CCR: Now & the Future
Supercomputing and Visualization at UB

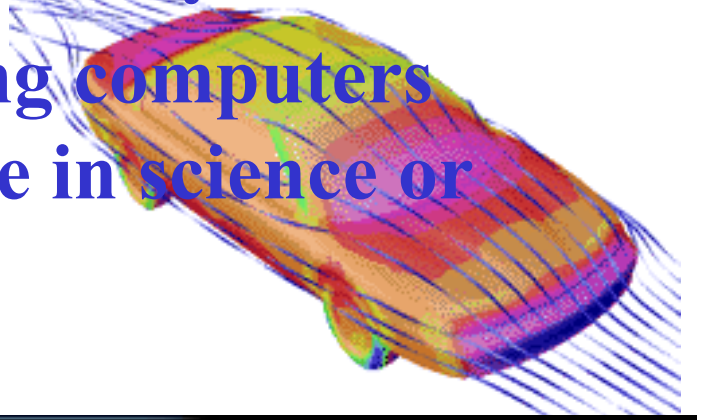
Russ Miller, Director
Center for Computational Research

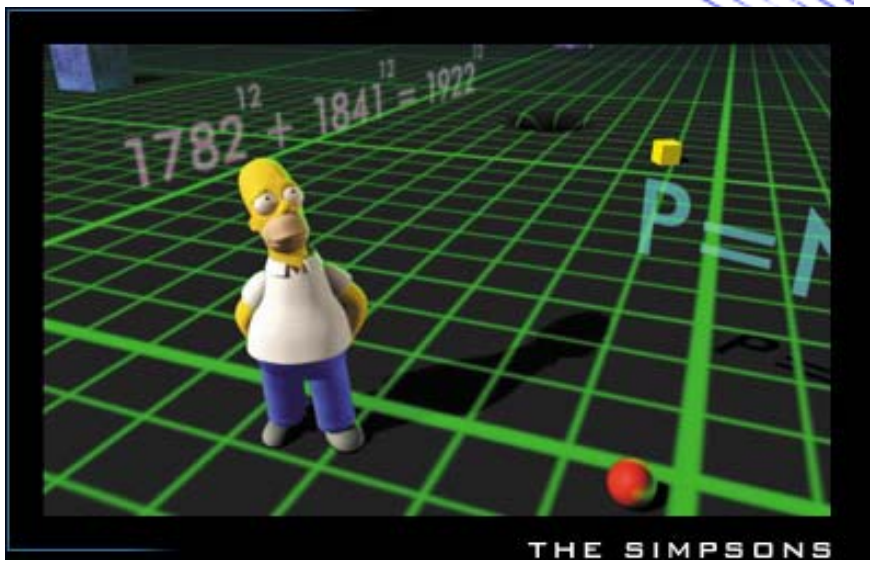
"Top 10 Worldwide Supercomputing Center"
- www.gapcon.com

University at Buffalo
The State University of New York

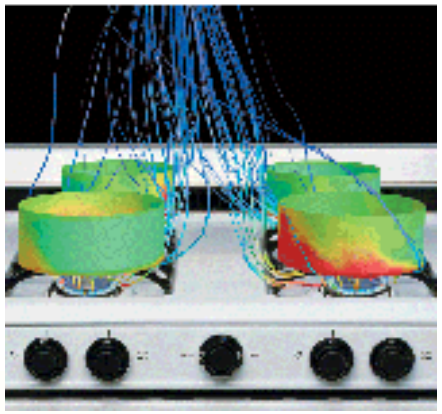
Introduction

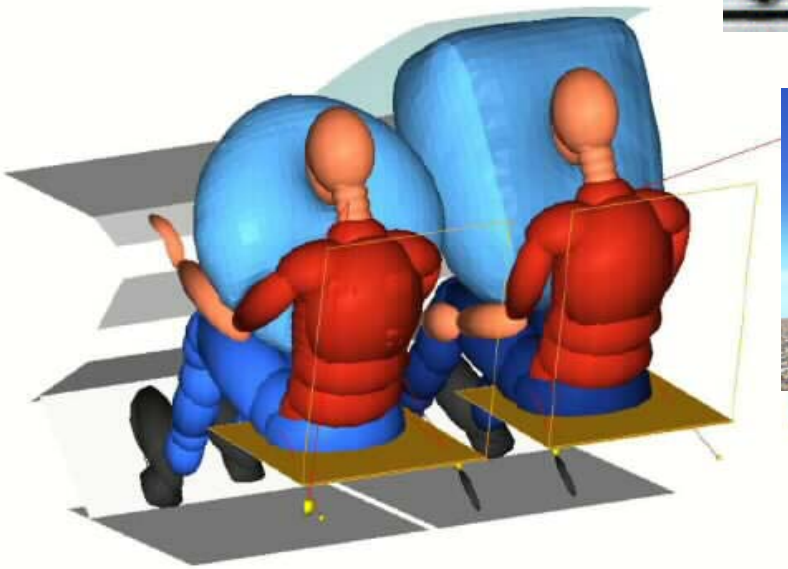
- Computers play an important role in your life
- There are many careers involving computers even for people without expertise in science or engineering





Computers Touch Every Aspect of Our Life....





.... including entertainment

Even during an Ice Age, things can get hot for Sid the sloth.

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

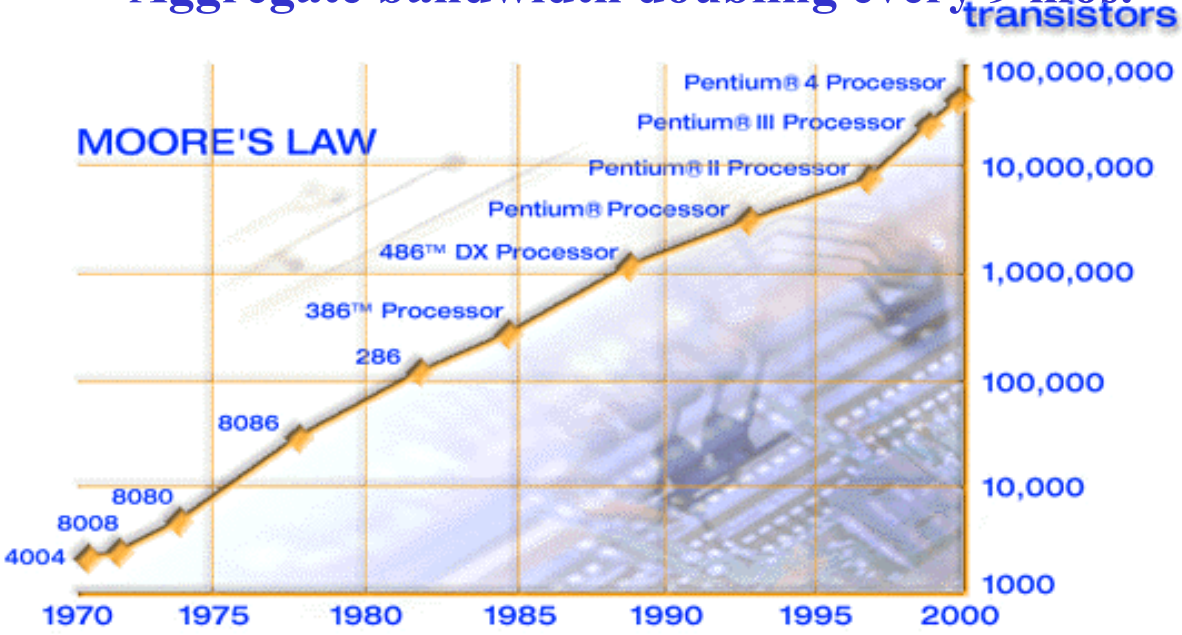
What is a CPU?

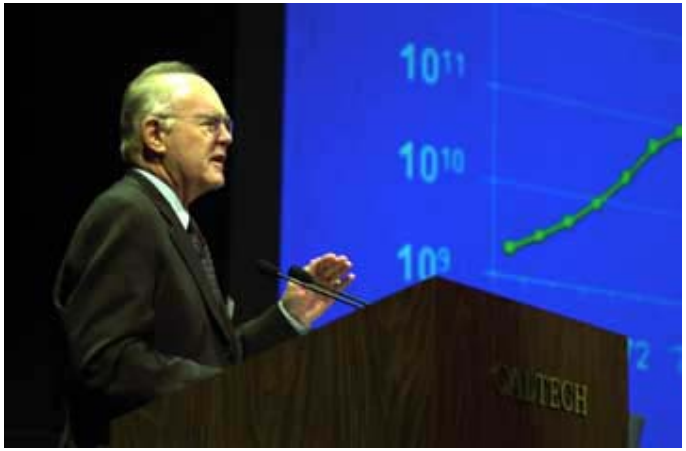
It's the computer's brain - it's the main *processor*

CPU stands for Central Processing Unit

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!

What is a Parallel Computer?

A computer that contains more than 1 processor (CPU)

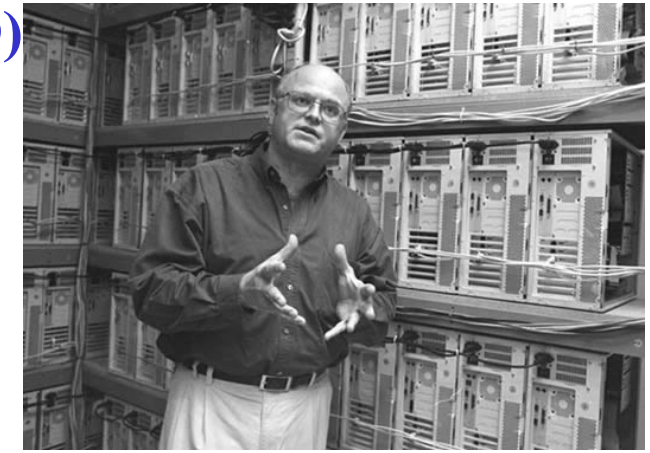
Why are they used?

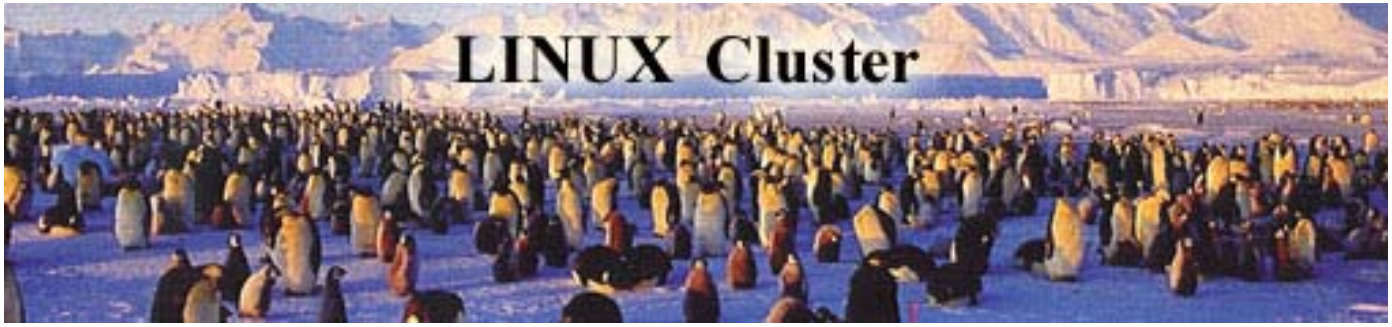
To solve problems faster than they could be solved using only 1 processor

What is a (Beowulf) Cluster?

- 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

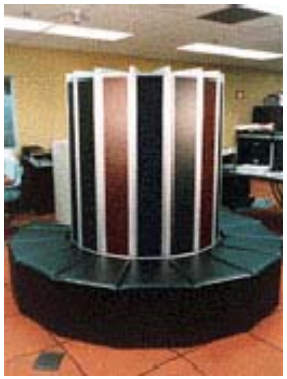
Thomas Sterling
Caltech



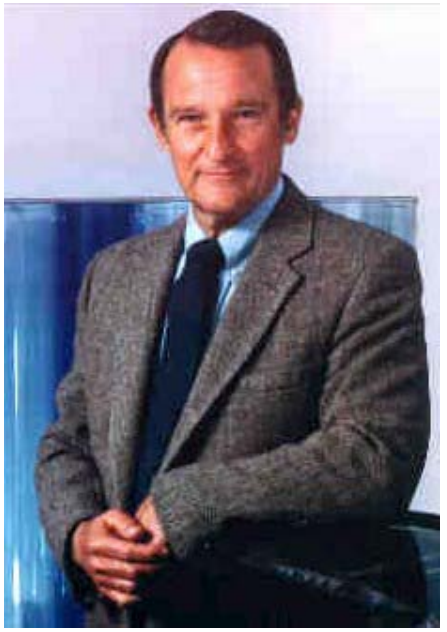


What is a Supercomputer?

- 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
1925-1996

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

Example

If you wanted to know what the weather will be like tomorrow, you could ...

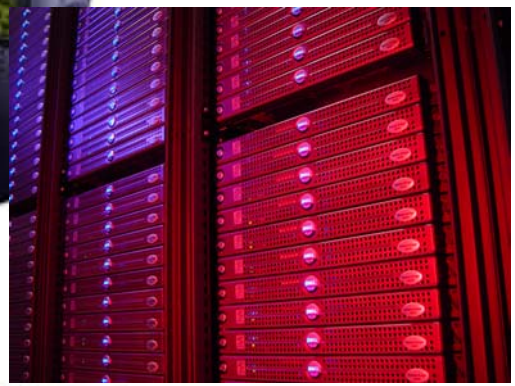
Solve the problem at home on your PC and wait one month to get the answer

or

Solve the problem on a supercomputer and have the answer in one hour!

Center for Computational Research

- High-Performance Computing and High-End Visualization
  - 110 Research Groups in 27 Depts
  - 13 Local Companies
  - 10 Local Institutions
  - External Funds: $108M
  - Vendor Contributions: $41M



- Sample Areas
  - Medical & Urban Visualization and Simulation
  - Computational Chemistry
  - Ground Water Modeling
  - Geophysical Mass Flows

- Deliverables
  - 350 Publications and Presentations
  - Hardware, Software, Algorithms, etc
  - Training: Workshops, Courses, Degree Programs

Computational Resources (10TF; 200TB)

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

- 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

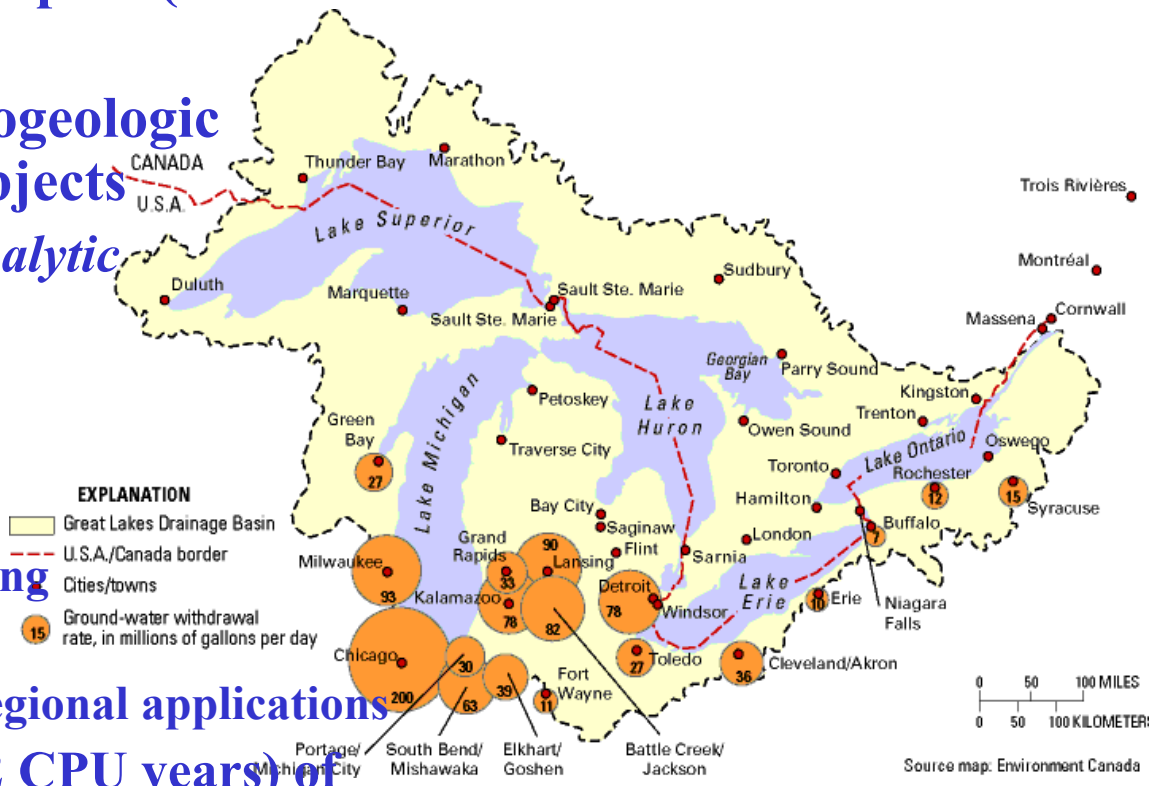
- SGI Intel Linux Cluster
  - 150 PIII Processors (1 GHz)
  - 75 GB RAM, 2.5 TB Disk Storage
- Apex Bioinformatics System
  - Sun V880 (3), 6800, 280R (2), PIIIs
  - Sun 3960: 7 TB Disk Storage
- HP/Compaq SAN (8/2003)
  - 25 TB Disk; 250 TB Tape

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

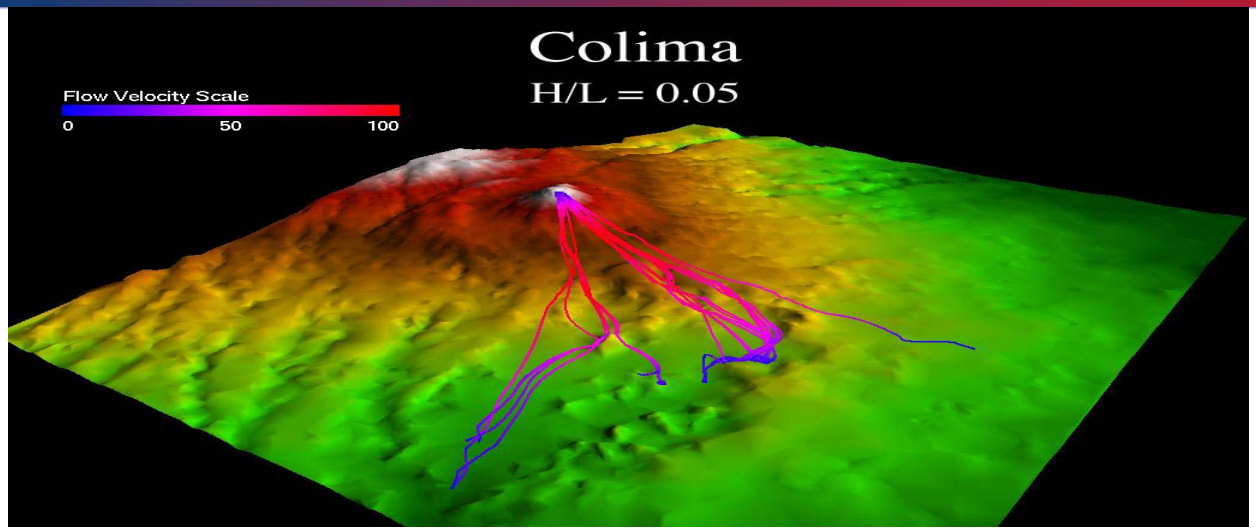
Groundwater Flow Modeling

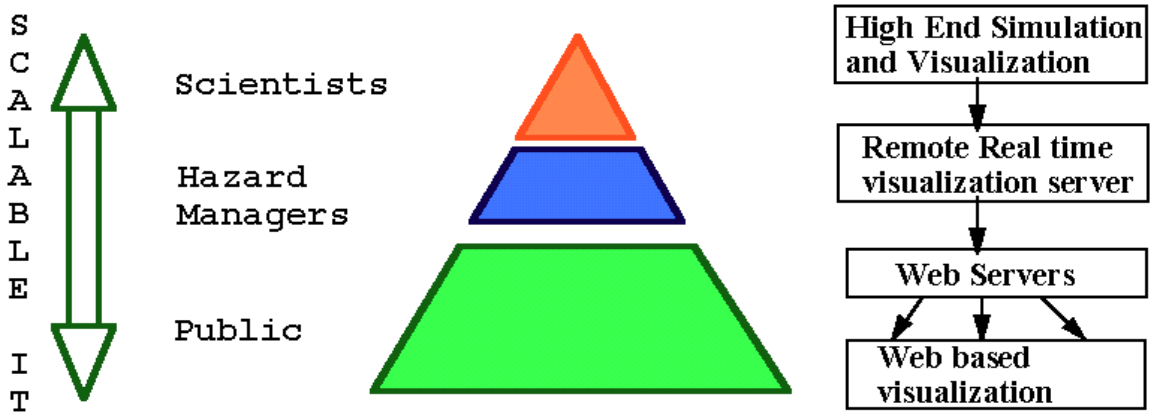
- Regional-scale modeling of groundwater flow and contaminant transport (Great Lakes Region)
- Ability to include all hydrogeologic features as independent objects
- Current work is based on *Analytic Element Method*
- Key features:
  - High precision
  - Highly parallel
  - Object-oriented programming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

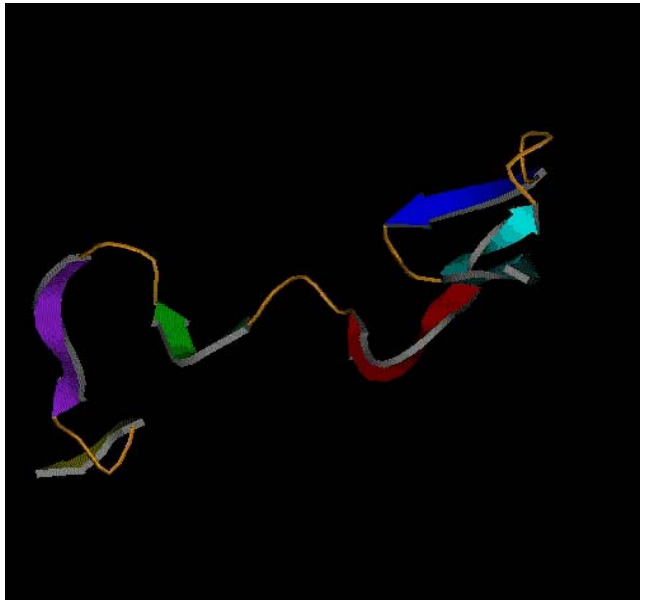
- Integrate information from several sources
  - Simulation results
  - Remote sensing
  - GIS data
- Develop realistic 3D models of geophysical mass flows
- Present information at user appropriate resolutions





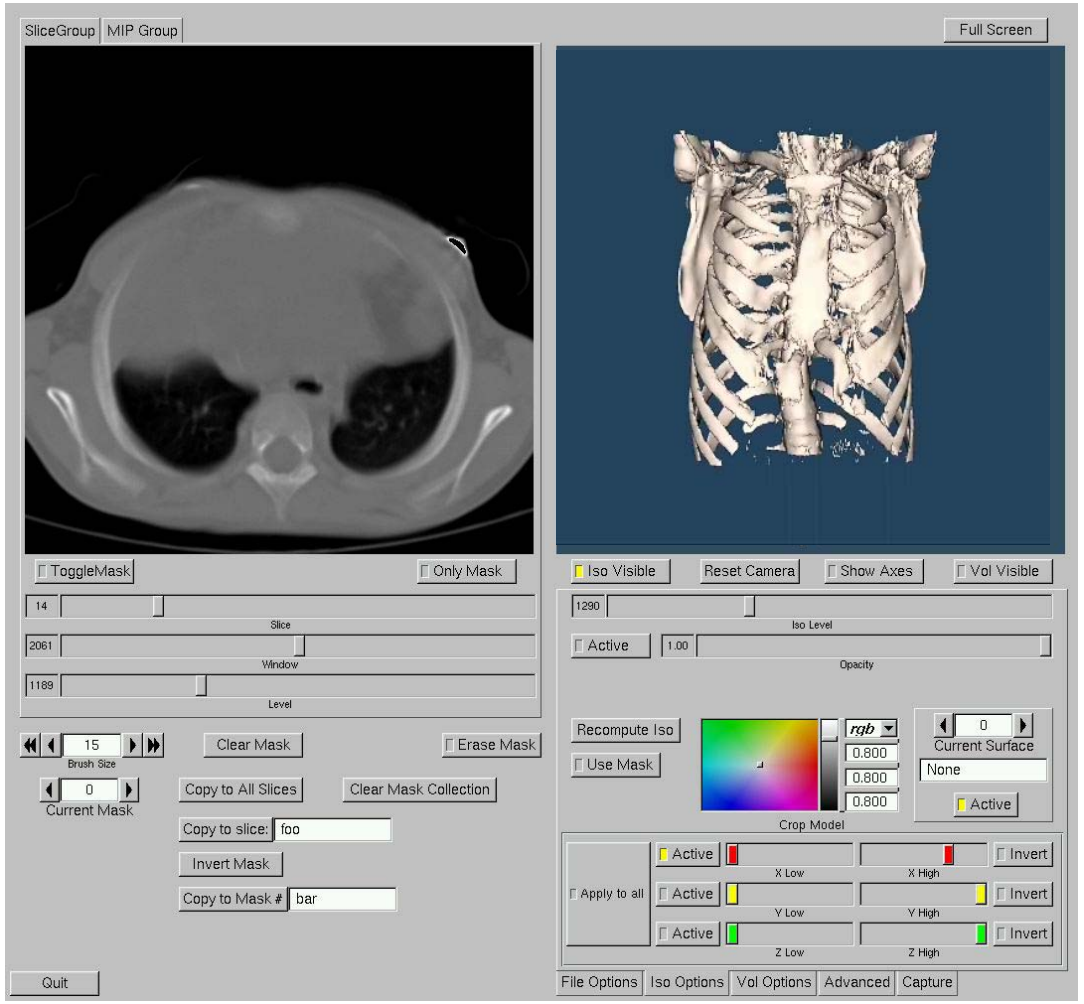
Protein Folding

- 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.



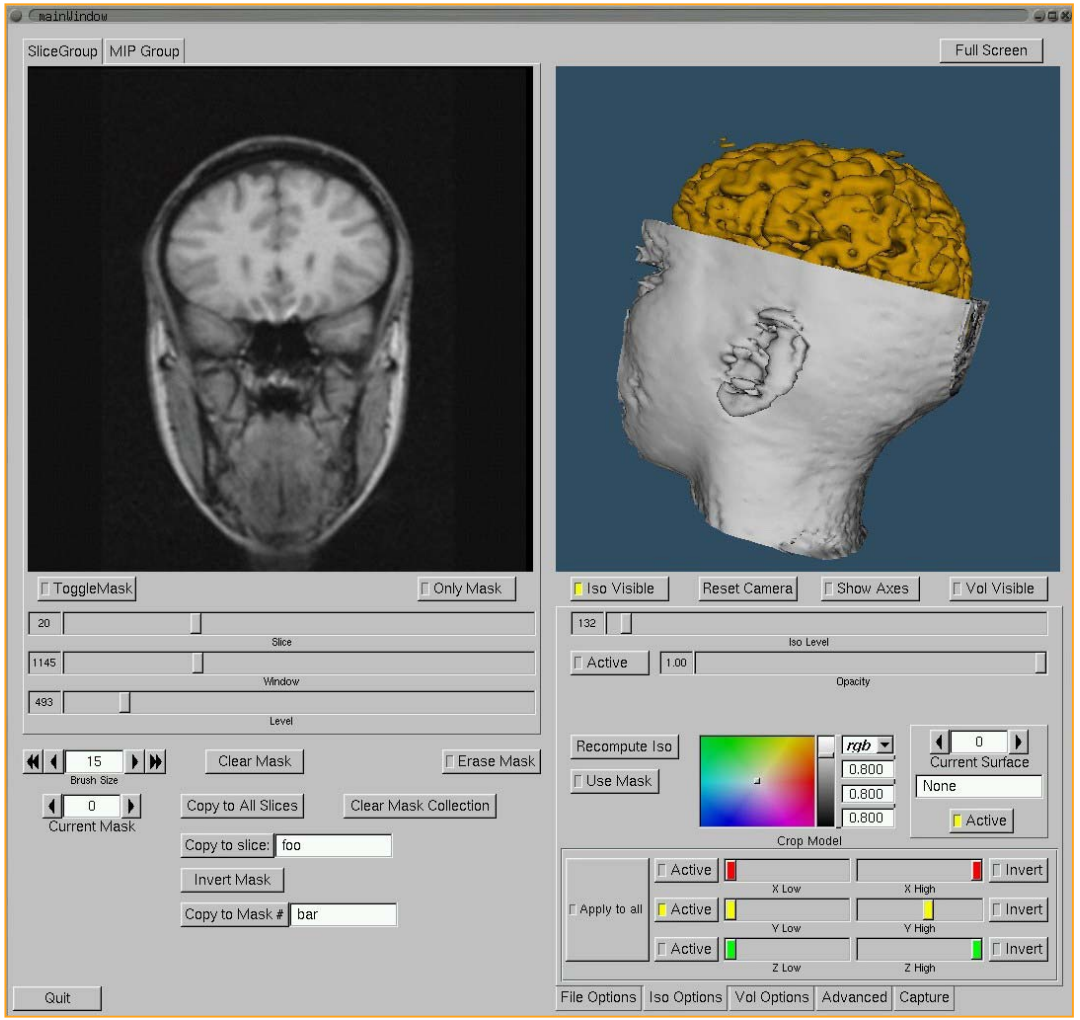
3D Medical Visualization App

- 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

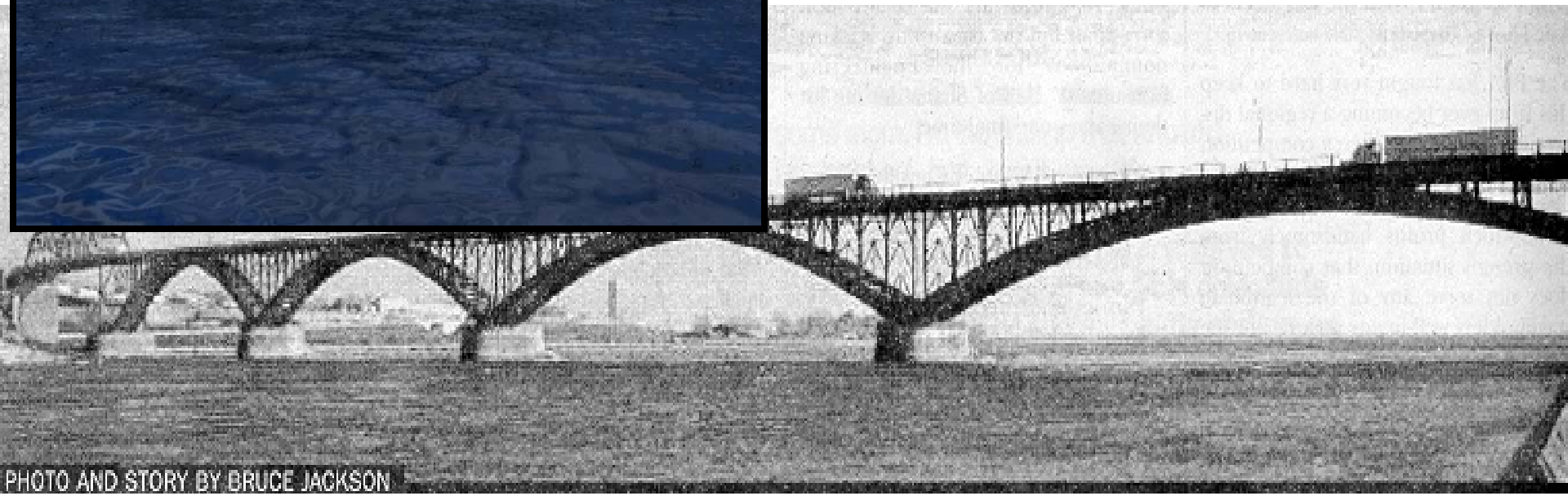


StreetScenes® Demo

- *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

Peace Bridge Visualization

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



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

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

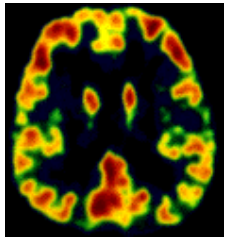
Gov. Pataki

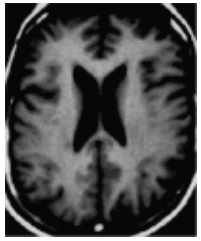
Congressman Reynolds

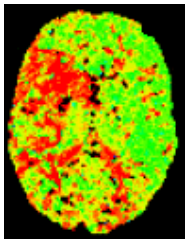
Senator Clinton

WNY Biomedical Advances

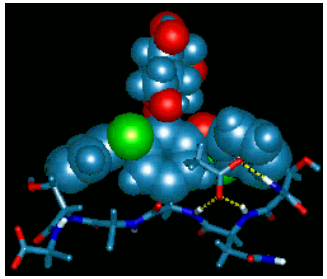
- PSA Test (screen for Prostate Cancer)
- Avonex: Interferon Treatment for Multiple Sclerosis
- Artificial Blood
- Nicorette Gum
- Fetal Viability Test
- Implantable Pacemaker
- Edible Vaccine for Hepatitis C
- Timed-Release Insulin Therapy
- Anti-Arrythmia Therapy
  - Tarantula venom







- Direct Methods Structure Determination
  - Listed on "Top Ten Algorithms of the 20th Century"
  - Vancomycin
  - Gramacidin A



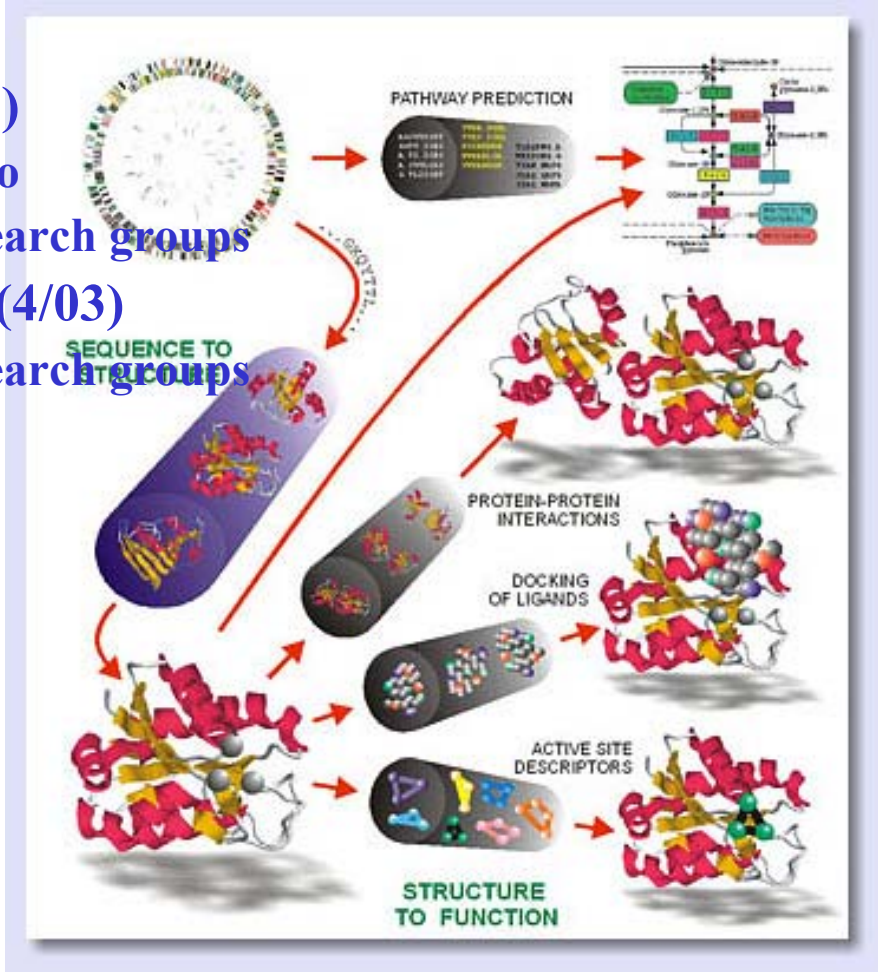
- High Throughput Crystallization Method: Patented
- NIH National Genomics Center: Northeast Consortium
- Howard Hughes Medical Institute: Center for Genomics & Proteomics

Bioinformatics in Buffalo
A $290M Initiative

- UB Center for Advanced Bioengineering & Biomedical Technologies
  - $1M/yr NYS
  - Med Tech for Product Dev & Commer.
- Center Disease Modeling & Therapy Discovery
  - UB, HWI, RPCI, Kaleida
  - $15.3M NYS
  - Software, device development, and drug therapies
- Buffalo Center of Excellence in Bioinformatics
  - UB, HWI, RPCI
  - $61M NYS
  - $10M Federal Government
  - $151 Corporate Funding
- UB Faculty Funding: $64M

UBCOEB 2002-03 Snapshot

- **Personnel**
  - Hired Jeff Skolnick as Director (7/02)
    - Brought 13 additional staff to Buffalo
    - Authorized to hire 10 additional research groups
  - Hired Norma Nowak as co-Director (4/03)
    - Authorized to hire 10 additional research groups
  - Additional members TBD
- **External Funding ($0)**
  - Applications submitted
- **Deliverables**
  - Six (6) scientific papers
- **Resources**
  - Building
  - 6TF → 10TF Compute Cluster



2003 H.S. Summer Workshop Bioinformatics

- June 30 – July 11
- Perl Scripts
- Public Databases
- Filtering Results
- Graphics & Visualization

- Contact
  - Dr. Bruce Pitman (pitman@buffalo.edu)

Outreach







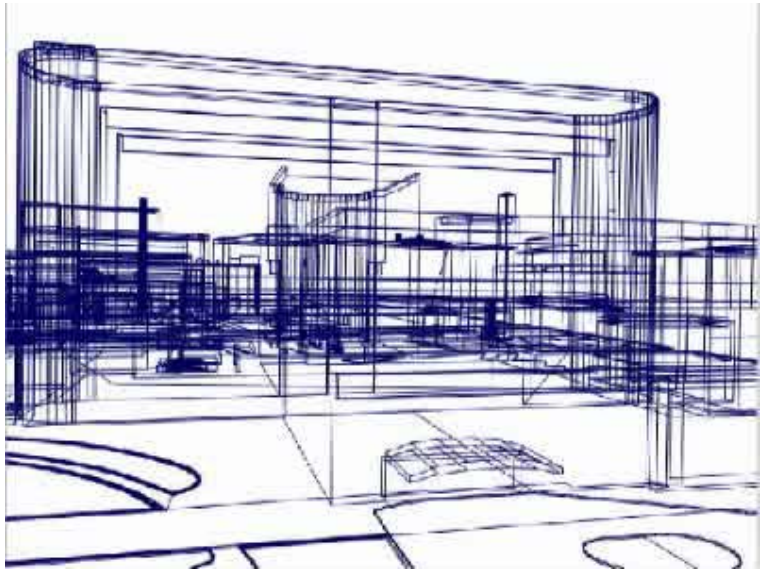








Contact Information



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