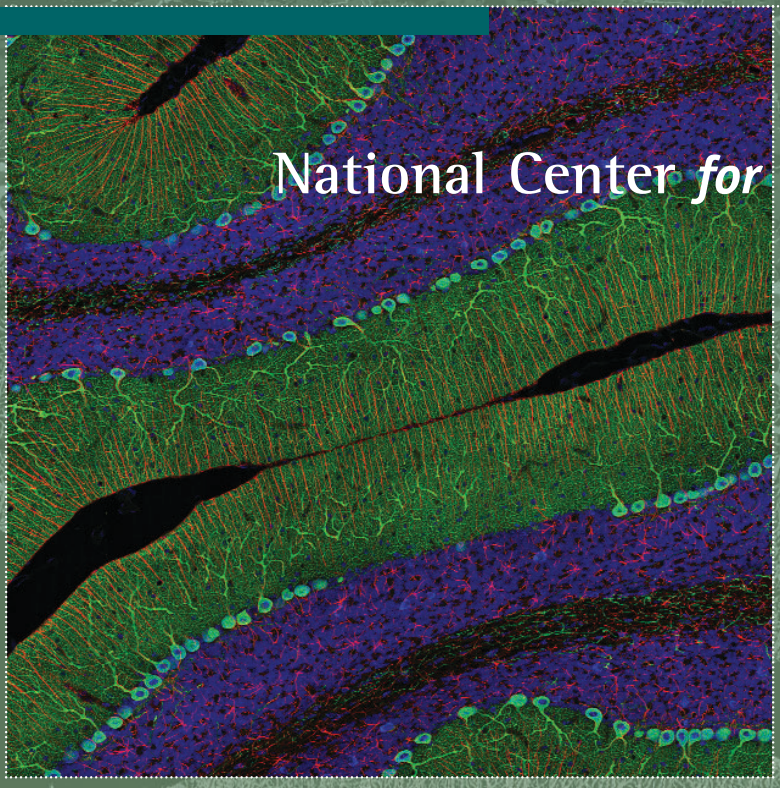
National Center for
Research Resources

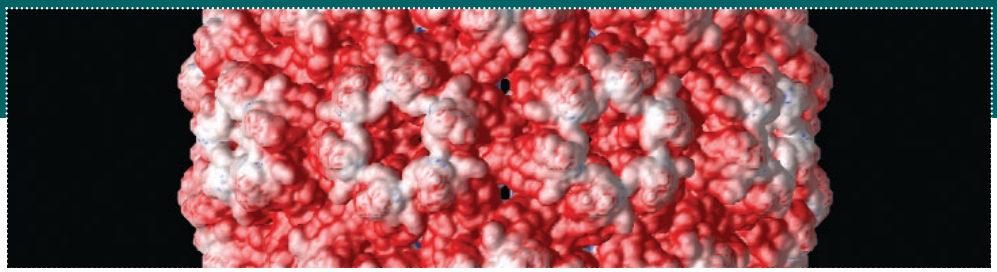
BIOMEDICAL COMPUTATION, VISUALIZATION, IMAGING, & INFORMATICS RESOURCES of the



National Center *for* Research Resources

National Institutes of Health

Participating Centers



BIOMEDICAL INFORMATICS RESEARCH NETWORK
University of California San Diego, Mark Ellisman

CENTER FOR BIOELECTRIC FIELD MODELING, SIMULATION, AND VISUALIZATION
University of Utah, Chris Johnson

HIGH-PERFORMANCE COMPUTING FOR BIOMEDICAL RESEARCH
Pittsburgh Supercomputing Center, Ralph Roskies

LABORATORY OF NEURO IMAGING RESOURCE
University of California Los Angeles, Arthur Toga

MULTISCALE MODELING TOOLS FOR STRUCTURAL BIOLOGY
The Scripps Research Institute, Charles Brooks III

NATIONAL BIOMEDICAL COMPUTATION RESOURCE
University of California San Diego, Peter Arzberger

NATIONAL CENTER FOR MACROMOLECULAR IMAGING
Baylor College of Medicine, Wah Chiu

NATIONAL CENTER FOR MICROSCOPY AND IMAGING RESEARCH
University of California San Diego, Mark Ellisman

NATIONAL RESOURCE FOR CELL ANALYSIS AND MODELING
University of Connecticut Health Center, Leslie Lowe

RESOURCE FOR BIOCOMPUTING, VISUALIZATION AND INFORMATICS
University of California San Francisco, Tom Ferrin

RESOURCE FOR MACROMOLECULAR MODELING AND BIOINFORMATICS
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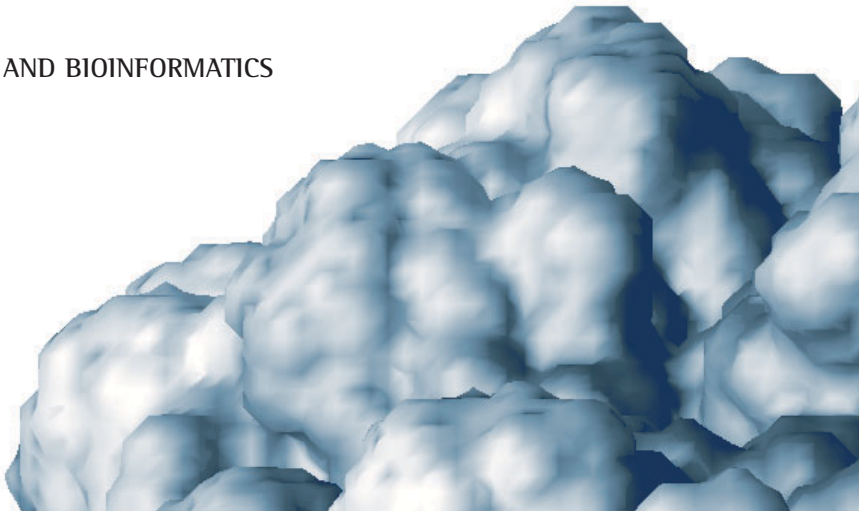


NCRR Mission

The National Center for Research Resources (NCRR) serves as a "catalyst for discovery" by creating and providing critical research technologies and shared resources. This infrastructure underpins biomedical research and enables advances that improve the health of our Nation's citizens.

Biomedical research investigators supported by the Institutes and Centers of the National Institutes of Health require a broad array of technologies, tools and materials critical to their research efforts. From the models required for research on diseases and disabilities, to the biomedical technology and instrumentation necessary to elucidate cellular and molecular structure, to the clinical settings in which to conduct studies to discern the cause of disease and in which novel clinical trials of new therapies can be developed, biomedical researchers must have access to the necessary resources in order to continue to make progress against human disease and disability.

The NCRR has a unique responsibility at the National Institutes of Health: to develop critical research technologies and to provide cost-effective, multidisciplinary resources to biomedical investigators across the spectrum of research activities supported by the NIH. This has four major facets:

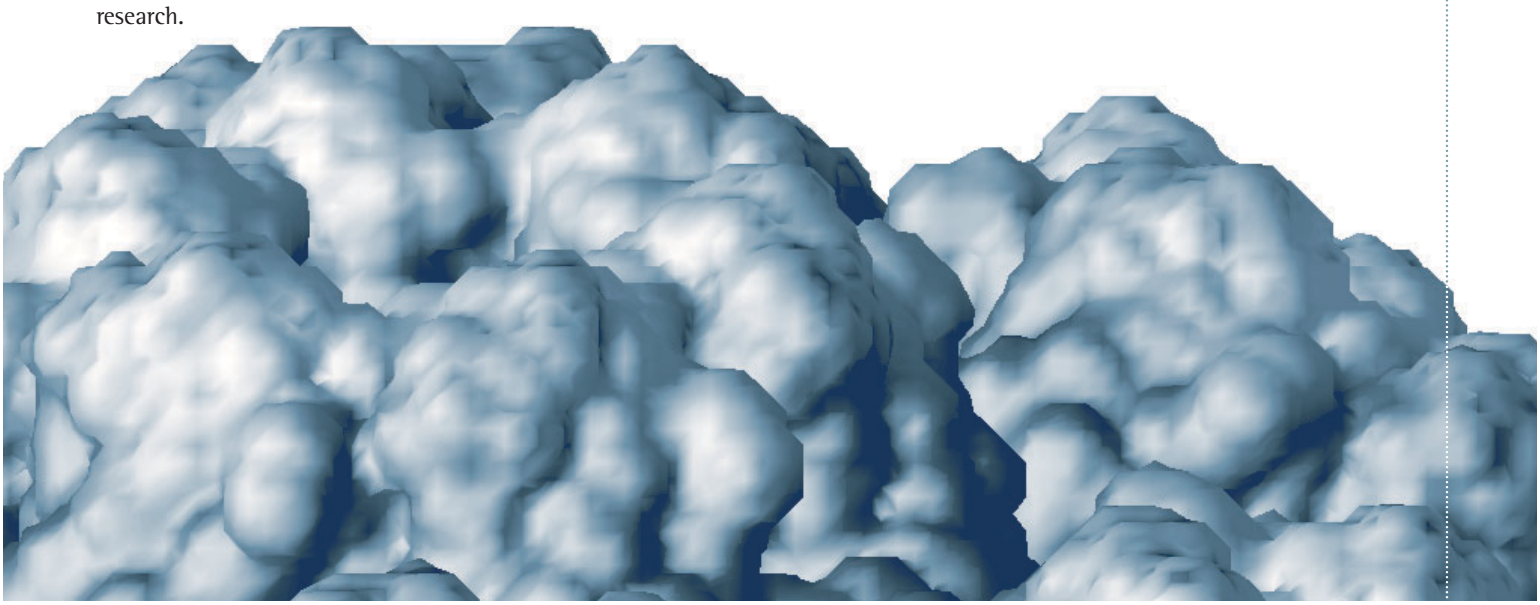
1. Create resources and develop technologies that are cost-effective, accessible and responsive to the research needs of the biomedical research community. To meet these needs the NCRR must be in the vanguard of evolving trends in basic and clinical research so that resources will be available to facilitate that research.

2. Provide shared clinical, primate and biotechnology resources for use by investigators supported by all the NIH Institutes and Centers. These resources, primarily centers, serve more than 10,000 researchers, supported through well over $1 billion of categorical research resource Institute funds, thus leveraging those funds for more cost-effective and efficient research.

3. Develop quick, flexible approaches to new and emerging biomedical research needs and opportunities. These innovations often involve high-risk research, but the payoffs may be substantial.

4. Strengthen the nation's biomedical research infrastructure through programs to develop and enhance the capacity of minority institutions and centers of emerging excellence to participate in biomedical research, to increase the exposure of K-12 students and their teachers to the life sciences, to improve the condition of research animal facilities, and to construct or renovate facilities for biomedical and behavioral research.

The NCRR plays a key role in addressing pressing trans-NIH research issues such as: access to state-of-the-art instrumentation and biomedical technologies; containment of the escalating costs of highly sophisticated clinical research; development of appropriate, specialized research models both animal and non-animal; and remedying the shortage of independent clinical investigators and the underrepresentation of minority investigators. Present and future program directions emphasize "smart," network-connected technologies, computer-aided drug design, development and testing of gene and molecular therapies, bioengineering approaches to decrease health care costs, and enhanced training and career development for patient-oriented research.



BIRN CYBERINFRASTRUCTURE SUPPORTS TEST BED COLLABORATIVE PROJECTS

Biomedical Informatics Research Network

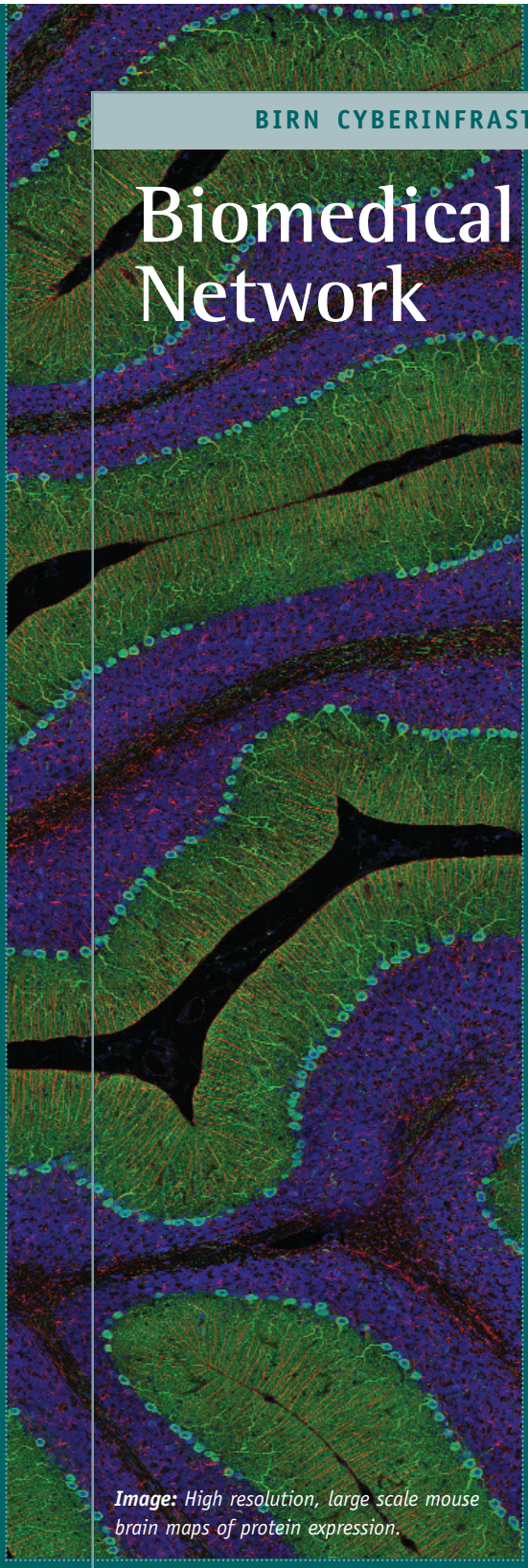


Image: *High resolution, large scale mouse brain maps of protein expression.*

The NIH National Center for Research Resources *(NCRR)*, the NSF National Partnership for Advanced Computational Infrastructure *(NPACI)* and the NSF Middleware Initiative *(NMI)* are pioneering the use of Grid infrastructure for medical research and patient care through the BIRN Initiative.

Established in 2001, BIRN developed and continues to evolve the hardware, software, and protocols necessary to share and mine data for both basic and clinical research. Central to the project is a scalable cyberinfrastructure consisting of advanced networks, federated distributed data collections, computational resources, and software technologies that are integrated to meet the evolving needs of collaborative test bed investigators. By pooling domain expertise, specialized research facilities, instrumentation, applications, and regional information, these investigators are tackling disease studies of greater scope and complexity than are independently possible.

The BIRN cyberinfrastructure is developed by the **BIRN Coordinating Center** and driven by the requirements of three research test beds. 1) **Function BIRN:** 12 universities studying regional human brain dysfunctions related to schizophrenia. 2) **Morphometry BIRN:** 6 research institutions investigating whether structural differences in the human brain distinguish diagnostic categories in unipolar depression, mild Alzheimer's disease, and mild cognitive impairment. 3) **Mouse BIRN:** 4 institutions studying animal models of disease at different anatomical scales to test hypotheses associated with human neurological disorders including schizophrenia, attention-deficit hyperactivity disorder, multiple sclerosis, and Parkinson's disease.

As additional biomedical research and clinical care test beds evolve, the BIRN will continue to stretch the boundaries of information technology infrastructure, enriching the Global Grid movement by providing "application pull" from these new domains.

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BIRN
BIOMEDICAL INFORMATICS RESEARCH NETWORK

www.nbirn.net

NIH CENTER FOR BIOELECTRIC FIELD MODELING, SIMULATION, AND VISUALIZATION

SCI Institute

The NIH Center for Bioelectric Field Modeling, Simulation, and Visualization is a collaboration between the Scientific Computing and Imaging Institute *(University of Utah)*, the Nora Eccles Harrison Cardiovascular Research and Training Institute *(University of Utah)* and the Biomedical Signal Processing Lab *(Northeastern University)*. This collaboration was formed to conduct research and development in advanced modeling, simulation, and visualization methods for solving bioelectric field problems. Modern medical imaging technologies such as magnetic resonance imaging, ultrasound, and positron emission tomography, provide a wealth of anatomical information to doctors and researchers. Measurements of the electric and magnetic fields from the body, such as electrocardiography *(ECG)* and magnetoencephalogrphy *(MEG)*, reflect the underlying bioelectrical activity of the tissues and organs. However, without equally advanced modeling and visualization technologies, much of the potential value of this information is lost. Our goal is to couple advanced medical imaging technology with state of the art computer simulation and modeling techniques to produce new methods and tools, which will allow doctors and researchers to tackle immediately important medical problems.

To accomplish this goal, we have created an integrated software tool for bioelectric field problems called “Bioelectric Problem Solving Environment” or more regularly, “BioPSE.”

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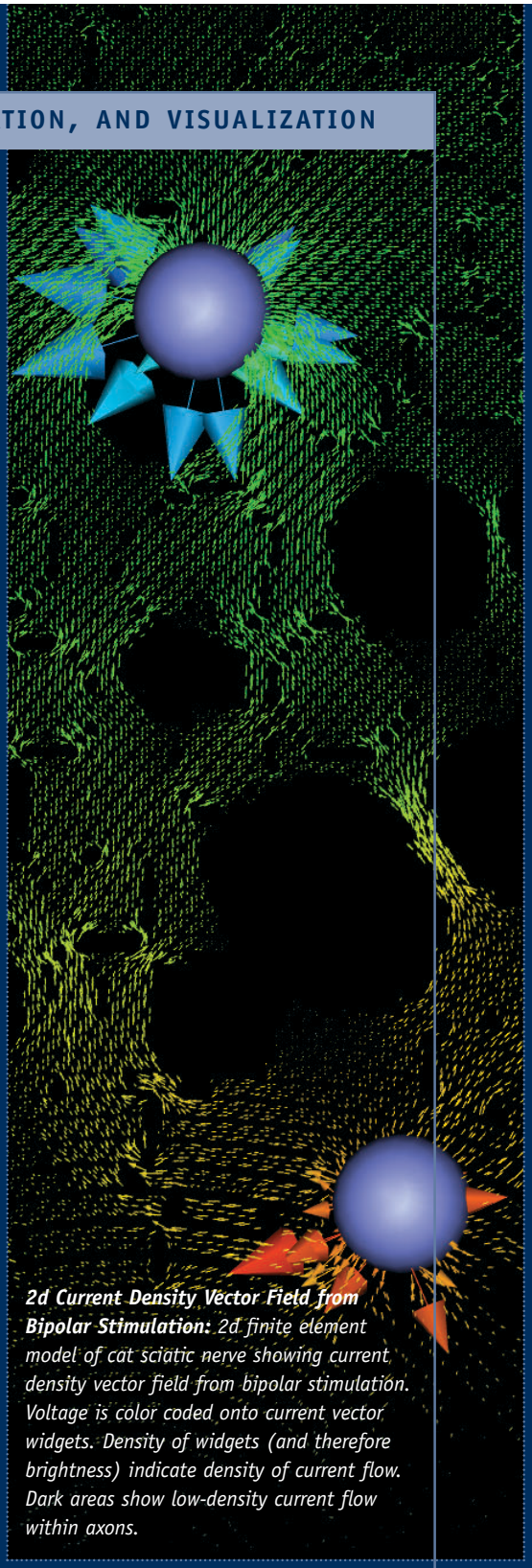
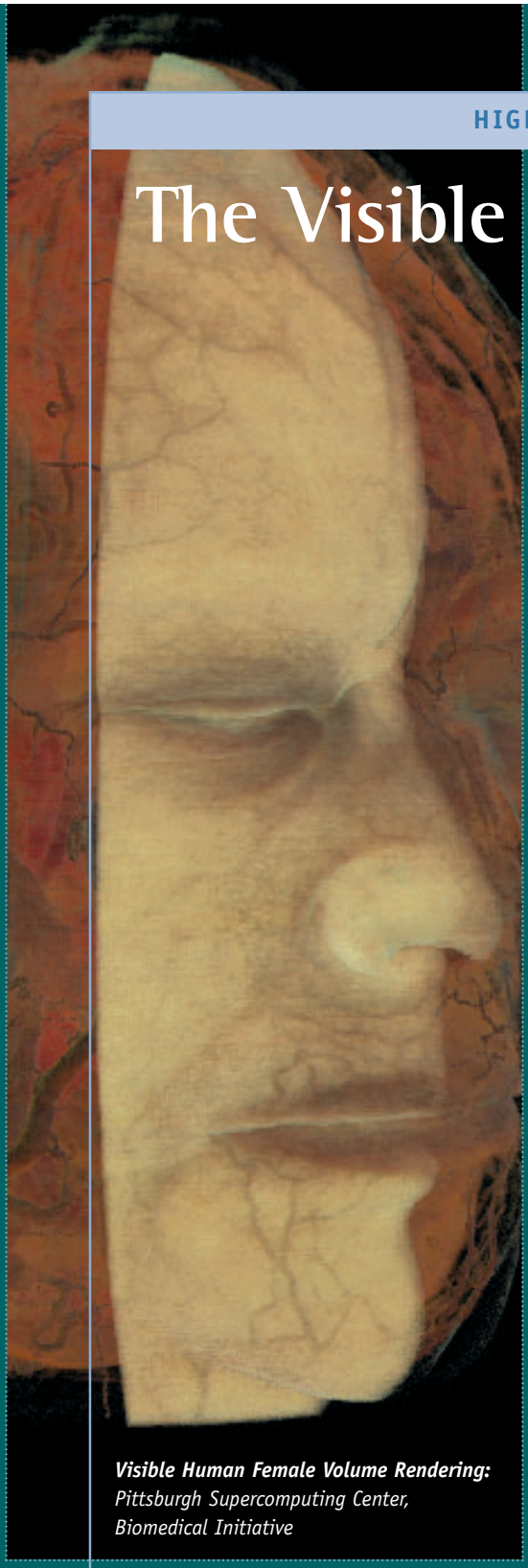


2d Current Density Vector Field from Bipolar Stimulation: *2d finite element model of cat sciatic nerve showing current density vector field from bipolar stimulation. Voltage is color coded onto current vector widgets. Density of widgets (and therefore brightness) indicate density of current flow. Dark areas show low-density current flow within axons.*

SCI INSTITUTE

www.sci.utah.edu/ncrr

The Visible Human



Visible Human Female Volume Rendering:
Pittsburgh Supercomputing Center, Biomedical Initiative

The resource mission is to develop new methods, optimize existing approaches, and undertake research projects in biomedical areas that require high-performance computing, broadly construed to include large-scale data management, high-speed networking, and visualization. The resource also identifies new biomedical application areas that could benefit from high-performance computing, and speed the introduction of high-performance computing techniques into these areas.

Current efforts are in structural biology, bioinformatics, cellular microphysiology, neural modeling, the Visible Human Project, and pathology. Specific projects include development and application of algorithms for sequence-sequence, sequence-structure, and multiple sequence alignment; classification and analysis of gene and protein superfamilies; understanding divalent metal ion binding sites in proteins and nucleic acids; incorporation of polarization effects in simulations of biopolymers; simulation of neural transmission *(Mcell)*; simulation of neural networks on parallel platforms *(NEOSIM)*; analysis of multi-electrode recordings of brain activity; display of anatomic *(visible human)* images; image analysis of pathology slides; databasing and retrieval of medically relevant images.

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PITTSBURGH SUPERCOMPUTING CENTER

LABORATORY OF NEURO IMAGING RESEARCH AT THE UCLA SCHOOL OF MEDICINE

The LONI Pipeline Processing Environment

The LONI Pipeline Processing Environment, created in Laboratory of Neuro Imaging at UCLA, was developed to address the increasingly complex analysis and growing computational processing needs of the brain mapping community. Data analysis in neuroimaging has become an arduous process entrenched in advanced mathematical, statistical, and computational concepts. There are large amounts of raw data that needs to be organized, classified, modeled, analyzed, and contrasted. Intermediate datasets are being formed that need to be stored and handled properly. Many of the processing programs have vastly different input and output requirements, employ different file formats, and often run on specific computer architectures. Additionally, there are often many ways to accomplish a given step in the analysis, each of which has its benefits for particular situations. The LONI Pipeline Processing Environment was developed to address these needs by providing a simple, platform-independent, visual programming interface that allows the linking together of many independently developed analysis programs into a processing pipeline. On execution of a pipeline the environment keeps track of temporary intermediate files and datasets for the user, automatically parallelizes data-independent sections of the analysis using a dataflow model, and provides the ability to save a complex analysis for later use on new datasets or for distribution to the rest of the brain mapping community. The pipeline environment also provides application and CPU cycle serving abilities from Pipeline Servers—providing an interface to programs, complete analyses, computer architectures, and even supercomputing facilities that the average scientist may not have access to.

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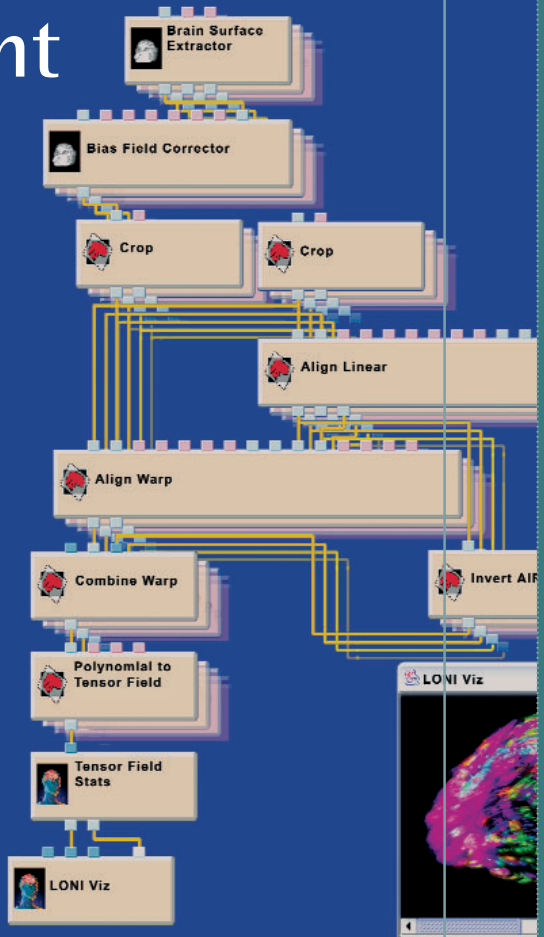

Analysis pipeline in the LONI Pipeline Processing Environment:: *Tensor based analysis of the structure of the human brain providing data about how regions of the brain vary across the given subject population. Volumetric whole-head MRI scans from the subjects are processed though multiple steps to extract the brains from the scans, compute a 6th order polynomial transformation aligning the subjects to a provided atlas space, and derive the statistics representing the anatomic variability for the population.*

www.loni.ucla.edu/Software

Multiscale Modeling Tools for Structural Biology

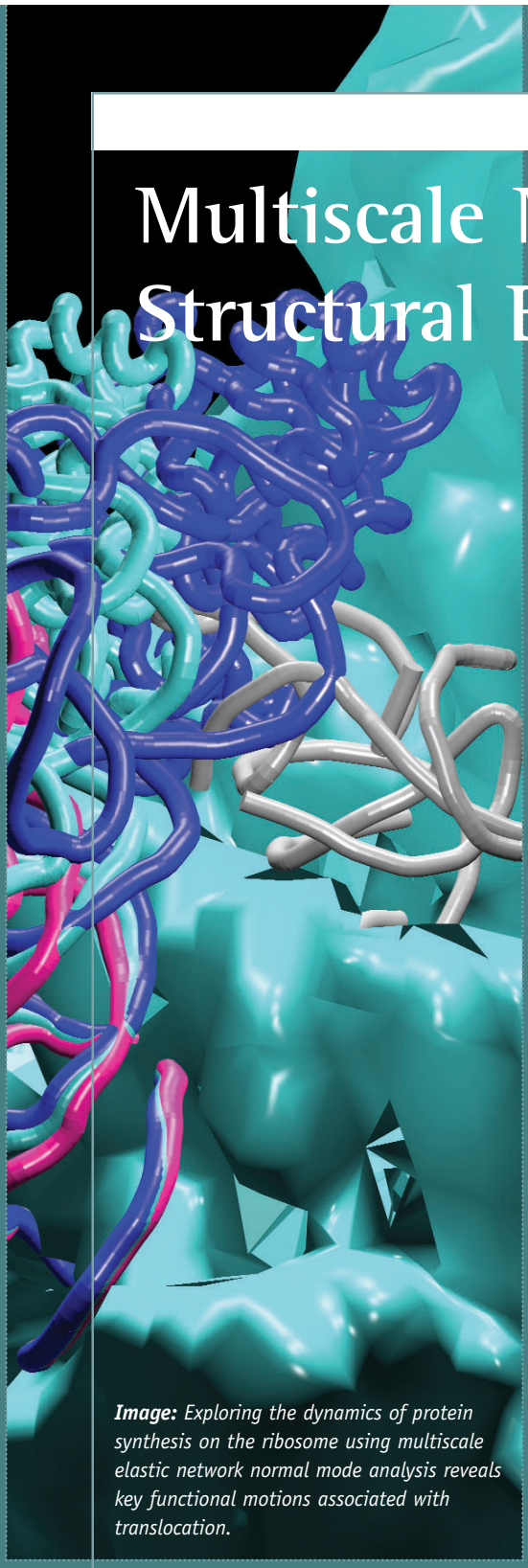

Image: *Exploring the dynamics of protein synthesis on the ribosome using multiscale elastic network normal mode analysis reveals key functional motions associated with translocation.*

Problems in structural biology increasingly require researchers to move between models of low-resolution and detailed atomic models to fully explore and exploit experimental information. This resource focuses on development of new and integrated approaches to multiscale modeling, with an emphasis on modeling large-scale assemblies of nucleic acids and proteins with nucleic acids; developing methods that combine lattice-based dynamic Monte Carlo and all atom molecular dynamics; studying physical processes involved in and developing models for the interactions associated with virus assembly; and establishing new tools for the combined treatment of crystallographic and low-resolution structural models from cryo-electron microscopy. These research threads are tied together through the development and distribution of computer codes to make such multiscale simulations and modeling readily accessible to the scientific community at large.

This group's research focus includes: Modeling very large conformational changes occurring in proteins, nucleic acids, and their assemblies; developing methods and models to explore virus swelling and associated large-scale capsid dynamics during viral maturation; exploring of meso-scale distortions of molecular assemblies using low-resolution data from electron microscopy, in the absence of any atomic level structural information; providing links between low-resolution images of functional states of the ribosome during translocation and the near-atomic structural distortions that comprise these motions; characterization of protein-protein interfaces in assembled virus capsids from an energetic and structural standpoint, providing a basis for understanding large-scale molecular assembly. Ongoing development of methods for, and applications to, protein folding, loop, and homology modeling, including participation in CASP5, to perfect physics-based approaches to structural genomics. Develop and test software to extend the range of atom-based modeling methods to larger systems.

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The Scripps Research Institute

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FOREFRONT COMPUTATIONAL, INFORMATION AND GRID TECHNOLOGIES

National Biomedical Computation Resource

The mission of the National Biomedical Computation Resource *(NBCR)* at the University of California, San Diego *(UCSD)* is to conduct, catalyze, and enable biomedical research by harnessing advanced computational technology. To fulfill this mission, NBCR efforts are focused on four key activities: integrate computational and visualization tools in a transparent, advanced computing environment to enhance access to distributed data, computational resources, and instruments; develop and deploy advanced computational tools for modeling, data query, linking of data resources, 3D image processing, and interactive visualization; provide access to and support of advanced computational infrastructure for biomedical researchers; and train a cadre of new researchers to have interdisciplinary knowledge of biology and the latest computation technologies.

The ultimate goal of the resource is to facilitate biomedical research by providing access to advanced computational and data grid capabilities via easy-to-use web portals, thereby enabling researchers to focus on the essential aspects of the biological/biomedical problem.

NBCR is part of UCSD's Center for Research on Biological Structure. Its technology development activities involve collaborations among researchers at UCSD, the San Diego Supercomputer Center, the California Institute of Telecommunications and Information Technology, and The Scripps Research Institute, with a general interest in performing basic biomedical research from atomic to organismic levels. Core research projects include methods for pattern recognition in protein and nucleic acid structure, parallel tomographic methods for reconstruction of 3D images, distributed database for cell-centered data, development/enhancement of cardiac electromechanics, parallel quantum mechanical modeling methods including environmental effects, development of platform-independent visualization tools, and the creation of portals for the biomedical community.

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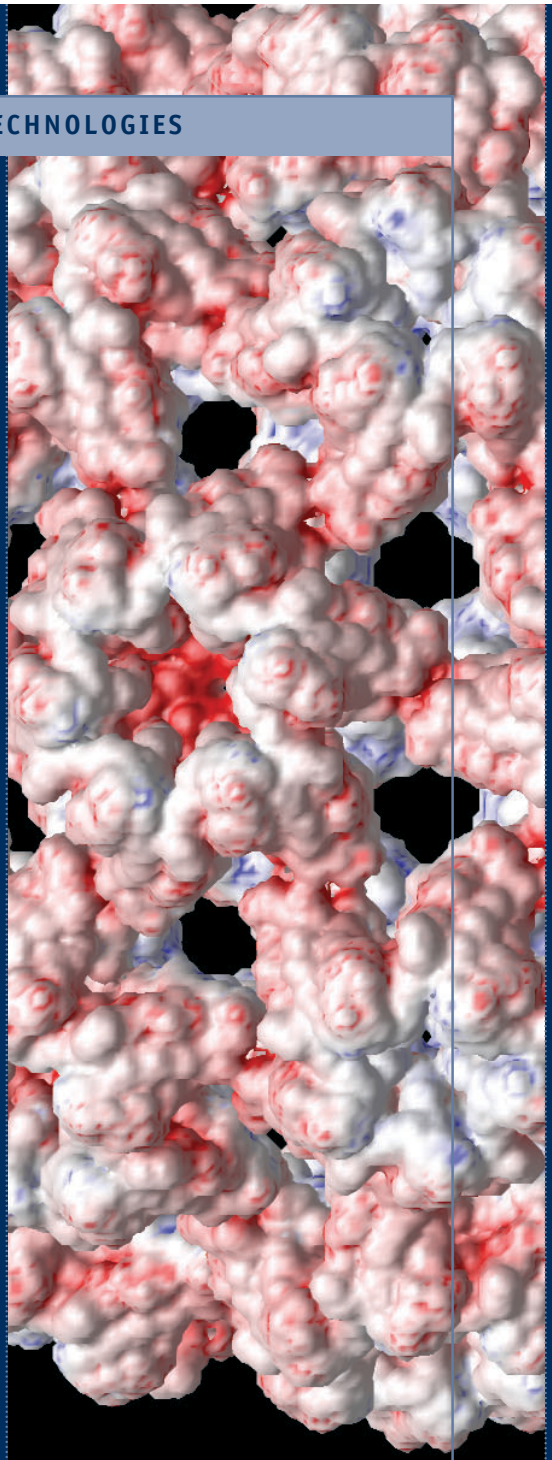

Electrostatic properties of CCMV viral capsid: *Calculated electrostatic potential of swollen CCMV capsid projected onto solvent accessible surface (negative potential in red, positive in blue).*

NBCR

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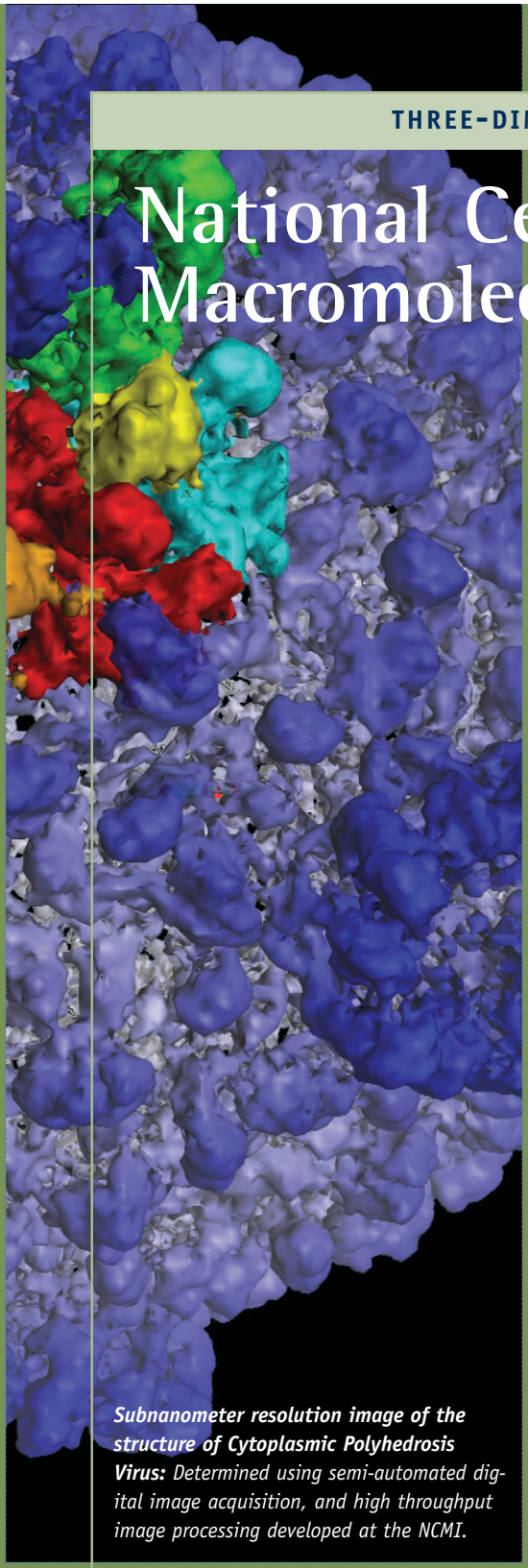
National Center for Macromolecular Imaging



Subnanometer resolution image of the structure of Cytoplasmic Polyhedrosis Virus: *Determined using semi-automated digital image acquisition, and high throughput image processing developed at the NCMI.*

Technology and research development efforts are focused on extending the resolution, speed, and flexibility of electron cryomicroscopy for three-dimensional structure determination of biological macromolecular assemblies. The resource tackles structural problems that are too complex or too difficult for X-ray crystallography and NMR spectroscopy. In the center, researchers have demonstrated the feasibility of visualizing secondary structure elements such as alpha helices and beta sheets of protein components in a number of large assemblies. They are developing technology for routine structure determinations at sub-nanometer resolution, approaching a resolution sufficient for tracing a polypeptide backbone. Generally they focus on macromolecular assemblies ranging from 300 kDa to 30 MDa and can produce structures from very small quantities of purified specimens.

Experimentally, researchers are involved in evaluation of new instruments for single particle imaging, development of automation techniques for high-throughput data collection, and improvements to cryo-preparation techniques. Computationally, they are developing algorithms and improving computational efficiency for the three-dimensional reconstruction of single particles toward atomic resolution. This software is embodied in EMAN and SAVR, which offer complete solutions for low symmetry and icosahedral single particles. In addition, they have produced SAIL, a set of specialized modules for producing professional-quality scientific animations. All three suites and a number of other tools are distributed free of charge.

The majority of efforts are focused on collaborative and service projects with a variety of groups around the world. Current biological projects include cytoskeletal filaments and bundles, ion channels, membrane transporters, icosahedral viruses, and large oligomeric proteins. In addition, the resource sponsors workshops and symposia on a regular basis to disseminate its imaging technology to a broader community.

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NCMI
National Center for Macromolecular Imaging

AN INTRODUCTION TO THE TELESCIENCE TOOL SUITE

National Center for Microscopy and Imaging Research

The National Center for Microscopy and Imaging Research *(NCMIR)*, a National Institutes of Health National Center for Research Resources-supported institution, developed Telescience as a comprehensive, platform independent, Grid-enabled system that allows researchers to perform end-to-end electron tomography. Telescience is performed through the "Telescience Portal," a web interface with a single user name and password that allows biologists to access the suite of tools that manage this process.

Users have access to resource scheduling; remote instrumentation; parallel tomographic Grid-based reconstruction; visualization, segmentation, and image processing tools; heterogeneous distributed file systems for data archiving; transparent deposition of data products into cellular structure databases *(e.g. NCMIR's Cell Centered Database)*; and utilities for shared "whiteboard" image annotations and "chatting" between multiple sites. Telescience provides the biologist with the power of the computational Grid while masking the complexity of its administration.

Telescience has been selected as one of the driving applications for the Pacific Rim Applications and Grid Middleware Assemblies *(PRAGMA)*. This association has led to international collaborations with facilities that include Osaka University, which assisted in the development of remote control for the high voltage electron microscope in San Diego and the ultra-high voltage electron microscope in Osaka through the IPv6; Taiwan's National Center for High Performance Computing *(NCHC)*, which allowed for the expansion of the Telescience visualization suite; and the Korea Basic Science Institute *(KBSI)*, which is implementing Telescience technologies with into their eScience program to facilitate remote use of their 1.25-million-volt ultra-high voltage electron microscope.

Advances in Telescience illustrate the benefits of producing a persistent infrastructure through the sharing of resources, technology, and experience.

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Reconstruction of Neuronal Spiny Dendrite: *Collaboration between NCMIR UCSD and Osaka University led to this imaging study of dendritic spines. Image created by combining electron tomography with high resolution light microscopy.*

NCMIR
NATIONAL CENTER for MICROSCOPY and IMAGING RESEARCH
A NIH-NCRR-supported resource center at UCSD

ncmir.ucsd.edu https://telescience.ucsd.edu

The Virtual Cell Project

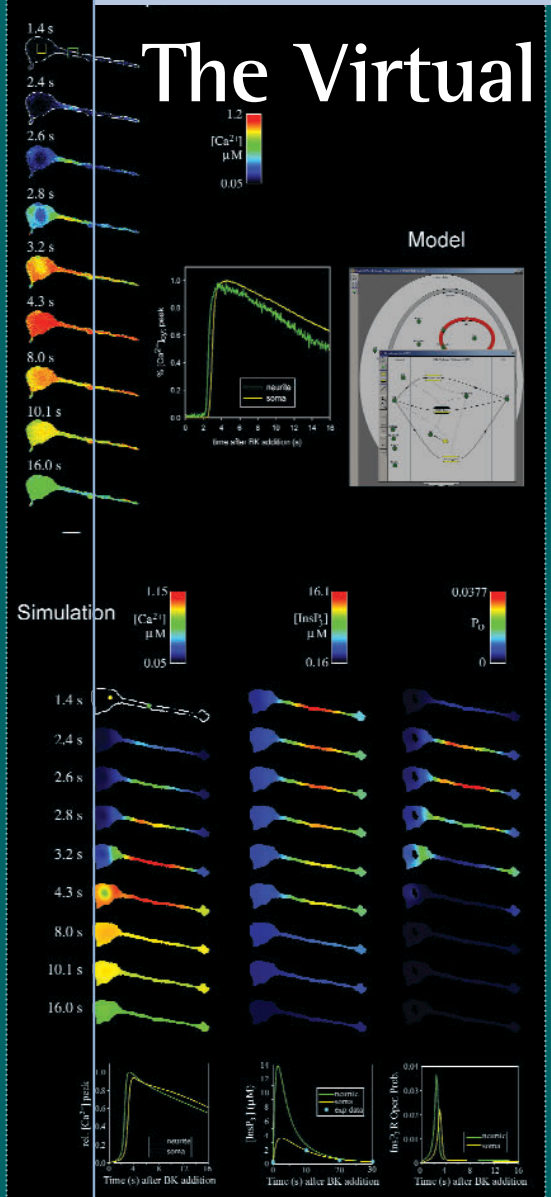

Image: *Bradykinin-induced calcium wave recorded in neuroblastoma cells (top left) simulated using the Virtual Cell (bottom left) by creating a model (top right) of receptor-induced signal transduction. Also shown are simulations of InsP3 concentration and channel open probability (bottom middle, right) that cannot be experimentally observed.*

The National Resource for Cell Analysis and Modeling is housed within, and is the principal venture of, the Center for Biomedical Imaging Technology at the University of Connecticut Health Center. The resource contains state of the art facilities for studying living cells, and has developed a new technology, the Virtual Cell, for analyzing and synthesizing this knowledge.

The Virtual Cell is a general software framework for modeling cell biological processes that is deployed as a freely accessible distributed application to be used over the Internet. Biochemical and electrophysiological data describing individual reactions are associated with experimental microscopic image data that describes their subcellular locations. Individual processes are integrated within a physical and computational infrastructure that will accommodate any molecular mechanism. Current development is focused on expanding the generalized mathematical descriptions of biological mechanisms, enhancing accessibility to non-mathematically savvy biologists, and integrating the interface with a database of experimental data and models, as well as other external databases. A wide range of applications of the Virtual Cell are being developed both as in-house research projects *(e.g. calcium dynamics in neuronal cells and RNA trafficking in oligodendrocytes)* and external collaborations. Additionally, to date more than 500 independent users worldwide have created and run simulations with the Virtual Cell.

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MULTISCALE STRUCTURAL MODELING WITH UCSF CHIMERA

Resource for Biocomputing Visualization and Informatics

The Resource for Biocomputing, Visualization, and Informatics *(RBVI)*, an NIH/NCRR Biomedical Technology Resource Center, creates innovative computational and visualization-based data analysis methods and algorithms; implements these as professional-quality, easy-to-use software tools; and applies these tools for solving a wide range of genomic and molecular recognition problems within the complex biological sequence -> structure -> function triad. Application areas include gene characterization and interpretation, drug design, understanding variation in drug response due to genetic factors, protein engineering, biomaterials design, and prediction of function from sequence and structure.

One of the software packages developed by the RBVI is UCSF Chimera, a highly extensible, interactive molecular graphics program. Chimera allows developers to quickly incorporate novel algorithms and analysis tools by providing many built-in sophisticated real-time graphics rendering and data management functions, allowing developers to focus on coding features unique to their application. About 30 extensions have been written to date, including ones focused on the display and manipulation of large volumetric data sets and multiscale molecular models as shown here.

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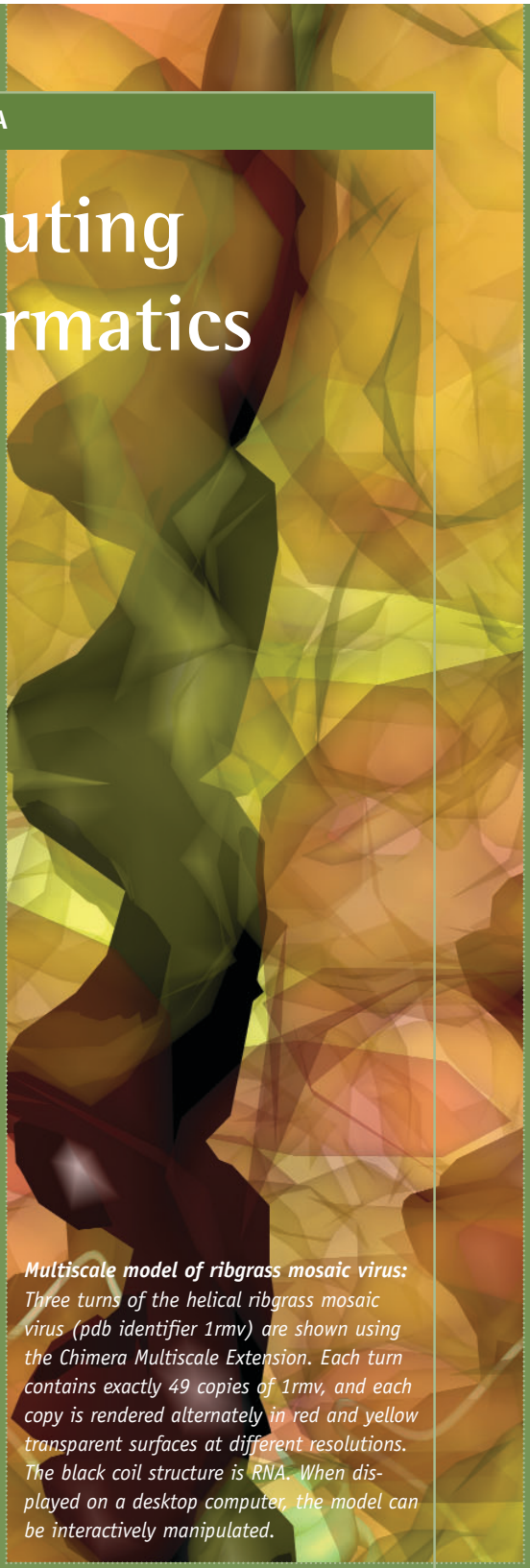
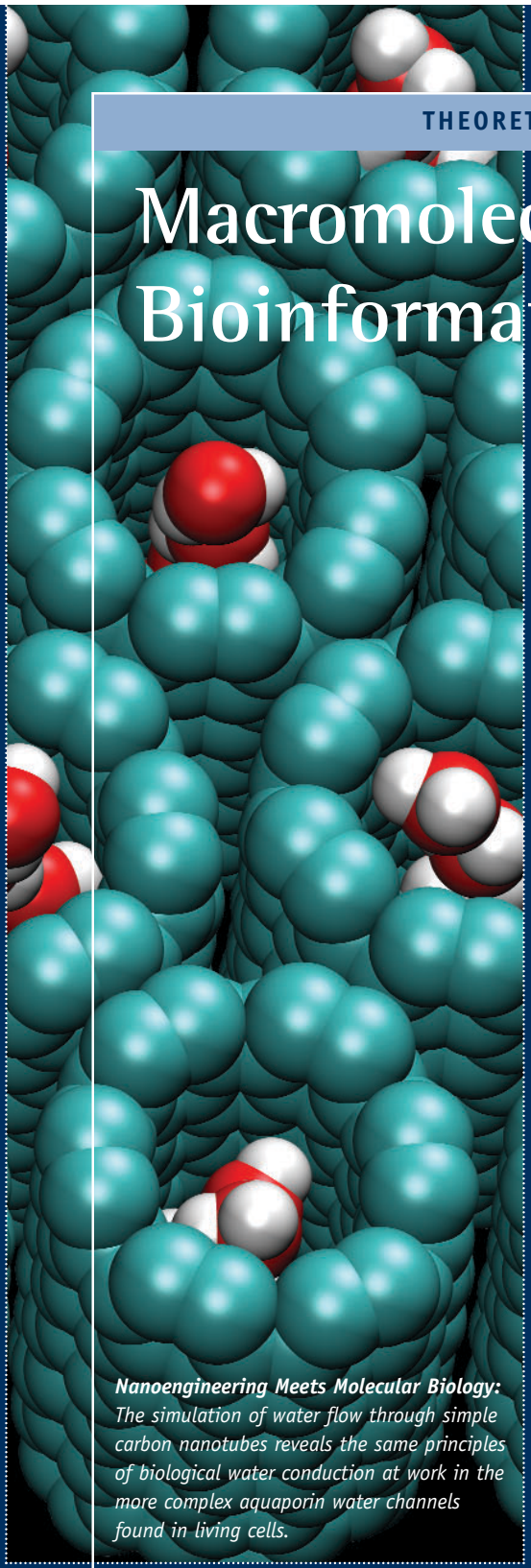


Multiscale model of ribgrass mosaic virus: *Three turns of the helical ribgrass mosaic virus (pdb identifier 1rmv) are shown using the Chimera Multiscale Extension. Each turn contains exactly 49 copies of 1rmv, and each copy is rendered alternately in red and yellow transparent surfaces at different resolutions. The black coil structure is RNA. When displayed on a desktop computer, the model can be interactively manipulated.*

Macromolecular Modeling and Bioinformatics



Nanoengineering Meets Molecular Biology: *The simulation of water flow through simple carbon nanotubes reveals the same principles of biological water conduction at work in the more complex aquaporin water channels found in living cells.*

The resource studies large biomolecular processes in living cells, focusing on membrane proteins that mediate the exchange of materials and information across, in particular, biological membranes as well as the conversion between electro-osmotic, mechanical, and chemical energy. It also develops software for large-scale simulations. Software tools include NAMD, a molecular dynamics simulation program used for classical, atomistic molecular dynamics simulations of large biomolecular aggregates; VMD, a molecular visualization program for displaying, animating, and analyzing both large and small biomolecular systems using 3-D graphics and built-in scripting; BioCoRE, a web-based, tool-oriented collaboratory for biomedical research and training.

Interactive molecular dynamics *(IMD)* for the manipulation of molecular simulations with real-time force feedback and interactive display; investigations of aquaporin channels, mechanosensitive channel, ATP synthase, chloride channel, photosynthetic proteins, visual receptors, and proteins with mechanical functions; efficient evaluation of force fields and integration schemes for simulation of very large biomolecular systems; efficient distributed molecular dynamics programs on workstation clusters and massively parallel machines; continued development of NAMD, VMD, and BioCoRE.

NAMD, VMD, and BioCoRE are the three flagship software packages developed by the NIH Resource for Macromolecular Modeling and Bioinformatics at the University of Illinois. NAMD, recipient of a 2002 Gordon Bell Award, is a parallel, object-oriented molecular dynamics code designed for high-performance simulation of large biomolecular systems. VMD is a molecular visualization program for displaying, animating, and analyzing large biomolecular systems using 3-D graphics and built-in scripting. BioCoRE is a collaborative work environment for biomedical research, research management and training.

Learn more about the NIH Resource for Macromolecular Modeling and Bioinformatics, visit www.ks.uiuc.edu.

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BioCoRE NAMD VMD

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