

Buffalo Center of Excellence in Bioinformatics

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**“Top 10 Worldwide
Supercomputing
Center”**

- www.gapcon.com



University at Buffalo

The State University of New York

WNY Biomedical Advances

■ PSA Test (screen for Prostate Cancer)

■ Avonex: Interferon Treatment for Multiple Sclerosis

■ Artificial Blood

■ Nicorette Gum

■ Fetal Viability Test

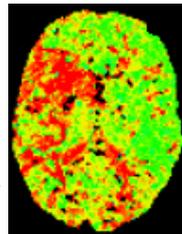
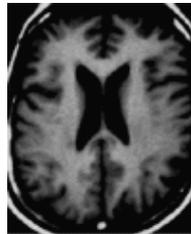
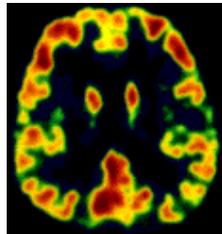
■ Implantable Pacemaker

■ Edible Vaccine for Hepatitis C

■ Timed-Release Insulin Therapy

■ Anti-Arrhythmia Therapy

□ Tarantula venom



■ Direct Methods Structure Determination

□ Listed on “Top Ten Algorithms of the 20th Century”

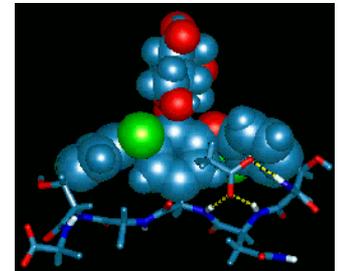
□ Vancomycin

□ Gramacidin A

■ High Throughput Crystallization Method: Patented

■ NIH National Genomics Center: Northeast Consortium

■ Howard Hughes Medical Institute: Center for Genomics & Proteomics



Bioinformatics in Buffalo

- **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
 - \$3M Federal Government
 - \$151 Corporate Funding



Buffalo Center of Excellence in Bioinformatics

- Act as a *research, development, education, and economic resource* for industries based on bioinformatics, including information technology, biotech, and pharmaceuticals.
- Combine state-of-the-art *computational facilities* with *high-throughput experimental facilities* to enable the development of new medical treatments.
- Develop and exploit new algorithms for data acquisition, storage, management, and transmission.



BCOEB Partners

■ Core Partners

- University at Buffalo
- Hauptman-Woodward Medical Research Institute
- Roswell Park Cancer Institute



■ Corporate Partners

- Amersham Pharmacia, AT&T, Beckman Coulter, BioPharma Ireland, Bristol Myers Squibb, Confederation of Indian Industries, Dell, General Electric, Human Genome Sciences, HP, Immco, InforMax, Invitrogen, Pfizer Pharmaceutical, Q-Chem, Sloan Foundation, SGI, Stryker, Sun, 3M, Veridian, Wyeth Lederle, Zeptomatrix

■ WNY Business Community



Life Sciences Complex (Buffalo-Niagara Medical Campus)

Training interspersed throughout 3 buildings

HWI \$20M to replace old building (not shown)



UB \$52M CoE in Bioinformatics

SUNY University at Buffalo

- Research and business partners
- 225 employees and business associates
- 150,000 sq ft: 50% labs, 50% computational facilities

RPCI \$60M Pharmacology/Genetics

Robert R. Parke Cancer Institute

- 60 PIs and 200 support staff
- 170,000 sq ft: 85% rsrch labs; 15% spprt

Life Sciences Complex



University at Buffalo

The State University of New York

Center for Computational Research

CCR

Experimental Facilities I

- **Molecular Targeting Laboratory**
 - ❑ Screen 30-50K compounds every 3 months
 - ❑ Apply compound to cell (different genes treated w fluor markers)
 - ❑ Rapidly identify effect on specific gene expression pathways
- **Gene Expression Laboratory**
 - ❑ High-throughput microarray and gene chip
 - ❑ Discover new genes, their functions, and pathways
- **Proteomics and Molecular Kinetics Lab**
 - ❑ Identify molecular targets found in Gene Expression Lab
- **Disease Modeling Laboratory**
 - ❑ In vivo testing (flies, mice, baboons,...)
 - ❑ Gene targeting and genetic mapping facilities

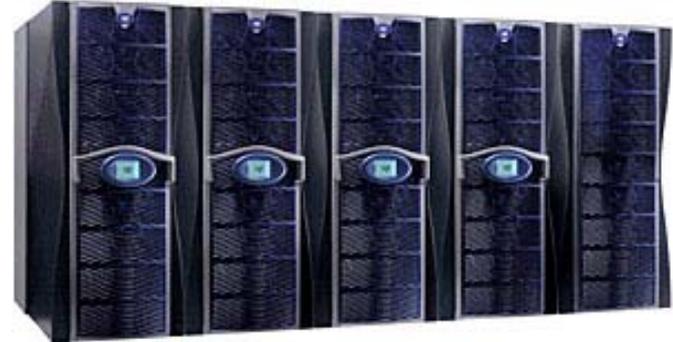
Experimental Facilities II

- **Bioengineering Support Laboratory**
 - Capabilities in photonics and nano-tech research
 - E.g., handheld devices to test for diseases
- **Protein Scale-Up and Purification**
- **High-Throughput Robotic Combinatorial Chemistry/Parallel Synthetic Chemistry Capabilities**
 - Drugs created robotically; Tested for interaction with target protein
 - Rapid identification of a large number of potential drugs
- **Public Health and Molecular Pathology**
 - Tissue repositories; disease gene maps; medical informatics
- **High-Throughput Search Process for Structural Biology**
 - Tests 1536 “chemical cocktails” to determine effective parameters for crystallization

Center for Computational Research

■ High-Performance Computing and High-End Visualization

- ❑ 70 Research Groups in 27 Depts
- ❑ 25 Companies and Institutions
- ❑ Ext Fund: \$108M; Vendor: \$41M

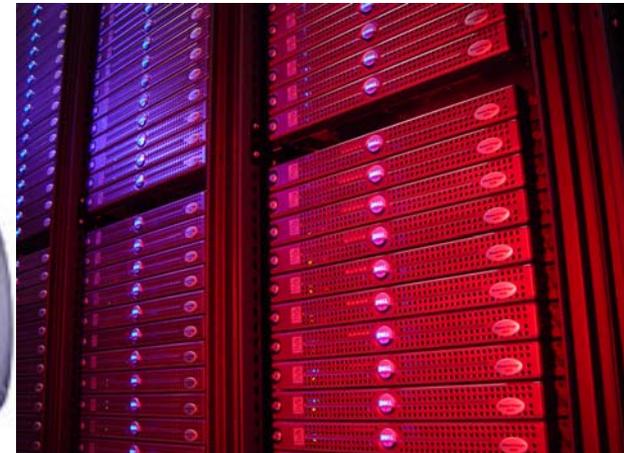
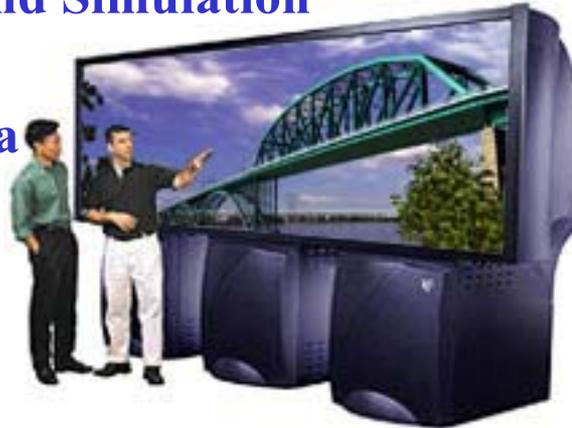


■ Sample Areas

- ❑ Computational Chemistry
- ❑ Ground Water Modeling
- ❑ Geophysical Mass Flows
- ❑ Urban Visualization and Simulation
- ❑ Medical Imaging
- ❑ Networked Multimedia

■ Training

- ❑ Workshops; Courses
- ❑ Degree Programs



Computational Resources

- **Dell Linux Cluster - #22 on top500**
 - 600 P4 Processors (2.4 GHz)
 - 600 GB RAM; 40 TB Disk
- **Dell Linux Cluster - #187 on top500**
 - 4036 Processors (PIII 1.2 GHz)
 - 2TB RAM; 160TB Disk; 16TB RD
- **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**
 - 25 TB Disk; 250 TB Tape



Visualization Resources

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

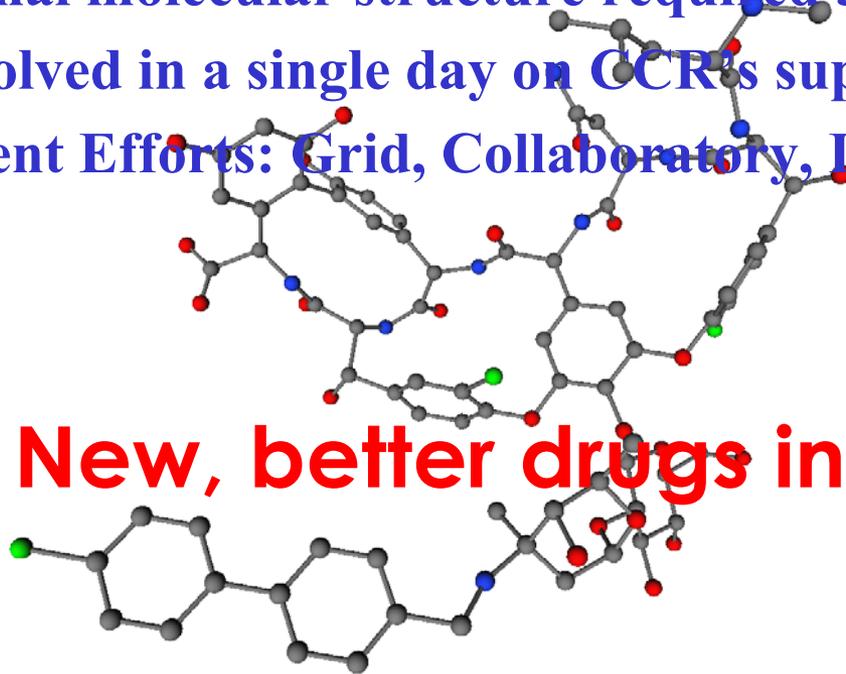


Antibiotics & Supercomputers

■ Vancomycin solved with *SnB* (UB/HWI)

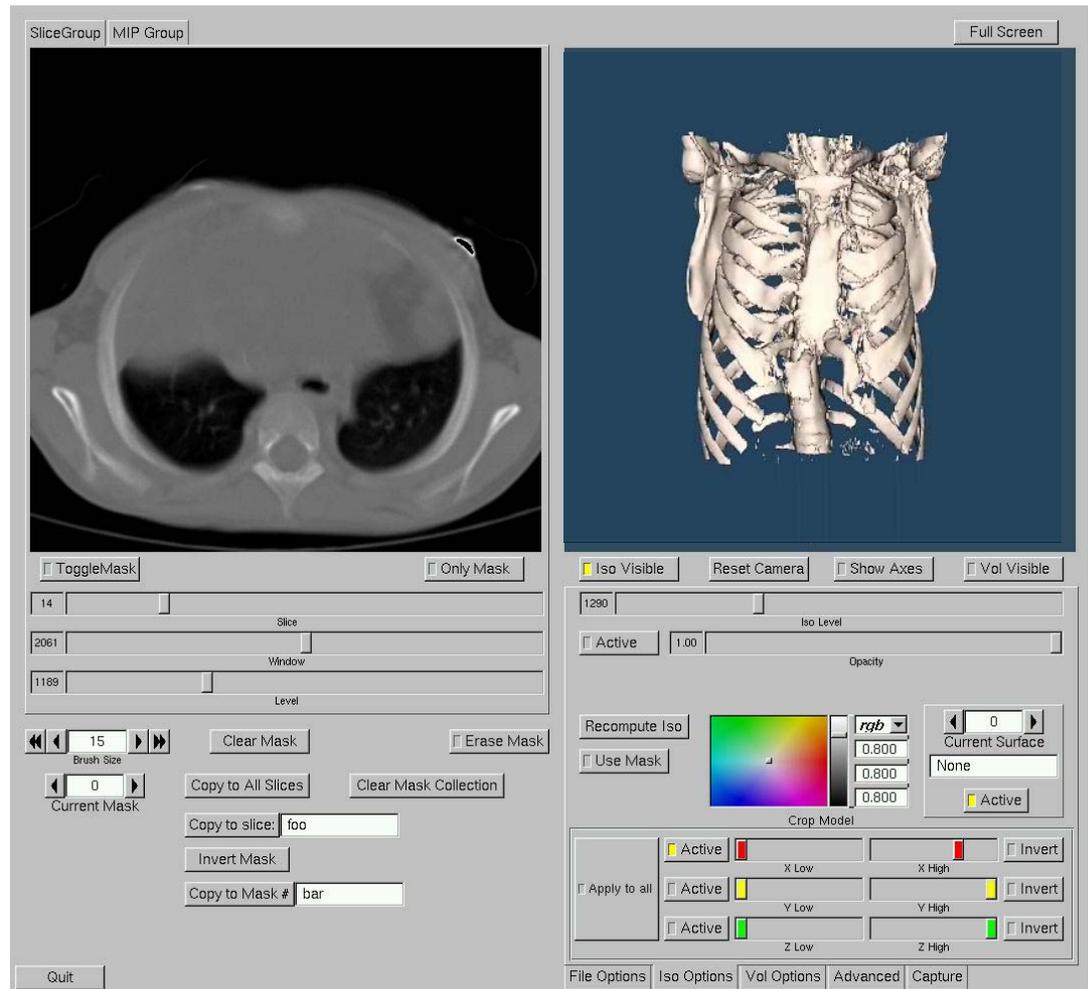
- ❑ *SnB*: “Top Algorithms of the Century”
- ❑ “Antibiotic of Last Resort”
- ❑ Original molecular structure required 5 months
- ❑ (Re)solved in a single day on CCR's supercomputers
- ❑ Current Efforts: Grid, Collaboratory, Intelligent Learning

Result: New, better drugs in shorter time



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

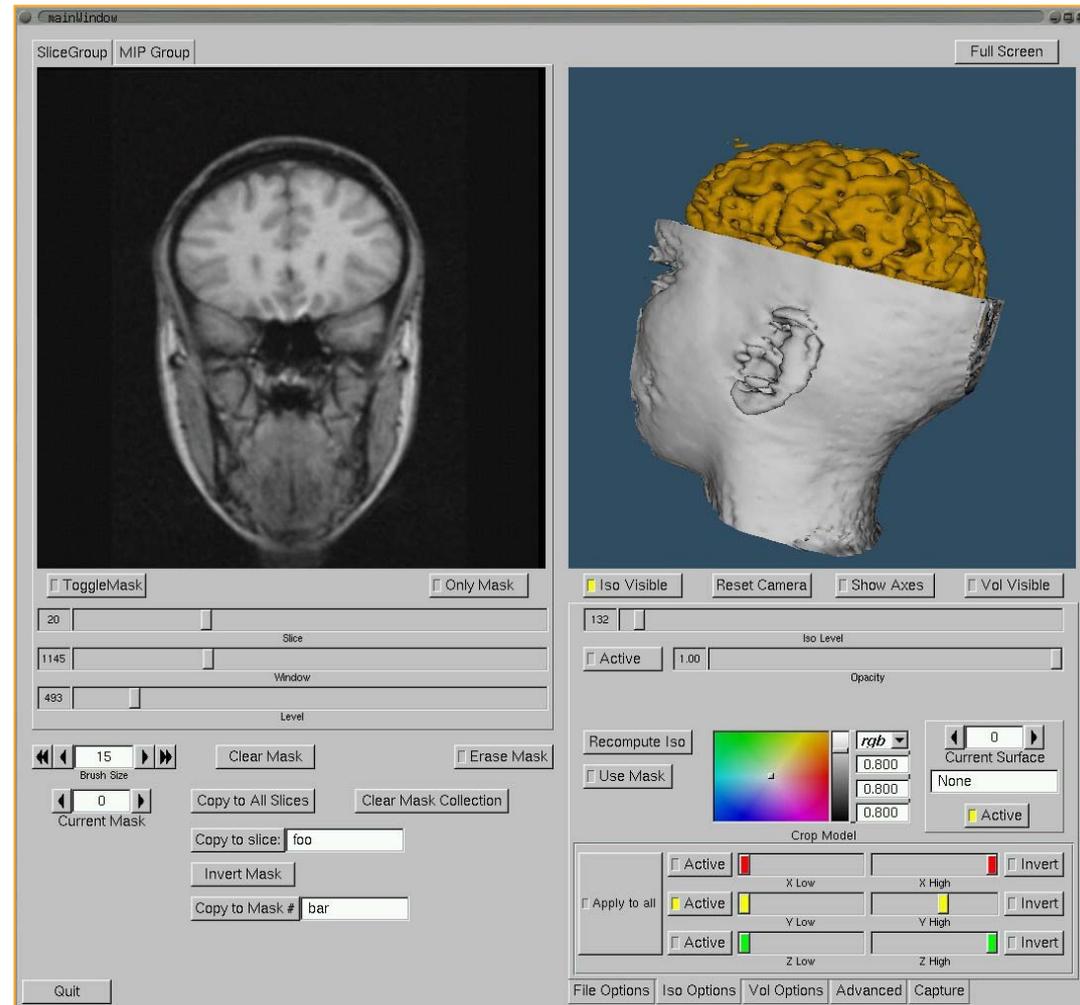


Multiple Sclerosis Project

- Collaboration with Buffalo Neuroimaging Analysis Center (BNAC)

- Developers of Avonex, drug of choice for treatment of MS

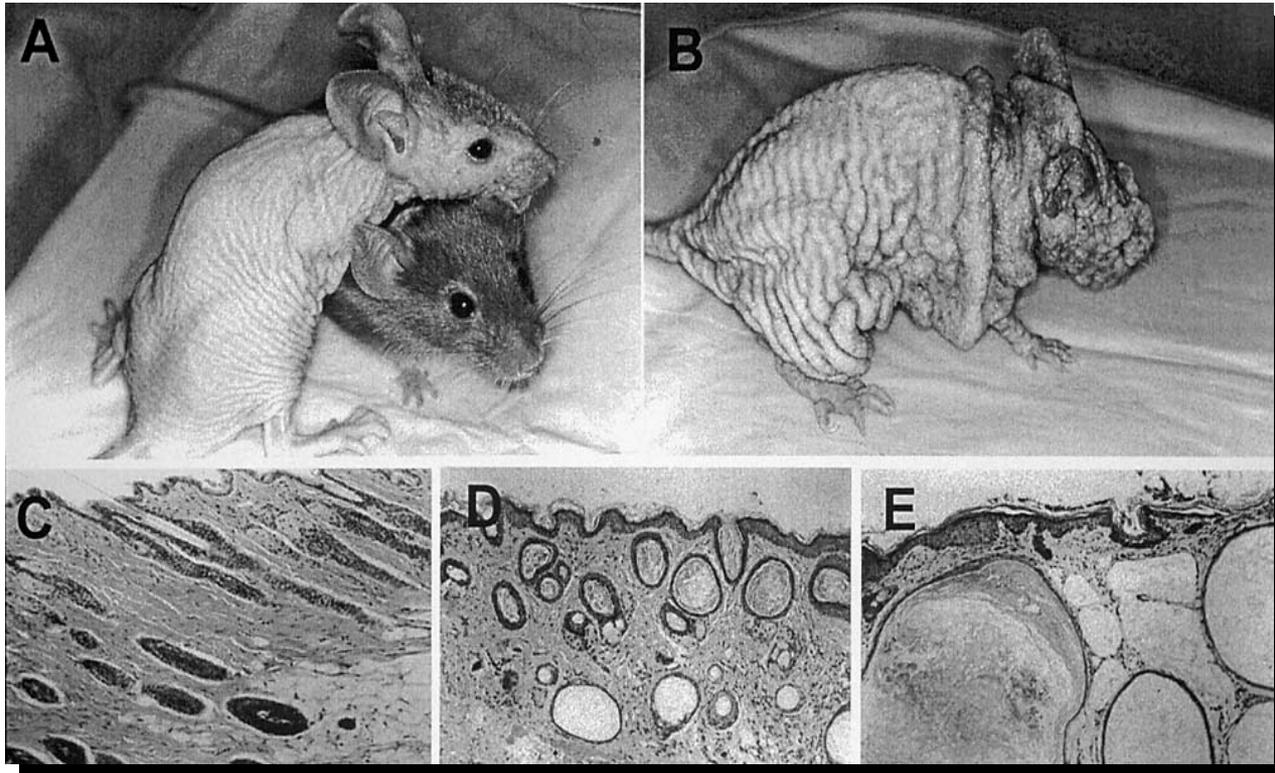
- MS Project examines patients and compares scans to healthy volunteers



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**

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