Center for Computational Research FSEC Status Report 2/2003

Russ Miller, Director

"Top 10 Worldwide Supercomputing Center"
  - www.gapcon.com

University at Buffalo

The State University of New York

Center for Computational Research

- **High-Performance Computing and High-End Visualization**
  - ❑ **70 (40+ active) Research Groups in 27 Depts**
  - ❑ **13 Local Companies**
  - ❑ **10 Local Institutions**
  - ❑ **External Funds: $108M**
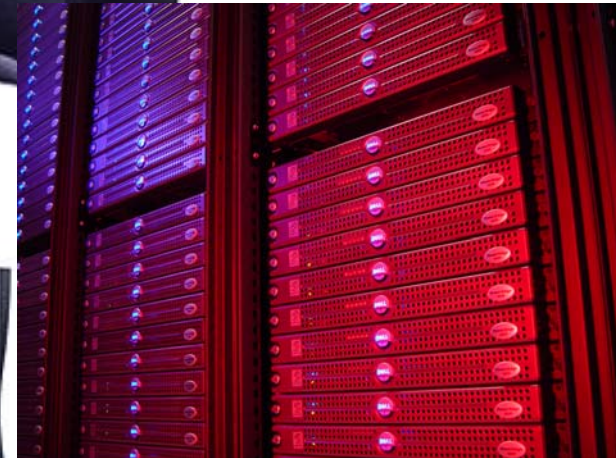 - ❑ **Vendor Contributions: $41M**
- **Deliverables**
  - ❑ **350 Publications and Presentations**
  - ❑ **Hardware, Software, Algorithms, etc**
- **Training**
  - ❑ **Workshops**
  - ❑ **Courses**
  - ❑ **Degree Programs**

Computational Resources

Dell Linux Cluster - #22 in World
- 600 P4 Processors (2.4 GHz)
- 600 GB RAM; 40 TB Disk

Dell Linux Cluster - #187 in World
- 4036 Processors (PIII 1.2 GHz)
- 2TB RAM; 160TB Disk; 16TB RD
- Private Use

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 (3/2003)
- 25 TB Disk; 250 TB Tape

Sample Computational Research

- **Computational Chemistry** (King, Kofke, Coppens, Furlani, Tilson, Lund, Swihart, Ruckenstein, Garvey)
  - ❑ **Algorithm development & simulations**
- **Groundwater Flow Modeling** (Rabideau, Jankovic, Becker, Flewelling)
  - ❑ **Predict contaminant flow in groundwater & possible migration into streams and lakes**
- **Geophysical Mass Flows** (Patra, Sheridan, Pitman, Bursik, Jones, Winer)
  - ❑ **Study of geophysical mass flows for risk assessment of lava flows and mudslides**
- **Bioinformatics** (Zhou, Miller, Hu, Szyperski – NIH Consortium, HWI)
  - ❑ **Protein Folding: computer simulations to understand the 3D structure of proteins**
  - ❑ **Structural Biology; Pharmacology**
- **Computational Fluid Dynamics** (Madnia, DesJardin, Lordi, Taulbee)
  - ❑ **Modeling turbulent flows and combustion to improve design of chemical reactors, turbine engines, and airplanes**
- **Physics** (Jones, Sen)
  - ❑ **Many-body phenomena in condensed matter physics**
- **Chemical Reactions** (Mountziaris)
- **Molecular Simulation** (Errington)

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**
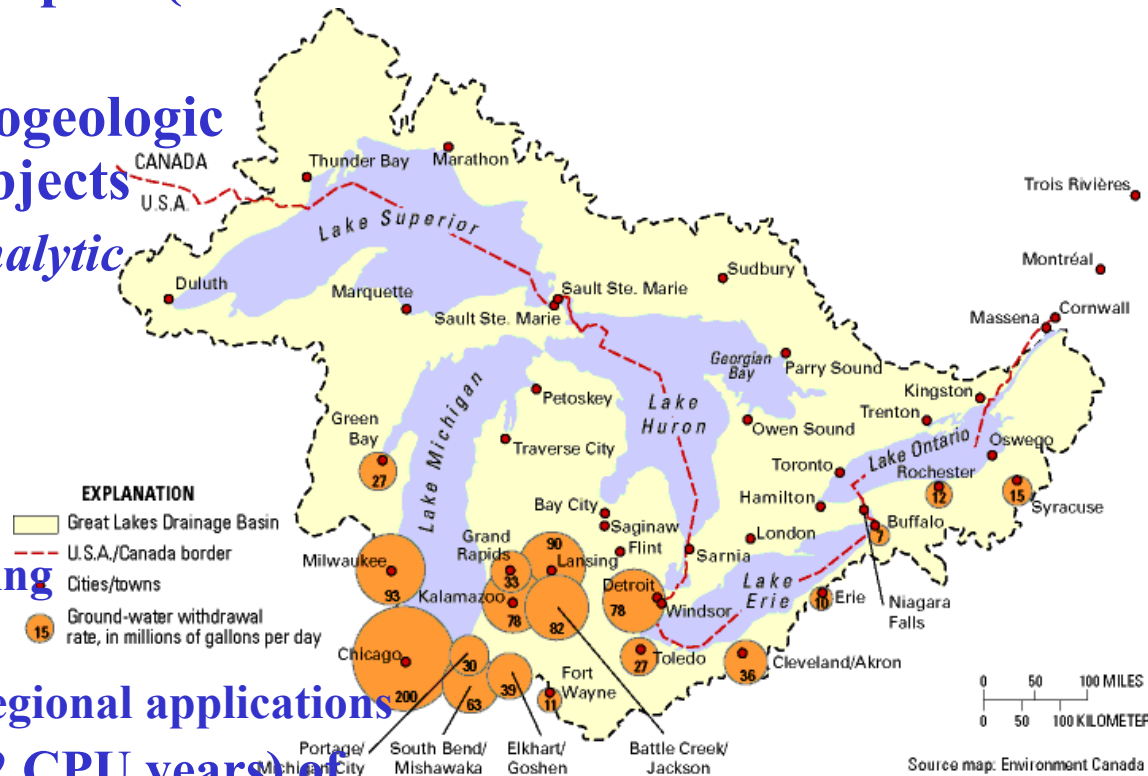 - ❑ **Portable projector works with PC**

Sample Visualization Areas

- **Computational Science** (Patra, Sheridan, Becker, Flewelling, Baker, Miller, Pitman)
  - ❑ **Simulation and modeling**
- **Urban Visualization and Simulation** (CCR)
  - ❑ **Public projects involving urban planning**
- **Medical Imaging** (Hoffmann, Bakshi, Glick, Miletich, Baker)
  - ❑ **Tools for pre-operative planning; predictive disease analysis**
- **Geographic Information Systems** (CCR, Bisantz, Llinas, Kesavadas, Green)
  - ❑ **Parallel data sourcing software**
- **Historical Reenactments** (Paley, Kesavadas, More)
  - ❑ **Faithful representations of previously existing scenarios**
- **Multimedia Presentations** (Anstey, Pape)
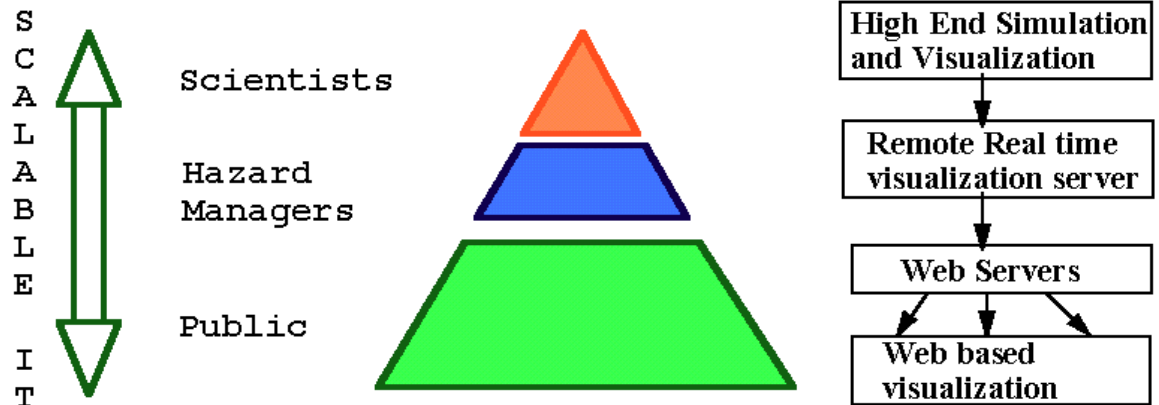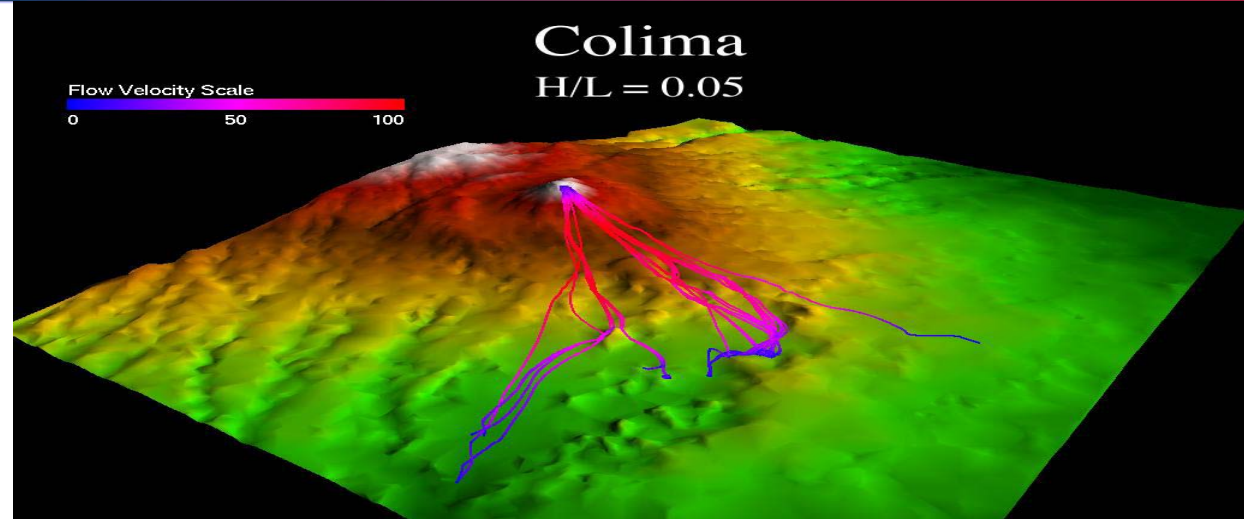 - ❑ **Networked, interactive, 3D activities**

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**

EXPLANATION

Great Lakes Drainage Basin
U.S.A./Canada border
Cities/towns
Ground-water withdrawal rate, in millions of gallons per day

Source map: Environment Canada

Risk Mitigation

Colima
H/L = 0.05
Flow Velocity Scale
0 50 100

- **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**

SCALABLE IT

Scientists

Hazard Managers

Public

High End Simulation and Visualization → Remote Real time visualization server → Web Servers → Web based visualization

Protein Dynamics

- **Dynamics of Hemoglobin (Example)**
- **50 Days of Processing on 16 Processors (800 CPU Days)**
- **Key**
  - ❑ **White – Heme Groups**
  - ❑ **Red – Phe97**
  - ❑ **Red – Oxygen (in the subunit at bottom)**
  - ❑ **Green – His 69 and 101**
  - ❑ **Blue – Tyr 72**
  - ❑ **Cyan (Ball) – Water Molecules**
  - ❑ **Yellow – Helix E/F**
- **Interest**
  - ❑ **Flip of the Phe97 ring at top**
  - ❑ **Water movement around Phe97**
  - ❑ **Heme-heme relative movement**
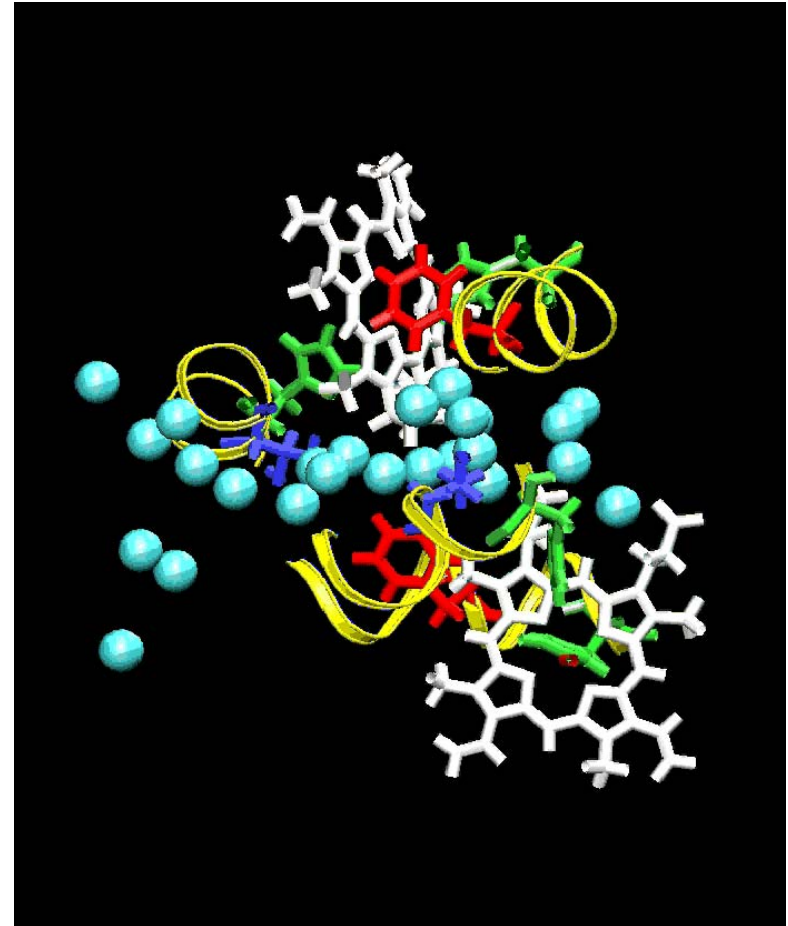
3D Medical Visualization App

- **Collaboration with Children's Hospital**
  - **Leading miniature access surgery center**
- **Application reads data output from a CT Scan**
- **Visualize multiple surfaces and volumes**
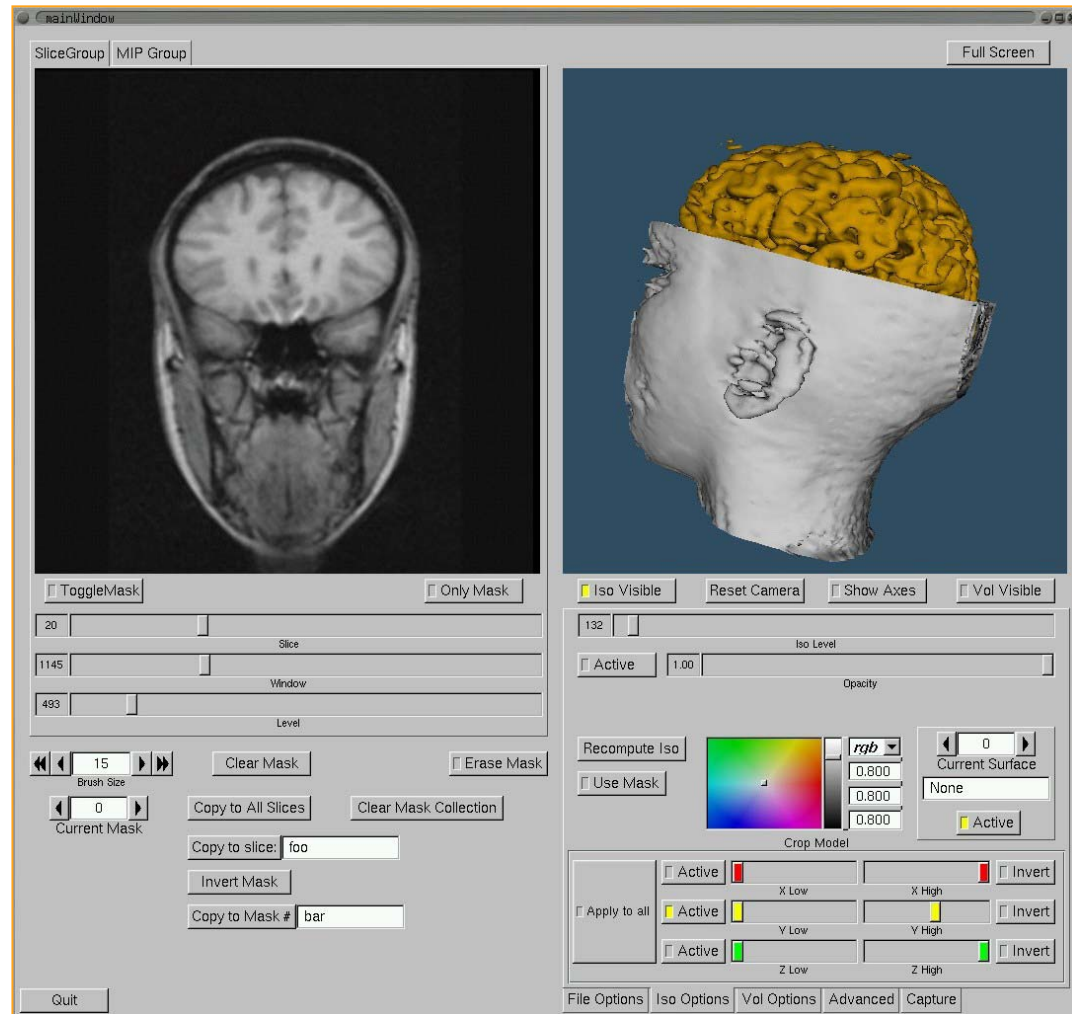- **Export images, movies or CAD representation of model**
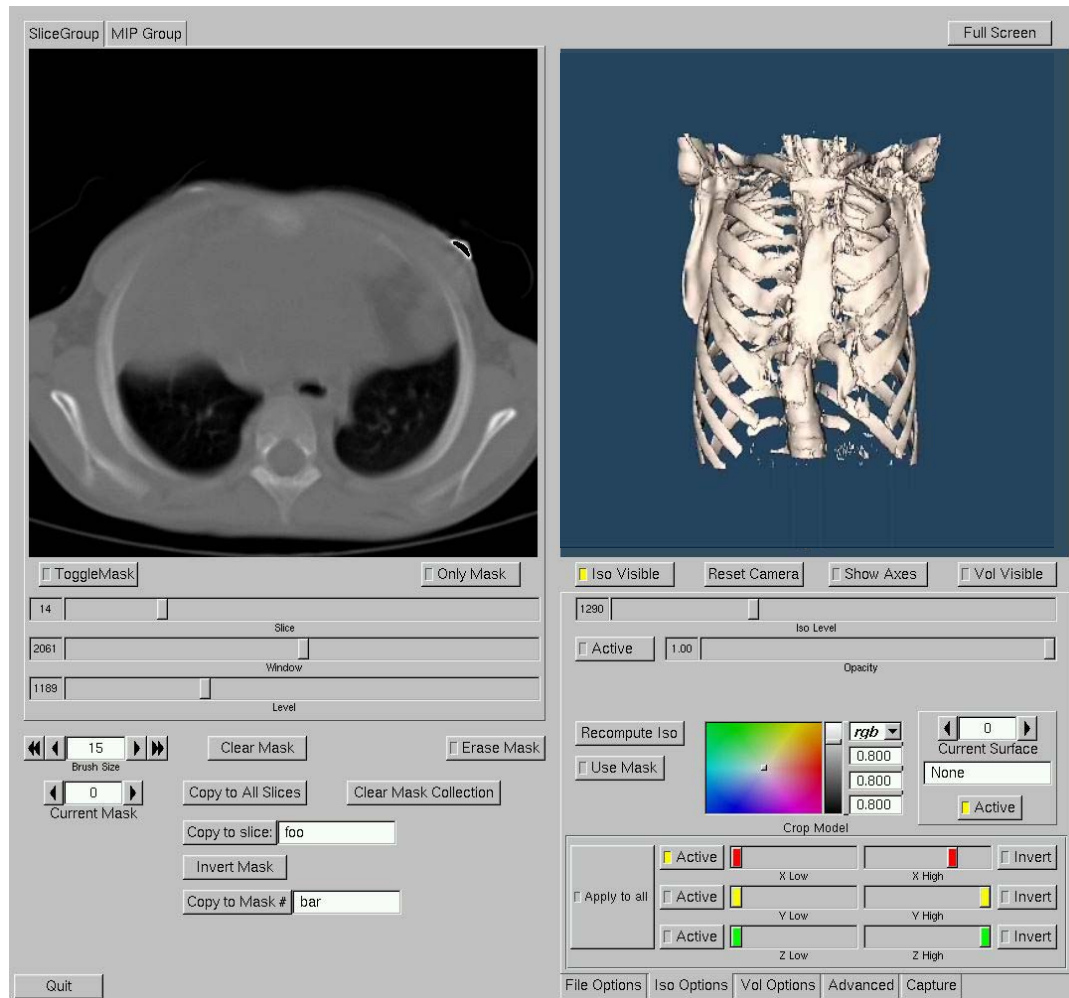
Multiple Sclerosis Project

- **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**

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**
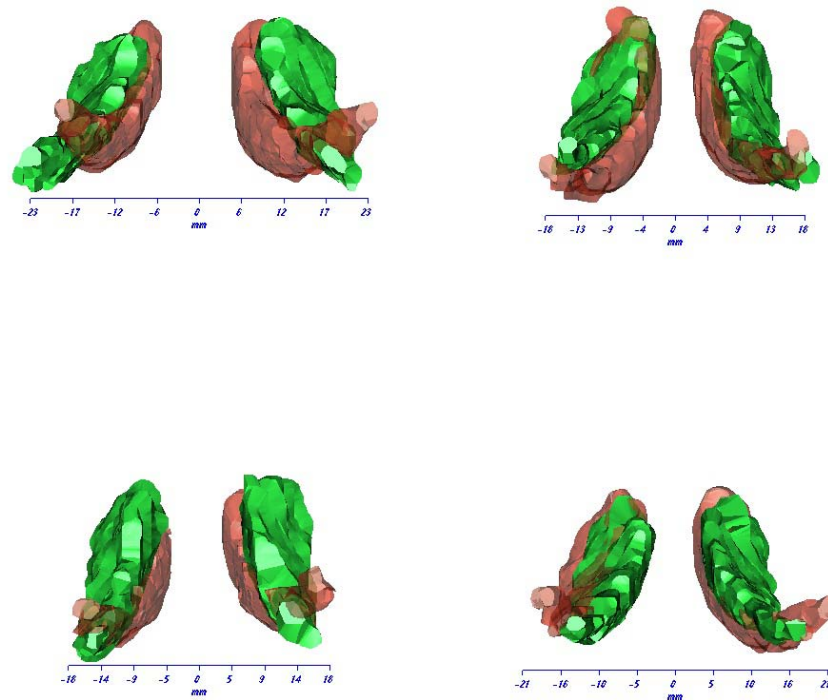
StreetScenes® Demo

- ***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**

Peace Bridge Visualization

Proposed Options
- ❑ Relocate US plaza
- ❑ Build a 3-lane companion span, rehab existing bridge
- ❑ Build a six lane signature span

PHOTO AND STORY BY BRUCE JACKSON

Sample UB Synergies

- **Media Study (Anstey, More)**
  - Donation of PCs
  - Courses, Students, UB Grant
  - "Alive on the Grid"
  - NSF ITR Grant
  - AVID Software
- **MAE (Kesavadas)**
  - Gov. Pataki Visit
  - Peace Bridge (Early)
  - Commodity Projection
- **Classics/MAE (Paley, Kesavadas)**
  - Virtual Site Museum, BBC2
- **H.S. Bioinformatics Program (Pitman)**
  - Verizon/Compaq
- **Buffalo Neuroimaging Analysis Center (Bakshi)**
  - MS Visualization

- **Children's Hospital (Glick)**
  - CT 3D Viz
- **Dent Neurologic Institute (Miletich)**
  - PET Imaging
- **Computer Science & Engineering**
  - Crash Lab
- **Library (Dilandro, Bertholf)**
  - Darwin Martin House
  - James Joyce Novel On-Line
- **Anthropology (Zubrow)**
  - Solar Powered Cluster
- **Management (Jain) & Math (Pitman)**
  - Tops Friendly Markets
  - M&T Bank
- **Access Grid Node (too numerous)**
  - Campus-Wide Outreach for Conf.
  - Center for Americas
    - Human Rights (China/Sweden)

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**

Personnel

- **Leadership**
  - Director & Associate Director
- **Clerical**
  - Office Manager; Budget; Receptionist;
- **Computational Scientists**
  - Comptutational Chemistry, Comptutational Physics
  - Bioinformatics, Scientific Visualization
- **Programmers**
  - Bioinformatics, Database, MultiMedia
- **System Administrators**
  - Sysadmins (5), SAN admin, Web/Help Desk
- **Soft Money**
  - Post-Docs (4)

Academic Programs

- **Bachelor's & Master's Program in Bioinformatics**
- **Related Disciplines**
  - ❑ **Chemical Biology**
  - ❑ **Computational Chemistry**
  - ❑ **Environmental Analysis (Sloan Support)**
  - ❑ **Medical Informatics (Sloan Support)**
- **Advanced Degrees under Development**
  - ❑ **Pharmacometrics, Biophotonics**
- **UB-HWI Department of Structural Biology**
- **Complementary Degrees**
  - ❑ **Canisius College**
  - ❑ **Niagara University**

Outreach

Bioinformatics in Buffalo

"This Center [of Excellence in Bioinformatics] will, through the University of Buffalo's Center for Computational Research, create academic and industrial partnerships …"
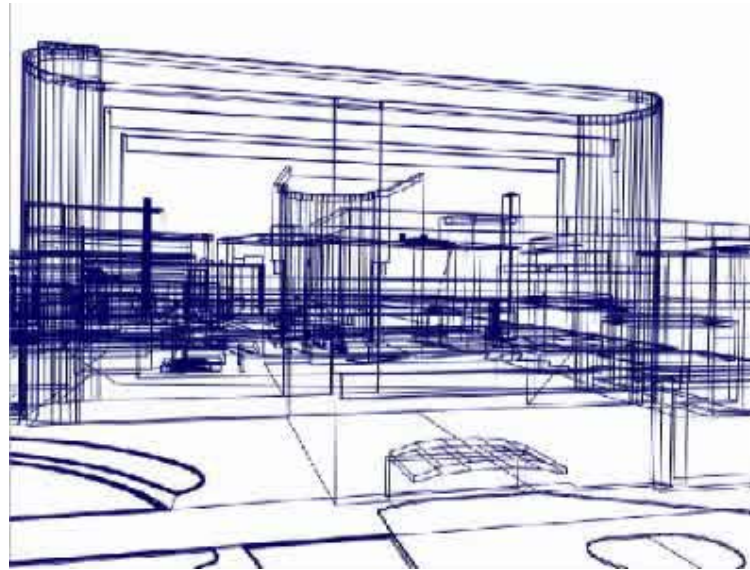— NYS Gov. George S. Pataki, January 2001

Gov. Pataki

Congressman Reynolds

Senator Clinton

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