# ENVIRONMENT, LIFE & COMPUTATIONAL SCIENCES
## ACCOMPLISHMENTS FY12

Biosciences | Environmental Science | Computational Science

BROOKHAVEN NATIONAL LABORATORY

**ON THE COVER**

Kewei Zhang and C.J. Liu are exploring ways to make plants easier to convert to biofuels.

Oak Ridge National Laboratory's new hybrid-architecture Cray XK6 system, named Titan, will have a peak theoretical performance of more than 20 petaflops. (Image courtesy of Oak Ridge National Laboratory)

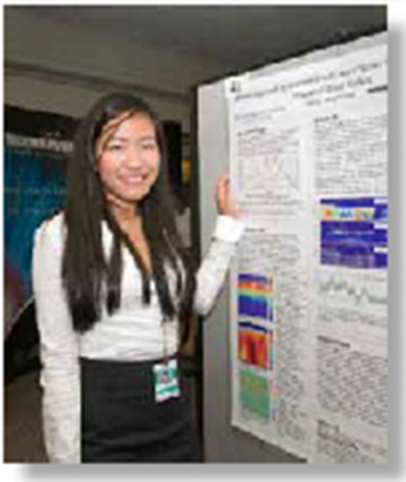
Biosciences Greenhouse

Brookhaven researchers Jilian Fan, Changcheng Xu, and Chengshi Yan with cultures of algae that were shown to increase oil production in response to excess carbon.

Conceptual drawings of the simultaneous PET/MRI breast imaging system being developed at Brookhaven Lab showing the how the PET insert (green) fits inside the MRI scanner and how it will be used with breast cancer patients.

Structural analysis of the MRI scans was performed using voxel-based morphometry (VBM).

# EDUCATION HIGHLIGHTS



## Brookhaven Lab's Office of Educational Programs offers a variety of learning opportunities for teachers and students from elementary to graduate level.

**Hands-on Science**
The Office of Educational Program's onsite Science Learning Center offers "Discovery Activities" for students in grades 1-8, featuring interactive exhibits and programs that demonstrate basic scientific principles and utilize the inquiry method of teaching. Learning Center staff also lead "Exploration Labs," either at the Lab or at schools, to engage middle and high school students in hands-on activities grounded in research conducted at Brookhaven. More than 35,000 students and teachers participate in Science Learning Center programs each year.

**Contests**
Students compete each year in a variety of Lab-run contests that foster appreciation for principles of science and engineering. These include an elementary school science fair, a middle school contest to design and test magnetically levitated (MagLev) vehicles, a high school bridge-building contest, a high school science-and-society essay contest, and regional science bowls sponsored by the Department of Energy for middle and high school students.

**Open Space Stewardship Program**
Through the Open Space Stewardship Program, the Lab fosters partnerships between schools and land stewards in their local communities. Students in grades K-12 participate in environmental research projects on undeveloped land owned by either a public or private agency. Lab scientists and educational staff help to train teachers and provide guidance, and host an annual celebration where participants share their experiences.

**Internships**
Each summer, high school students work side-by-side with scientists in Brookhaven's world-renowned facilities on cutting-edge research in physical science, life science, and technology development. Students can also participate in research-based classes and lectures. College and graduate-level programs are also available for students interested in furthering their exploration of science and possibly pursuing careers.

**Teacher Workshops**
A wide variety of professional development workshops are available to teachers.

**For More Information**
Office of Educational Programs, (631) 344-4503, http://www.bnl.gov/education/

# INTRODUCTION

## Environment, Life and Computational Sciences at Brookhaven National Laboratory

This brochure highlights selected accomplishments in fiscal year 2012 by researchers in environmental, biological, and computational sciences at Brookhaven National Laboratory (BNL). Much of our work involves cross-disciplinary teamwork at BNL and with our partners at other national labs and in academia and industry. 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 (NIH) 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 biological imaging. For our work, we leverage special and often unique capabilities across BNL, and facilities such as the National Synchrotron Light Source (NSLS) and by 2014, the next-generation light source, NSLS-II, the Center for Functional Nanomaterials (CFN), the NASA Space Radiation Laboratory (NSRL), and the Center for Computational Science. FY12 was a productive year for this directorate, and I look forward to sharing future discoveries and advances as they emerge from these disciplines.



**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.

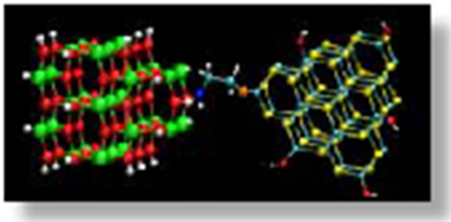
http://www.bnl.gov/cfn/

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

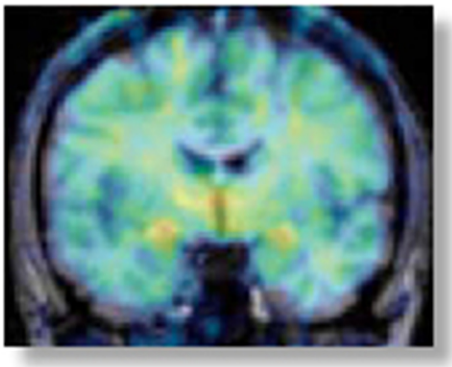
The **NASA Space Radiation Laboratory (NSRL)** at Brookhaven was built through a partnership between NASA and the DOE Office of Science to study the effects of space radiation on biological and physical systems. Scientists use beams of heavy ions provided by a particle accelerator to simulate space radiation 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.

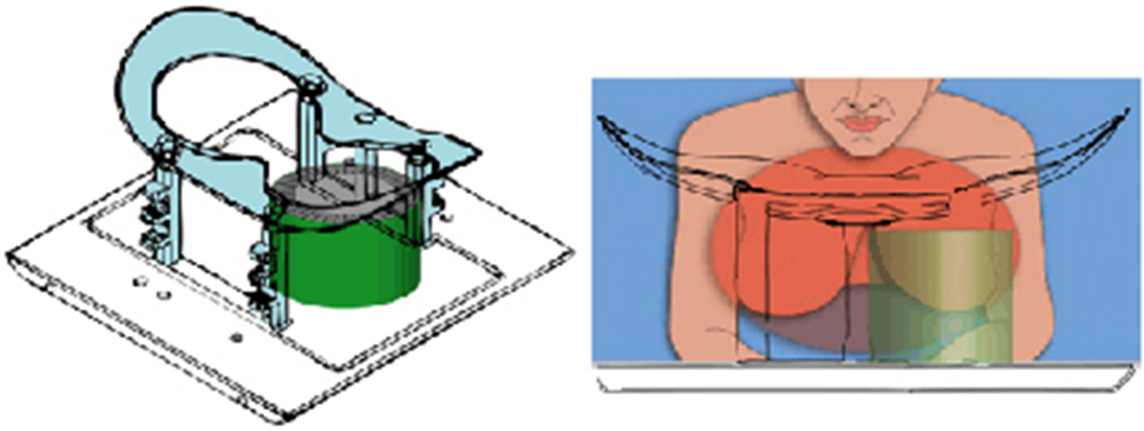
http://www.bnl.gov/csc/



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/

## Combined PET/MRI Breast Scanner Shows Promise



Conceptual drawings of the simultaneous PET/MRI breast imaging system being developed at Brookhaven Lab showing the how the PET insert (green) fits inside the MRI scanner and how it will be used with breast cancer patients.

Recent tests of a device combining positron emission tomography (PET) and magnetic resonance imaging (MRI) to detect breast cancers have shown promising results, including the ability to detect breast lesions smaller than 5 millimeters. Tests of the device — which is under development by researchers at Brookhaven Lab and Aurora Imaging Technology — were conducted at Taipei Medical University in Taiwan.

The technique collects both anatomical and functional information with the same scan, combining the sensitivity of MRI with the selectivity of PET, which could be a very valuable diagnostic tool for detecting very small lesions, and provide the ability to distinguish between malignant and benign growths.

The device is a spin-off of a miniaturized, wearable PET scanner Brookhaven researchers have been developing for imaging brain function in fully awake mice. Brookhaven partnered with Aurora, know for breast imaging technologies, to combine the small-scale PET scanner with MRI technology in a single device.

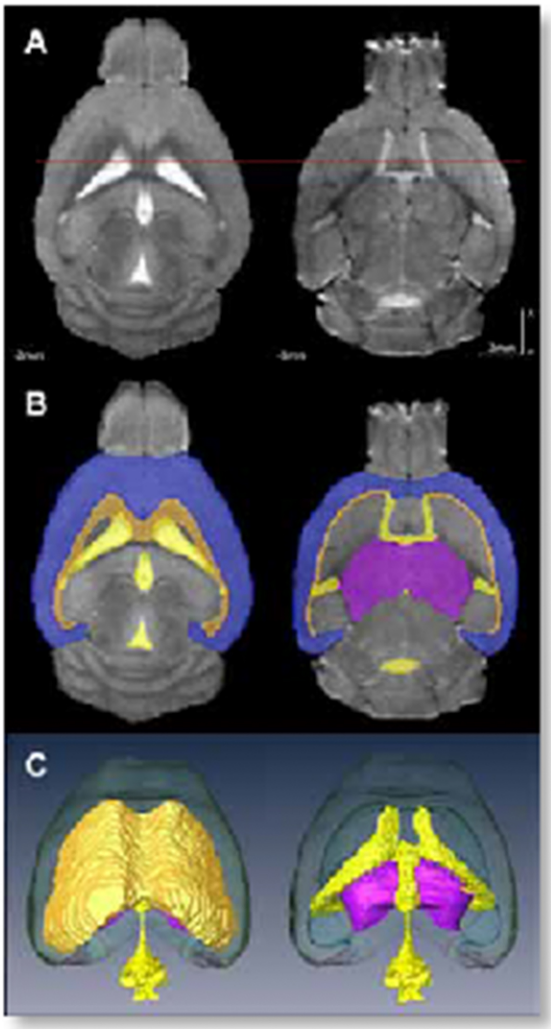
The current design allows a patient to lie facedown on an exam table for an MRI scan with no breast compression as in a mammogram. If the MRI scan detects anything suspicious, the small PET scanner can be brought in right next to and around the breast to produce a simultaneous image of metabolic activity. The technique may help rule out the need for biopsies by being able to distinguish between malignant and benign lesions.

The researchers see the technique as particularly valuable for high-risk patients. It might also be expanded in the future to other clinical applications such as prostate cancer.

The tests in Taiwan were done with a one-ring detector system. Brookhaven and Aurora are currently building and testing a four-ring system that would provide a larger field-of-view and greater sensitivity.

http://www.bnl.gov/newsroom/news.php?a=1975

# Drinking Alcohol Shrinks Critical Brain Regions in Genetically Vulnerable Mice




The scientists used MRI data mapped onto an existing atlas of the mouse brain to compare the effects of drinking ethanol and water on brain volume overall and region-by-region in mice with and without dopamine D2 receptors. Alcohol-drinking mice that lacked dopamine receptors had lower overall brain volume and reduced volume in the cerebral cortex (blue) and thalamus (purple) compared with D2 receptor-deficient mice drinking water. Alcohol-drinking mice with dopamine receptors did not show these deficits in response to drinking alcohol, suggesting that dopamine receptors may be protective against the brain atrophy associated with chronic drinking.

Brain scans of two strains of mice imbibing significant quantities of alcohol reveal serious shrinkage in some brain regions — but only in mice lacking a particular type of receptor for dopamine, the brain's "reward" chemical. The study provides new evidence that these dopamine receptors, known as DRD2, may play a protective role against alcohol-induced brain damage.

The study specifically explored how alcohol consumption affects brain volume — overall and region-by-region — in normal mice and a strain of mice that lack the gene for dopamine D2 receptors. Half of each group drank plain water while the other half drank an ethanol solution for six months.

Magnetic resonance imaging (MRI) scans comparing the groups showed that chronic alcohol drinking induced significant overall brain atrophy and specific shrinkage of the cerebral cortex and thalamus in the mice that lacked dopamine D2 receptors, but not in mice with normal receptor levels.

This pattern of brain damage mimics a unique aspect of brain pathology observed in human alcoholics. In humans, these brain regions are critically important for processing speech, sensory information, and motor signals, and for forming long-term memories.

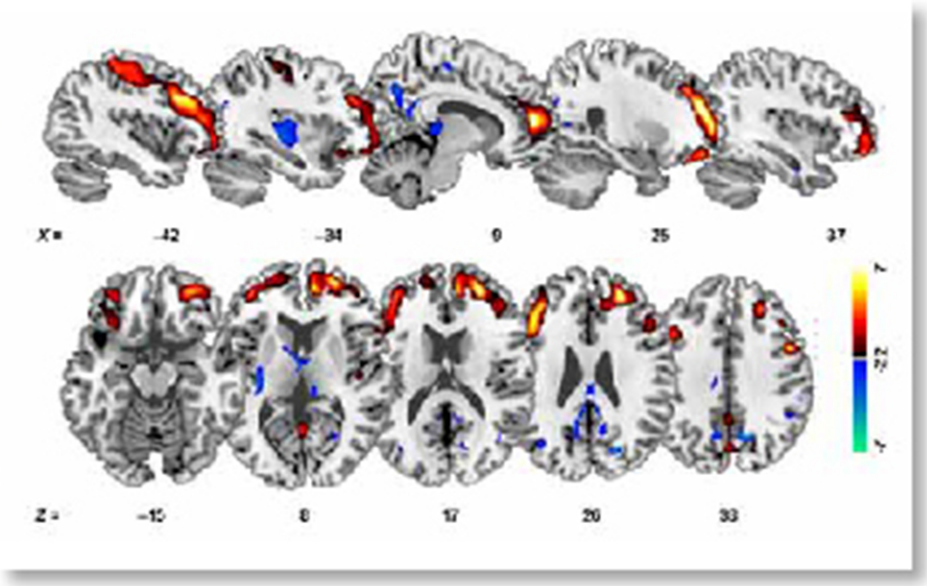
The fact that only mice that lacked dopamine D2 receptors experienced brain damage suggests that DRD2 may be protective against brain atrophy from chronic alcohol exposure. Conversely, the findings imply that lower-than-normal levels of DRD2 may make individuals more vulnerable to the damaging effects of alcohol.

http://www.bnl.gov/newsroom/news.php?a=11383

# Gray Matter in Brain's Control Center Linked to Ability to Process Reward

**The more gray matter you have in the decision-making, thought-processing part of your brain, the better your ability to evaluate rewards and consequences. A new study published in the *Journal of Cognitive Neuroscience* is the first to show this link between structure and function in healthy people — and the impairment of both structure and function in people addicted to cocaine.**

**The study documents for the first time the importance to reward processing of gray matter structural integrity in the parts of the brain's prefrontal cortex that are involved in higher-order executive function, including self-control and decision-making.**




**Differences in gray matter volume — the amount of brain matter made up of nerve cell bodies, as opposed to the "white matter" axons that form the connections between cells — have been observed in a range of neuropsychiatric diseases when compared with healthy states. To explore the structure-function relationship in healthy individuals and in drug-addicted individuals, the scientists performed magnetic resonance imaging (MRI) brain scans. The scans collect structural (brain volume) measurements for the entire brain, and can also be analyzed to get detailed measurements for individual brain regions.**

**Within a short period of the MRI scans, the scientists also used electrodes placed on the research subjects' scalps to measure a particular electrical signal that can index brain activity related to reward processing while the subjects performed a timed psychological task. The scientists used statistical methods to look for correlations between brain activity under various reward conditions and the gray matter volume in different parts of the brain.**

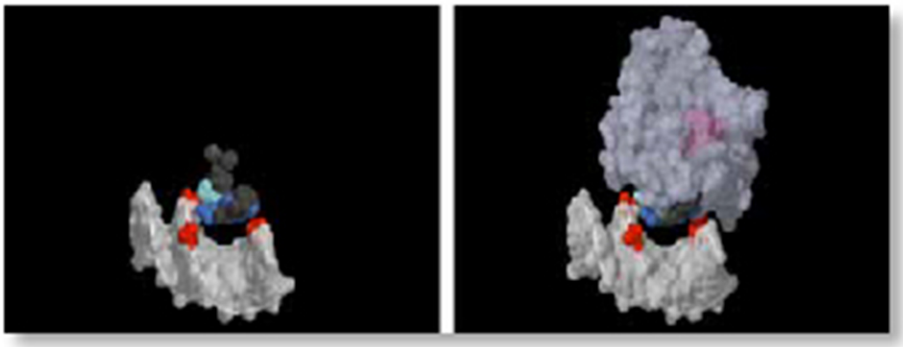
**Their findings suggest that impaired reward processing may be attributed to deficits in the structural integrity of the brain, particularly in prefrontal cortical regions implicated in higher order cognitive and emotional function. The implications are important for understanding the potential loss of control and disadvantageous decision-making that can occur in people suffering from drug addiction, especially in high-risk situations — for example, when craving or under stress — leading individuals to use drugs despite catastrophic consequences. Such multimodal imaging techniques may open new ways to address these and other questions relevant to understanding human motivation in both health and disease states, with particular relevance to treating drug addiction.**

http://www.bnl.gov/newsroom/news.php?a=11355

Structural analysis of the MRI scans was performed using voxel-based morphometry (VBM). VBM is a whole-brain, fully automated, unbiased and operator-independent MRI analysis technique that is commonly used to detect regionally specific differences in brain tissue composition using voxel-wise comparisons. The gray matter tissue probability from each voxel was then correlated with the P300 amplitude difference between the highest monetary reward (45 cents per correct response) and no money (0 cents) conditions of a sustained attention task. The red/orange/yellow highlights on these brain scans indicate the regions where the correlation between gray matter volume and differential P300 response was quite strong in healthy control subjects but weak or nonexistent in cocaine-addicted individuals — the dorso-lateral and ventro-lateral prefrontal cortex, anterior cingulate cortex, and the orbitofrontal cortex, which are known to be functionally involved in reward processing and decision-making. These results suggest that the structural integrity of the prefrontal cortex modulates electrocortical sensitivity to monetary reward. Impairments in these regions may also be related to decreased ability to assess and respond to other modulated rewards and consequences, such as those associated with using addictive drugs.

# Biologists Describe Details of New Mechanism for Molecular Interactions

A group of scientists including Brookhaven Lab biologists has discovered a new mechanism by which two proteins of the human adenovirus use DNA as an efficient form of transportation inside a newly synthesized virus particle. The proteins use what the scientists are calling a "molecular sled," which slides along the DNA double helix—much like a train running along its tracks—to find and interact with other proteins. The research raises the possibility that all proteins in the nucleus of cells interact by sliding along DNA in this fashion.



Model of the "molecular sled" mechanism. Left: The sled (dark gray and blue) sits in a groove on the DNA (white with four phosphate groups colored red). The blue parts of the sled are what interact with and slide along the DNA. Right, the adenovirus protease (light gray) is attached to the sled, with its active site (pink) exposed to interact with other proteins.

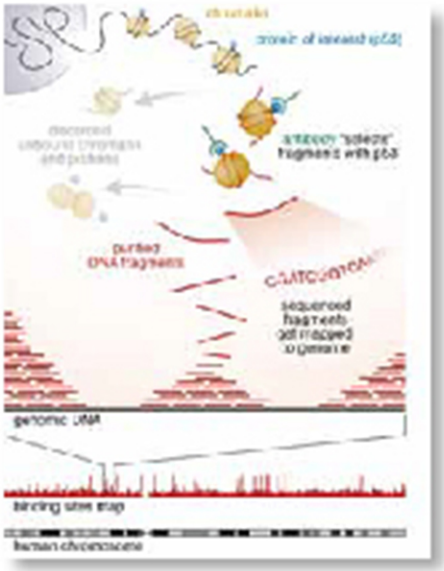
The new mechanism builds of years of exploration that began with the question of how a protease (an enzyme that cleaves other proteins) is involved in the replication of adenoviruses—a virus with features related to many other infectious agents, which may point the way to new treatments.

The interactions of the protease with DNA, first observed in the early 1990s, were a surprise. The recent work describes the process in detail. The simplest, but unprecedented, interpretation of the results was that the protease was sliding on the DNA to look for and cleave its proteins. But the protease alone does not slide. It must first be attached to an 11-amino acid fragment from a different adenovirus protein. Interestingly, the fragment by itself slides on DNA. Could this fragment be a "molecular sled," which can slide along the DNA "track" carrying any cargo, not just the protease?

Proof of this 11-amino-acid fragment acting as a vehicle came when the group attached other proteins to the sled, even ones that by themselves do not bind to DNA, and discovered that those slid too. The concept of the "molecular sled" is the subject of a provisional patent that was just filed with the intent that the idea can be commercialized to deliver desired cargoes (for example, healthy genes for gene therapy).

These first experimental examples of proteins sliding along DNA solely to interact with each other, rather than the DNA, raise the possibility that *all* proteins in the nucleus of cells interact by sliding on DNA. Many proteins that enter the nucleus contain the DNA-binding portion of the sled, lending support to this idea. A protein sliding along the DNA could easily move around the DNA-dense environment within a cell nucleus to find its targets. Such a mechanism might also greatly improve the efficiency of molecular interactions by controlling the alignment and speed of molecular interactions, the researchers said.

http://www.bnl.gov/newsroom/news.php?a=11458




Where proteins bind: Scientists used the "ChIP-seq" technique to identify where p53, an important tumor suppressor protein, binds across the entire genome in normal human cells. After cross-linking the protein to DNA, they split open the cells and used a specific antibody to identify and isolate the chromatin fragments containing the bound protein. Then they purified those DNA fragments and used high-throughput sequencing techniques and computational analysis to map millions of sequenced fragments to the genome. The main finding — that p53 has a different binding pattern in normal human cells compared with that previously observed in cancer cells — may have implications for understanding the suppressor protein's function.

## Tumor-Suppressor Interactions Reveal Key Differences Between Normal and Cancer Cells

**Scientists at Brookhaven and Cold Spring Harbor laboratories investigating the binding patterns of a major tumor-suppressor protein known as p53 with the entire genome in normal human cells have turned up key differences from those observed in cancer cells. The distinct binding patterns reflect differences in the chromatin (the way DNA is packed with proteins), which may be important for understanding the function of the tumor suppressor protein in cancer cells.**

p53 modulates a cell's response to a variety of stresses (nutrient starvation, oxygen level changes, DNA damage caused by chemicals or radiation) by binding to DNA and regulating the expression of an extensive network of genes. Depending on the level of DNA damage, it can activate DNA repair, stop the cells from multiplying, or cause them to self-destruct — all of which can potentially prevent or stop tumor development. Malfunctioning p53 is a hallmark of human cancers.

Most early studies of p53 binding explored its interactions with isolated individual genes, and all whole-genome studies to date have been conducted in cancer-derived cells. This was the first study to present a high-resolution genome-wide p53-binding map for normal human cells, and to correlate those findings with the "epigenetic landscape" of the genome, including a published high-resolution map of DNA methylation — one of the most important epigenetic modifications to DNA.

In the normal cells, p53 binding sites were located in close proximity to genes and particularly at transcription start sites. In earlier studies of cancer-derived cell lines, p53 binding sites were *not* close to genes and transcription start sites.

Additionally, nearly half of the newly identified p53 binding sites in the normal cells (in contrast to about five percent of the sites reported in cancer cells) reside in under-methylated portions of the genome known as CpG islands.

This is important because, during cancer development, many CpG islands are subjected to extensive methylation while the bulk of the genomic DNA contains fewer methyl groups than normal. These major epigenetic changes may contribute to the differences observed in the p53-binding-sites' distribution in normal and cancer cells.

http://www.bnl.gov/newsroom/news.php?a=11351

# Chemistry Building at Brookhaven Lab Named Historic Chemical Landmark

On Friday, October 19, 2012, the New York Section of the American Chemical Society (ACS) designated the Chemistry Building at the U.S. Department of Energy's Brookhaven National Laboratory as an Historic Chemical Landmark in recognition of the synthesis of $^{18}$FDG, a radiotracer that has had a revolutionary and global impact on cancer diagnosis and management and brain research. Originally synthesized at Brookhaven Lab in 1976 for positron emission tomography (PET) scanning, $^{18}$FDG is now the world's most widely used radiotracer for cancer diagnosis, with more than 1.5 million $^{18}$FDG PET scans performed annually.

BNL chemist Joanna Fowler with an early $^{18}$FDG synthesis apparatus.

The development of $^{18}$FDG is a testament to one of the key strengths of the national laboratories, which bring together scientists from a range of disciplines in an environment that fosters collaborative approaches to address some of our nation's toughest challenges. The achievement drew on BNL expertise in organic synthesis and radiochemistry, input from other chemists, physicists, and engineers, as well as external collaborators at the National Institutes of Health (NIH) and the University of Pennsylvania.

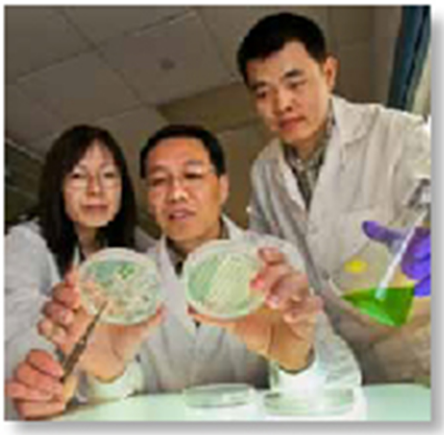
Attaching a radioactive fluorine-18 tag to deoxyglucose — a molecule closely related to glucose, the body's main source of energy — gave scientists a way to track this energy source's location and concentration in the body. The synthesis was tricky and had to be accomplished in a short period of time so the $^{18}$FDG molecules could be transported from Brookhaven to Philadelphia, where the first scanner capable of mapping brain glucose metabolism in humans was located and before the radioactive signal disappeared.

By using positron emission tomography (PET) scanners to track $^{18}$FDG over time, scientists can monitor site-specific metabolic activity under a variety of conditions. This groundbreaking technique opened a window to the exploration of a wide range of diseases and conditions, including drug addiction, eating disorders, attention deficit hyperactivity disorder (ADHD), neurodegenerative diseases such as Alzheimer's, epilepsy, and coronary artery disease. $^{18}$FDG PET imaging has also emerged as a revolutionary tool for cancer diagnosis and treatment, by picking out tumors as "hot spots" of high metabolic activity that stand out from surrounding healthy tissue, even before anatomical changes are detected, and helping to monitor patients' response to treatment.

http://www.bnl.gov/newsroom/news.php?a=11461

# New Strategies for Using Plants, Algae for Energy

*With expertise in plant biology, chemistry, computational modeling, environmental interactions, and biofuel conversions, Brookhaven scientists are exploring new ways to engineer Nature's green factories to efficiently store and release energy. Their research explores how plants and other organisms such as algae accumulate biomass, oils, and other products, and how to influence and optimize these processes. Some recent examples:*



Brookhaven researchers Jilian Fan, Changcheng Xu, and Chengshi Yan with cultures of algae that were shown to increase oil production in response to excess carbon.

## Carbon gets algae to pump out more oil

Algae could be an excellent resource for producing raw materials for alternative fuels. They grow very quickly and efficiently convert carbon dioxide into carbon-chain molecules like starch and oils. But they have a "preference" for starch production. Starving the algae of certain key nutrients could tip the balance in favor of oil, but the algae would stop growing.

A team of Brookhaven scientists set out to learn all they could about oil production in algae, including the factors that control metabolic switching between starch and oil. By growing the microbes under a variety of nutrient conditions, with and without inhibitors of certain biochemical pathways, and studying a mutant strain that lacks the capacity to make starch, the scientists learned why carbon preferentially partitions into starch rather than oil, and how to affect the process.

The main finding was that feeding the algae more carbon (in the form of acetate) quickly maxed out the production of starch to the point that any additional carbon was channeled into high-gear oil production. And, most significantly, under the excess carbon condition and *without* nutrient deprivation, the microbes kept growing while producing oil. The researchers hope to use what they've learned to increase the yield of commercial algal strains for the production of raw materials for biofuels.

http://www.bnl.gov/newsroom/news.php?a=11424

Jordan Hay and Jörg Schwender are modeling plant metabolism to improve oil production.

## Model IDs potential pathways for increasing oil output

A computational model developed at Brookhaven to incorporate detailed information about plants' interconnected metabolic processes has recently helped its designers identify key pathways that appear to "favor" the production of either oils or proteins. The research may point the way to new strategies to tip the balance and increase plant oil production.

The model incorporates 572 biochemical reactions that play a role in rapeseed plants' central metabolism and/or seed oil production, as well as information on how those reactions are grouped together, are organized in subcellular compartments, and how they interact. Using it the researchers identified which metabolic pathways are likely to increase in activity—and which have to decrease—to convert a "low-oil" seed into a "high-oil" seed. The results narrowed down the large list of enzyme reactions to a relatively few possible targets for future genetic manipulation to tip the balance in favor of greater seed oil production.

http://www.bnl.gov/newsroom/news.php?a=11457

Former Brookhaven postdoc Carl Andre and Brookhaven biochemist John Shanklin.

## Identifying 'stop' signal suggests ways to increase oil production

Biochemical feedback loops regulate a wide range of metabolic processes — similar to the way a thermostat turns a home heating system off and on as the temperature rises and falls. Brookhaven biochemists have just identified such a biochemical feedback system for plant oil production — how plants "know" when they've made enough oil and how they slow down production. Now that they understand how this system operates, they can look for ways to break the feedback loop to get plants to make more oil.

The scientists performed their biochemical tests using a plant embryo cell culture. With assistance from the Radiotracer Chemistry and Biological Imaging group at Brookhaven, the team synthesized "labeled" forms of the fatty acids that occur as intermediates along the metabolic pathway that leads to oil production, and step-by-step tested to see which added intermediates would inhibit oil production.

Through this painstaking process, they identified the key intermediate that puts the brakes on oil production — a molecule produced fairly late in the production process that, when accumulated, inhibits an enzyme at the very first step.

The team is now exploring biochemical schemes to keep the "slow-down" signaling metabolite from accumulating, ways to block its effects on the enzyme, and more. If they can interrupt the feedback signaling, they might trick the cells into making more oil.

http://www.bnl.gov/newsroom/news.php?a=11418

Kewei Zhang and C.J. Liu are exploring ways to make plants easier to convert to biofuels.

## Engineered enzyme alters cell wall composition

Looking for ways to make plants easier to convert to biofuels, Brookhaven scientists have engineered an enzyme that effectively reduces the amount of lignin in plant cell walls. Today's industrial processing methods require cell wall biomass to be pretreated to remove lignin, which significantly adds to the cost of biofuel production. Incorporating the new enzyme into plants could substantially reduce the cost of that step.

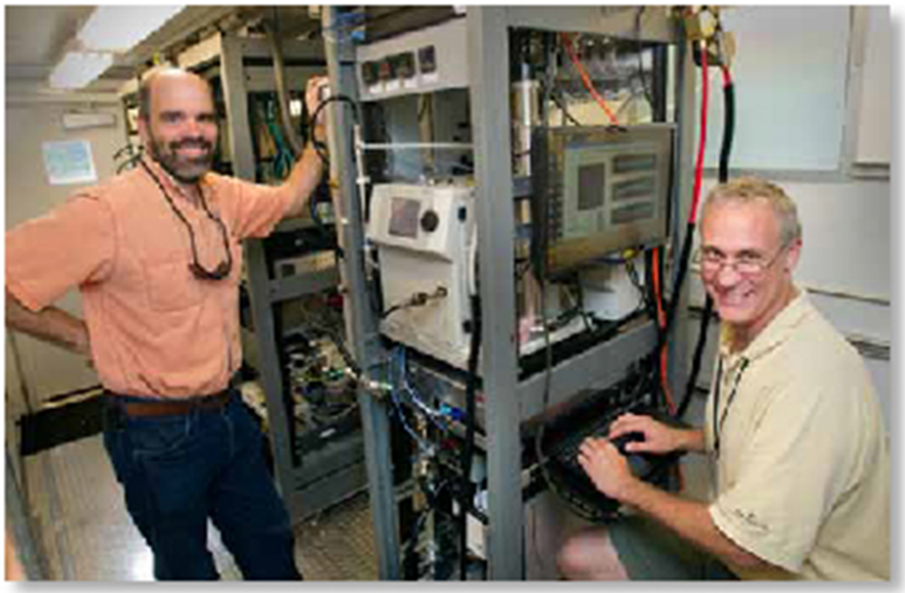
The new enzyme modifies lignin precursors so they can't link up to form the lignin polymer. The first version worked well in the lab, but not in plants. By using Brookhaven's National Synchrotron Light Source to determine the enzyme's x-ray crystal structure, the scientists were able to identify additional tweaks in the amino acid sequence that did the trick. The new enzyme reduced the lignin content of the test plants by up to 24 percent, leading to a 21 percent increase in the release of cell wall sugars. Furthermore, it did so without compromising the plant's development or significantly reducing the biomass yield.

The next step is to test the enzyme's function in poplar trees or other DOE-dedicated energy crops.

http://www.bnl.gov/newsroom/news.php?a=11439

## Built-To-Go Aerosol Observing Laboratories: Just Add Power and Internet

Aerosol Chemical Speciation Monitor modified for installation in shock-mounted rack of MAOS-A



Stephen Springston and Art Sedlacek at system console

AMF2 AOS on a mountain at Steamboat Springs, CO

Remote accessible screen with common user GUI

**Brookhaven Lab researchers have completed construction of four mobile Aerosol Observing Systems for the Department of Energy's (DOE) Atmospheric Radiation Measurement (ARM) program, and two more are on the way. These units — shipping containers filled with more than twenty commercial and laboratory-built instrument systems for measuring atmospheric aerosols and their precursors — can be deployed around the world for on-location sampling. Built with funds from the American Recovery and Reinvestment Act (ARRA), each unit is self-contained with redundant data acquisition, a 10-meter sampling tower, shock-mounted instrument racks, and climate-control systems sufficient for operation in extreme environments. A custom, Brookhaven-designed Graphical User Interface (GUI) gives a common look and feel to the wide range of instruments, which greatly facilitates on-site staff training and operations. Only one or two technicians are required for running even the more advanced instruments, and on-site set up can be done in half a day. Brookhaven provides intensive technical support for field campaigns. Remote monitoring and control allows mentors to supervise multiple units deployed globally. Since 2010, the units have participated in six campaigns ranging in duration from two to nine months at locations from snowy mountaintops to the rolling deck of a cargo ship. Data collected will help improve understanding of aerosols' effects on weather and climate.**

# Understanding Ecosystem-Climate Feedback in the Arctic

Measuring CO2 uptake, Barrow, AK

When it comes to projecting our future climate, understanding the response of high latitude ecosystems is essential. The Arctic is globally important and climatically sensitive. As the permafrost thaws in response to rising temperature, carbon dioxide ($CO_2$) released from the huge reserves of frozen organic carbon has the potential to dramatically increase the rate of climate change. However, the processes that govern the carbon cycle at high latitudes are understudied and poorly represented in Earth System Models.

Brookhaven researchers are participating in one of a coordinated set of investigations that target improved process understanding and model representation of important ecosystem-climate feedbacks in the Arctic. Their research on the processes and interactions that take place within Arctic terrestrial ecosystems will improve how these variables and interactions are represented in climate models, and increase our confidence in climate projections for high-latitude regions of the world.

The work is part of a new multidisciplinary project, Next Generation Ecosystem Experiments – Arctic, which involves more than fifty scientists from eight institutions, and is aimed at improving the representation of the Arctic in Earth System Models. Researchers in Brookhaven's Environmental Sciences Department have begun to characterize the variables that influence photosynthesis and the uptake of nutrients such as nitrogen by Arctic plants. Data collected in Barrow, Alaska, during the first field season of this project show that current models greatly underestimate the potential for plants to take up $CO_2$ through photosynthesis. These new measurements will be used to update and improve the models.

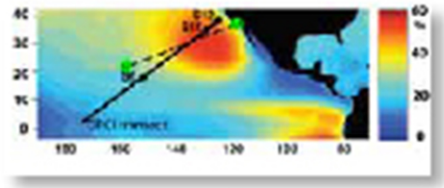
http://ngee.ornl.gov/

# Yearlong MAGIC Climate Study Launches

The Horizon Spirit makes the round trip between Los Angeles and Hawaii every two weeks.

Brookhaven scientist Ernie Lewis and one of the mobile SeaTainer units now installed aboard the Horizon Spirit, a 272-meter cargo ship that will take atmospheric measurements during a yearlong cloud/climate study.


A radar unit being installed on Horizon Spirit.



Horizon Spirit's route from Los Angeles to Hawaii (dashed line) lies adjacent to the GPCI transect that is used to compare climate models (solid line), which also contains specific locations used for other modeling efforts (labeled points). The color scale representing the annual average percentage of low-level cloud cover over the region shows that the route is ideal for assessing the effects of changing cloud conditions.

A Horizon Lines container ship outfitted with meteorological and atmospheric instruments installed by Department of Energy (DOE) national laboratory scientists from Argonne and Brookhaven began taking data in October 2012 for a yearlong mission aimed at improving the representation of clouds in climate models. The study, a collaborative effort between DOE's Atmospheric Radiation Measurement (ARM) Climate Research Facility and Horizon Lines, marks the first official marine deployment of the second ARM Mobile Facility, AMF2, and is likely the most elaborate climate study ever mounted aboard a commercial vessel.

The Horizon *Spirit* makes a roundtrip journey from Los Angeles to Hawaii every two weeks, which allows for repeated measurements over the same transect at different seasons. Collecting data on a wide range of atmospheric conditions over an entire year, including the transitions among cloud types along this particular route, will give the scientists a large amount of data to help refine and validate models of Earth's climate.

The project—dubbed MAGIC, for the Marine ARM GPCI Investigation of Clouds, where GPCI is a project comparing results from major climate models—will take place through September 2013. It will focus on factors that affect low marine boundary layer clouds over the ocean, which exert a large influence on Earth's climate through reflection of sunlight and by mediating interactions between the atmosphere and the ocean.

Instruments housed mainly in three 20-foot cargo containers outfitted for marine deployment—including one designed, built, and outfitted at Brookhaven—will monitor properties of clouds and precipitation, aerosols, atmospheric radiation, other standard meteorological variables, and atmospheric structure (with weather balloon launches four times daily). The data will be used by several global-modeling groups, and are expected to greatly enhance understanding of clouds, aerosols, Earth's energy and water balance, and the interactions among them in the marine environment—which should improve the representation of these variables and reduce uncertainties in global climate models.

http://www.bnl.gov/newsroom/news.php?a=11455

100 new BATSII samplers being readied for Tracer Technology Group field testing

# New generation, state-of-the-art, Brookhaven Atmospheric Tracer Samplers

How do pollutants move through different kinds of environments? How far would toxic chemicals released in a terror attack travel? These are the kinds of questions that have motivated "atmospheric dispersion studies" of the Tracer Technology Group (TTG) within Brookhaven's Environmental Sciences department for more than 30 years.

Using unique techniques for analyzing harmless perfluorocarbon tracers (PFTs), scientists can track air movement over regions measuring mere meters to hundreds of kilometers to:

Checking operation of the new Brookhaven Atmospheric Tracer Samplers (BATS II)

- track the long range transport of pollutants, such as coal-fired power plant emissions
- monitor residential air quality and energy efficiency
- model the transport of toxic materials in urban environments and other issues relevant to homeland security, such as building vulnerabilities
- identify leaks in gas lines and dielectric power lines
- monitor air in nuclear power plant control rooms

The group recently overhauled and upgraded their programmable air samplers—the Brookhaven Atmospheric Tracer Sampler (BATS) system, developed at the Lab more than 30 years ago—to improve sampling flexibility, accuracy, and reliability. 100 of the new, state-of-the-art tools, dubbed BATS II, are now ready for their first deployment in a large urban dispersion study.

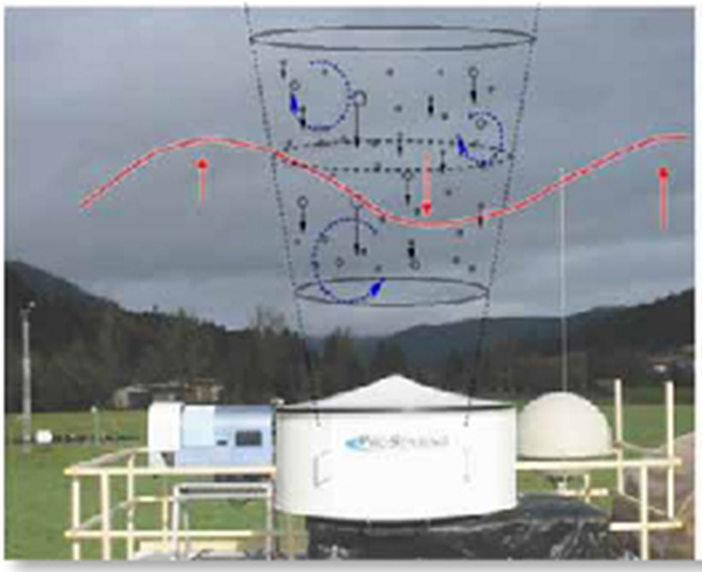
The compact BATS II devices now include WiFi, GPS, flow rate monitoring, on-the-fly flow control, data logging, and low power electronics and peripherals. This newest version uses a single board computer and is capable of taking air samples at pre-programmed dates and times, varying flow rates, and varying sample intervals from seconds to hours and more. Each sampler can accommodate up to 24 capillary adsorption tubes (CATS) optimized for PFT sampling.

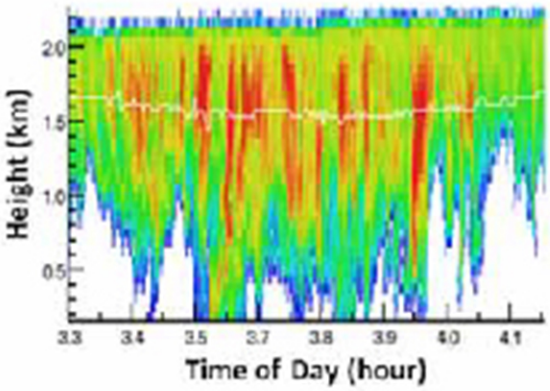
Environmental scientists complete final testing of new BATS II samplers.

This flexibility allows samples to be taken more frequently initially with lower frequency over time, as tracers decay and concentrations diminish, resulting in a better understanding of the rise and decay rates of tracer concentrations and the ability to extend overall monitoring periods.

WiFi enables changes in programming after deployment—for example, to adapt to unexpected weather conditions, rather than postponing a study—without having to remove samplers from difficult-to-reach locations (e.g., high on rooftops). WiFi also allows rapid and reliable programming prior to testing and easy checking in the field. GPS marks deployment location, and also serves for time synchronization, allowing all samplers to be precisely activated simultaneously (within less than half a second).

## Advanced Targeted Cloud Science






Innovative techniques, made possible by new, state-of-the-art cloud radar systems, enable a novel look at the inner workings of cloud processes.

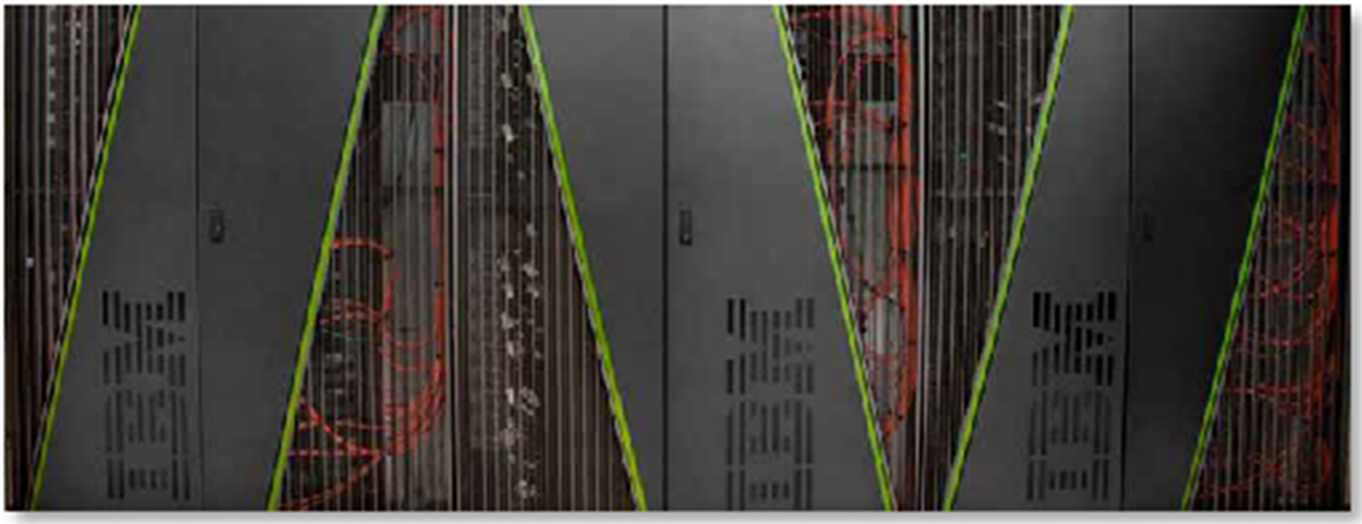
New eyes lead to new discoveries — this is the central tenet of Brookhaven Lab's effort aimed at improving the representation of cloud properties and processes in climate models, known as Advanced TArgeted Cloud Science, or ATACS.

The "Advanced" within ATACS is made practical by observations from new Department of Energy (DOE) Atmospheric Radiation Measurement (ARM) instruments such as dual-band radars — installed with funding from the American Recovery and Reinvestment Act — that are used with newly developed innovative analyses to study important cloud-related phenomena in unprecedented detail.

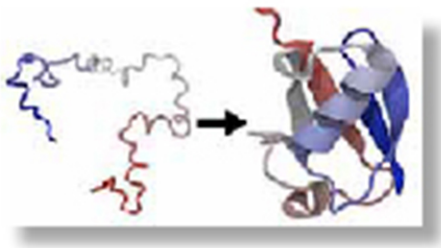
"TArgeted" refers to the marriage of these observations with theory and modeling, such that they are woven together to work in concert and inform each other for maximum benefit to target processes that are most important to the improvement of the models. This marriage distinguishes ATACS from approaches typically used within this research community, which usually treat observations and models as separate entities with observations used merely to compare with the models.

At the heart of ATACS is Brookhaven's long-standing core expertise in remote sensing technique development (particularly with multiple types of cloud radars), cloud process analysis, theoretical development, and the infusion of these data and theory into climate models.

# Brookhaven Lab Installs Blue Gene/Q Supercomputer



The above is an image of the Blue Gene/Q computer at BNL



Different molecular forces cause proteins to fold into unique, complex shapes. Supercomputers like the BNL Blue Gene/Q and the Cray XK6 system Titan at Oak Ridge National Laboratory allow researchers to calculate such shapes and determine molecular properties with important applications to Bioscience. (Image courtesy of Justin MacCallum, Stony Brook University)

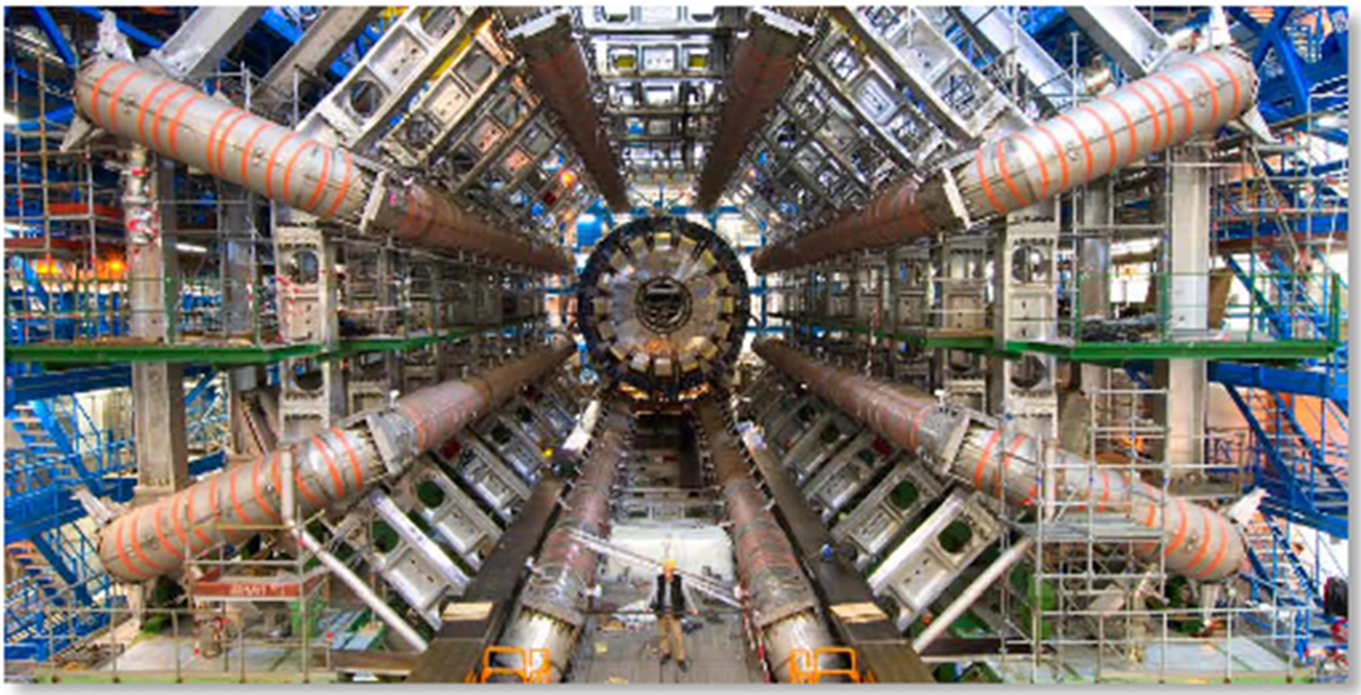
Brookhaven Lab now hosts one of the world's most powerful supercomputers, IBM's Blue Gene/Q. This latest version in the IBM supercomputer series adds 600 teraflops, or floating operations per second, of processing power to the Lab. The three racks of the new Blue Gene/Q can complete six times as many operations as the 18 racks of Blue Gene/L that was previously installed. The system consists of two racks for the RIKEN BNL Research Center (RBRC) operated with Japan, and a third belonging exclusively to Brookhaven and run by the Computational Science Center (CSC).

The new system will be unleashed to push the boundaries of data intensive applications associated with Brookhaven Lab's Relativistic Heavy Ion Collider, Center for Functional Nanomaterials, the upcoming National Synchrotron Light Source II, and CERN's Large Hadron Collider.

Blue Gene/Q excels at critical data-intensive processes because of its leading energy efficiency and system density, placing it on the top of the Green 500 list of the world's most energy efficient computer rated by flops per watt. Each of Brookhaven's three racks has 1,024 computational nodes and 16,384 cores, or individual processing units that read and execute programs. These cores are linked by an advanced interconnect system that allows data to flow with limited bottlenecks when handling data intensive tasks.

Brookhaven Lab was one of the first customers to acquire Blue Gene/Q, and its three high-performing racks are actually pre-production hardware. As such, the primary challenge of the installation was the successful assembly and configuration of such a complex computer without the benefit of IBM support nor official documentation. Lab engineers overcame these challenges and the system went into operation in the spring of 2012. At that time, the staff successfully configured and ran the Graph 500 benchmark for data-intensive calculations, earning fifth place honors in the June 2012 global ranking.

## PanDA: Next Generation Workload Management and Analysis System for 'Big Data'



ATLAS detector

This year, the Department of Energy's Office of Advanced Scientific Computing Research provided funding to Brookhaven Lab and collaborators to develop a universal version of a "workload management system" that was originally built to process huge volumes of data from high-energy physics research. The new project could expand the use of the Production and Distributed Analysis System (PanDA) to other areas of science that rely on "big data," including medicine, astrophysics, and more.

Originally funded by the National Science Foundation and DOE, PanDA uses 250,000 central processing unit (CPU) cores to process data from the ATLAS experiment at the Large Hadron Collider in Geneva, Switzerland. The computing hardware associated with ATLAS is located at 100 computing centers around the world that manage more than 50 petabytes, or 50 million gigabytes, of data. PanDA links the computing centers and allows scientists to efficiently analyze the tens of millions of particle collisions taking place at ATLAS each day.

PanDA was cited as an example of a successful technology already in place during a recent White House announcement of its "Big Data Research and Development Initiative," a $200 million investment in tools to handle huge volumes of digital data needed to spur science and engineering discoveries. Expanding PanDA's use could help bolster science and engineering research in a wide range of fields.

http://www.bnl.gov/newsroom/news.php?a=11451

# New Smart Grid: Enhanced Power System Operation and Control

Northeastern Power Grid

Brookhaven Lab computational scientists are embarking on a new collaborative project with the State University of New York (SUNY) and the New York Power Authority (NYPA) to improve the performance of New York State's electricity transmission grid. This is one step toward the ultimate goal of developing a "smarter" grid—one that will automatically respond to changes in generation and load profiles and provide more efficient electricity delivery.

The computational project will use advanced numerical algorithms and high performance computing for solving power-flow, state-estimation, and system-stability control problems. These efforts will make use of extensive data collected by emerging Smart Grid technologies, including telecommunication networks and a new generation of sensors, such as phase measurement units (PMUs), to assist in grid-control decisions.

The main objective is to investigate how these problems can be solved 10 to 100 times faster than currently possible by using recent algorithmic and software developments for parallel supercomputers, and software packages optimized for massively multi-core supercomputing facilities. These new computational methods are now being applied and tested on data provided by NYPA.

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

# AWARD HIGHLIGHTS

**Nelly Alia-Klein**, a clinical psychologist with expertise in forensic psychology and neuroimaging, was named Woman of the Year in Medicine by the *Village Beacon Record* newspaper of Long Island. Her research focuses on understanding the neurological mechanisms that underlie aggression and violent behavior. The award recognizes her creative approach to tackling a major public health issue that is tough to study and that could improve many lives.

**F. William Studier**, a Brookhaven biologist credited with developing the Lab's most successful technology—the T7 protein expression system used by researchers around the world to produce proteins for basic biomedical research and applications including medical diagnosis and treatment—received recognition from Brookhaven Town for two recent patents. These patents describe methods to simplify the production of target proteins in the T7 expression system, increase the amounts of protein produced in a given volume of culture, enable convenient production of many different proteins in parallel, and improve overall reliability.

**Rita Z. Goldstein** of Brookhaven's Biosciences Department has won the Joel Elkes Research Award for her work on how drugs affect the brain and behavior. The award is given annually by the American College of Neuropsychopharmacology to a scientist 50 years of age or younger to recognize outstanding clinical contribution to the field. Goldstein was selected for her research advancing understanding of self-regulatory processes, or one's ability to control and evaluate their actions, as they affect mental function and behavior in both healthy individuals and those suffering from disease, particularly drug addiction.

**Arokiasamy J. (A.J.) Francis**, a Scientist Emeritus in the Environmental Sciences Department, was recognized with an award for outstanding service as an online mentor of the American Society for Microbiology Minority Mentoring Program. During his nearly 37 years at Brookhaven, he has concentrated on the realm of microbial interactions with organic and inorganic contaminants—and their remediation. Francis' investigations have ranged from nitrogen cycling and the control of nitrate pollution to the transformation of radioactive contaminants in the environment. The award recognizes his contributions guiding graduate students, post-docs, and research staff scientists on: the remediation of uranium, strontium, and cesium contaminated soils and water; the influence of ionic liquids on biotransformation of uranium; biodegradation of organic compounds in nuclear wastes; and microbial gas generation from low- and intermediate-level radioactive wastes.

**Chang-Jun Liu**, a Brookhaven plant biologist, was granted tenure for his creative original research elucidating the molecular mechanisms by which plant cell-wall components are synthesized and transported, and using that knowledge to manipulate cell-wall structures and properties with the aim of improving the efficiency of converting plant biomass to energy.

**Chongai Kuang**, a Brookhaven Lab environmental scientist, received the 2012 Sheldon K. Friedlander Award from the American Association of Aerosol Research (AAAR), in recognition of his doctoral dissertation on the formation of aerosol particles in the atmosphere. Kuang's 2009 thesis, "Atmospheric Nucleation: Measurements, Mechanisms, and Dynamics," was chosen for its combination of "elegant, theoretical descriptions of key processes with much needed observational constraints." The AAAR cited Kuang, who conducts comprehensive studies of aerosol particle formation and develops predictive models and measurement techniques, as one of the most accomplished and talented aerosol scientists in the world.

**Laurie Gregory**, a data system engineer in the Environmental Sciences Department, earned a Distinguished Alumni Award from Stony Brook University for her work on the design, development, and operation of the External Data Center for the Department of Energy's Atmospheric Radiation Measurement (ARM) Climate Research Facility. She has experience with data acquisition and analysis of surface, model, and satellite data, which is used to augment data generated within ARM. In recent years, she has also taken on the responsibilities of ARM instrument mentor, overseeing and coordinating instrument calibration, data quality, maintenance, upgrades, troubleshooting, deployment, and instrument development.

**Allen Orville**, a biophysicist, was awarded tenure for his creative, original work in integrating several research techniques to understand how specific enzymes affect biochemical reactions involved in metabolism, light emission, photosynthesis, and DNA repair. His creative original research makes use of physical-biochemical, spectroscopic, crystallographic, and mathematical modeling techniques.