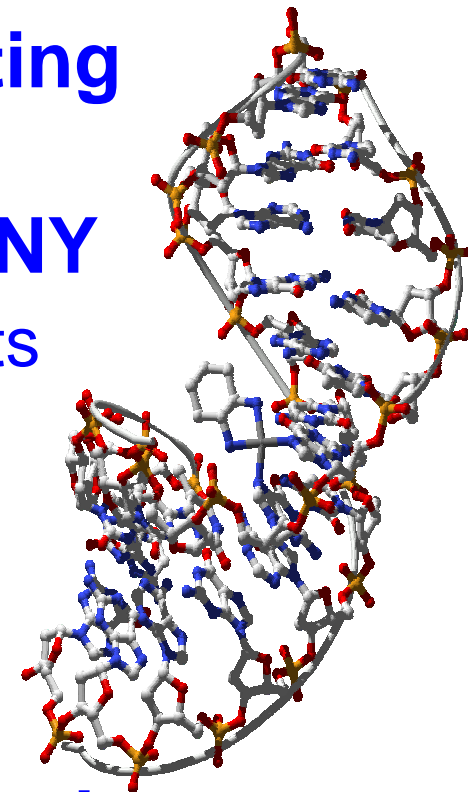**Supercomputing**

- **Leading Academic Supercomputing Center in the U.S.**
- **Enable Research at UB and in WNY**
  - 90 Research Groups/25 Departments
- **Industrial Outreach**
- **Education, Outreach & Training**
  - High Schools and Middle Schools
  - Local Colleges
- **Total Aggregate Computing Capacity**
  - **13** Teraflops (13 Trillion operations/sec)
  - Can do in 1 day what a PC would take 6 years to do

CCR Computing Resources (13 Tflop)

Supercomputing

- **Dell Linux Cluster (10TF)**
  - 1600 P4 Processors (3.2 GHz)
  - Myrinet High-Speed Interconnect
  - 2000 GB RAM; 60 TB Local Disk
  - 30 TB SAN
- **Dell Linux Cluster (3.0TF)**
  - 512 P4 Processors (3.0 GHz)
- **EMC SAN**
  - 35 TB Storage
- **HP/Compaq SAN**
  - 75 TB Disk; 190 TB Tape
  - 64 Alpha Processors (400 MHz)
  - 32 GB RAM; 400 GB Disk

- **SGI Altix3700 (0.4TF)**
  - 64 Processors (1.3GHz ITF2)
  - 256 GB RAM,2.5 TB Disk
- **BioACE: Bioinformatics System**
  - Sun V880 (3), Sun 6800
  - Sun 280R (2)
  - Intel P4's
  - Sun 3960: 7 TB Disk Storage

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CCR Visualization Resources

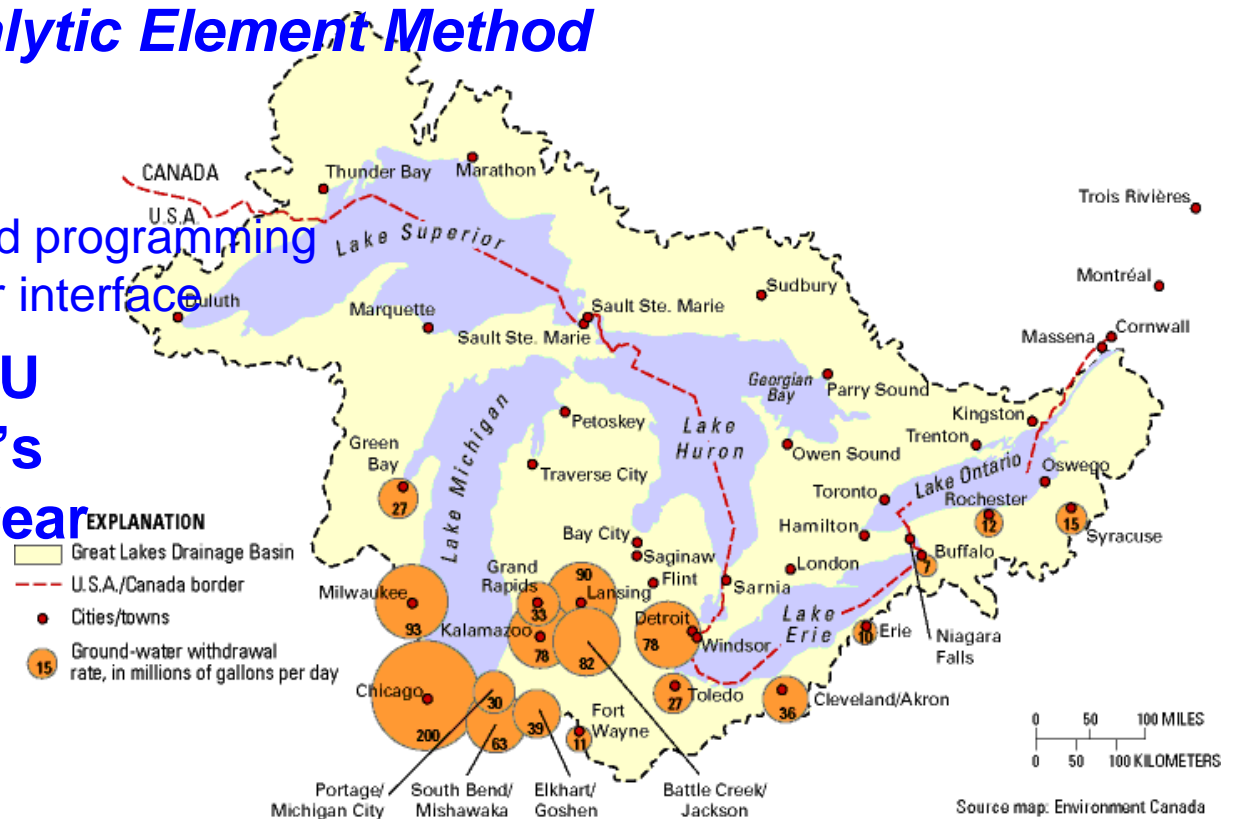**High End Visualization**

- **Tiled-Display Wall**
  - 20 NEC projectors: 15.7M pixels
  - Screen is 11'×7'
  - Dell PCs with Myrinet2000

- **Access Grid Nodes (2)**
  - Group-to-Group Communication
  - Commodity components

- **3D Passive Stereo Display**
 - VisDuo ceiling mounted system

Groundwater Flow Modeling

- **Regional scale modeling of groundwater flow and contaminant transport (Great Lakes)**

- **Ability to include all hydrogeologic features as independent objects**

- **Based on *Analytic Element Method***

- **Key features:**
  - Highly parallel
  - Object-oriented programming
  - Intelligent user interface

- **Utilized 42 CPU years on CCR's clusters last year**

A. Rabideau, I. Jankovic, M. Becker
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Groundwater Dispersion
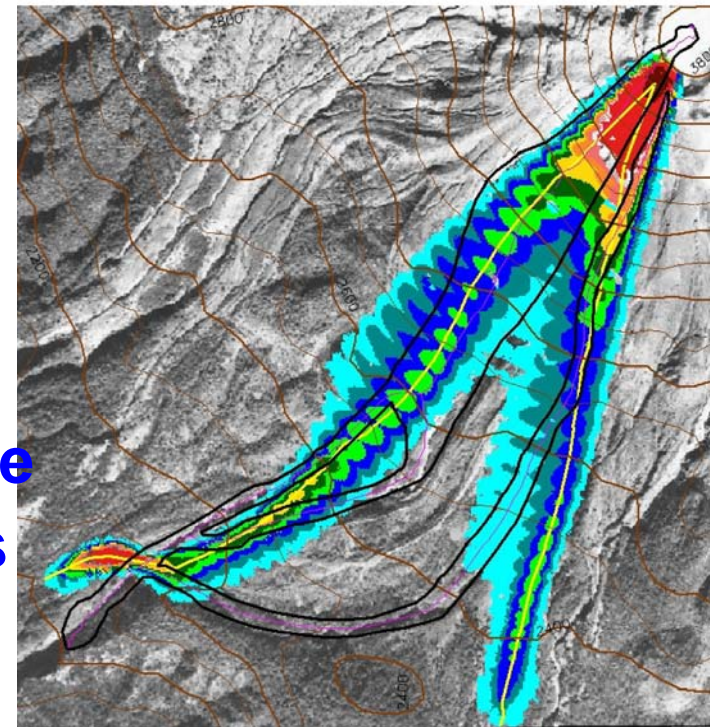
Environmental Engineering

- **Basic research on contaminant spreading in aquifers**
- **Collaboration with leading scientists from Israel and Italy**
- **Designed to improve characterization of existing and future contaminant plumes**
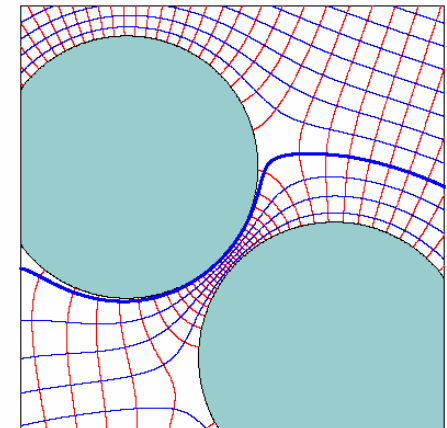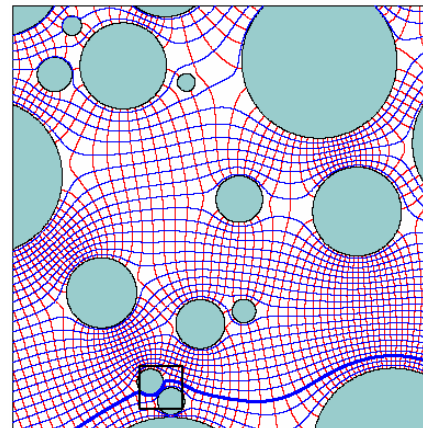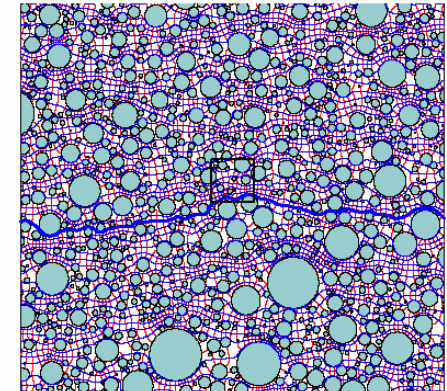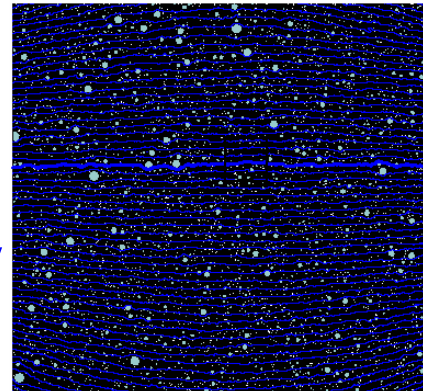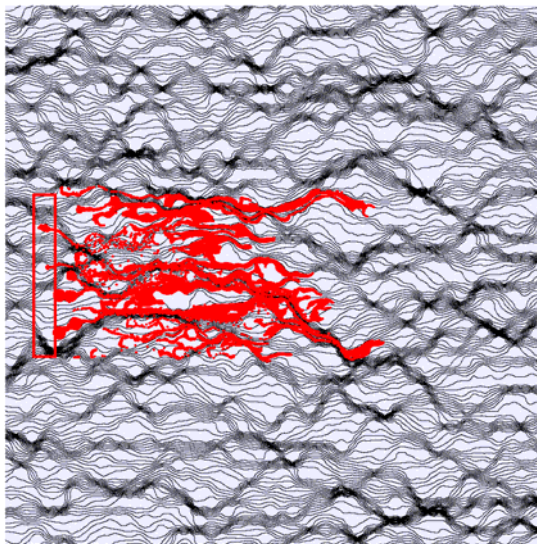
- **Analytic and numerical modeling with up to 10 billion cells in 2D and 3D**

Avalanches, Volcanic and Mud Flows

- **Modeling of Volcanic Flows, Mud flows (flash flooding), and Avalanches**
- **Integrate information from several sources**
  - Simulation results
  - Remote sensing
  - GIS data
- **Present information to decision makers using custom visualization tools local & remote**
- **GRID enabled for remote access**
- **Key Features**
  - Parallel Adaptive Computation
 - Integrated with GIS System for flows on natural terrain

Flow models of Colima volcano
In Mexico – courtesy Rupp et. al.'06

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A. Patra, B. Pitman, M. Sheridan, M. Jones
Center for Computational Research

Cardiac Arrhythmia

Center for Cellular and Systems Electrophysiology

- **Comprehensive models of cardiac cells**

- **Modeling multicellular cardiac tissues and mechanisms of arrhythmias in the heart**

- **Simulation of genetic heart disease and arrhythmia suppression by drug application**
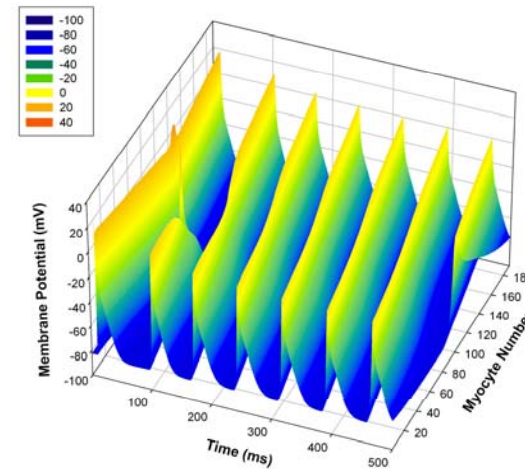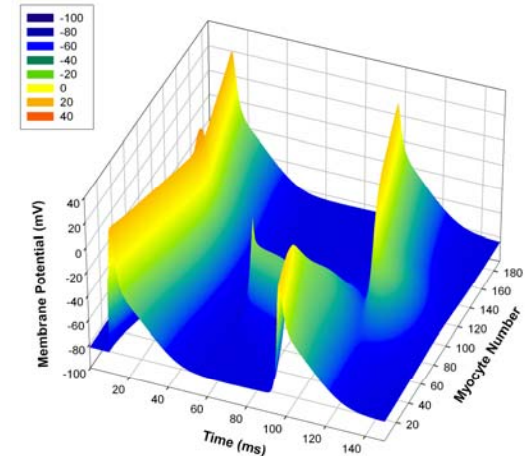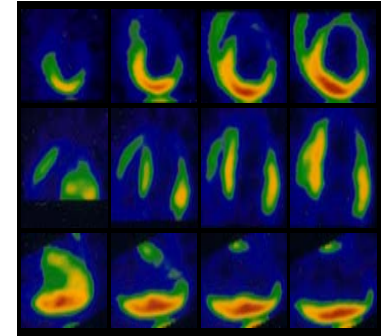

Non-sustained and sustained arrhythmia

Cardiovascular Research

Cardiology

- ## Molecular Imaging – PAREPET Clinical Study

  Analysis of cardiac PET (Positron Emission Tomography) scans aims to revolutionize assessment of an individual's risk for sudden cardiac death.
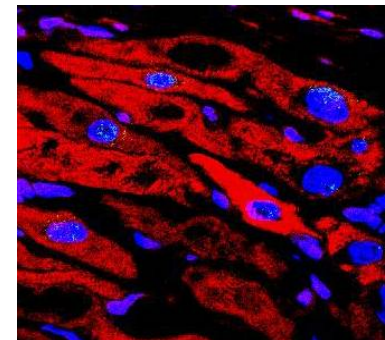
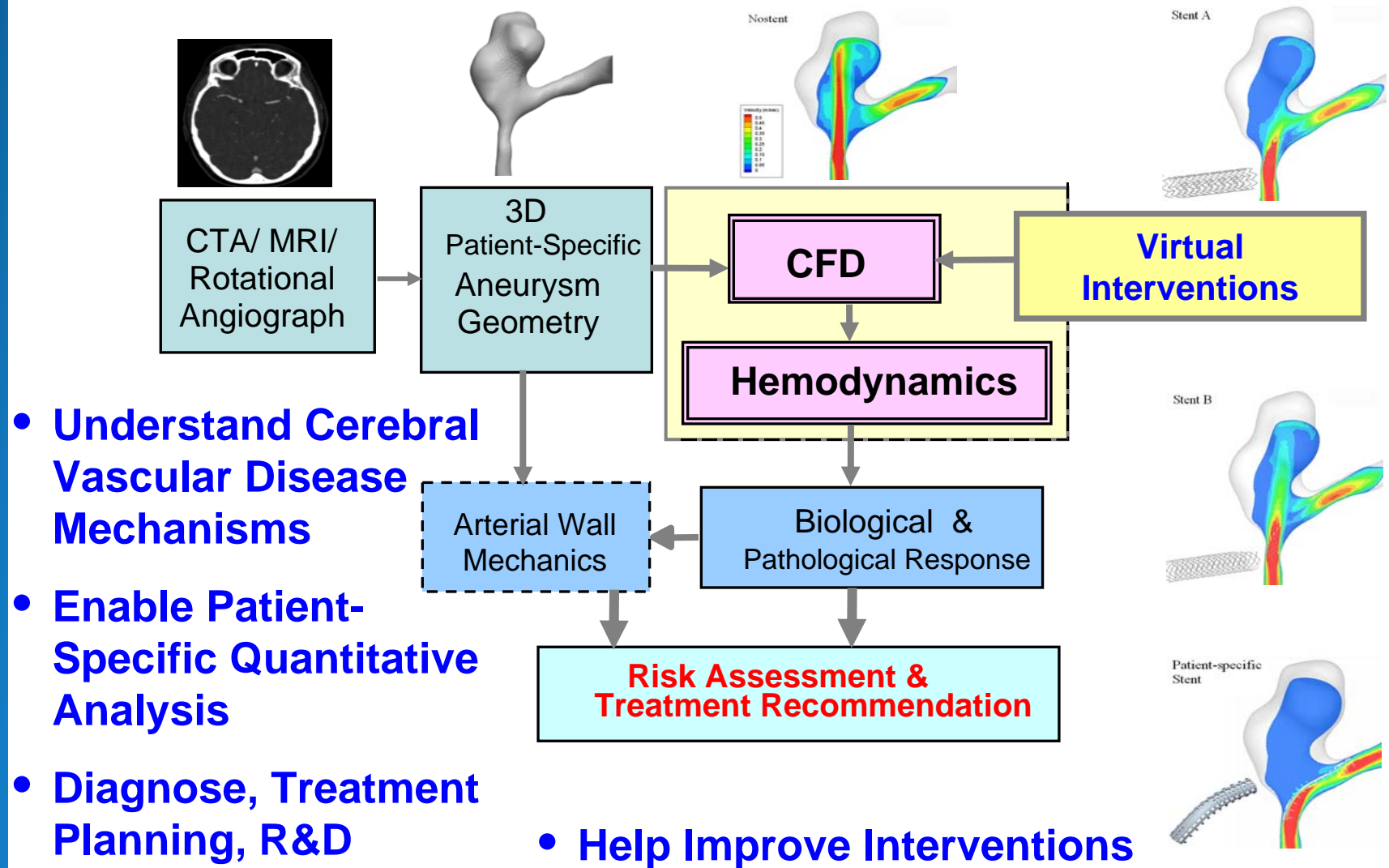- ## High-Throughput Discovery – Proteomics and Genomics

  Protein and gene expression profiling using differential in-gel electrophoresis and microarray technology provides a blueprint for the cellular mechanisms involved in hibernating myocardium.
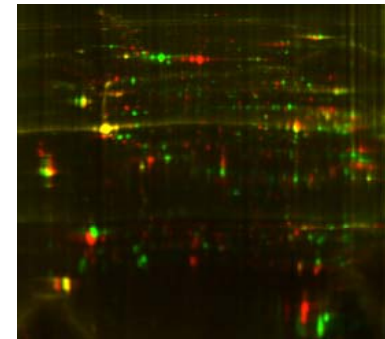
  Translate results to identify gene and other therapeutic targets aimed at improving heart function and survival.
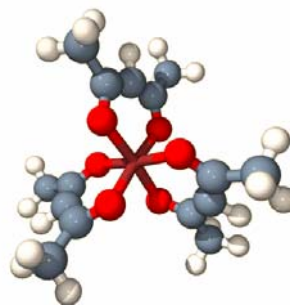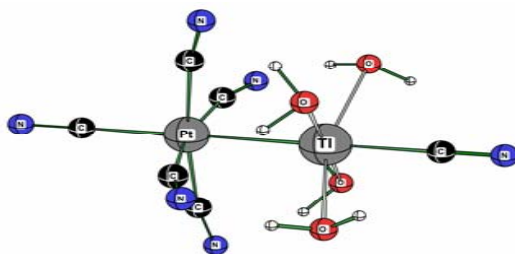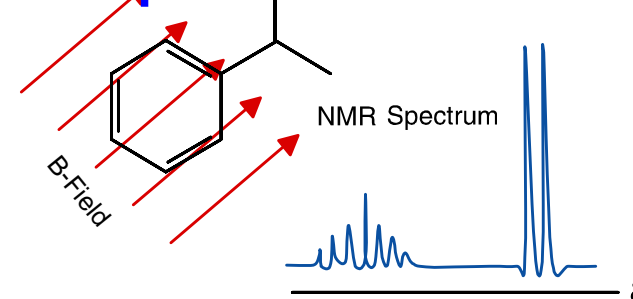
Cerebral Aneurysm: Virtual Intervention

CTA/ MRI/ Rotational Angiograph → **3D Patient-Specific Aneurysm Geometry**

CFD ← **Virtual Interventions**

Hemodynamics

Arterial Wall Mechanics ← **Biological & Pathological Response**

Risk Assessment & Treatment Recommendation

- **Understand Cerebral Vascular Disease Mechanisms**
- **Enable Patient-Specific Quantitative Analysis**
- **Diagnose, Treatment Planning, R&D**
- **Help Improve Interventions**

Nostent

Stent A

Stent B

Patient-specific Stent

Theoretical and Computational Chemistry

Chemistry

Applied to:
- **Polypeptides**
- **Carbon Nanotubes**
- **Fullerenes**
- **Cluster Compounds**
- **Transition metal Chemistry**

Computational NMR

NMR Spectrum

B-Field

δ

Magnetic Properties of Molecules

Software Development

Theory and Calculation of Optical Activity

Optical Rotation
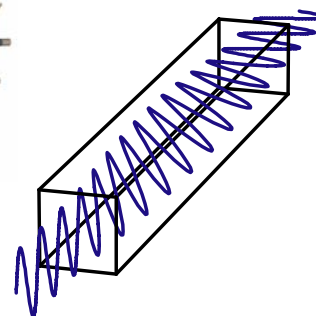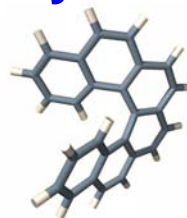
Circular Dichroism Spectra

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J. Autschbach

University at Buffalo
The State University of New York

Center for Computational Research
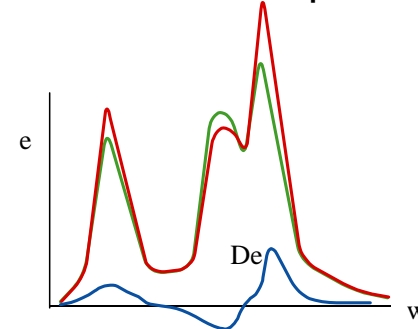
3D Structure of Proteins

- **Direct Methods for Crystal Structure Determination**
  - Listed on "Top Ten Algorithms of the 20th Century"
- **UB/HWI collaborative software development**
  - SnB – determine protein heavy-atom substructures
    (http://www.hwi.buffalo.edu/SnB/)
  - BnP – determine complete protein structures
    (http://www.hwi.buffalo.edu/BnP/)
- **Applications to drug design**
  - AIDS
  - Arthritis
  - Cancer
  - Heart disease
  - SARS

BIOCHEMISTRY

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Hauptman-Woodward
Institute

R. Miller, C. Weeks
Center for Computational Research
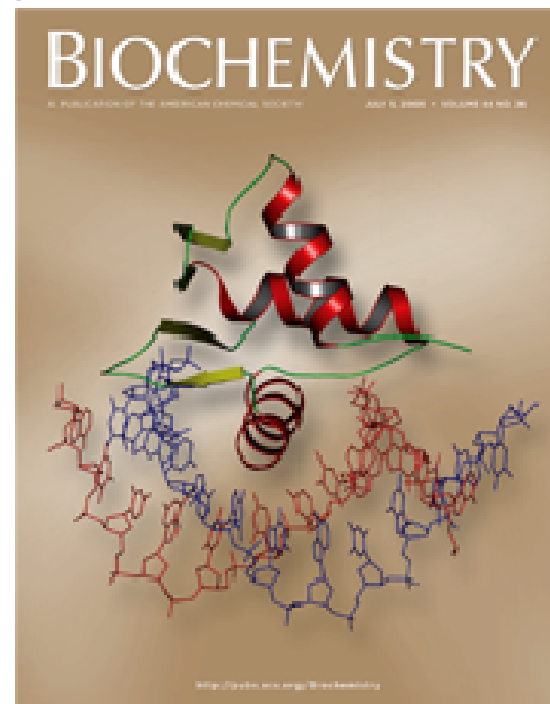
Understanding How Proteins work

Collaboration with Merck Pharmaceutical Company

Chemistry

Modeling:
- **DNA-Protein Interaction (understanding cancer)**
- **Drug-Protein Interaction (understanding blood clotting)**

Movie shows a chemical reaction between a protein and DNA, which is responsible for some types of cancer.

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M. Freindorf, T. Furlani
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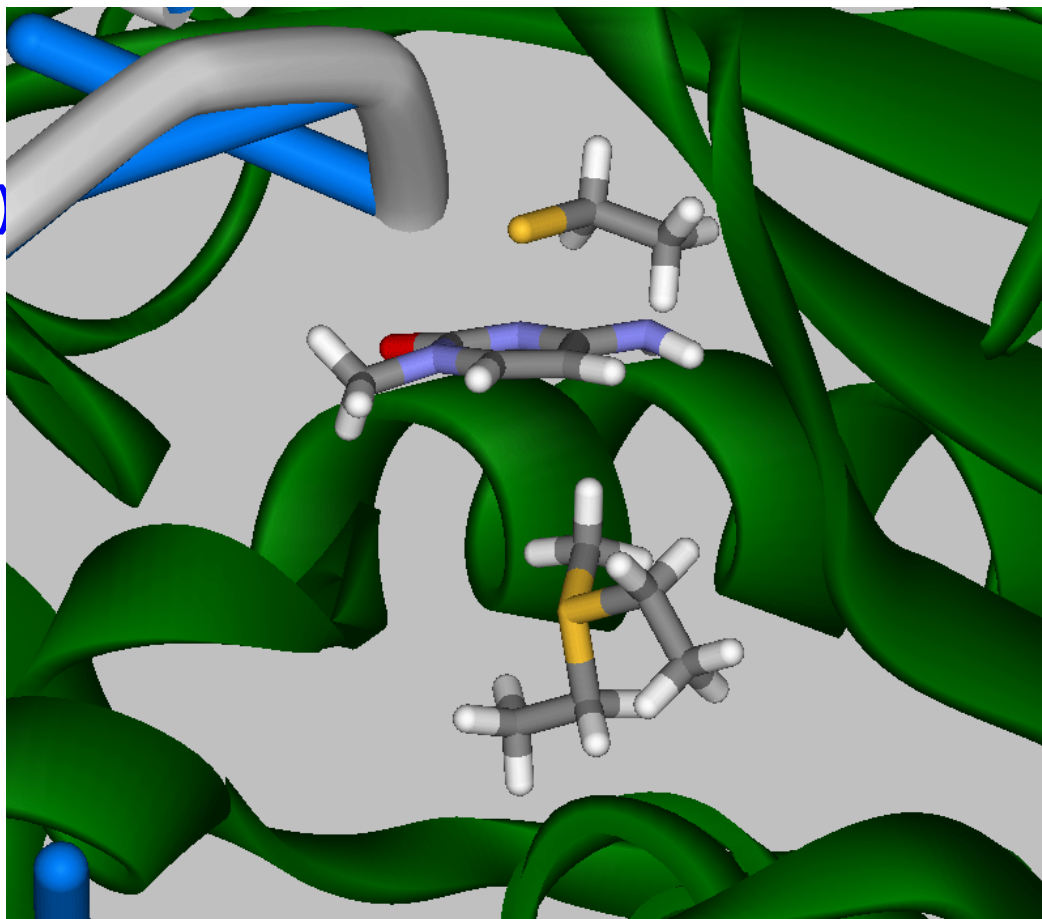
Computational Biology & Bioinformatics

- **Development of Bioinformatic Tools**

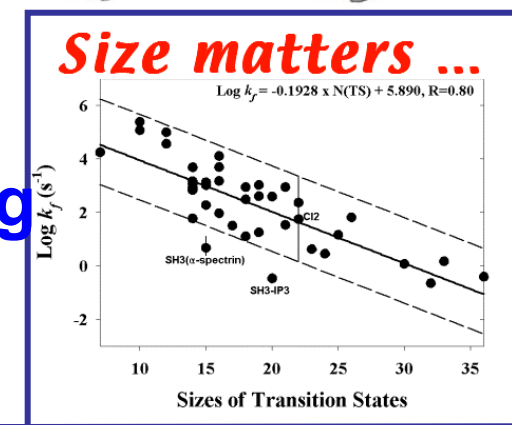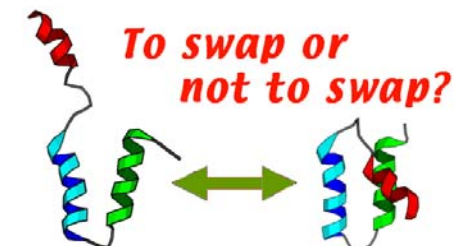 SPEM – align multiple sequences for discovering hidden evolution information of genes.

  SPARKS/SP^3 – predict three-dimensional structures of proteins by matching a query sequence with known structural templates.

  DFIRE – predict binding affinities of protein-protein, protein-ligand, and protein-DNA complexes for structure-based drug design.

- **Mechanistic study of protein folding and binding**

  http://theory.med.buffalo.edu

M. Halfon

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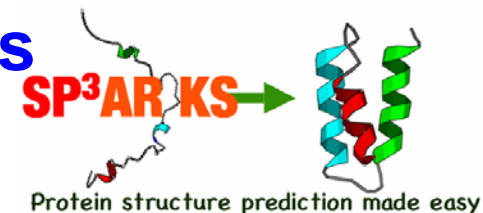
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Computational Chemistry

- **UB Software development in Quantum Chemistry**
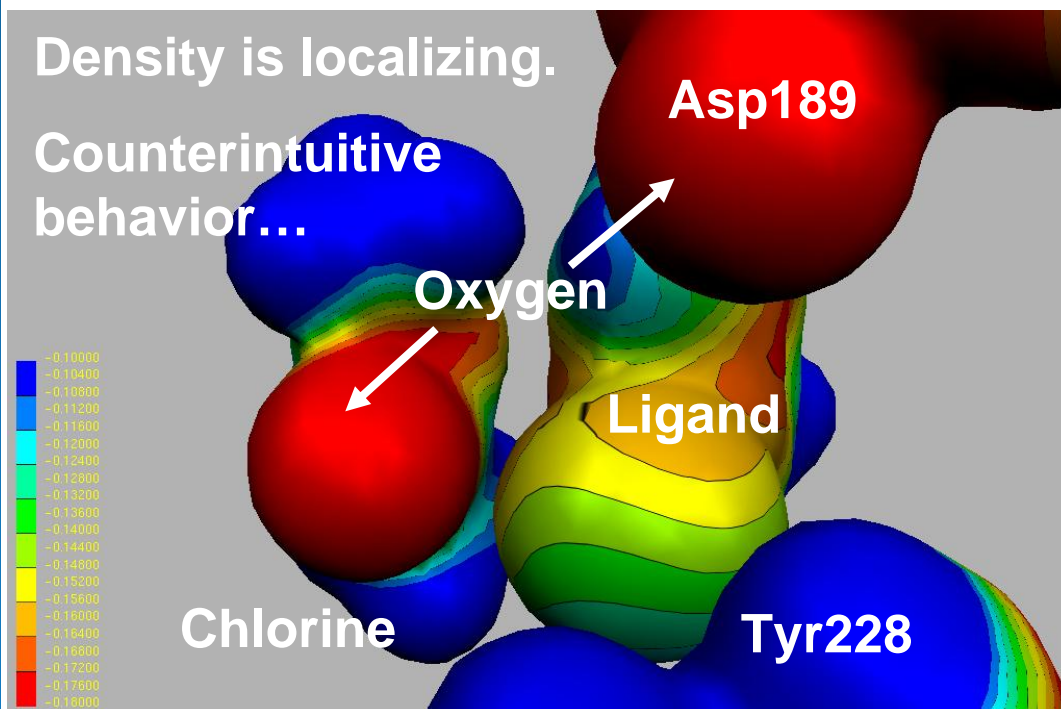 - **Q-Chem** – development of combined QM/MM methods for large molecular systems such as proteins
  - **ADF** – development of algorithms to calculate magnetic and optical properties of molecules
- **Used to determine**
  - 3D Molecular Structure
  - Electronic Spectra
  - Chemical Reactivity
- **Applications**
  - Pharmaceutical Drug Design
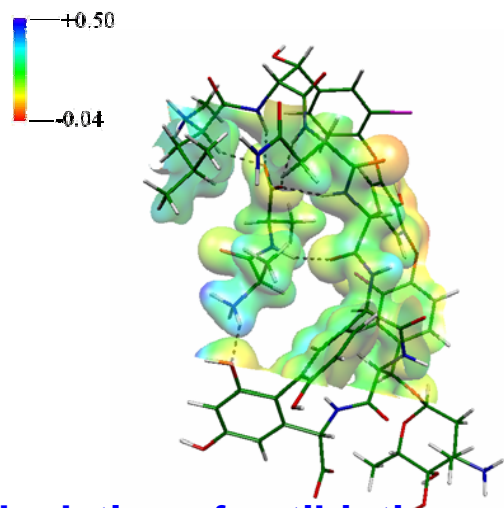 - Industrial Catalysis
  - Materials Science
  - Nanotechnology

Chemistry

SIGMA-ALDRICH: NEW PLAN INVIGORATES COMPANY

CHEMICAL
& Engineering News

OCTOBER 8, 2001

Computational Chemistry
Scenes from the cutting edge

Binding in a Drug-Receptor Complex

Pharmaceutical Drug Design

Density is localizing.

Counterintuitive behavior…
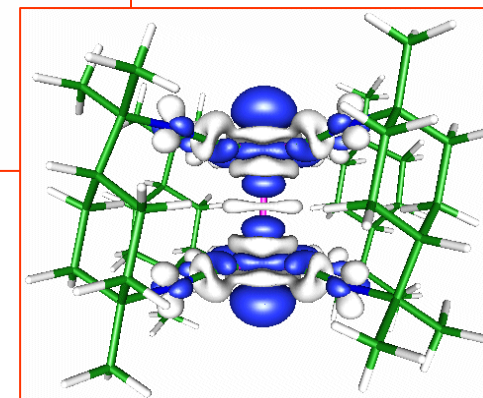
Asp189
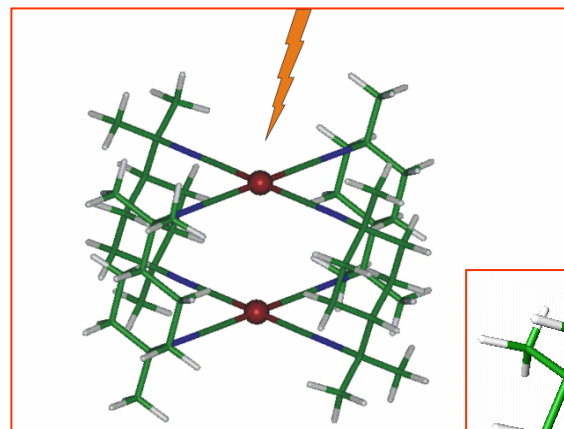
Oxygen

Ligand

Chlorine

Tyr228

- **Ligand docked with residues of the active site of thrombin. Electrostatic potential map superimposed onto the electron density isosurface.**
- **The goal is to elucidate the thermodynamics of molecular recognition in binding.**

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D. Hangauer, M. Freindorf
Center for Computational Research

Understanding Large Molecules and Fleeting Species

Chemistry

+0.50
−0.04

**Calculation of antibiotic molecules:
electrostatic potential of vancomycin**

A molecule changes on excitation by light

A supramolecular solid

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P. Coppens
Center for Computational Research
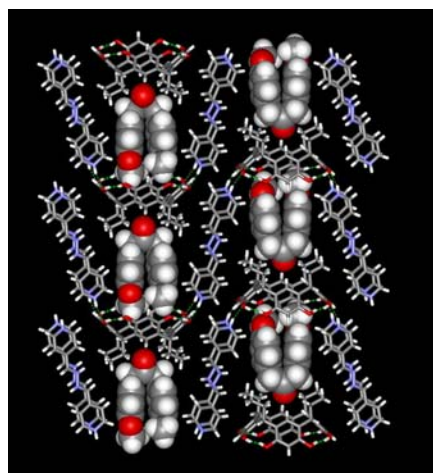
# 3D Medical Visualization

- **Reads data output from a CT or MRI Scan**
- **Collaboration with Children's Hospital**
- **Visualize multiple surfaces and volumes**
- **Export images, movies or CAD file**
- **Pre-surgical planning**
- **Runs on a PC**

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M. Innus
Center for Computational Research

Mapping Brain Activity

Medical Imaging
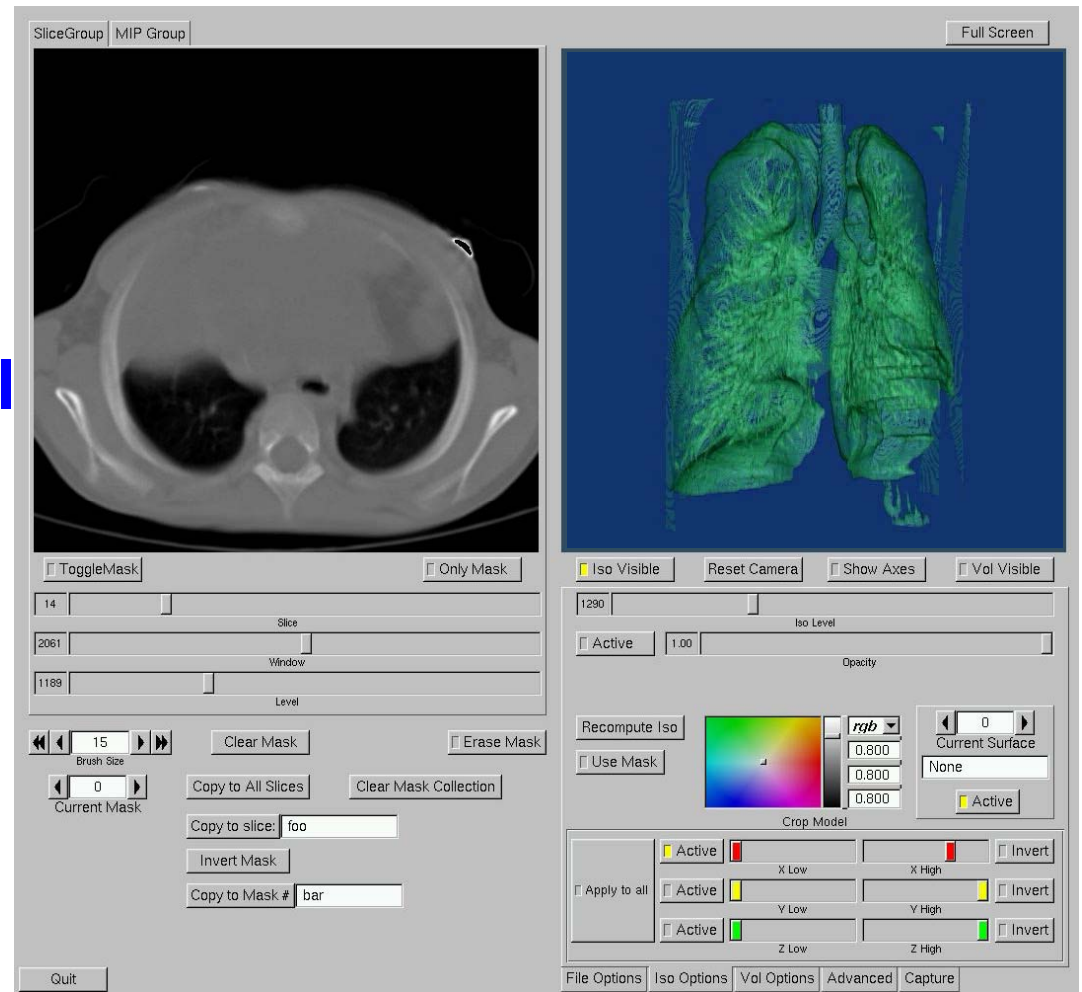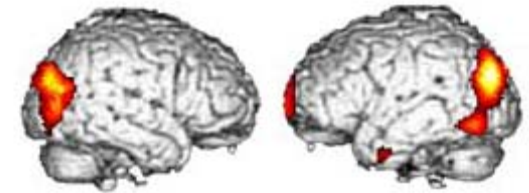
Positron emission tomography (PET), shows sites activated and deactivated as subjects decide whether a sound is a target or not.
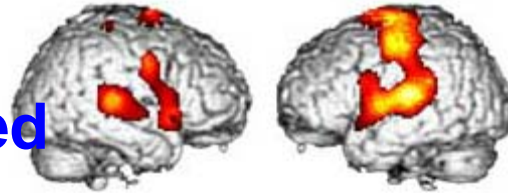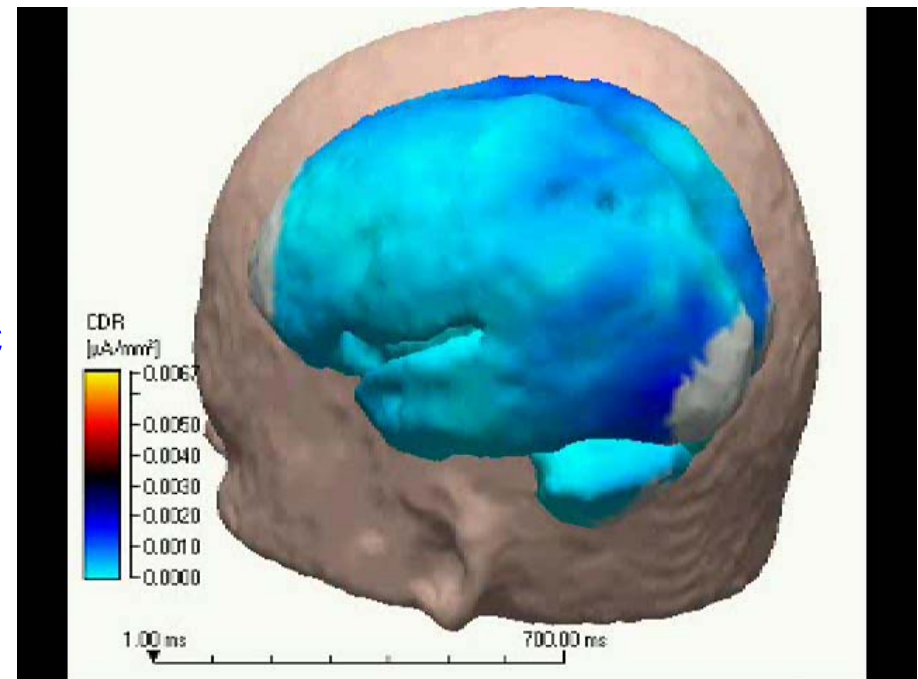
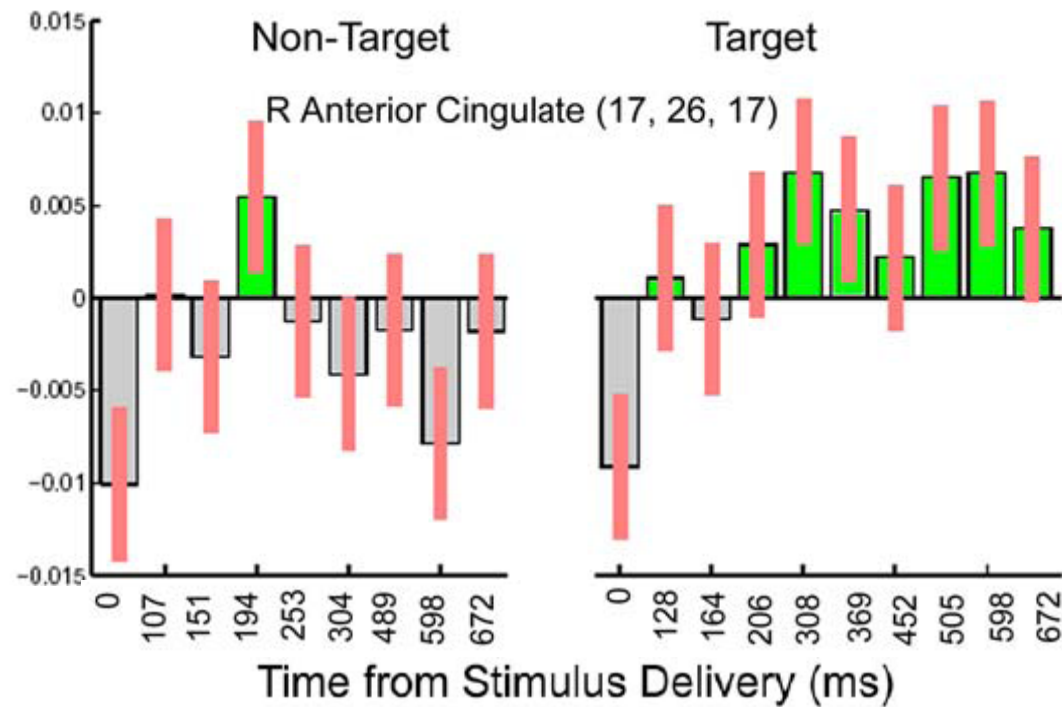**Current density maps of brain surface (1–700 ms after target) show dynamic pattern of brain activity during decision-making process.**

Sites Activated

Sites Deactivated

CDR
[μA/mm²]

- 0.0067
- 0.0050
- 0.0040
- 0.0030
- 0.0020
- 0.0010
- 0.0000

1.00 ms   700.00 ms

Mapping Brain Activity

Temporal sequence of anterior cingulate cortex activation in response to targets and non-targets. This brain region controls attention-related neural activity. Green bars indicate significant differences compared to T = 0, the time of stimulus presentation.

Nuclear Medicine

- ## Monte Carlo simulation
  - for modeling imaging system characteristics, optimizing system design, and validating data correction algorithms.

- ## Image reconstruction
  - for development of high resolution image reconstruction algorithm and software for both human and animal nuclear emission tomographic systems.
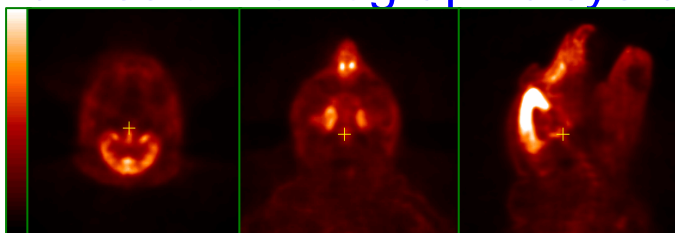
Transverse, coronal and sagittal views of a monkey brain scanned on a dedicated brain PET using the radioligand ^{18}F-FCWAY.
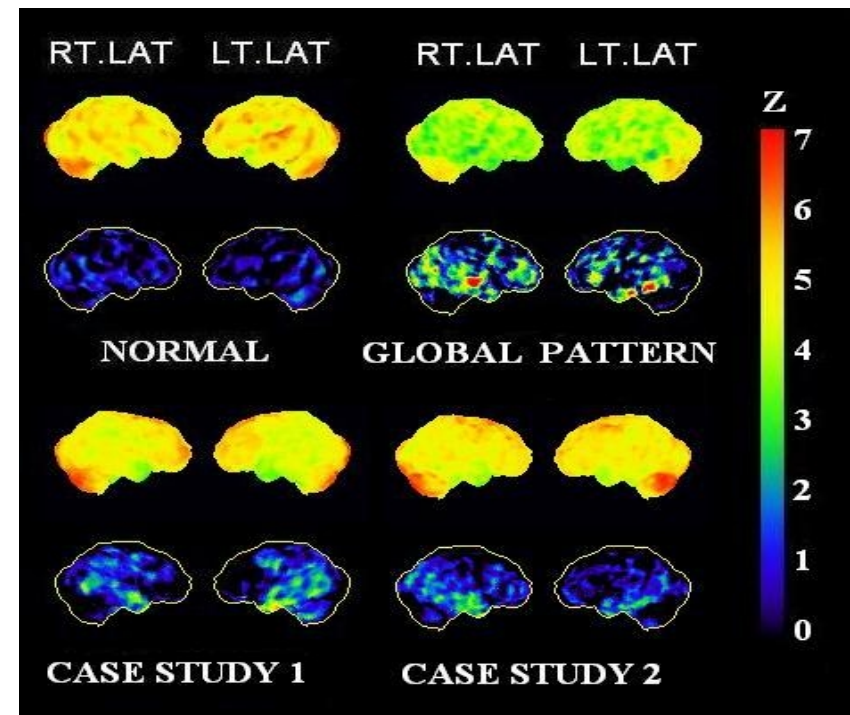
Medical Imaging
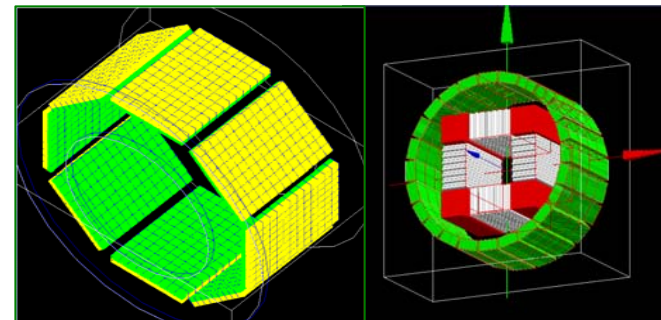
Two virtual imagers simulated for system modeling and design evaluation.
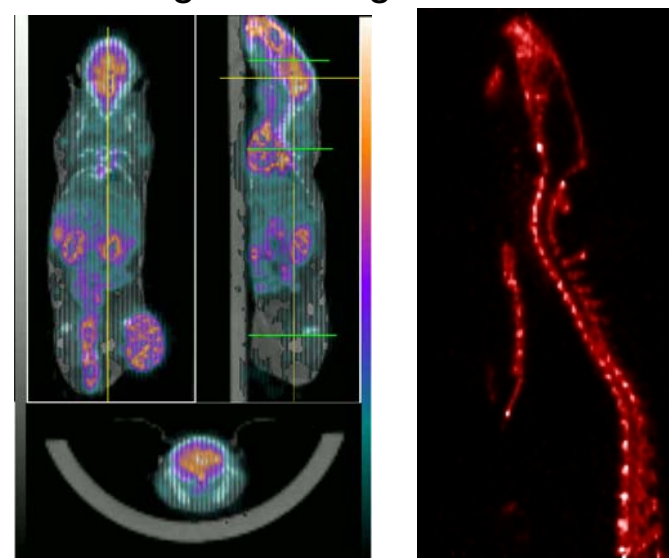
Co-registered ^{18}F-FDG PET and CT mouse images (left) and a ^{18}F-Fluorine bone image of a 250 gram rat.

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Y. Yao, M. Jones
Center for Computational Research

Vascular Dementia Imaging

- **Early diagnosis of dementia from cerebral small vessel disease using computer analysis of SPECT Images**

- **Collaboration between Nuclear Medicine, CCR, Neurology, and Kaleida Stroke Center**

- **Funded by the Pfeiffer Foundation**

- **<u>Fractal scores</u>:**
  - Normal   0.75
  - Global Pattern   1.13
  - Case Study 1   0.96

- **<u>Case Study 1</u> Moderate white matter and cortical hypo-perfusion with visual memory, speed of processing, and verbal fluency deficits**

Medical Imaging

University at Buffalo
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J. Baker, M. Innus
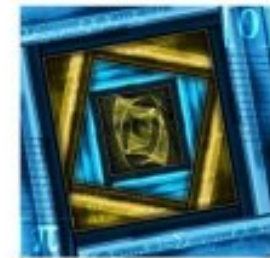Center for Computational Research

Parallel Algorithms

- **String pattern matching searches for word processors, Web, molecular biology**
- **Image processing**
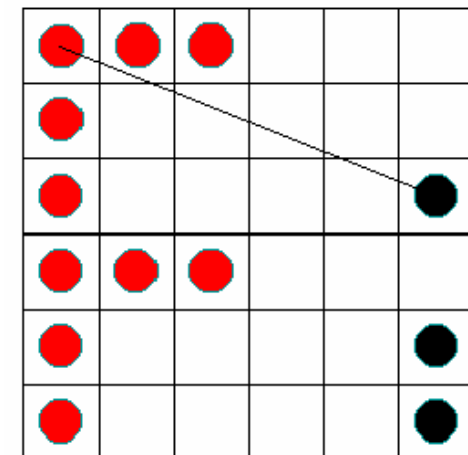- **Computational geometry**
- **Fundamental operations**
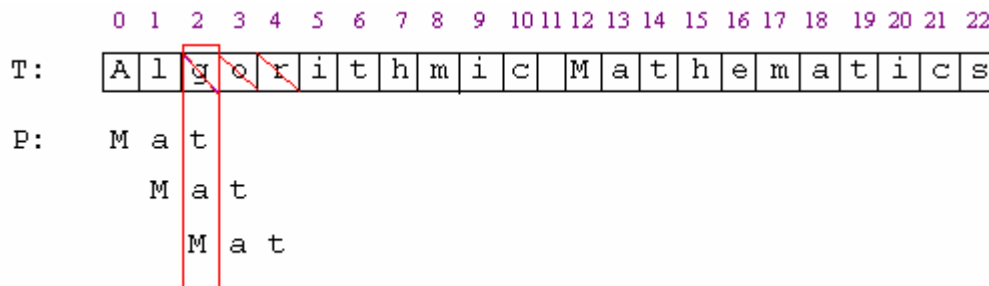
Collaborative Visualization Environments

Visualization

- Enable distributed collaboration via software developed at CCR

- Enable visualization and interaction with data across a geographically disparate network topology

- Integrate multiple data sources:
  - Scientific, Multimedia

- Research topics:
  - Distributed databases
  - OpenGL 3D programming
  - 3D Modeling
  - Character animation
  - User interaction
  - Virtual Reality

A. Ghadersohi, R. Miller, M. Green
Center for Computational Research

University at Buffalo
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Literacy & Disability in Canada

- **Exploring the relationship between illiteracy & disability across the Canadian landscape**
- **Social Systems GIS Lab in the Dept. of Anthropology is working with researchers from York University & the Canadian Abilities Foundation.**
- **Sponsored by The Adult Learning & Literacy Directorate of the Ministry of Human Resources & Social Development Canada.**

E. Zubrow
Center for Computational Research
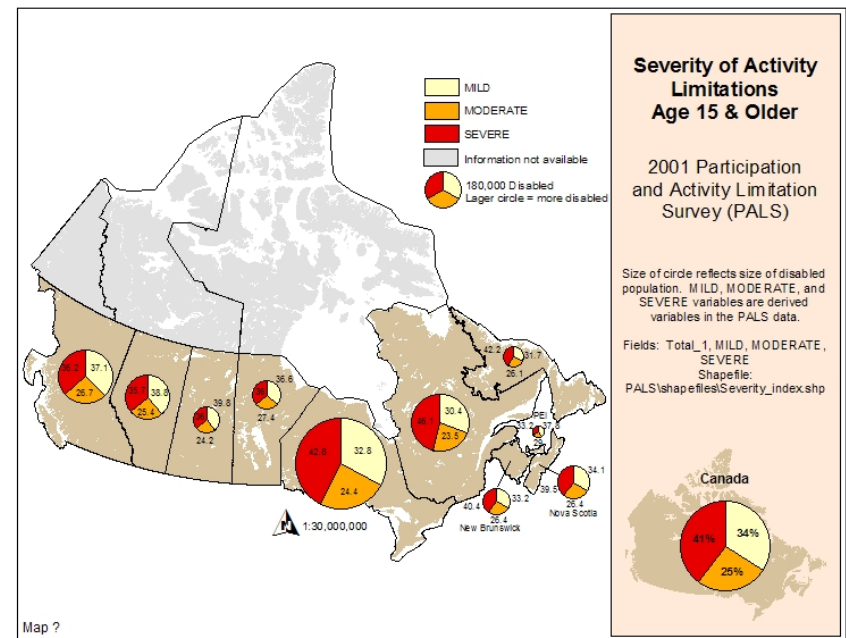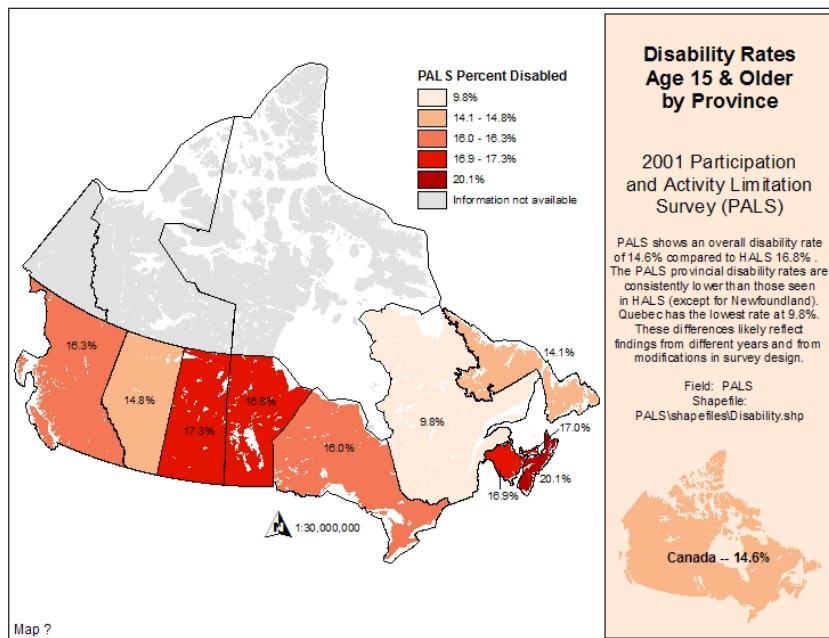
Verberie Paleolithic Site in France

- **Intrasite spatial analysis and 3D modeling of the a Late Upper Paleolithic archaeological site in the Paris Basin of France**
- **Social Systems GIS Lab in the Dept. of Anthropology is working with researchers from the CNRS in Paris**
- **Sponsored by the National Science Foundation**

Anthropology
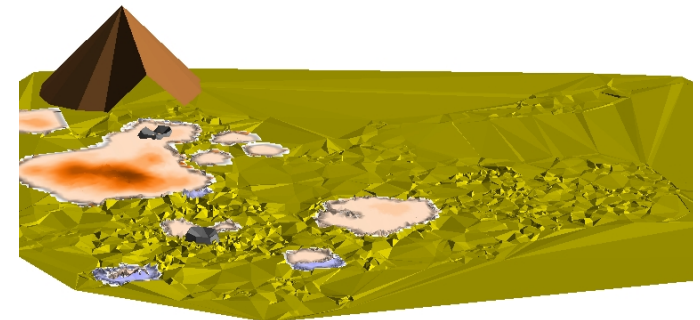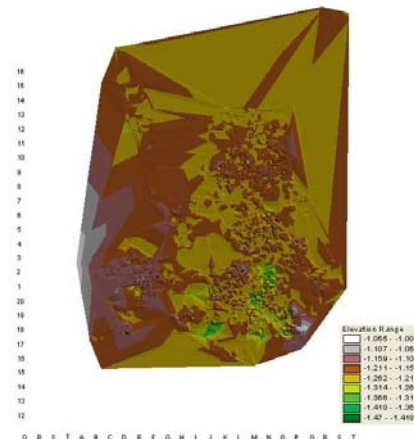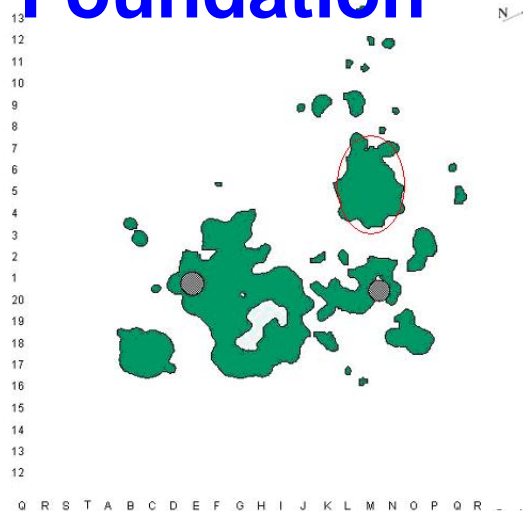
Cosmological Parameter Estimation
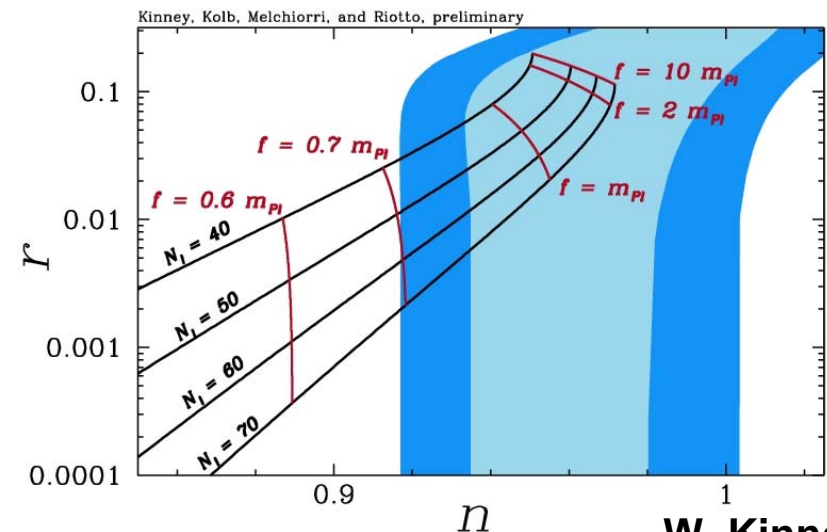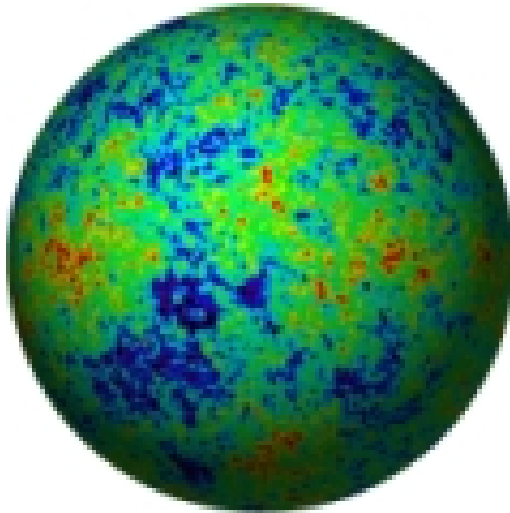
Cosmology

- **Wealth of new precision cosmological data**
- **WMAP Cosmic Microwave Background Measurement**
- **Sloan Digital Sky Survey: 3-D map of a million galaxies**
- **Interpret implications of data for models of the first trillionth of a second of the universe: _inflation_**
- **_Monte Carlo Markov Chain data analysis: stochastic exploration of many-dimensional parameter spaces_**
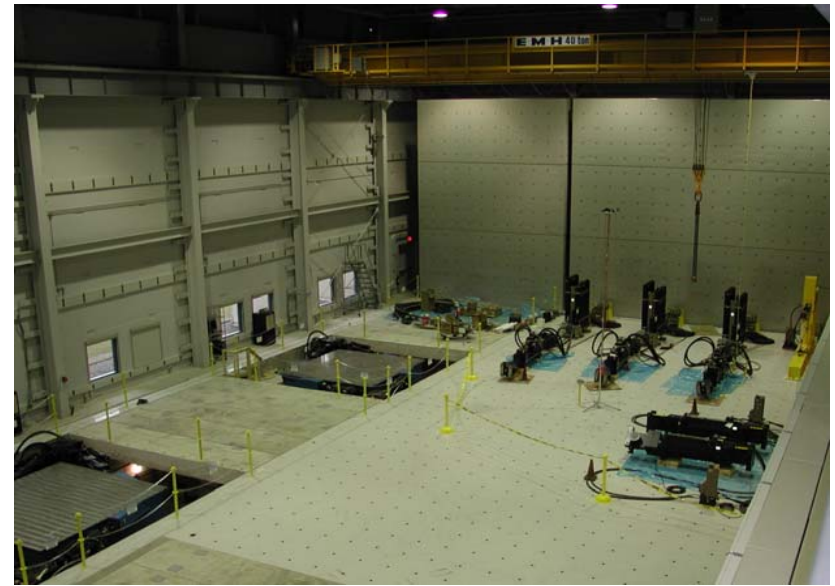

Kinney, Kolb, Melchiorri, and Riotto, preliminary

$f = 10\ m_{Pl}$
$f = 2\ m_{Pl}$
$f = 0.7\ m_{Pl}$
$f = 0.6\ m_{Pl}$
$f = m_{Pl}$
$N_I = 40$
$N_I = 50$
$N_I = 60$
$N_I = 70$
r
n

W. Kinney

UB's Structural Engineering and Earthquake Simulation Laboratory (SEESL)

Structural Engineering

- **World Class Center for Earthquake Engineering**
- **Flagship lab for the (National) Multidisciplinary Center for Earthquake Engineering Research - (N)MCEER since 1986**
- **Upgraded in 2000-2004 under the NSF George E. Brown *Network for Earthquake Engineering Simulation (NEES): ($21.2M)***
- **Commissioned in 2004 and funded through 2014 under NSF's 10-Year "Management, Operation and Management" Award ($15M)**

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M. Bruneau, A. Reinhorn, G. Lee
Center for Computational Research

UB's Structural Engineering and Earthquake Simulation Laboratory (SEESL)

Structural Engineering

- ## Equipment
  - Twin 6-DOF shake tables (50 m-ton capacity); 7mx7m platforms,
  - Three 100-ton dynamic actuators and two 200-ton static actuators
  - Non-structural component Simulator (NCS)
  - 2-D Geotechnical Laminar Box

M. Bruneau, A. Reinhorn, G. Lee
Center for Computational Research

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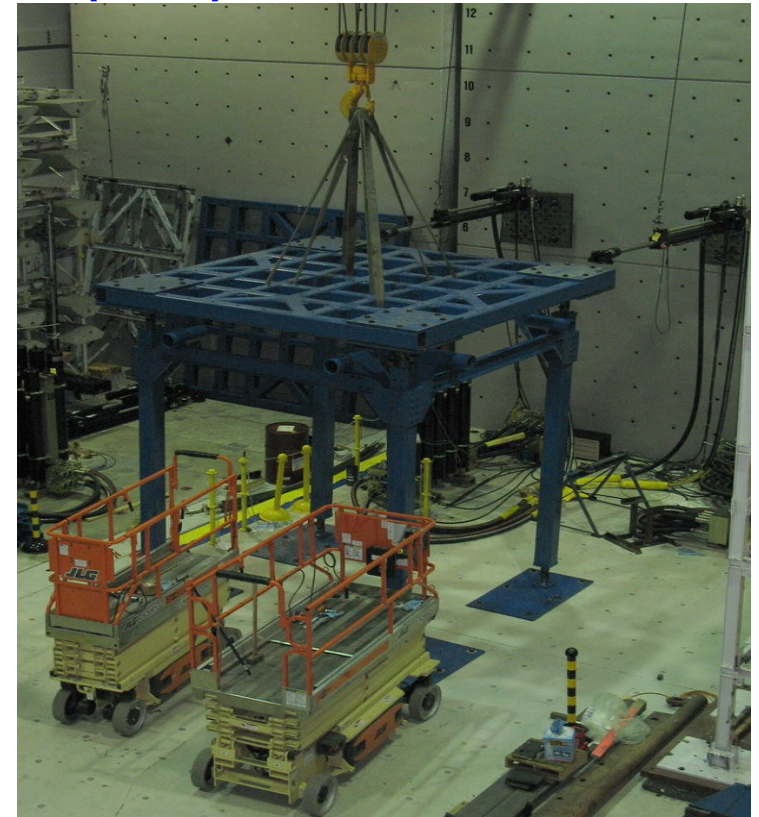
UB's Structural Engineering and Earthquake Simulation Laboratory (SEESL)
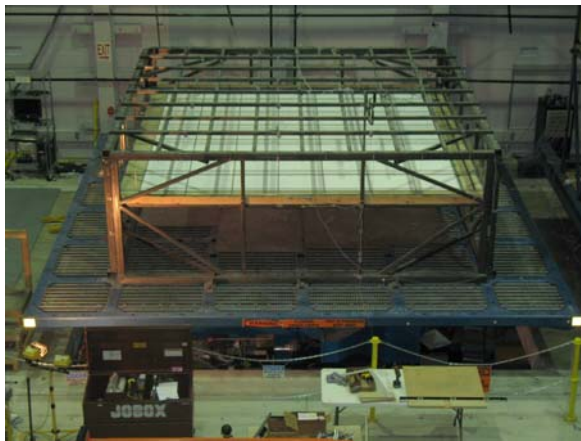
Projects

Seismic Qualification and Fragility Tests of a 230KV-3 Phase Switch Assembly

Seismic Fragility Tests of a Centrifugal Liquid Chiller and Restraint System

Dynamic Seismic Response of Steel Braced Frames

Suspended Ceiling Tile Tests
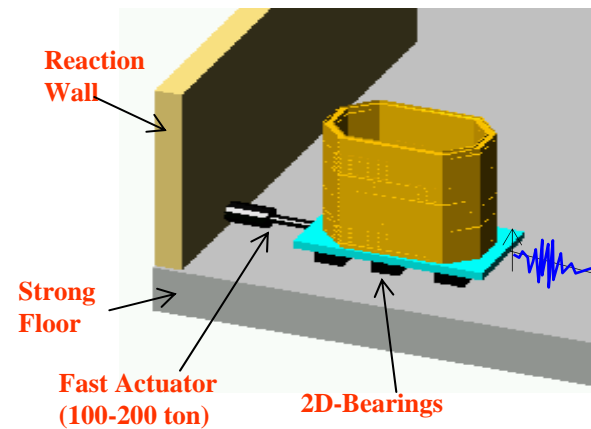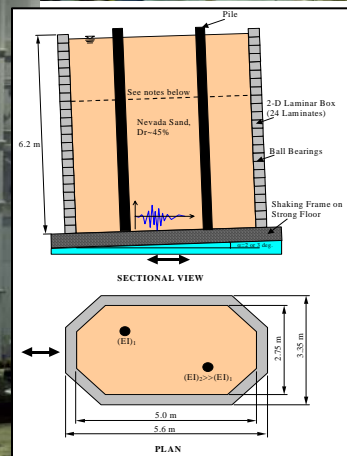

Ridge-U-Rak Inventory Storage System Tests

Structural Engineering

University at Buffalo
The State University of New York

M. Bruneau, A. Reinhorn, G. Lee
Center for Computational Research

Structural Engineering

Projects

NEESWood: Development of a Performance-Based Seismic Design for Woodframe Construction:

**Two-story Townhouse on Twin Shake Tables**

2-D Geotechnical Laminar Box Tests of Pile Foundations Subjected to Soil Liquefaction

Reaction Wall

Strong Floor

Fast Actuator (100-200 ton)

2D-Bearings

University at Buffalo
The State University of New York

M. Bruneau, A. Reinhorn, G. Lee
Center for Computational Research

Cyberinfrastructure in STEM Education

- **Developing a scalable, multi-site cyber-infrastructure for Science, Technology, Engineering and Mathematics (STEM) education and training called *MyDesignSpace*.**

- **Implementing a digital design repository to enhance instruction and learning in STEM education.**

- ***MyDesignSpace* will also help bridge existing gaps between secondary and collegiate STEM education.**
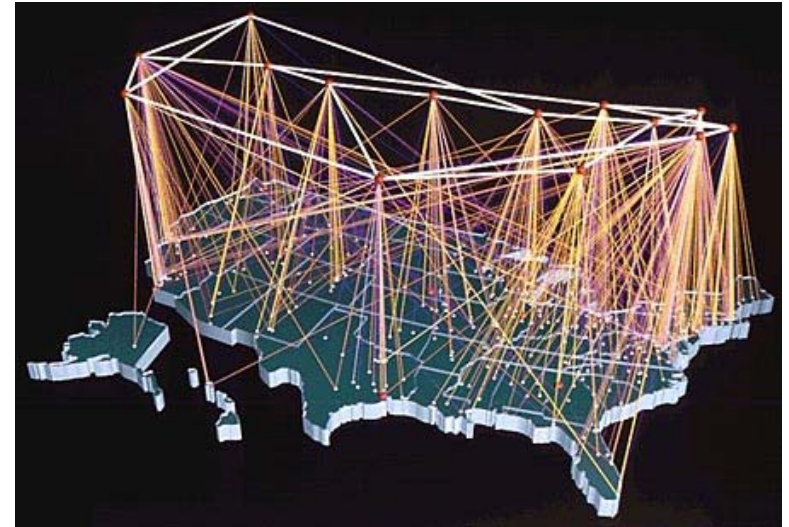
NYSCEDII
New York State Center for Engineering
Design and Industrial Innovation

www.nyscedii.buffalo.edu

K. Lewis

University at Buffalo
The State University of New York

Center for Computational Research

Determining 3D Protein Structure

- **NMR-based Structural Biology and Structural Genomics**
- **Bio-NMR Methodology**
- **NMR-based Metabonomics in Cancer Research**

BUFFALONEWS

HIGH TECHNOLOGY
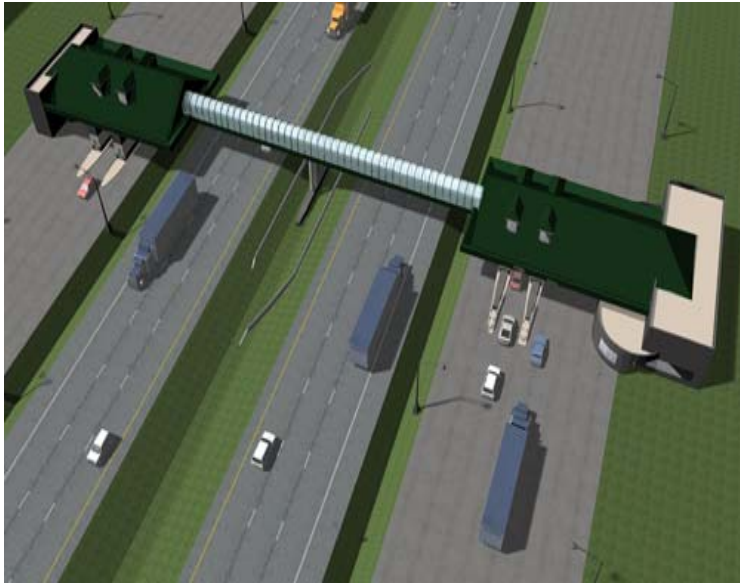**Breakthrough at UB**

Structural Biology

Propelled by Recent Advances, NMR Moves Into the Fast Lane

A speedy new NMR technique could finally help structural genomics groups achieve their goal of devising factory-style approaches to mapping protein structures at high speeds

Urban Modeling & Visualization

- **Peace Bridge Gateway Improvement Project**
- **Olmsted Park Conservancy**
- **Williamsville Toll Barrier Relocation**
- **Buffalo Niagara Medical Campus**

3D Visualization

University at Buffalo
The State University of New York

M. Innus, A. Koniak, A. Levesque, T. Furlani
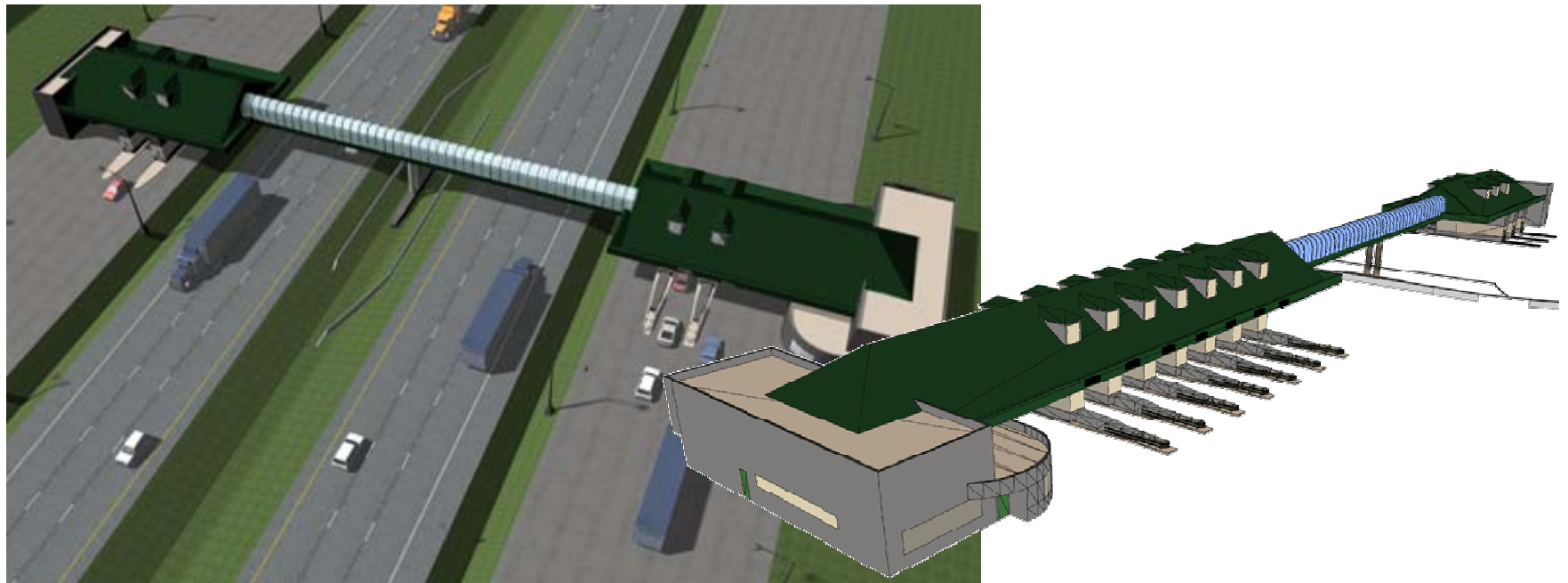**Center for Computational Research**

CCR Model Development

- ***StreetScenes*®** is a Virtual Reality (VR) software solution for 3D interactive visualization of surface traffic.

- Import data from most traffic simulation packages
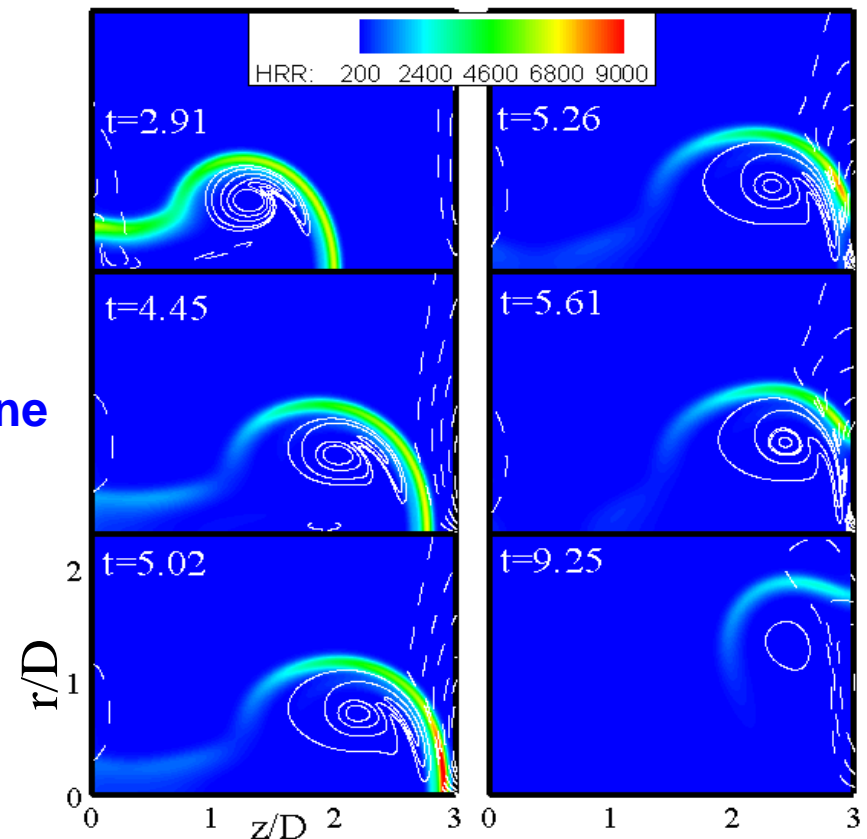   – Corsim
    – Synchro
    – Vissim

Urban Modeling & Visualization

- **High Speed EZPass**
- **Planning tool for NYS Thruway Authority**
- **Visualization of real traffic data**
- **Interactive model for public meetings and demonstrations**

University at Buffalo
The State University of New York

M. Innus, A. Koniak, A. Levesque, T. Furlani
**Center for Computational Research**

Understanding Combustion

- **Flame-wall interaction modeling for a non-premixed flame propelled by a vortex ring. CFD lab, SUNY, Buffalo.**

- **In this figure different time instants are shown during the interaction. White line contours and color contours represent vortex ring and flame, respectively.**

- **Key Features:**
  - Modeling of Detailed GRI3.0 Mechanism for Methane Combustion
  - Parallel algorithm using mpi
  - 85-90% Parallel efficiency for up to 64 processors

- **FWI study is important to determine**
  - Engine Design
  - Quenching Distances
  - Flame Structure
  - Unburned hydrocarbon
  - Maximum Wall heat fluxes

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**C. Madnia**
Center for Computational Research

Molecular Simulation Software

- Molecular simulation has wide application in existing and emerging technologies
- Recent advances in information technology make simulation more broadly accessible
- *Etomica* development environment permits easy construction of simulations
- Object-oriented, Extensible, Interactive, Portable and Adaptable
- Stand-alone simulations can be constructed as a teaching tools
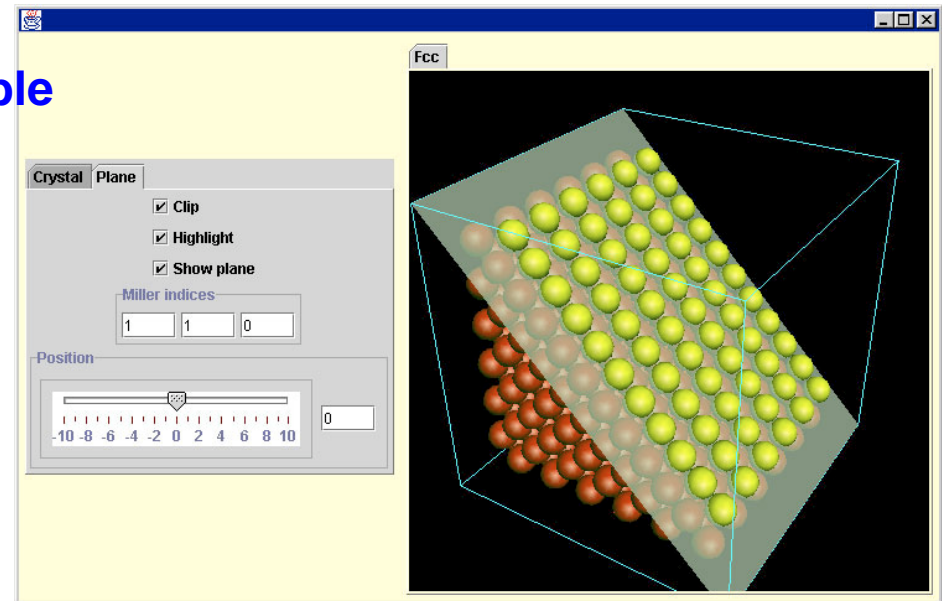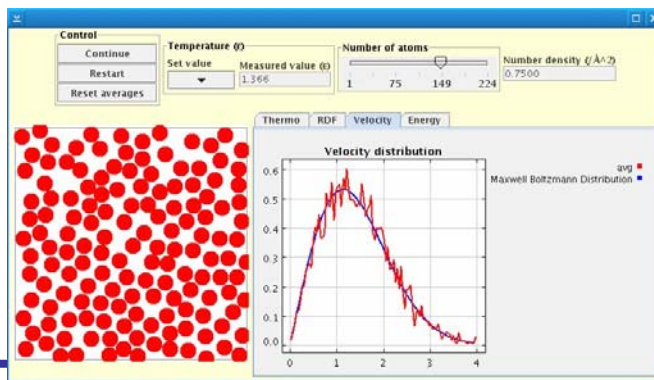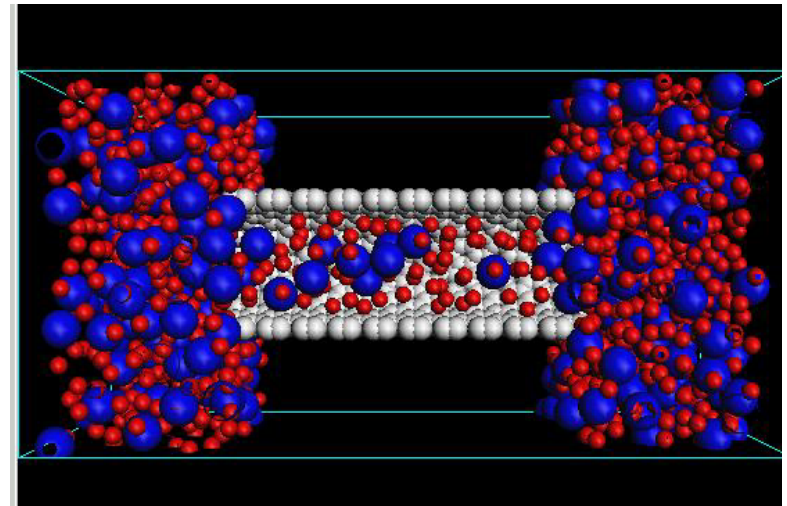
Computational Materials Science

- **Molecular and mesoscale modeling used to understand the behavior of materials**
- **Example application: Electromigration**
- **Strong electrical currents cause movement of atoms in metal**
- **Result is large defects that lead to failure of electrical connection**
- **Consequences can be catastrophic**
- **Interdisciplinary experimental/ modeling studies leading to understanding of behavior**
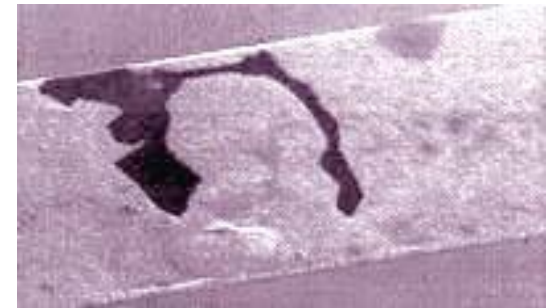
Photos of metal lines that have developed voids (above) and hillocks (below) due to electromigration. (source: www.nd.edu)

MV   DV

MV   DV
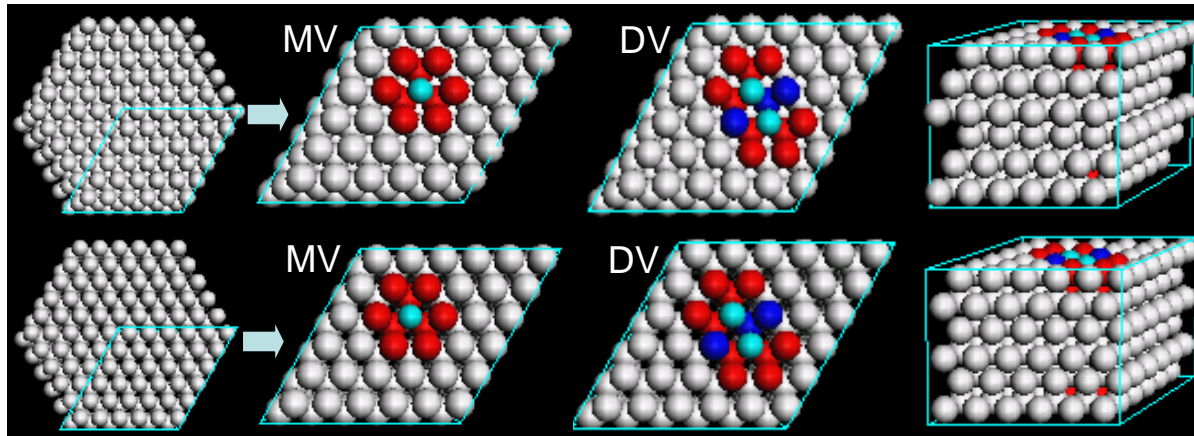
Simulation cells of solids with mono- and di-vacancies (light blue spheres), highlighting atoms neighboring the defects.

Nano Confinement of Fluids

- Fluids in the presence of one or more surfaces exhibit rich phase behavior that can be strikingly different than that observed for bulk fluids

- A fundamental understanding of the relationship between a system's microscopic interactions and the phase behavior of a system is essential for the development of novel materials

- Molecular simulation is a useful tool for developing these relationships through the use of model systems that mimic the behavior of real fluids


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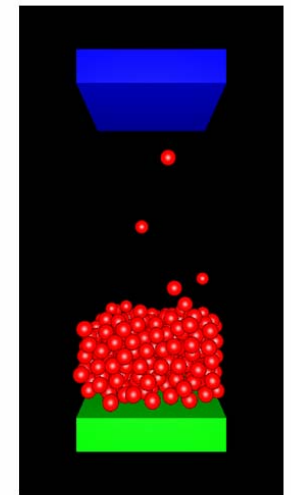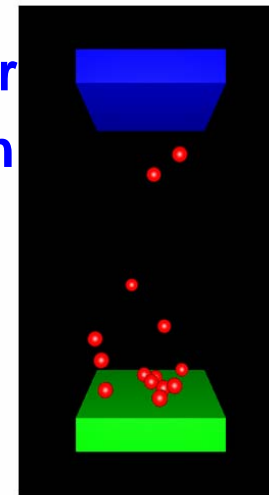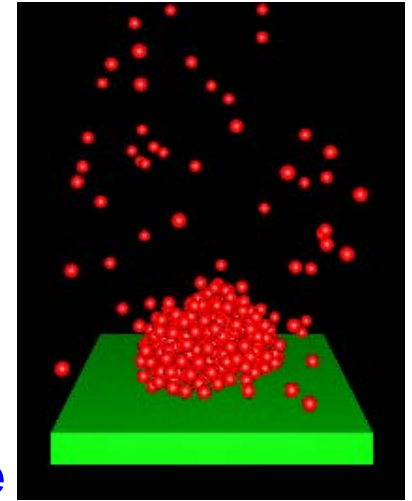
J. Errington
**Center for Computational Research**

Aqueous Solutions

- The behavior of water and aqueous mixtures plays a key role in biology, chemistry, physics, and the design of many chemical and biological processes

- To gain a fundamental understanding of aqueous solutions, one must consider the effect the microscopic hydrogen-bond network has on the macroscopic properties of the system

- The goal of our program is to obtain a more complete understanding of aqueous systems using this molecular approach

- The diagram is a snapshot from a molecular dynamics simulation that depicts the organization of water molecules within 3.5 Å of a trehalose molecule
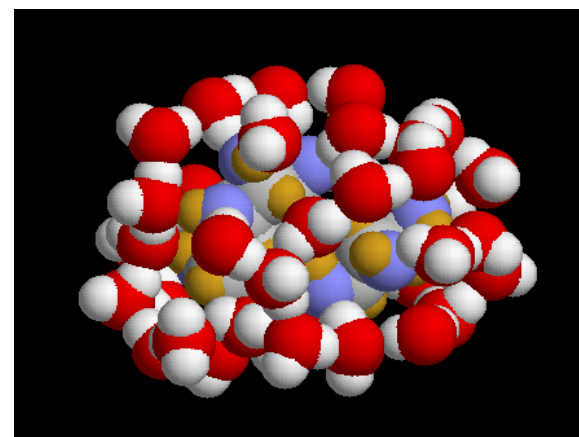
# UB/WNY Biomedical Advances

Inventions

- **PSA Test 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 for Crystal Structure Determination**
  - Listed on "Top Ten Algorithms of the 20th Century"
  - Vancomycin, Gramacidin A
- **Patented High Throughput Crystallization Method**
- **NIH National Genomics Center: Northeast Consortium**
- **Howard Hughes Medical Institute: Center for Genomics & Proteomics**
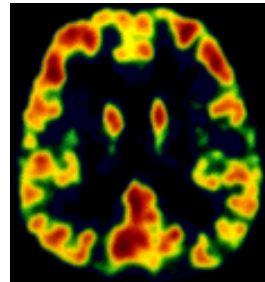
Genome-wide Study of Iron Homeostasis

- **Physiological and Hepcidin-hormonal regulators are involved in iron homeostasis**

- **Intestinal iron transport controls overall body iron homeostasis**

- **Computational biology to discover new genes involved in iron homeostasis**

- **Systems biology to reveal regulatory pathway responding to iron status**

- **Known and novel genes are regulated according to iron status**

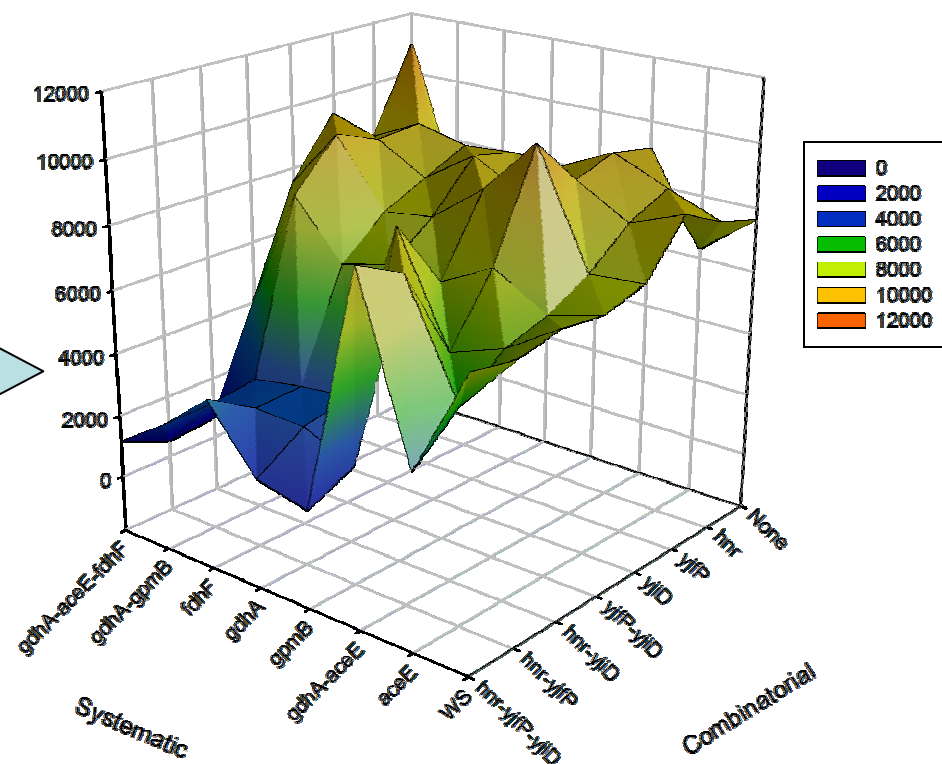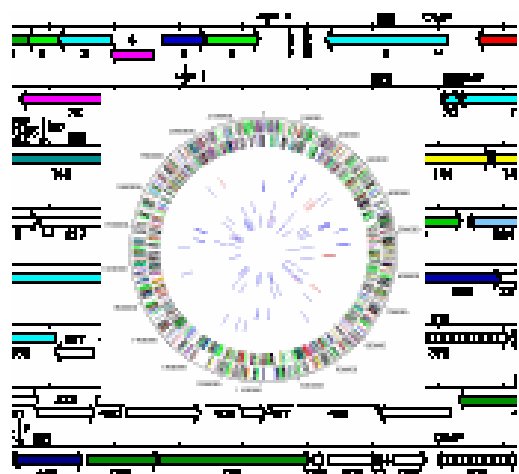- **Sp1 or related TFs may be involved in regulating expression of some genes during iron-deficiency**
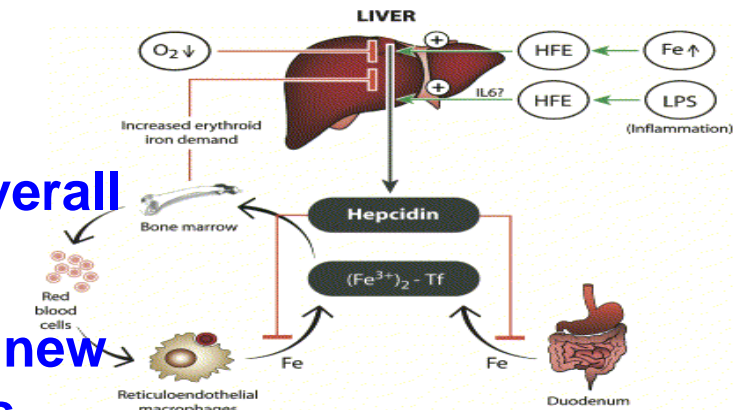
Hentze M.W., *et. al.* Cell 117(3):285-97, 2004

Bioinformatics
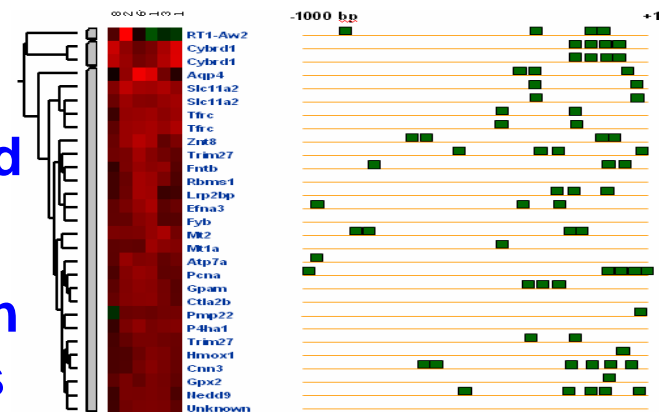
Distribution of SP1 on promoters of genes induced during iron-deficiency

Designing Cellular Phenotypes

- **Genome-wide metabolic models of sequenced microorganisms**
- **Optimization of metabolic and cellular phenotypes**
- **Goal is to design biocatalysts for the production of pharmaceuticals and high-value chemicals**

Regulation of Gene Expression

- *REDfly* (Regulatory Element Database for Fly) Database of verified transcriptional regulatory elements
- Over 650 entries
- Most comprehensive resource of animal regulatory elements
- Fully searchable, has DNA sequence and gene expression data, link-outs to other databases

Bioinformatics

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M. Halfon, S. Gallo
Center for Computational Research

Data Mining and Analysis

Bioinformatics

- **GeneChips hybridized with cRNAs of biological interest**

- **Many probe set algorithms for summarizing expression intensity**

- **Significant differences of differentially expressed genes generated by different algorithms from the same dataset**

dChip 853 466 876 *RMA*
274
327 375
789
MAS5.0
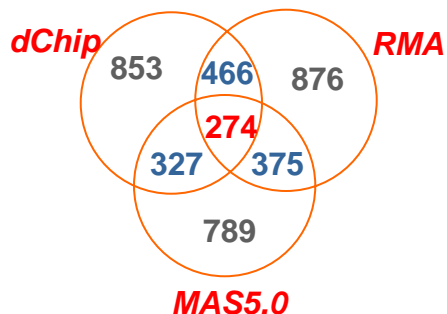
31% - 55% overlap

Which algorithm is best?

Great impact on subsequent expression data analysis

- **Novel statistical approach for data variance and result bias analyses**

- **No external reference data needed**

- **Algorithm evaluation with direct applications to experimental datasets of interest**
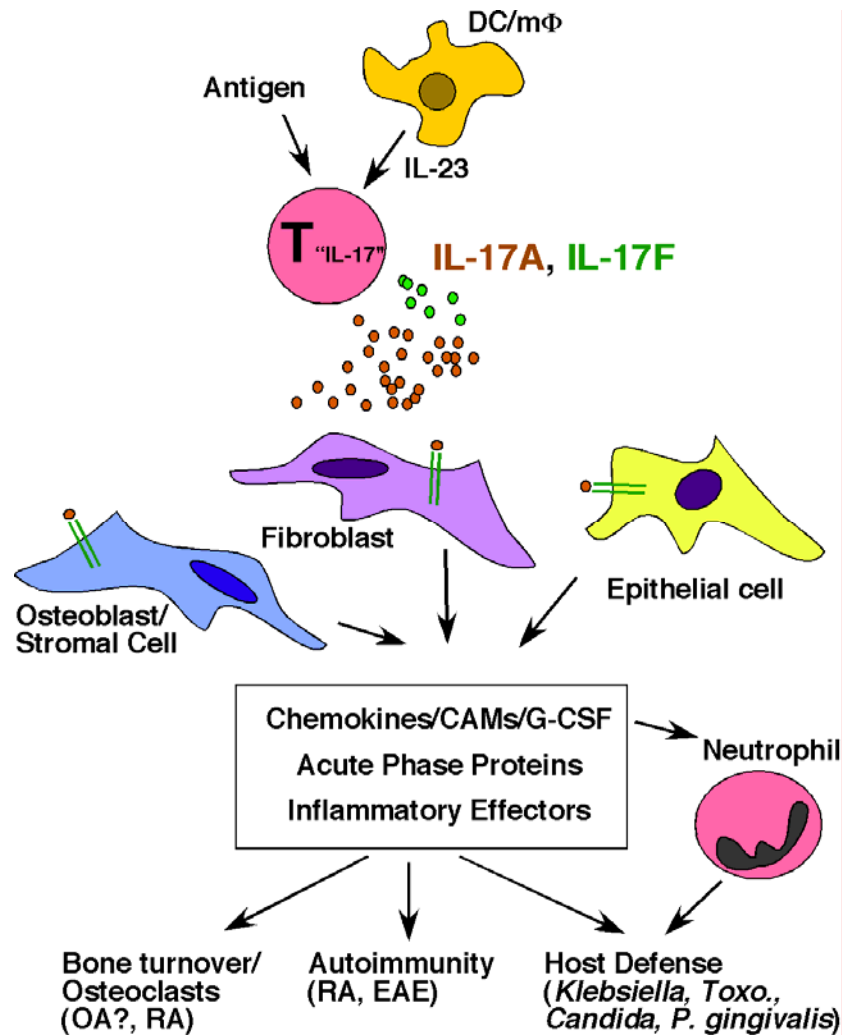

GeneChip® Expression Analysis Process
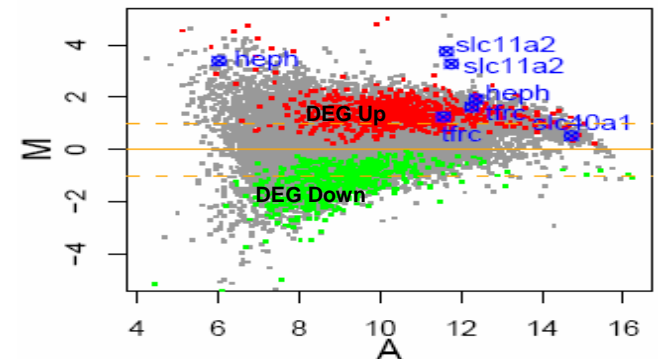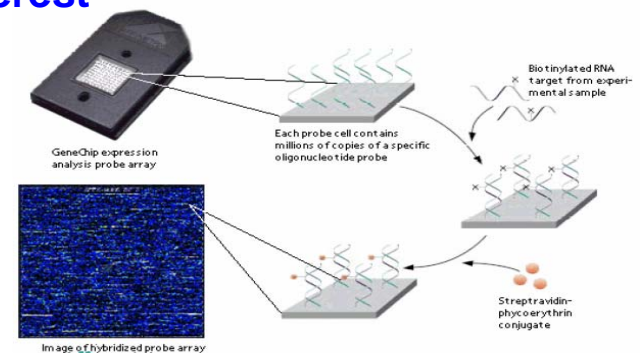
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Z. Hu, G. Willsky
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Defining Cytokine Signaling Mechanisms

-T cells secrete cytokines such as IL-17 to promote host defense and/or autoimmunity

-Microarrays used to define IL-17 gene targets in various cell types

-Computational and statistical approaches used to compare the promoters of IL-17 target genes in mouse and human genomes to identify conserved transcription factor binding sites (TFBS), with the ultimate goal of understanding how IL-17 mediates molecular signals
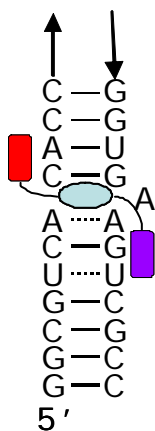
- IL-17 target promoters contain conserved TFBSs, including NF-kB and C/EBP

Computational Biology

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S. Gaffen, Z. Hu
Center for Computational Research

Prediction of RNA Structure to Facilitate Design of Drugs Targeting RNA

aggtccctcg cggatggagc tgaaatcagt cgaagatacc agctggctgc aactgtttat
taaaaacaca gcactgtgca aacacgaaag tggacgtata cggtgtgacg cctgcccggt
gccggaaggt taattgatgg ggttagcgca agcgaagctc ttgatcgaag ccccggtaa
cggcggccgt aactataacg gtcctaaggt agcgaaattc cttgtcgggt aagttccgac
ctgcacgaat ggcgtaatga tggccaggct gtctccaccc gagactcagt gaaattgaac
tcgctgtgaa gatgcagtgt acccgcggca agacggaaag accccgtgaa cctttactat
agcttgacac tgaacattga gcctgatgt gtaggatagg tgggaggctt tgaagtgtgg
acgccagtct gcatggagcc gaccttgaaa taccacccttt taatgtttga tgttctaacg
ttgacccgta atccgggttg cggacagtgt ctggtgggta gtttgactgg ggcggtctcc
tcctaaagag taacggagga gcacgaaggt tggctaatcc tggtcggaca tcaggaggtt
agtgcaattgg cataagccag cttgactgcg agcgtgacgg cgcgagcagg tgcgaaagca
ggtcatagtg atccggtggt tctgaatgga agggccatcg ctcaacggat aaaaggtact
ccggggataa caggctgata ccgcccaaga gttcatatcg acggccggtgt ttggcacctc
gatgtcggct catcacatcc tggggctgaa gtaggtccca agggtatggc tgttcgccat
ttaaagtggt acgcgagctg ggtttagaac gtcgtgagac agttcggtcc ctatctgccg
tgggcgctgg agaactgagg ggggctgctc ctagtacgag aggaccggag tggacgcatc
actggtgttc gggttgtcat gccaatggca ctgcccggta gctaaatgcg gaagagataa
gtgctgaaag catctaagca cgaaacttgc cccgagatga gttctccctg accctttaag
ggtcctgaag gaacgttgaa gacgacgacg ttgataggcc gggtgtgtaa gcgcagcgat
gcgttgagct aaccggtact aatgaaccgt gaggcttaac ctt

23s rRNA Sequence

RNA Secondary Structure Prediction →

23s rRNA 2D Structure

RNA 3D Structure →

30S

Search Small-Molecule-RNA Ligand Database for RNA motifs to which we have identified an organic ligand ↓

Modular Assembly to increase affinity ←

$$\Delta G_{ligand} = \Delta G_1 + \Delta G_2 + \Delta G_3 + \Delta G_{linker(s)}$$

```
C — G
C — G
A — U
C — G
      A
A ···· A
C — G
U ···· U
G — C
C — G
G — C
G — C
5′
```
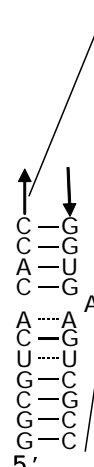
A-site
Aminoglycoside target

```
        A
A ···· A

A — U
C — G

C — G
U ···· U
```
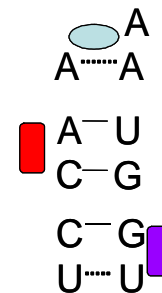
Results from ligand database search

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M. Disney
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Chemistry

Stem Cells and Tissue Engineering

Bioengineered Skin
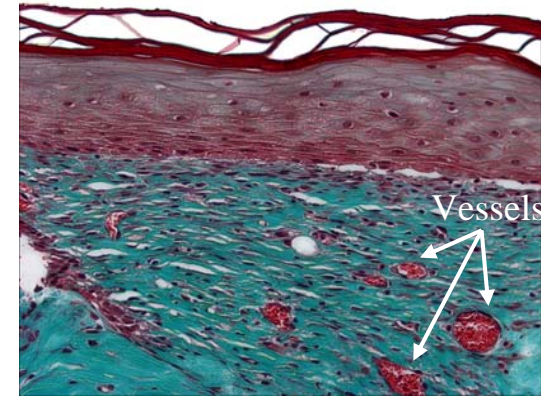
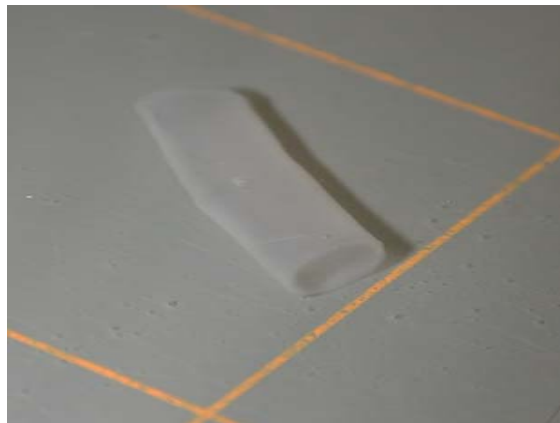Bioengineered Skin Transplanted onto mouse

SC
GL
SL
BL

Vessels
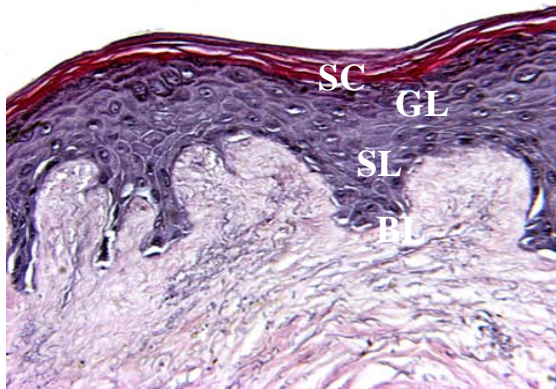
Genetically modified tissue engineered skin:
1. Wound healing e.g. burns, chronic wounds
2. Insulin delivery for treatment of diabetes
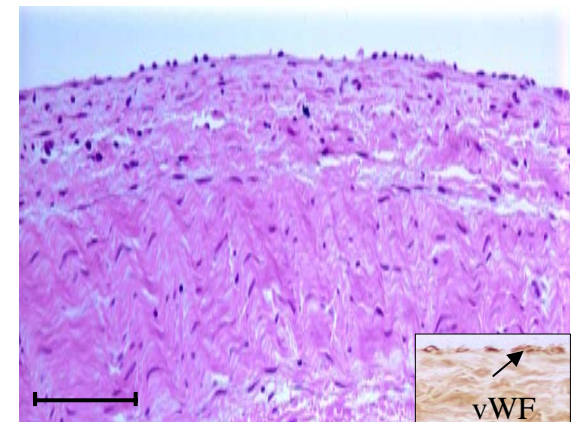**3. Development of a model to study tumor invasion**

Bioengineered Blood Vessel

TEV Transplanted in jugular vein of lambs

Tissue engineered blood vessels (TEV):
**1. Bypass surgeries**
2. Model to study mechano transduction and vascular biology
3. TEVs from bone marrow stem cells

vWF

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S. Andreadis
Center for Computational Research

Designing new materials

- **Understand and predict materials properties**
- **Materials design from first-principles**
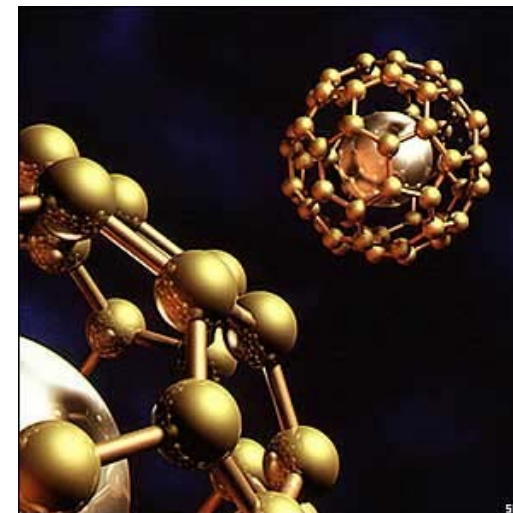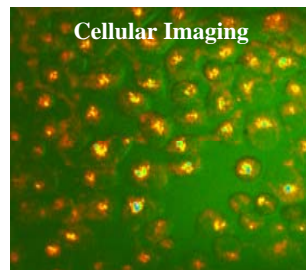- **Development of new theoretical and computational techniques**
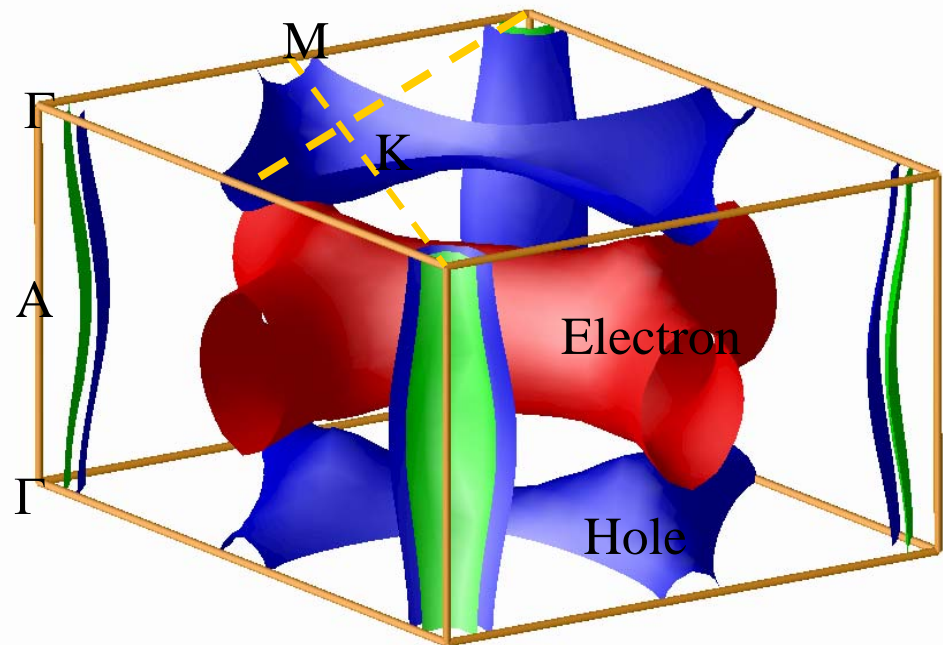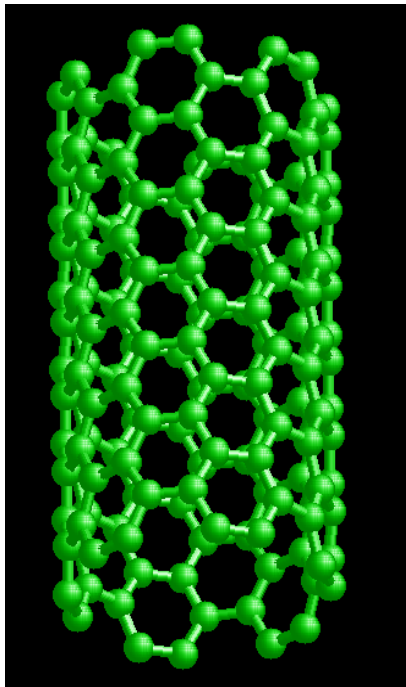
Nanomedicine Program

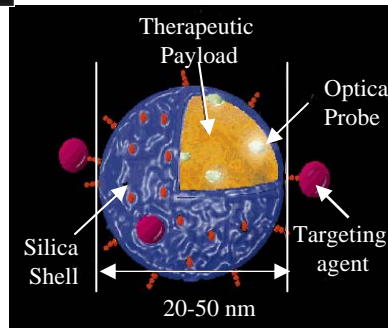**World class Research Program Melding Nanotechnology with Biomedical Sciences**

In Vivo Imaging

Tumor site:

Multi-Modal Imaging

Cellular Imaging

BioCompatibility/ Distribution

Therapeutic Payload

Optical Probe

Silica Shell

Targeting agent

20-50 nm

In Vivo Sensing

Gene Delivery

Targeted Therapy

Drug Delivery

Building from the Bottom Up

State of the Art Molecular Imaging and Nanocharacterization Facilities
- Multiphoton Laser Scanning System
- Confocal Imaging including FRET, FLIM & FRAP analysis
- Coherent Anti-Stokes Raman Imaging
- Optical Trapping/Dissection
- Advanced Laser Systems

www.biophotonics.buffalo.edu

"Leading the Way to Technology through Innovation"

University at Buffalo
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P. Prasad

Center for Computational Research

Molecular Imaging

"Lighting the Way to Technology through Innovation"

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Complete Air Sterilization

B3

Buffalo Bio Blower

sterilized air exhaust

contaminated air inlet

compressive heating of flowing air destroys ANY & ALL airborne pathogens, 99.9999% killed in a single pass through the BioBlower air pump

Can completely protect any enclosed area (plane, train, bus, building) from:
anthrax spores, smallpox, SARS, MARS, influenza, tuberculosis, avian flu, mold, fungi, allergens, etc

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J. Garvey, J. Lordi
Center for Computational Research
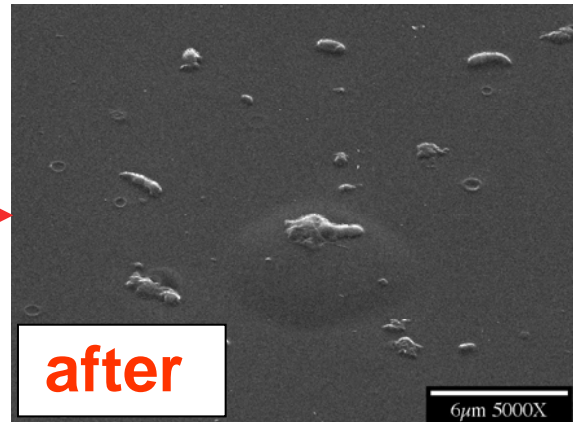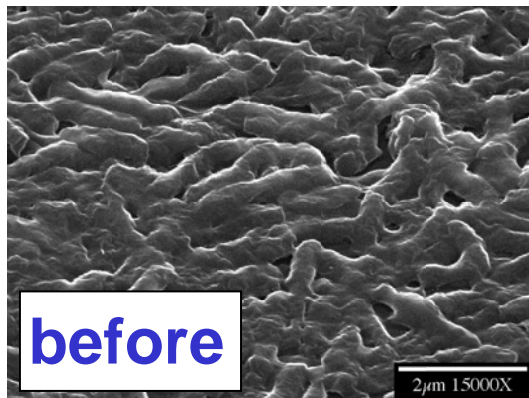
Complete Air Sterilization

**Buffalo
Bio
Blower**

compressive heating of flowing air destroys ANY & ALL airborne pathogens, 99.9999% killed in a single pass through the BioBlower air pump

heat treated *Bacillus globigii* (*Bg*) spores, an anthrax surrogate, are continuously injected upstream of BioBlower, then sampled downstream

before

2μm 15000X

after

6μm 5000X

"Everything from hospitals, first-responder units, and postal facilities -- to government buildings and mass-transit systems could benefit enormously from the security and peace of mind generated by this device" Rep. L. Slaughter, Business First, 8/16/05

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Center for Computational Research

Industrial 3D Flow Analysis

- **Modeling of Complex 3D and Mixing Flows for Part Analysis and Design**