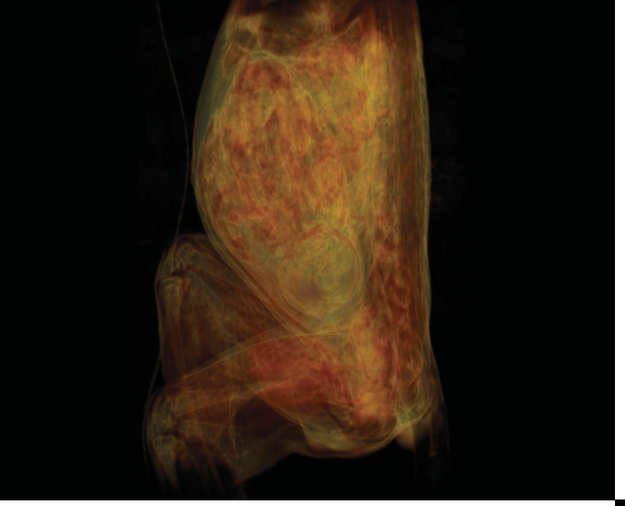


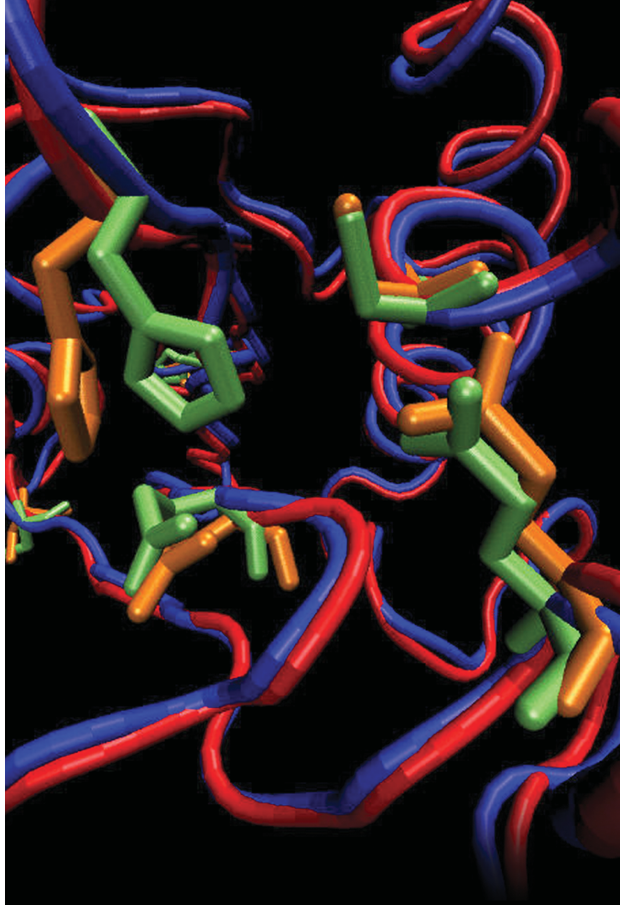
## X- Ray Computed Microtomography

**(Astrophysics)**

A microtomography facility at the Brookhaven National Synchrotron Light Source (NSLS) combines rapid image reconstruction using high speed parallel computing resources, with theoretical modeling and high-bandwidth networking. Three-dimensional volumes with a spatial resolution as small as 3 microns are used as input to quantitative calculations to improve our knowledge in a variety of disciplines. Shown below is a micrometeorite (279 microns diameter) with its outer surface (blue) made transparent. The red mass is a metal nugget; the yellow regions represent metal oxides.

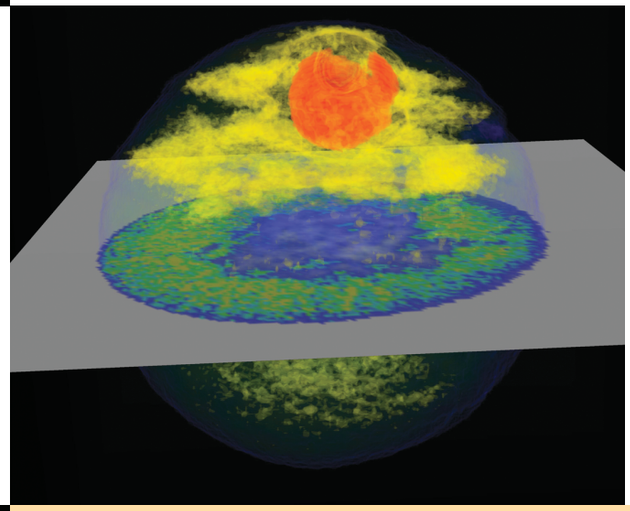
## Computational Biology

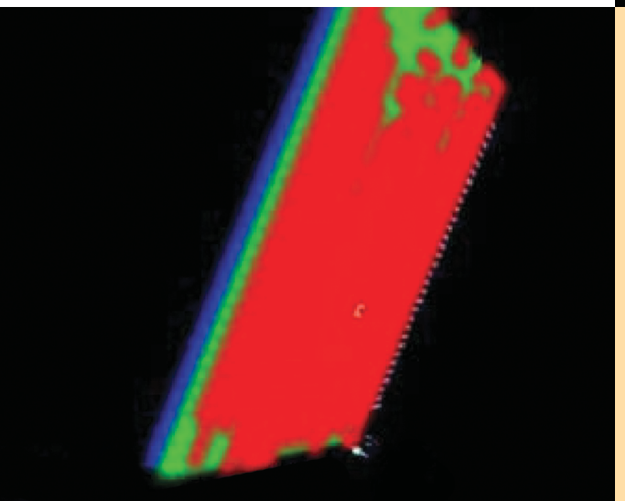
Computational biology has become an essential ingredient in the process of new drug design. The structure of the adenovirus proteinase (AVP) bound to a peptide cofactor (pVIc) was solved to atomic resolution at Brookhaven National Synchrotron Light Source. To obtain the structure of AVP in the absence of pVIc, molecular simulation was initiated. The cover image shows the structure AVP with pVIc removed, at zero time and after 1 nsec simulation, which took 10 days of computation. Whereas most of the strands in the two structures have not moved in that time period, a histidine residue (five membered ring in orange and in green) has moved. This explains why the enzyme is inactive without the peptide cofactor and why it is active with pVIc.



## Medical Science

Noninvasive medical imaging using high resolution MRI can show small details of the anatomy that would otherwise go undetected. The MRI of a third-trimester pregnant macaque Radiata generated on the BNL 4-Tesla Magnet is shown above. The spatial resolution is 0.78 x 0.625 x 2 $mm^3$. Three-dimensional visualization is used to safely highlight the development. In the future, biochemical PET data as well as physiological data will be incorporated in the image. BNL collaborates with NIH, National Cancer Institute and FDA to use visualization and data-mining for cancer detection. Below is a visualization of proteomic mass spectrometer data from blood samples. Different colors discriminate different stage cancers for early detection.





Brookhaven National Laboratory (BNL) is a U. S. Department of Energy (DOE) scientific research laboratory located on Long Island, New York. As a non-defense research institution, BNL is dedicated to basic and applied investigation in a multitude of scientific disciplines. Experimental and theoretical physics, medicine, chemistry, biology, environmental research, engineering and many other fields are represented here by our 3,000 member staff and over 4,000 visitors who come to BNL every year to use our world-class facilities.

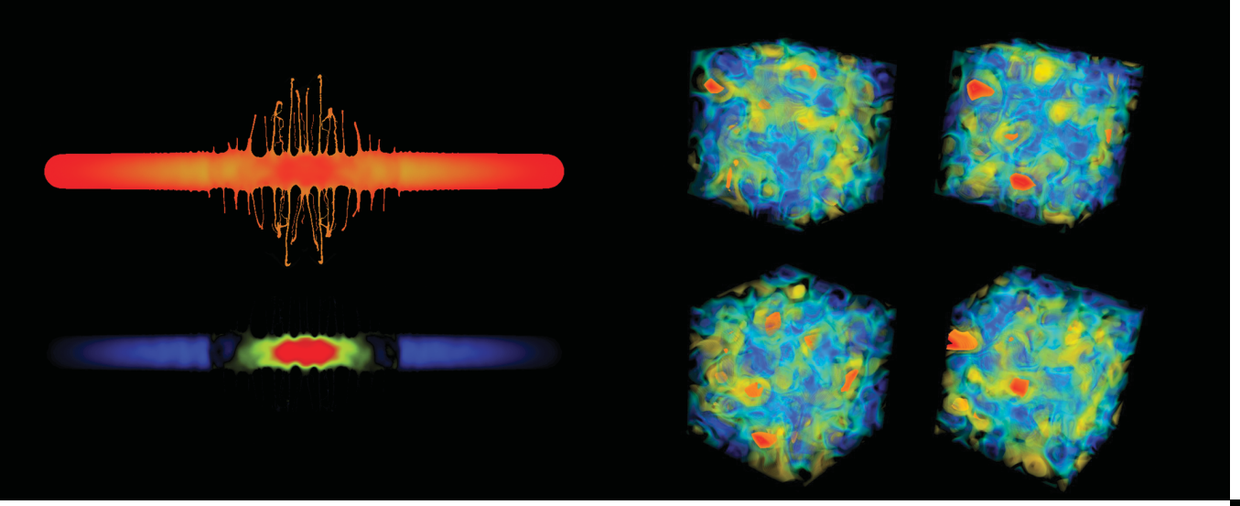
The Information Technology Division (ITD) works closely with BNL's scientific departments and other divisions to provide high quality service in computing, networking and telecommunications. The Stereoscopic Visualization Theatre and the projects represented here are but a part of ITD's efforts to support research and industrial partnerships at BNL.

**For more information contact:**


Michael McGuigan
Information Technology Division
Brookhaven National Laboratory
Upton NY 11973-5000
(631) 344-2695 mcguigan@bnl.gov
http://www.itd.bnl.gov/visualization/

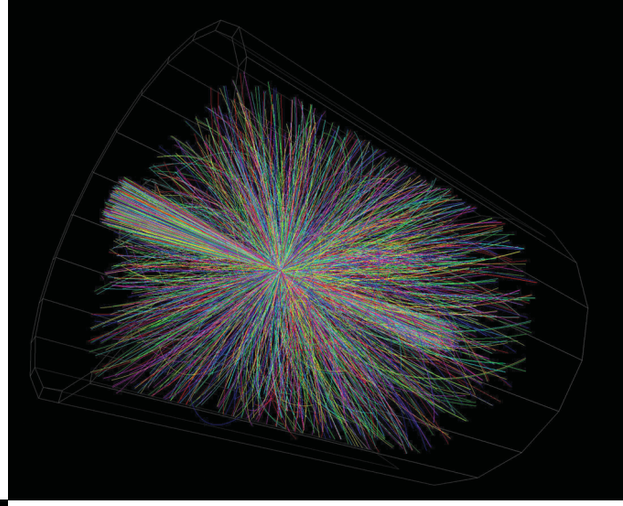

# Scientific Visualization at

BROOKHAVEN NATIONAL LABORATORY



## Environmental Science

Shown below is a 3-D volume rendering of the sulfate mixing ratio (moles sulfate/mole air) in the Northern Hemisphere. Mixing ratios were calculated with the BNL atmospheric chemical transport and transformation model. Simulations were driven by archived numerical weather forecast data; results were evaluated using observations taken at the same time and location. Mixing ratio values go from blue (small) to red (large). The "slicing" plane highlights the influence of the plume from Popocatepetl, a volcano near Mexico City. Sulfate (an atmospheric aerosol species derived from natural and anthropogenic sources) contributes to human health impairment, visibility reduction, acid deposition, and climate change. The image was created using Vis5D, a software package for visualizing meteorological data.

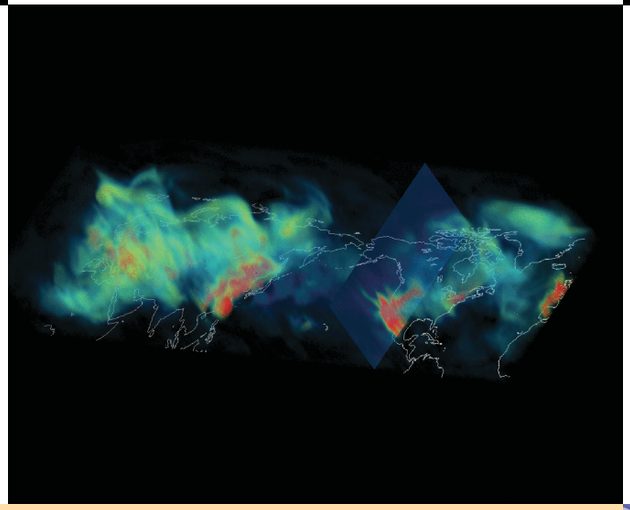


## Nuclear Physics (Accelerator Design)

The design of targets to generate high-flux particle beams has been an important problem in the design of advanced accelerators such as the Spallation Neutron Source (SNS) and the Muon Collider/Neutrino Factory. The Muon Collider target has been proposed as a pulsed free mercury jet interacting with proton pulses in the presence of a strong magnetic field. The expected disintegration of the jet into droplets due to this interaction creates complications for machine operation. The collapse of cavitation bubbles in the SNS mercury target, has been the most critical problem reducing target lifetime. Large-scale numerical simulations of hydro- and magnetohydrodynamic processes in high power liquid mercury targets improve target design while reducing costs of target tests. Shown above is a simulation of a Muon Collider target, showing distributions of density (top) and pressure (bottom) in the mercury jet after interaction with a proton pulse.

## Nuclear and Particle Physics

The RIKEN BNL Research Center's QCDSP super-computer (12,288 nodes, .6 Teraflops) is used for a variety of Quantum Chromodynamics (QCD) calculations, typically in four dimensions (3 for space, one for time). Shown above are four three-dimensional slices of the topological charge density of a lattice QCD gauge configuration with red indicating high values of the topological charge.

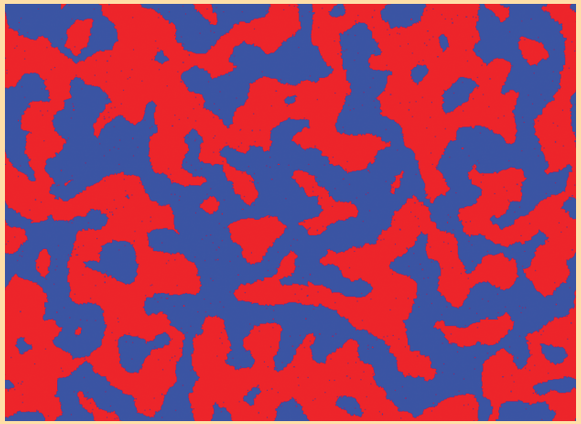
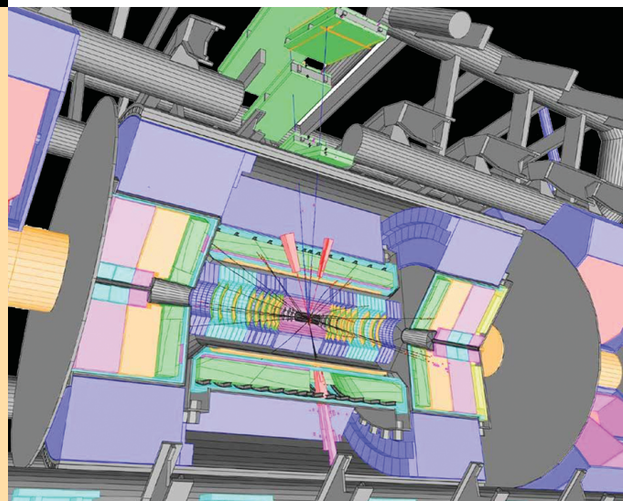


## Nuclear and High Energy Physics

Shown above is an image from a collision at RHIC (Relativistic Heavy Ion Collider) located at BNL. There are approximately 2000 particle tracks detected after a collision of two gold nuclei. Shown below is a visualization of the ATLAS (A Toroidal LHC ApparatuS) detector currently under construction at the Large Hadron Collider facility at CERN. BNL will be the US Tier 1 Computing Center for ATLAS. BNL researchers are collaborating with scientists from around the world to develop and deploy large scale computing Grids that will allow ATLAS physicists to conduct their research efficiently on a widely distributed set of computing resources.

## Scientific Visualization Facilities at BNL

The Information Technology Division (ITD) maintains two visualization facilities at BNL: a stereoscopic theatre and a central graphics cluster. Both facilities are available to all research groups at BNL. The display system in the stereoscopic theatre is driven by a SGI Onyx2 rack system. The stereo effect is achieved in a conference room setting by projecting two polarized images on a specially designed 10 foot screen (treated to retain light polarization), then viewed through polarized glasses. The viewing algorithm makes the image of the object appear to float into the center of the room.



The high performance and low cost of graphics cards has led to computational research at BNL to see if ordinary numerical simulations can be performed on Graphics Processing Units (GPUs). The GPU processor on the graphics card is the graphics analog of the CPU and accelerates the graphics computations. To the left is shown a result from an Ising model simulation performed on an Nvidia GPU. The Ising model is a Monte Carlo type simulation for magnets. The red/blue coloring corresponds to electron spins pointing up/down. Our main research interest is in using multiple GPUs in parallel simulations with applications to QCD, fluid and gas flows.