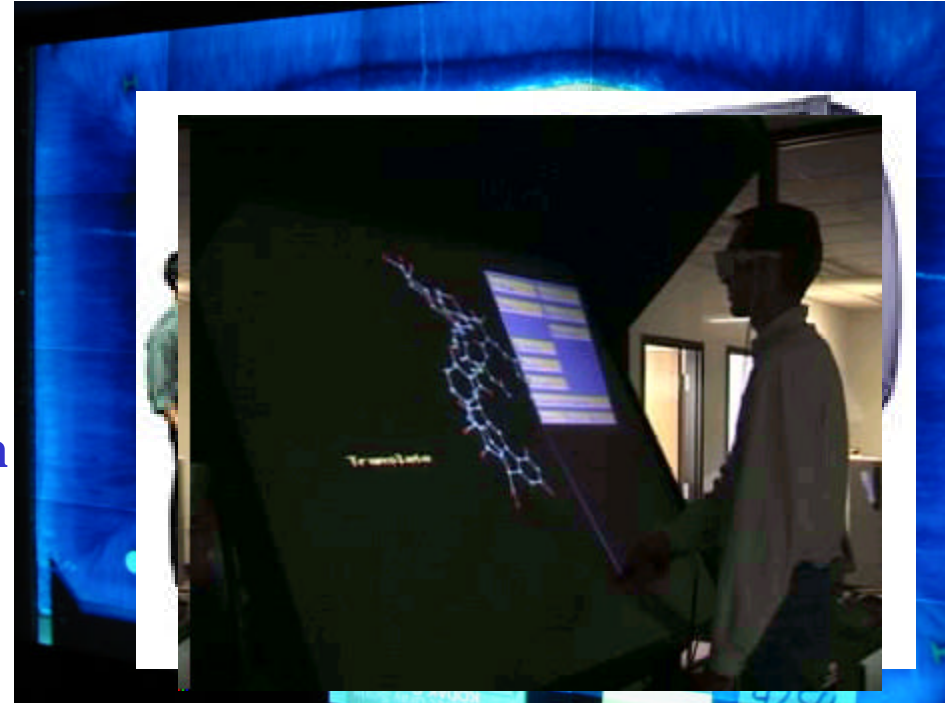
- Group-to-Group Communication
- Commodity components

## ■ 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



# Williamsville Toll Barrier Improvement Project



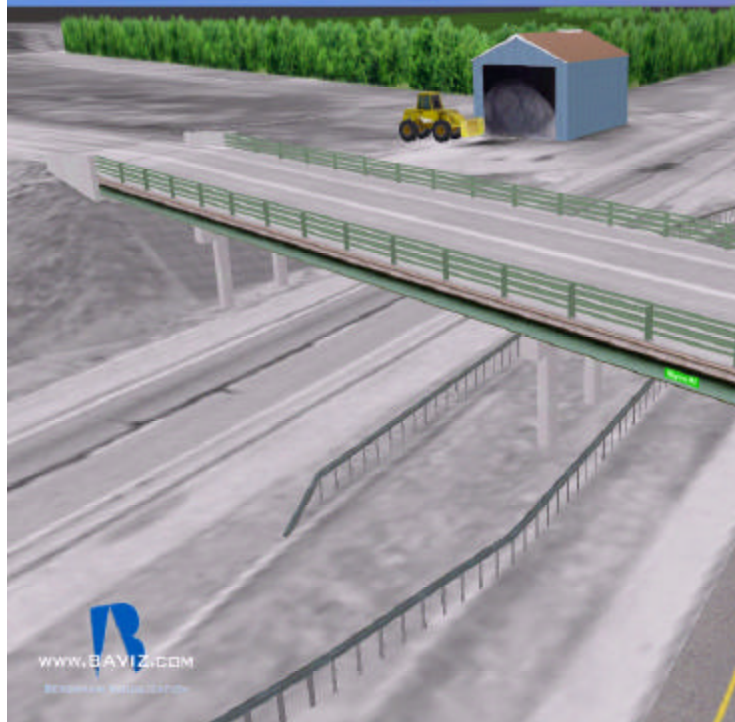
**Initial Photo Match incorporating real and computer-generated components**



# Real-time Simulation

Westbound  
Distance to Barrier: 1.33 mi. (7029 feet)

TVGA  
CONSULTANTS



Westbound  
Distance to Barrier: 1.18 mi. (6147 feet)

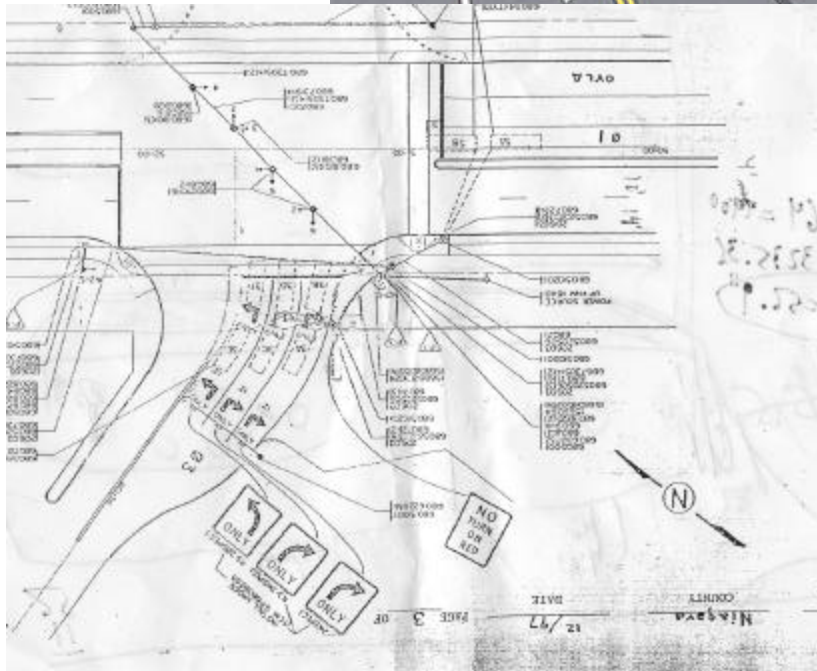
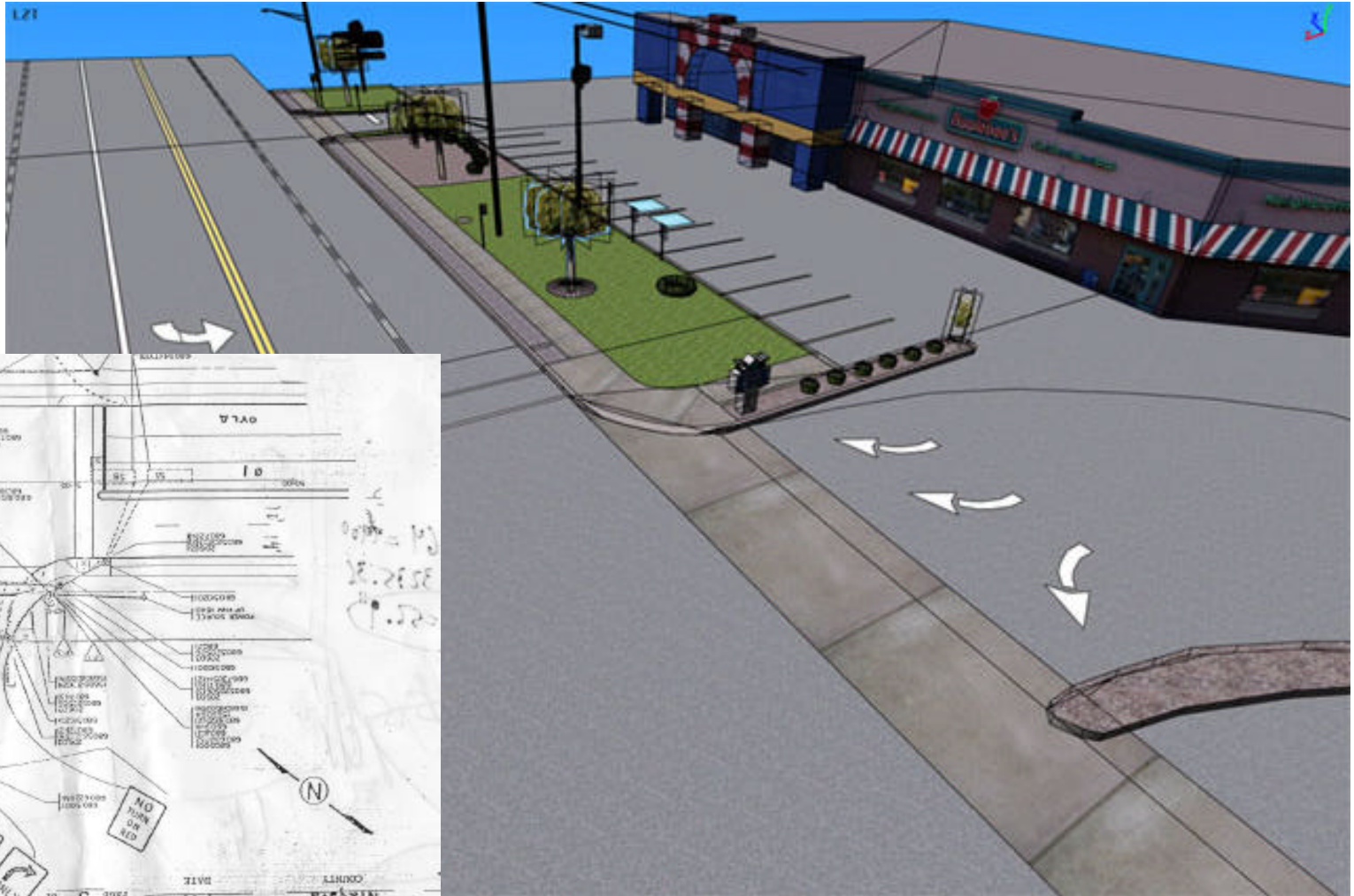
TVGA  
CONSULTANTS



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

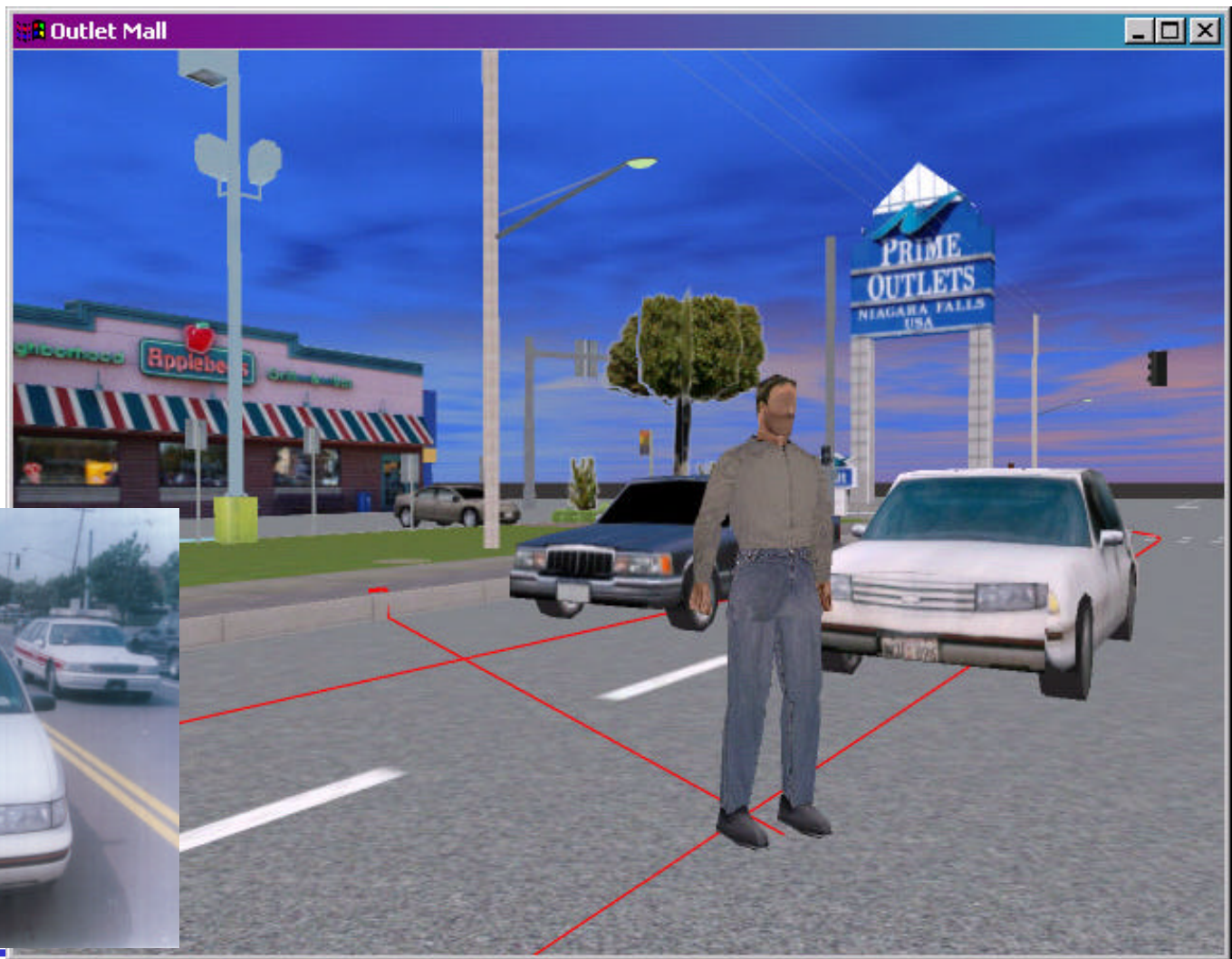


# Accident Reconstruction



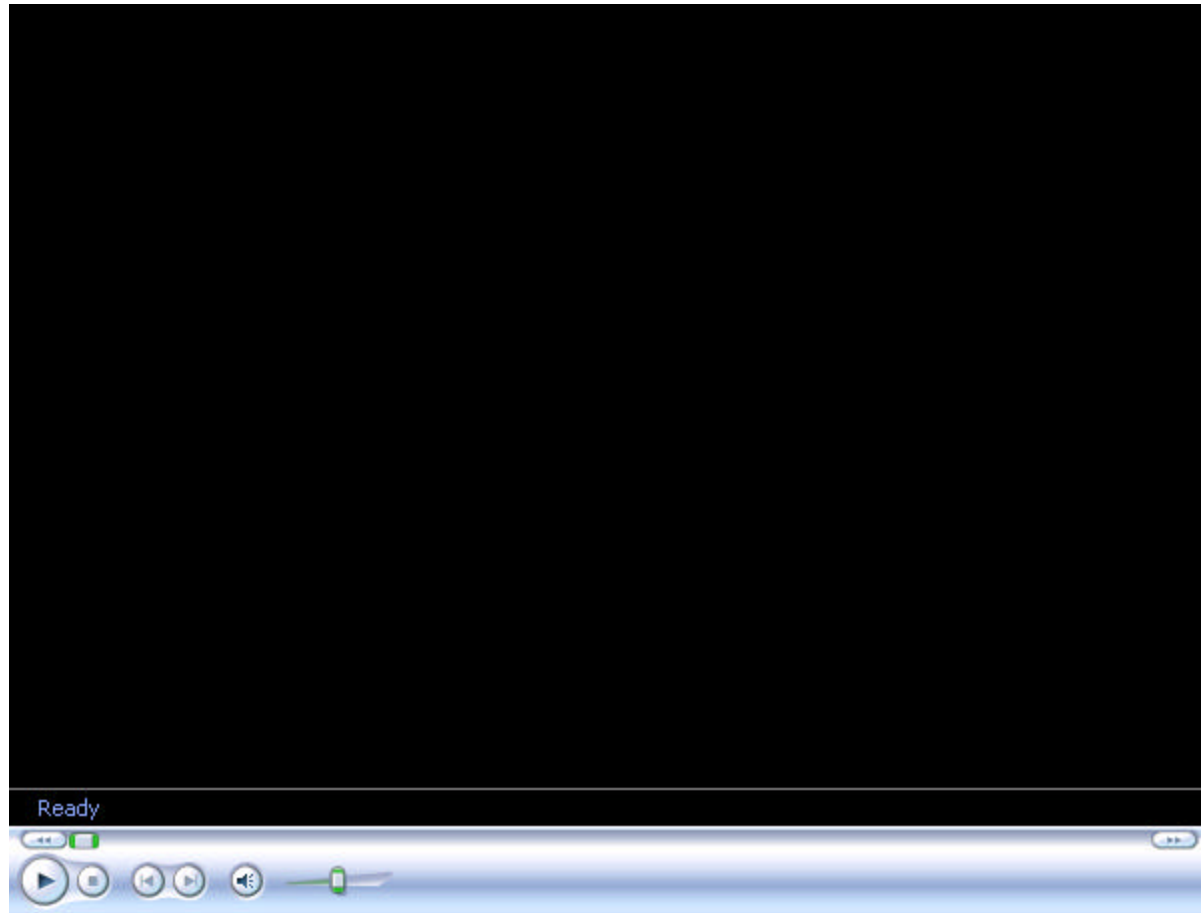


# The Accident



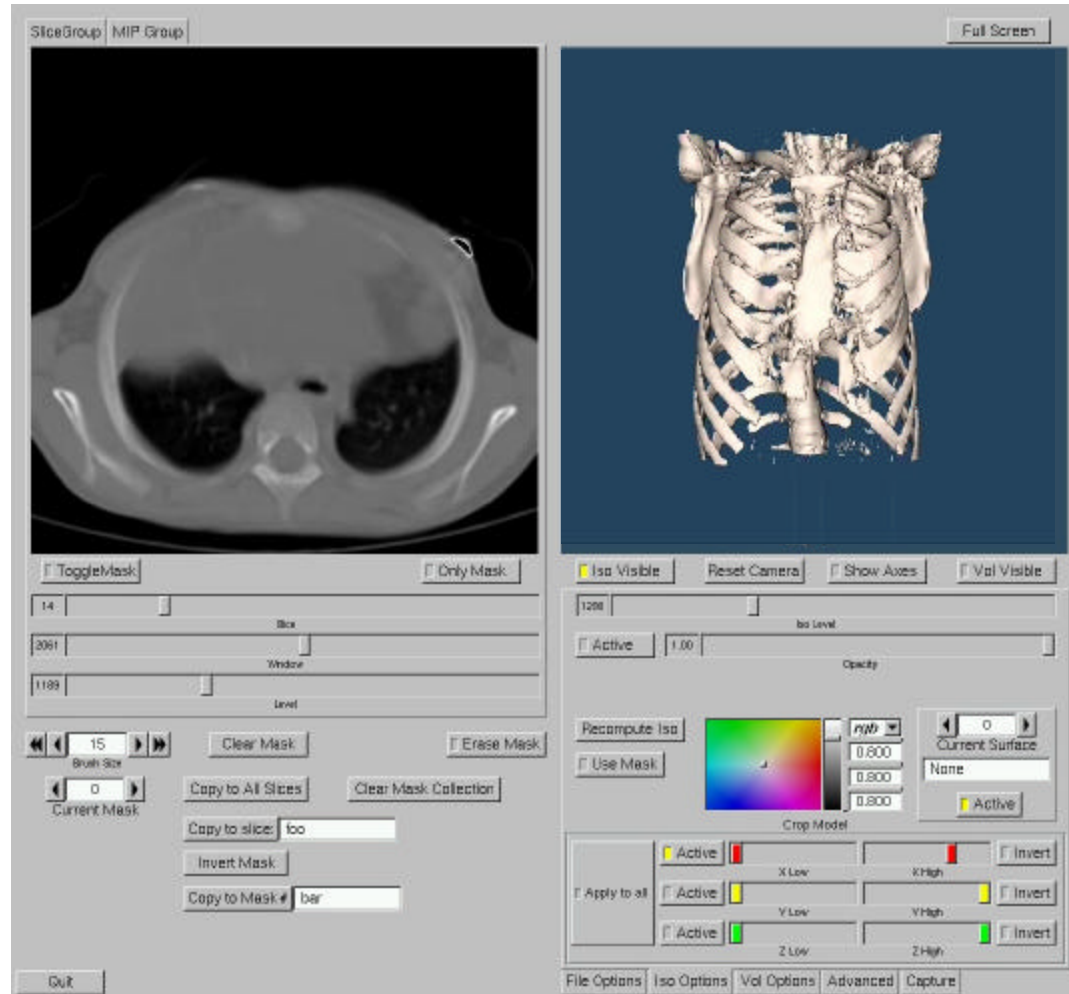


# Accident Animation (Driver's View)



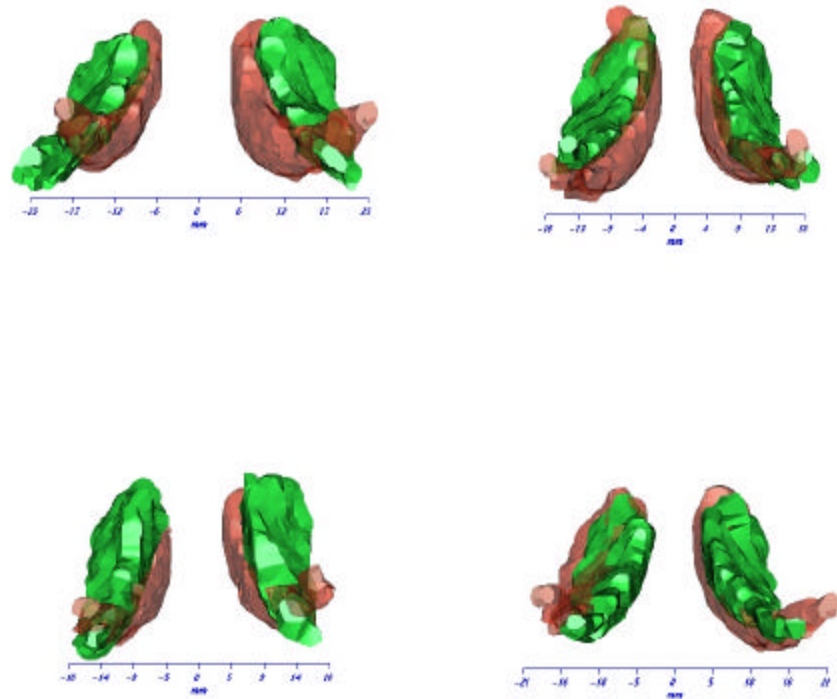
# 3D Medical Visualization App

- 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<sup>®</sup> Demo

- *StreetScenes*<sup>®</sup> is a Virtual Reality (VR) software solution for 3D visualization of surface traffic
- 3D model of proposed soccer stadium in Rochester
- Used *StreetScenes*<sup>®</sup> 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



UNIVERSITY OF BUFFALO NEWS

EDUCATION

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

ROBERT A. COLLAMORE/UNIVERSITY OF BUFFALO

## An early look at bioinformatics

By EMMA D. SAPIONG  
New Northwest Bureau

For most of Darcy Brown's educational career, science classes have been instructive but somewhat abstract. They've been steeped in theories and ideas that she left behind in the classroom.

But that's not the case anymore for the senior at Mount St. Mary Academy. The world of science has come alive and is practical.

She's in her second year of a University at Buffalo Center for Computational Research bioinformatics program geared to high school students. And when she studies DNA in biology class, she can bring that lesson to life by writing a DNA program.

The innovative and rigorous pilot program, called "Next Generation Scientists: Training for Students and Teachers," merges life sciences and

computational science. It is being taught at Mount St. Mary, Orchard Park High School and City Honors School. About two dozen students are involved in the program; they work on smaller versions of the computers used at the research center.

Brown and the three other students in the program demonstrated and spoke about the program Thursday at Mount St. Mary, Annandale, where officials from UB and Vassar, which launched the program with a \$50,000 grant.

"When you take science in school, it's really not practical," Brown said. "Bioinformatics has shown me how to apply science in real life. It has really opened doors for me."

L. Bruce Pritikin, associate dean for research and sponsored programs at UB, said the program aims at bringing bioinformatics to high schools by developing a curriculum and training

teachers. It will expand into other schools in upcoming years.

The students work with a couple of selected teachers in their schools who also are receiving training and three UB undergraduate students.

Senior Courtney Kosenzki, who plans to major in mechanical engineering at Clarkson University, said bioinformatics has prepared her for her field of study. She said it's "going to give me a stronger background in engineering."

Because the students are all graduating, Brown said they are trying to recruit students for the program.

"Bioinformatics is really a different experience," she said. "You think of computers and computer programs and the way they are, and now you know the work that goes behind them."

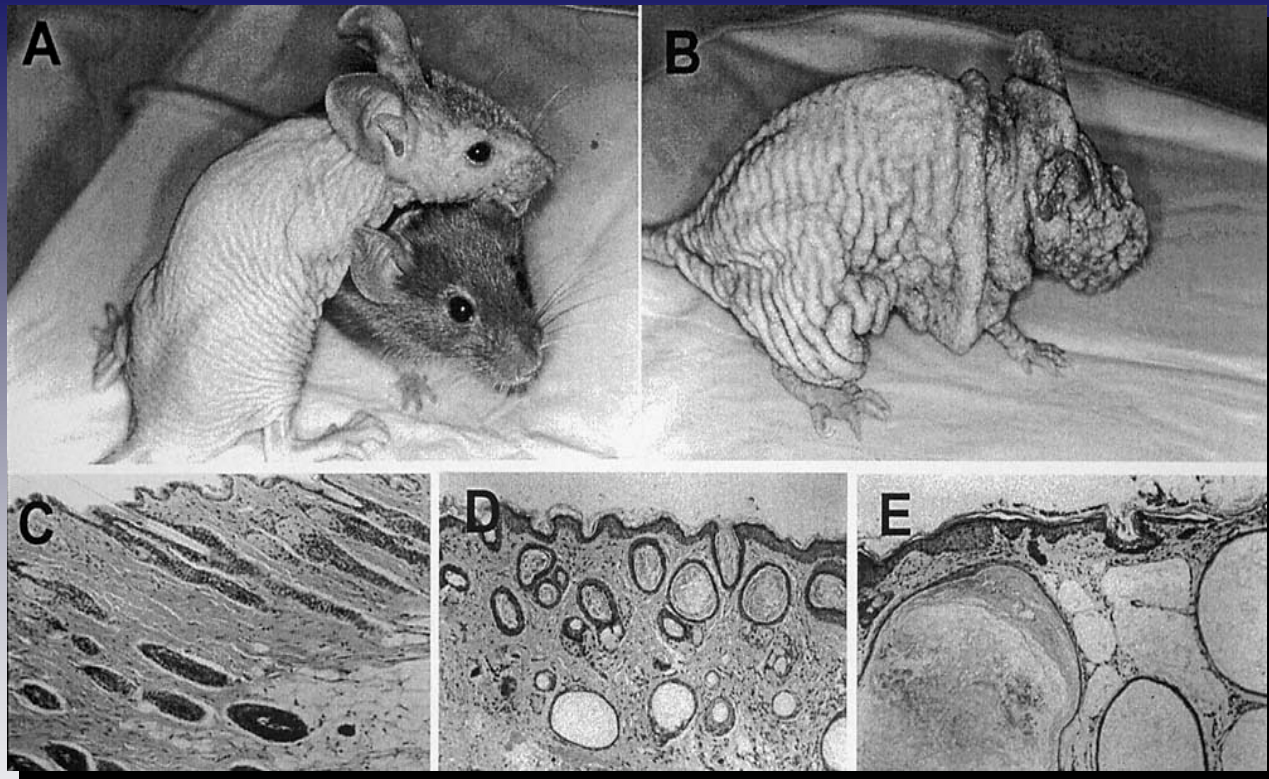
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