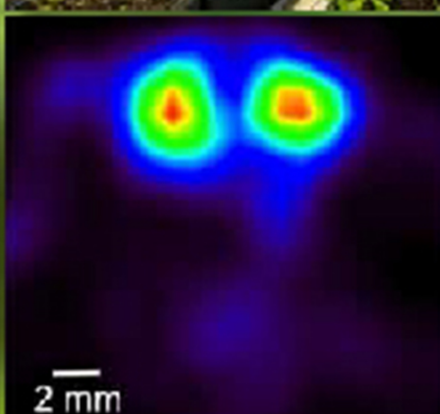
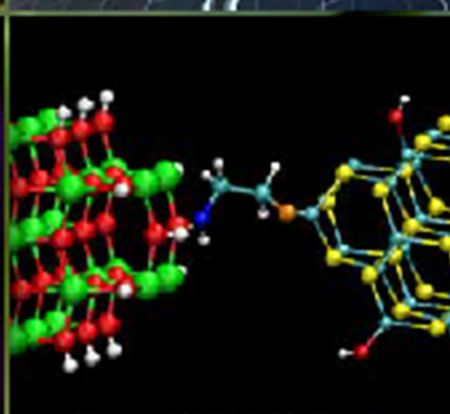
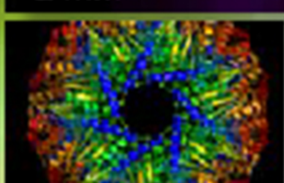
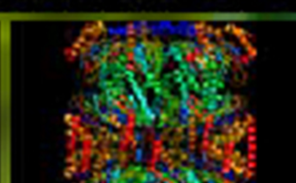
ENVIRONMENT & LIFE SCIENCES
ACCOMPLISHMENTS

Environmental Science | Biology | Medical | Computational Science







BROOKHAVEN NATIONAL LABORATORY

INTRODUCTION

Biology, Environmental Science, and Computational Science at Brookhaven National Laboratory

The biology and environmental sciences program at Brookhaven National Laboratory (BNL) features cross-disciplinary efforts that seek to understand relationships among climate change, sustainable energy, and ecosystems. Our efforts are aligned with the U.S. Department of Energy (DOE) missions and goals in energy and environmental research. In addition, we perform cutting-edge research for other agencies — including the National Institutes of Health and the National Aeronautics and Space Administration (NASA) — and for non-governmental organizations.

We have world-leading, distinctive expertise and capabilities in atmospheric science, plant systems biology, genetics, structural biology, radiobiology, radiochemistry, and bio-imaging. For our work, we leverage special and often unique capabilities across BNL and facilities including the National Synchrotron Light Source (NSLS) — and by 2014 the next generation light source, NSLS-II; the Center for Functional Nanomaterials; the NASA Space Radiation Laboratory (NSRL); and the New York Center for Computational Science (NYCCS).

Another critical component in our mission is to educate new generations of scientists, engineers, technicians, and teachers. The Environment & Life Sciences Directorate uses a wide variety of mechanisms to advance this initiative, including programs run by Brookhaven Lab's Office of Educational Programs.

Strategic partnerships with other research institutions are also important to accomplish our ambitious goals. Among those are nearby Stony Brook University (SBU) and Cold Spring Harbor Laboratory, as well as the core universities associated with the contract under which Brookhaven Science Associates manages BNL for the DOE (Columbia, Harvard, Massachusetts Institute of Technology, Princeton, and Yale) and the New York State High Performance Computing Consortium (SBU, Rensselaer Polytechnic Institute, and the State University of New York at Buffalo).

Computing and computational science have become a more integral part of the R&D program portfolio across BNL. The Computational Science Center provides a focal point for this growing core capability. In particular, the BNL distinguishing signature in this area has been in lattice quantum chromodynamics, accelerator science and technology, and large-scale data analytics in high-energy and nuclear physics. Our efforts in biology, environmental science, materials science, and advanced energy applications are expanding.

This brochure highlights selected recent accomplishments by researchers in the program. In total, the dedicated work by the 225 staff members in the program resulted in more than 230 refereed journal papers and 90+ invited presentations during fiscal year 2011 (October 2010 – September 2011).

Reinhold Mann, *Associate Laboratory Director*

CAPABILITIES / FACILITIES

Scientists in the Environment & Life Sciences Directorate at Brookhaven National Laboratory make use of many of the Lab's unique research facilities including:

The **Center for Functional Nanomaterials (CFN)** provides state-of-the-art capabilities for the fabrication and study of nanoscale materials — materials with dimensions on the order of *billionths* of a meter. The emphasis is on atomic-level tailoring to achieve desired properties and functions. One of five Nanoscale Science Research Centers funded by the Department of Energy's (DOE) Office of Science, the CFN supports Brookhaven's goal of leadership in the development of advanced materials and processes for selected energy applications. In addition to research programs aimed at understanding electronic nanomaterials, interfaces and catalysis, there are focus areas for developing new capabilities and uses for electron microscopy, theory and computation, and nanofabrication approaches based on soft and biological nanomaterials.

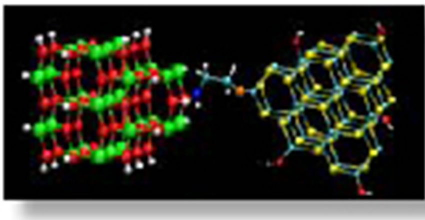
http://www.bnl.gov/cfn/

The **National Synchrotron Light Source (NSLS)** is one of the world's most widely used scientific research facilities, each year hosting more than 2,000 researchers from 400+ universities, laboratories, and companies. These researchers use beams of x-ray, ultraviolet, and infrared light along with an array of sophisticated imaging techniques to capture highly detailed "pictures" of a wide variety of materials, from biological molecules to semiconductor devices. The Lab is currently constructing a new light source, **National Synchrotron Light Source II (NSLS-II)**, which will produce x-ray beams 10,000 times brighter than NSLS. The new facility will be a key resource for researchers at Brookhaven's CFN and will have broad impact on a wide range of disciplines and scientific initiatives, including the National Institutes of Health's structural genomics initiative, DOE's Genomics:GTL initiative, and the federal nanoscience initiative. Of particular interest will be efforts to mimic nature to assemble nanomaterials into useful devices, improved capabilities for imaging complex protein structures, and the development of the next generation of sustainable energy technologies.

http://www.nsls.bnl.gov/ and http://www.bnl.gov/ps/nsls2/about-NSLS-II.asp

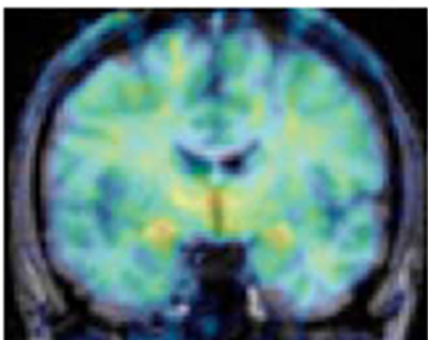
The **NASA Space Radiation Laboratory (NSRL)** at Brookhaven was built through a partnership between NASA and the DOE Office of Science to study the effects of space radiation on biological and physical systems. Scientists use beams of heavy ions provided by a particle accelerator to simulate space radiation and study its effects on biological specimens — including cells, tissue, and DNA — as well as industrial materials and detectors that might one day travel through space. This research will help scientists develop methods and materials to reduce the risks for humans exposed to ionizing radiation on future long-term space missions.

http://www.bnl.gov/medical/NASA/NSRL_description.asp



The **Brookhaven Computational Science Center (CSC)** brings together researchers in biology, chemistry, physics, and medicine with applied mathematicians and computer scientists — from Brookhaven, Stony Brook University, Columbia University, and other collaborating institutions — to exploit the remarkable opportunities for scientific discovery that have been enabled by modern computers. These opportunities are especially great in computational biology and nanoscience, but extend to many other areas including sustainable energy, environment, and homeland security. Some examples include modeling protein structures, brain physiology, and atmospheric chemistry. These data-intensive programs make use of the Center's two supercomputers with collectively more than 45,000 core processors, as well as new tools developed specifically for interactive visual and statistical data analysis.

http://www.bnl.gov/csc/



Brookhaven Lab is home to a suite of tools for **Radiotracer Chemistry, Instrumentation and Biological Imaging (RCIBI)**, including small and clinical scale positron emission tomography (PET) and magnetic resonance imaging (MRI) scanners and facilities for the production of radioisotopes and incorporating them into small precursors and complex molecules including nanomaterials. These radiotracers are designed to image specific biochemical transformations and the movement of molecules including environmental toxicants in vivo, and have been used to make numerous advances in neuroimaging, drug development, and studies of plant metabolism aimed at assessing genetic and environmental effects to improve carbon sequestration and energy crop growth.

http://www.bnl.gov/medical/RCIBI/

BNL-Led Effort Pursues Innovative Ways to Improve Climate Modeling

With FASTER Project leader Yangang Liu (front, left) of BNL's Atmospheric Sciences Division (ASD) in the Environmental Sciences Department (ESD) are Kiran Alapaty (front right) of DOE's Atmospheric System Research Program, and (back, from left) Peter Daum, acting ESD Chair, and FASTER team member Bob McGraw, ASD acting head.

50 scientists from more than 10 leading climate research centers in Europe and the U.S., led by Brookhaven Lab, have begun a new multi-institutional project aimed at accelerating the evaluation and improvement of fast physics processes in climate models. The overall goal of this initiative — known as the "FASTER" (FAst-physics System TEstbed & Research) project — is to build a fast physics testbed and perform research to identify and fix climate model deficiencies.

Fast physics refers to climatic processes that occur on scales of time and space that are too small to be portrayed by most global climate models, particularly processes related to clouds and precipitation. This lines up nicely with Brookhaven scientists' traditional areas of expertise — namely, a process-level understanding of meteorological, microphysical, and chemical aspects of aerosols and clouds — which, through the new program, will be directed toward the improvement of models for climate simulation.

The FASTER project is a major effort of the Earth System Modeling Program of DOE's Office of Biological & Environmental Research (BER) to bridge the research undertaken within BER's Atmospheric System Research Program to fully utilize the decade of measurements collected by Brookhaven researchers and others as part of the DOE Atmospheric Radiation Measurement Program. Since the early 1990s, ARM scientists have gathered data on clouds, radiation, and many other geophysical variables that are critical to climate modeling at locations from the tropics to the southern Great Plains to the Arctic.

http://www.bnl.gov/today/story.asp?ITEM_NO=1541, and
http://www.deixismagazine.org/2010/11/in-climate-modeling-speed-matters/

Assessing How Storm Clouds Contribute to Climate

An anvil cloud looms over the Southern Great Plains site.

Scientists from Brookhaven Lab recently headed to *Oklahoma!* — where the *clouds* come sweepin' down the plain, and . . . the wind comes right behind the rain — to take atmospheric measurements aimed at improving global climate models. Working with DOE's Atmospheric Radiation Measurement (ARM) Climate Research Facility in collaboration with NASA's Global Precipitation Measurement Mission, the scientists collected data on many factors that contribute to the formation and lifecycle of convective clouds — those towering masses formed by rising heat that can produce thunderstorms and other severe weather.

The findings from this Midlatitude Continental Convective Cloud Experiment will lead to a better representation of convective storm systems in global climate models, and also improve the fidelity of satellite observations of precipitation.

Using the full range of atmospheric measuring equipment at the ARM Southern Great Plains site in central Oklahoma, including a new, state-of-the-art dual-band scanning radar — installed with funding from the American Recovery and Reinvestment Act — the scientists performed the most-comprehensive-ever three-dimensional observations of clouds. The ground-based observations were supplemented by observations from NASA aircraft flying within and above the cloud systems.

The experimental approach is to document, in three dimensions, not only precipitation, but also clouds, winds, and moisture in an attempt to provide a holistic view of convective clouds and their feedback with the environment.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1262

Solar panels at the Long Island Solar Farm

Monitoring and Predicting Solar Energy Variability at the Long Island Solar Farm

The Long Island Solar Farm — a 200-acre array of photovoltaic panels installed at Brookhaven Lab — will be the largest solar energy generating facility in the Northeastern U.S. Generating up to 32 megawatts (MW) of power for the Long Island grid, it will bring a significant source of renewable energy to homes and businesses, and provide Brookhaven scientists with unique research opportunities. In addition to the large array, a smaller dedicated research array will be built at BNL to expand research capabilities.

The initial research project is a collaborative endeavor to evaluate and model the efficiency of the facility and examine issues of systems integration. Scientists will install a large array of field sensors across the solar farm to monitor available solar radiation and meteorological conditions in real time. When paired with information on power output and quality, these data will help scientists evaluate the efficiency of the large photovoltaic array, identify potential challenges associated with maintaining stability of the electric grid, and assess the feasibility of large photovoltaic energy generating facilities in the Northeast.

The group is also developing the ability to predict, up to 30 minutes in advance, the output of the large array based on observation, tracking, and evaluation of cloud conditions. This technique, known as "now-casting," uses optical imaging of the clouds and sophisticated software to identify shapes, track movements, and evaluate the optical density of the clouds — that is, how much light is filtered by clouds overhead. This type of near-term forecasting will help utilities anticipate changes — such as dips in solar-generated power at times of cloud cover — and make adjustments before they occur to maintain constant power on the grid.

http://www.bnl.gov/today/story.asp?ITEM_NO=2413

A FACE research site in Wisconsin

Sowing the Seeds for Sustainability

Plants may hold the secret to a sustainable energy future. Even today they are subsidizing our use of fossil fuels by absorbing approximately 30 percent of manmade carbon dioxide (CO_2) emissions. When we use the plants themselves as fuels, the CO_2 released during combustion is balanced by the CO_2 they take up during growth, resulting in a nearly carbon-neutral situation. But what if the CO_2 released from biofuels could be captured and stored? Then biofuels could provide an alternative energy source *and* remove CO_2 from the atmosphere.

Understanding the CO_2 subsidy provided by plants is key to improving our ability to project the future global change. At Brookhaven, environmental scientists have been exploring these relationships, particularly how photosynthesis responds to rising CO_2, in large field experiments where circular systems of pipes expose vegetation to the levels of CO_2 predicted to occur in the middle of this century. These Free Air CO_2 Enrichment (FACE) experiments have found that a sustained maximal response of photosynthesis to rising CO_2 is dependent on the ability of plants to use the extra products of photosynthesis (sugar), and on an adequate supply of nitrogen, an essential plant nutrient.

The FACE experiments have also shown that the few crop lines that have been tested in their production environment had a less than maximal response to elevated CO_2. With the aim of increasing the ability of future crop plants to respond maximally to CO_2, scientists are planning quantitative genetic, molecular, and biochemical analyses of collections of different varieties of crops. At Brookhaven they are developing a platform for high-throughput biochemical phenotyping that will aid this effort and help identify the most CO_2-responsive crops and highly productive but sustainable biofuels.

http://www.bnl.gov/des/ERTD/CarbonScience/PlantPhysiology.asp

Scientists Decipher Structure of Nature's 'Light Switch'

Above: Atomic model of a light-sensing protein that helps plants know when to flower, produce chlorophyll, and grow.

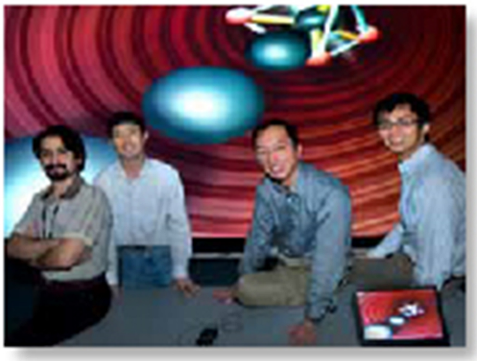
Right: Biophysicist Huilin Li

When the first warm rays of springtime sunshine trigger a burst of new plant growth, it's almost as if someone flicked a switch to turn on the greenery and unleash a floral profusion of color. Opening a window into this process, scientists at Brookhaven Lab and collaborators at the University of Wisconsin have deciphered the structure of a molecular "switch" known as a phytochrome that is much like the one plants use to sense light. They used a combination of electron microscopy, cryo-electron microscopy, and computational techniques to produce a 3-D map of the full structure. They then used this map to piece together the detailed structures of small phytochrome fragments that had been previously determined using x-ray crystallography.

The new structure revealed a long twisted area of contact between two individual "sister" units, with a good deal of flexibility at the untwisted ends. This structure supports the idea that the absorption of light somehow adjusts the strength or orientation of the contact, and through a series of conformational changes, transmits a signal down the length of the molecular interface. Understanding how these changes in shape send signals that tell plants when to flower, produce chlorophyll, and grow may help scientists design new ways to modify plant growth.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1143

Uptake Protein Acts as Zinc's Doorway to the Cell



Brookhaven biologists Babak Andi, Jin Chai, Dax Fu, and Wei Lin discovered how a particular protein (molecular structure) helps zinc ions (spheres) move through a membrane channel into cells.

A recent Brookhaven Lab study details how zinc, an element fundamental to cell growth, enters the cell via zinc-specific uptake proteins. The researchers were the first to purify this kind of protein and study its role in zinc uptake.

While there are six classes of known proteins that act as transporters or channels enabling zinc to cross the cell membrane, scientists have identified one metal-specific family of proteins whose purpose is to facilitate the cell's zinc uptake. These are called ZIP proteins, a reference to their resemblance to zinc-regulated and ion-regulated transporter proteins.

The exact mechanism by which ZIP proteins facilitate zinc uptake has been a mystery. A long-held belief has posited that ZIP proteins work like elevators, pumping zinc across the cell membrane and into the cell. But the Brookhaven team found no evidence to support this explanation. Instead, the Brookhaven team found evidence of electrodiffusion.

When ions diffuse, they move from a region with a high concentration to one of a lower concentration — like diners who relocate from a crowded dining hall to an adjoining, empty coffee room. In electrodiffusion, the diffused ions also change the electric charge of the space that they occupy. The imbalance in charge created by zinc ions moving into the cell builds during zinc uptake and acts against the concentration gradient, eventually causing zinc uptake to stop.

The researchers postulate that the ZIP protein allows zinc ion diffusion by providing an opening that is specifically shaped for zinc coordination chemistry. This hypothesis will eventually be confirmed in studies that crystallize and examine the ZIP protein at the atomic level.

Aside from satisfying scientific curiosity, this understanding could have a big impact. Zinc uptake at the cellular level is implicated in a range of biomedical and energy research.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1198

Modeling Plant Metabolism to Optimize Oil Production

Scientists at Brookhaven Lab have developed a computational model for analyzing the metabolic processes in rapeseed plants — particularly those related to the production of oils in their seeds. Their goal is to find ways to optimize the production of plant oils that have widespread potential as renewable resources for fuel and industrial chemicals.

Plant seed oil represents the most energy-dense form of biologically stored sunlight, and its production is controlled, in part, by the metabolic processes within developing seeds. Prior efforts to monitor these processes have been compared to assessing traffic flow on roads in the United States by measuring traffic flow only on the major highways. The new model — which includes 572 biochemical reactions that play a role in the seed's central metabolism and/or seed oil production, and incorporates information on how those reactions are grouped together and interact — aims to get a more detailed view.

This large-scale model is a much more realistic network, like a map that represents almost every street, with computational simulations to predict what's going on. Scientists can use it to simulate complicated metabolic processes under varying conditions — for example, looking for changes in oil production or the formation of oil precursors in response to changes in available nutrients, light conditions, and other variables. The scientists can now try to simulate the effect of "road blocks" or where to add new roads to most effectively eliminate traffic congestion on the path to biofuel production.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1308

Scientists Unravel Details of Plant Cell-Wall Construction

Biologist Chang-Jun Liu is exploring ways to make plant cell walls that are easier to convert to biofuels.

One big challenge in converting plant feedstocks to biofuels is that the complex biopolymers that keep plants standing up make it hard to break them down. Plant biochemists at Brookhaven are unraveling details of how plant cells' structural supports — their cell walls — are made, with the hope of finding ways to change their composition for more efficient biofuel production.

The primary focus is to explore the molecular basis for cell wall construction and to develop new methods and technologies to manipulate cell wall biopolymers, particularly the natural aromatic polymer lignin, which hinders the release of simple sugars from cell wall biomass and their subsequent conversion to liquid fuels. Being able to manipulate lignin biosynthesis would have a great influence on the ability to produce renewable biofuels, and could also have a large effect on many other agricultural and industrial processes.

One recent project explored the details of how precursors to lignin are transported across cellular membranes or stored prior to linking up. The key finding, that the process requires a class of energy-dependent transporter molecules, known as ABC-like transporters, may provide a "chink in the armor" that opens a way to alter plants' lignin content.

The group is also working to elucidate the catalytic mechanisms involved in cell wall construction, so that knowledge and the tools of molecular biology and protein engineering can be used to create novel catalysts to control the process. By mimicking the process of evolution in the laboratory, the group obtained a set of novel enzymes that can modify lignin precursors. They found that the modified precursors were unable to be processed for polymerization, which substantially reduced the lignin content of the cell wall. With less lignin, the cellulosic biomass was more easily converted to simple sugars under enzymatic digestion.

Developing embryos after being excised from a growing rapeseed plant. The embryos accumulate seed oils, which represent the most energy-dense form of biologically stored sunlight, and have great potential as renewable resources for fuel and industrial chemicals.

Another project aims to understand the synthesis of the aromatic domains of the specific cell-wall biopolymers suberin and cutin, which act as a barrier to keep harmful substances and infectious microorganisms from entering plant cells, while facilitating the intake and storage of water and other nutrients. Knowledge of how these polymers are produced could eventually be used to modify plants for agricultural purposes, including improved biomass production and sustainability. The group identified a key enzyme responsible for suberin biosynthesis, and demonstrated that plants deficient in this enzyme were much more permeable to salt than wild-type plants. This suggests that suberin, ubiquitous in root tissues, plays an important role in plants' adaptation to their habitats. Understanding and controlling its biosyntheis might therefore help scientists tailor crops to thrive in specific, even harsh, environments — an important milestone on the road toward economically efficient biofuel production.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1209
http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1021
http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=997

Brookhaven/NASA Summer School Trains Future Space Scientists

At NSRL, scientists study the effects of space radiation and test strategies designed to protect astronauts.

Students and scientists from around the world come to Brookhaven Lab each summer to participate in the NASA Space Radiation Summer School. Working in medical labs and at the NASA Space Radiation Laboratory (NSRL) — a unique facility that simulates the harsh radiation environment of outer space — the students study the possible risks astronauts may face during future long-term space flights, and ways to mitigate these risks.

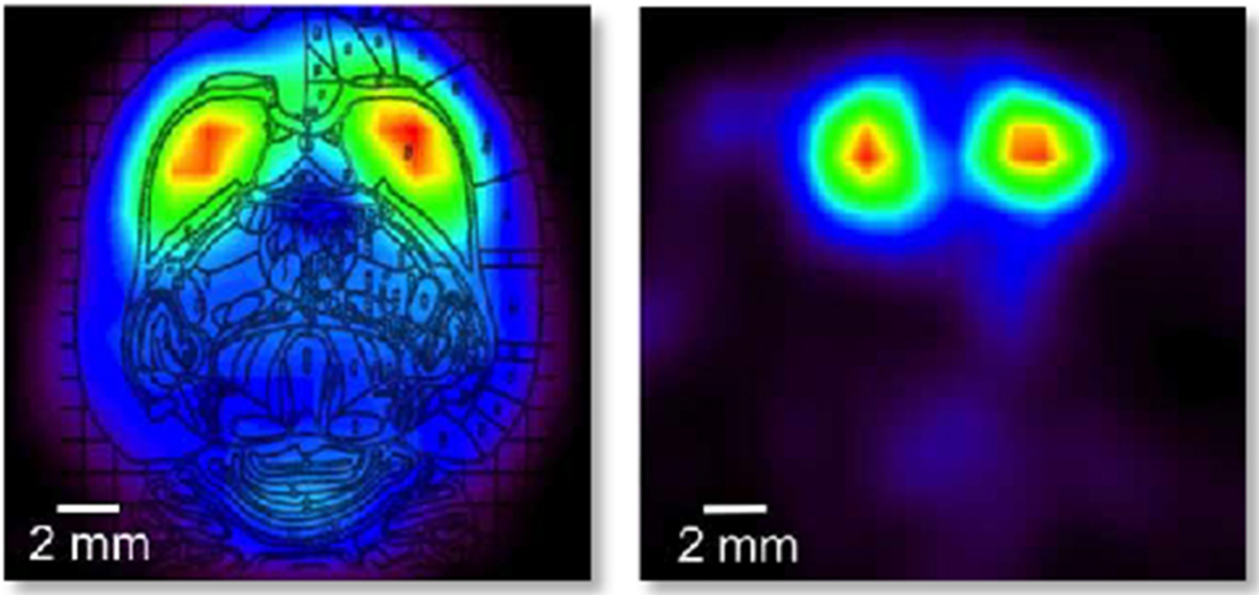
While there is a wealth of data describing the effects of conventional radiation like x-rays, the same is not true for the types of radiation present in space. It is essential to define the potential risks of exposure to space radiation and, if necessary, develop effective countermeasures to permit safe missions of longer durations than in the past.

Scientists are particularly interested in understanding how intense cosmic rays may promote the development of cancer, as well as how this radiation can affect the central nervous system and other organ systems of the body. NSRL researchers are also looking at ways to protect against these dangers through shielding and other strategies to minimize risks.

The summer program is sponsored by NASA and organized and managed by Brookhaven Lab, Loma Linda University Medical Center, and Universities Space Research Association (a consortium of universities, research organizations, and governmental groups involved in space research).

http://www.bnl.gov/medical/nasa/NSRSS/default.asp and http://www.bnl.gov/medical/NASA/LTSF.asp

Miniature "Wearable" PET Scanner



PET scans of a rat's brain made with the RatCAP scanner (horizontal view superimposed on a rat brain atlas figure, left, and a coronal slice, right). The rainbow scale (red = high, violet = low) indicates the level of a radiotracer that binds to receptors for dopamine, which are concentrated in the striatum, a brain region involved in reward and motivation.

Positron emission tomography (PET) is a powerful tool for studying the molecular processes that occur in the brain. But studying animals with PET has required general anesthesia or other methods to immobilize the animals, making it impossible to simultaneously study neurochemistry and the animals' behavior – the actions resulting from what goes on in the brain.

Scientists from Brookhaven Lab and Stony Brook University and collaborators have overcome this limitation by developing a "wearable" portable PET scanner. The idea was to eliminate the need for restraint by developing a PET scanner that would move with the animal, thus opening up the possibility of directly correlating the imaging data with behavioral data acquired at the same time.

Weighing only 250 grams, the device — dubbed RatCAP, for Rat Conscious Animal PET — can be "worn" like a collar on a rat's head, and is counter-balanced by a system of springs and motion stabilizers to allow the animal significant freedom of movement.

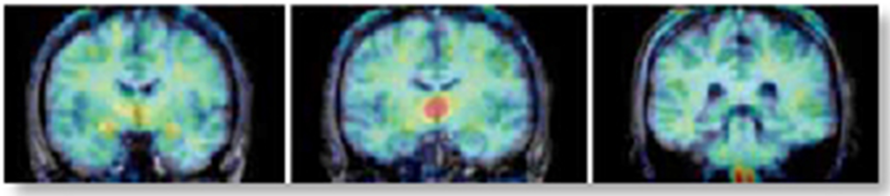
Validation tests clearly demonstrate that RatCAP can correlate brain function measurements with behavioral measures in a useful way. Brookhaven scientists are also developing ways to combine RatCAP with magnetic resonance imaging (MRI) for simultaneous multimodal imaging studies.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=1235

http://www.nature.com/nmeth/journal/v8/n4/full/nmeth.1582.html

http://iopscience.iop.org/0031-9155/56/8/009/

Scans Reveal Estrogen-Producing Hotspots in Human Brain



In these PET scans, from the front to the back of the head, red indicates the highest level of vorozole, a molecule that binds to the enzyme responsible for estrogen production in the brain (blue is the lowest level). These "hotspots" have the highest levels of estrogen production.

Brookhaven scientists have opened a gateway to new research on estrogen in the brain by using a molecule "tagged" with a radioactive form of carbon and a positron emission tomography (PET) scanner to monitor levels of aromatase, an enzyme responsible for the hormone's production.

Estrogen is implicated in a range of conditions, from breast cancer to Alzheimer's disease. So studying its production using noninvasive imaging techniques can be a useful diagnostic and investigative tool.

The study was designed to expand use of the radiotracer N-methyl-11C vorozole. Vorozole binds to aromatase, an essential catalyst in the biosynthesis of estrogen. This is the first study to demonstrate that vorozole is a useful radiotracer for studying estrogen-producing hotspots in the human brain.

The scientists found a surprise in the anatomical distribution of aromatase, with the highest levels in the thalamus and then the medulla, which differs from animal studies, where aromatase was concentrated in smaller regions, principally the amygdala and preoptic areas. Future studies will investigate this distribution and monitor aromatase levels related to a range of factors — including age, sex, personality, and memory — and conditions such as unusual aggression, breast cancer, and Alzheimer's disease.

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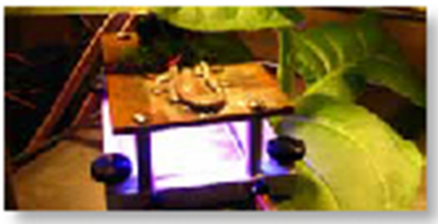
Radiotracers Track Plant Biochemistry



Scientists monitor the uptake and distribution of radiolabeled nitrogen in plants.

Researchers at Brookhaven are now using radiotracer technology developed for brain scans to study the allocation of nutrients and hormones in plants. This unique application of bio-imaging technology gives scientists a non-invasive way of investigating how plants accumulate biomass, respond to changing environments, fight off pests, and many other factors that can play a role in improving biofuel production, carbon sequestration, crop yields, or pest resistance.

These studies have revealed, for example, how plants "harden" their cell walls to fend off attacks from pests. Finding a way to push this process in reverse might make plants easier to digest when making biofuels.

Scientists monitor radiolabeled compounds — produced from "tagged" carbon dioxide or nitrogen — using positron emission tomography (PET), autoradiography, and other techniques. Also, through extensive radiochemistry, scientists can make and administer complex biomolecules to study plant signaling. Unlike cell-culture and/or destructive techniques, this approach enables the study of integrated plant responses with repeated measurements of the same plant over time. It also allows studies at an organismal scale, where key regulatory controls within plant metabolism are communicated across scales of the whole plant via long-distance transport of hormones and/or metabolites acting as signals.

These studies will help unravel the complex physico-chemical and biochemical processes that exist both within plants — across scales from the whole-plant down to cellular metabolism — and between plants and their surrounding environment. Information gained can then be applied to a system-level understanding of plant growth relevant to global issues of sustainable energy, environment, and agriculture.

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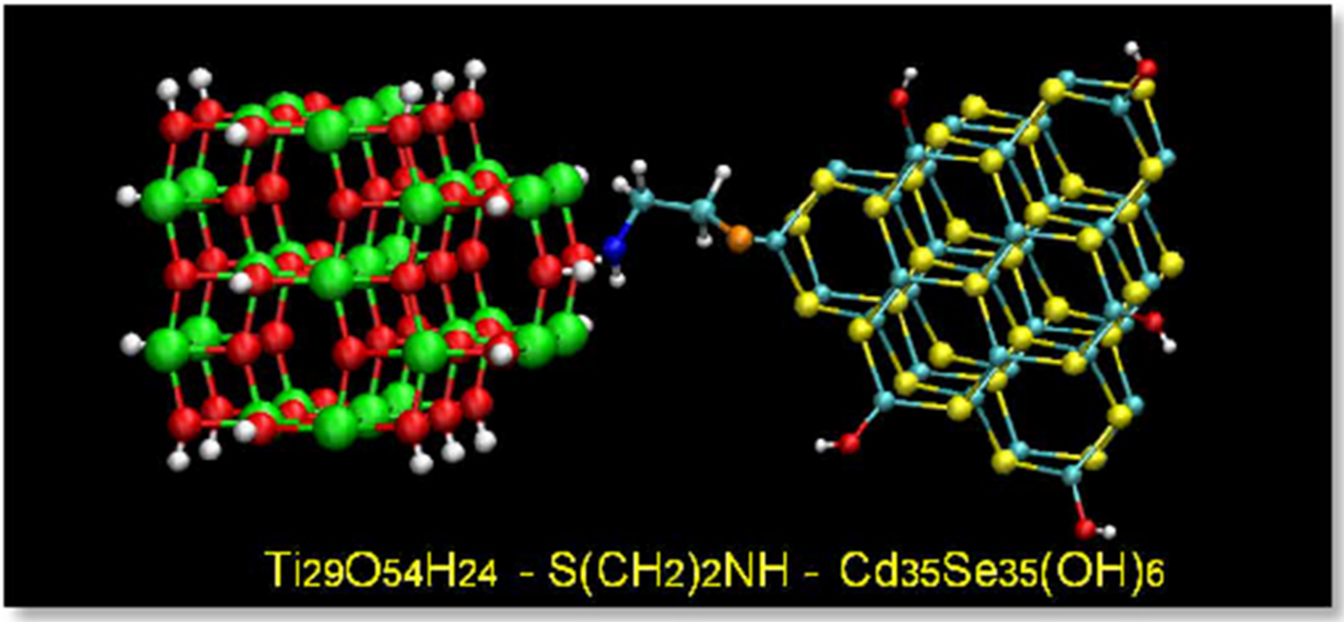
NY Blue Helps Advance Research in Many Fields



Cadmium-selenium (CdSe) quantum dot solar cells are simulated on New York Blue and may lead to efficient photovoltaic solar cells that are needed to make solar energy cost-competitive with other energy sources.

Brookhaven National Laboratory and Stony Brook University have formed the New York Center for Computational Sciences (NYCCS) with a 36,000-processor IBM Blue Gene supercomputer known as New York Blue as its centerpiece. Under this umbrella organization, NY Blue — jointly managed by Stony Brook and Brookhaven — serves more than 350 authorized users from institutions around New York State, including Stony Brook, Columbia University, NYU, Cornell, Mount Sinai Medical Center, and General Electric.

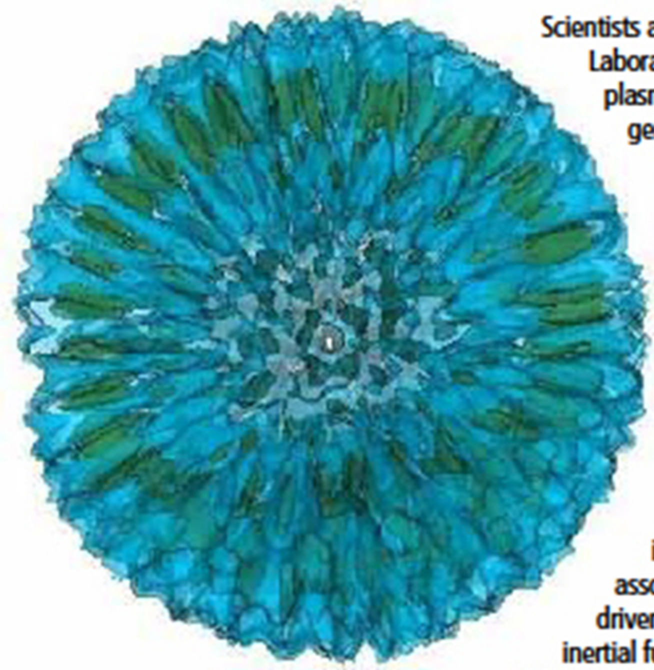
Capable of performing 100 trillion calculations per second, NY Blue is about 10,000 times faster than a personal computer. The broad-based science program for NY Blue includes drug design, protein molecular dynamics, quantum physics of quarks and gluons, fluid dynamics of energy related processes, climate modeling, accelerator design, and materials design.

As an example, one Stony Brook University computational biologist is using the supercomputer to model the molecular behavior of viruses. Areas of interest include modeling the structural changes in biomolecules, recognition and repair of damaged DNA, understanding why and how proteins fold, the role of protein dynamics in ligand binding and drug resistance, and the development of new algorithms and models for biomolecular simulations. This research may assist scientists studying potential new drugs to treat diseases including HIV-AIDS, tuberculosis, and cancer.

In addition, Brookhaven and RIKEN (the Japanese laboratory for physical and chemical research) are acquiring three racks of Blue Gene Q in 2011, which will add 600 Teraflop/s of computational capability of the latest supercomputer architecture.

http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=07-69
http://www.bnl.gov/bnlweb/pubaf/pr/PR_display.asp?prID=906

Simulations to Evaluate New Approach to Fusion



FronTier simulation of the implosion of a plasma liner formed by the merger of 625 jets.

Scientists at the Computational Science Center at Brookhaven National Laboratory are conducting large-scale simulations to explore plasma-jet driven magneto-inertial fusion, a novel approach to generating energy via nuclear fusion. Like the fusion reactions that power our Sun, this process has the potential to release enormous amounts of energy — ideally, more than is required to run the reaction. If realized, such fusion power could have enormous impact on meeting our ever-growing energy needs.

In plasma-jet driven magneto-inertial fusion (PJMIF), a large number of radial, highly supersonic plasma jets merges to form a plasma liner, which then implodes on a magnetized deuterium-tritium plasma target and compresses it to ignite the fusion process. The PJMIF technique combines the best features of magnetic and inertial confinements of plasma and avoids major difficulties associated with other approaches — for example, traditional laser driven inertial confinement fusion and solid liner driven magneto-inertial fusion. It therefore has the potential for providing a low-cost and fast R&D path toward the demonstration of practical fusion energy.

An advanced multiphysics code, FronTier, has been used for the computational evaluations of the PJMIF concept. These simulations have demonstrated the successful formation of the plasma liner by the merger of 625 jets. As highly supersonic jets collide to form a liner, strong oblique shock waves are generated that induce perturbations and heat the liner. The simulations have estimated the uniformity and thermodynamic state of the liner after the jet merger. The uniformity of the liner is critical for the reduction of hydrodynamic instabilities in the target, while maintaining a low temperature in the liner is necessary to achieve high target compression rates.

These simulations support the Department of Energy's program in High Energy Density Laboratory Plasmas, in particular the Plasma Liner Experiment at Los Alamos National Laboratory.

High-Performance File-Transport Protocols and Tools

FTP 100: a high performance data transport tool to move data across optical networks between data centers, clouds, and supercomputers

Some of today's most compelling scientific problems — from climate modeling and genomics, to studies of the cosmos, interactions among subatomic particles, and properties of materials at the nanoscale — are expected to generate exabytes of data (that's *quintillions* of bytes) over the next five years. To make sense of all that data, teams of scientists around the globe need tools to transfer it, visualize it, and analyze it from their distant geographic locations — all in a transparent, easy-to-use manner and at high speed without overwhelming available computing resources.

Scientists at Brookhaven Lab's Computational Science Center are working to meet this challenge by developing high-performance file-transport protocols and tools for data-intensive applications. Their latest advance is a Remote Direct Memory Access (RDMA) based File Transfer Protocol (FTP) and associated tools that allow direct access from the memory of one computer into that of another without involving either one's operating system. Data transfers continue in parallel with other system operations, and data is delivered directly to the network. This can reduce latency and enable faster message transfer.

The flexible design has allowed the computational scientists to investigate the application-level performance of different implementations of RDMA offload engines over Local Area Networks and Wide Area Networks. Their experiment results show that bandwidth performance is greatly improved with much lower central processing unit (CPU) consumption on a local data center platform.

However, some existing RDMA over TCP (Transmission Control Protocol) techniques like iWARP demonstrate performance loss compared to its TCP counterpart in a high-bandwidth high-latency Internet. This performance loss is caused by the difficulty of tuning network parameters in network cards and the overhead induced by the complex layered structure of the iWARP stack.

To mitigate this performance problem, the scientists proposed solutions, based on an advanced architecture, to maximize the parallelism of RDMA operations to achieve a satisfactory performance over long-haul links in the network. Furthermore, a science data network provided by DOE ESnet offers dedicated network circuits to allow network users to use lightweight transport protocols along with RDMA for high-speed data access. Such improvements should enhance the ability of global scientific collaborations to share, copy, and access complex datasets without overtaxing computing resources.

AWARD HIGHLIGHTS

Nelly Alia-Klein, a scientist in Brookhaven's Medical Department, was honored by Brookhaven Town for her accomplishments in science as part of a public ceremony to celebrate the significant achievements of local women during Women's History Month. Initially trained as a clinical psychologist, with expertise in forensic psychology, Alia-Klein has specialized in neuroimaging, together with DNA and behavioral analyses, to study the mechanisms that underlie aggression and violent behavior.

Huilin Li, of Brookhaven's Biology Department, was named Man of the Year in Health/Medicine by *The Village Beacon Record*, a local weekly newspaper. Li was a key member of a team of scientists from Brookhaven, Stony Brook University, and Weill Cornell Medical College whose research revealed how a proteasome — a structure essential to the tuberculosis (TB) bacterium's survival — is put together and how it works. These details could assist in the development of new anti-TB drugs.

Rita Goldstein, a scientist in the Medical Department at Brookhaven, has been named a member of the American College of Neuropsychopharmacology, the nation's premier professional society in brain, behavior, and psychopharmacology research. Goldstein, a clinical psychologist, specializes in the neuropsychology and neuroimaging of drug addiction, with the particular aim of understanding how cocaine addiction affects brain function and behavior so as to influence the development of new modalities for treatment.

Jacob Hooker, an assistant chemist in Brookhaven's Medical Department and Director of Radiochemistry at the Athinoula A. Martinos Center for Biomedical Imaging in Massachusetts, has been named as a recipient of the Presidential Early Career Award for Scientists and Engineers. Hooker, an organic chemist, was recognized for his work in adapting modern synthetic chemistry to create new tools for studying the chemistry of living systems. Working from basic chemical principles, Hooker has focused his research on advancing fundamental radiochemistry and developing new radiolabeled compounds for biomedical imaging.

Paul Kalb, a leading engineer in environmental research in Brookhaven's Environmental Sciences Department, was honored as Brookhaven's "Inventor of the Year" by Battelle, the global science and technology company that, together with Stony Brook University, manages Brookhaven Lab. Kalb has specialized in developing and applying technologies for hazardous- and radioactive-waste management, environmental cleanup, decontamination and decommissioning, and environmental security. He played a key role in developing a new method to passively concentrate and remove toxic mercury from soil, sediment, sludge, and other industrial waste. The method allows mercury to be removed without excavating and replacing large volumes of toxic soil or other material, thereby reducing cleanup cost and environmental impact.

Gene-Jack Wang, chair of Brookhaven Lab's Medical Department, was honored at the 2011 Asian Pacific American Heritage Month Celebration as a "distinguished Asian American professional." Wang oversees approximately 70 employees. And conducts research using imaging technologies, such as positron emission tomography (PET) and magnetic resonance imaging, to track and understand the brain mechanisms associated with addiction, alcoholism, obesity, and eating disorders.

Joanna Fowler, a senior chemist and director of radiotracer chemistry, instrumentation, and biological imaging at Brookhaven Lab, received a Distinguished Women in Chemistry/Chemical Engineering Award from the American Chemical Society (ACS) as part of the United Nations' International Year of Chemistry 2011. Fowler, a member of the National Academy of Sciences (NAS) and 2009 recipient of the National Medal of Science, has made significant contributions to brain research and to understanding diseases such as addiction through brain-imaging studies using positron emission tomography (PET). She is co-inventor of FDG, a PET radiotracer used in hospitals and research centers throughout the world to diagnose and study neurological and psychiatric diseases and to diagnose cancer.