Creating Opportunity

UT-ORNL Science Alliance

July 1, 2010–June 30, 2011

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Science Alliance Span of Operation
July 1984–2011

Cover photo of switchgrass plots along the Tennessee River by Jack Rose.

2011 JDRD Projects

First-Year Awards

Gajanan Bhat, *Materials Science and Engineering,* Monolayer polymeric coatings to enhance the performance and service life of membranes for high temperature biomass pretreatment (Nanoporous inorganic membranes for selective separations in high temperature flow-through recycle pretreatment of lignocellulosic biomass, Ramesh Bhave)*

Qing Cao, *Electrical Engineering and Computer Science,* Distributed computational framework for massive heterogeneous data fusion: a location-centric approach (Distributed computational framework for massive heterogeneous data fusion, James Horey)

Shane Foister, *Chemistry,* Catalytic degradation of lignin to low molecular weight organics (Biomass production and conversion for energy and materials, Wei Wang and Tommy Phelps)

Jens Gregor, *Electrical Engineering and Computer Science*, Iterative image reconstruction for neutron tomography (Neutron imaging of fluids within plant-soil-groundwater systems, Hassina Z. Bilheux)

Lee Han, *Civil and Environmental Engineering,* Distributed computation framework for faster-than-real-time microscopic traffic simulation (Distributed computational framework for massive heterogeneous data fusion, James Horey)

Qiang He, *Civil and Environmental Engineering,* Lignocellulose bioconversion in anaerobic digestion, as a unique model (Harnessing nitrogen and sulfur cycles to develop microbial consortia for consolidated bioprocessing, David Graham)

David Jenkins, *Chemistry,* Well-defined tetra-carbene complexes for metal deposition in zeolites for catalytic alcohol production (Novel zeolitic carbon support for catalytic bioethanol production, De-en Jiang and Sheng Dai)

Shih-Lung Shaw, *Geography,* Integration of space-time GIS with climate informatics for climate change research (Enhancing climate impact integrated assessment for water through climate informatics, William Lenhardt)

Second-Year Awards

Paul Crilly and Seddik Djouadi, *Electrical Engineering and Computer Science*, Integrated navigation system for GPS-denied environments (LDRD title same as above, Stephen Smith)

Joshua Fu, *Civil and Environmental Engineering,* Downscaling of global chemistry and climate predictions: regional analysis and local impacts (Real-time simulation of power grid disruptions, Steven Fernandez)

Ivan Maldonado, *Nuclear Engineering,* Revolutionary radiation transport for next-generation predictive multi-physics modeling and simulation (LDRD title same as above, John C. Wagner)

Stephen Paddison, *Chemical and Biomolecular Engineering, Ab initio* studies of Li+ mobility in solid electrolytes and their interfaces (Tough electrolytes for batteries—composites inspired by nature, Nancy Dudney)

Edmund Perfect, *Earth and Planetary Sciences,* Neutron imaging of fluids in rocks and soils (Neutron imaging of fluids within plant-soil-groundwater systems, Hassina Z. Bilheux)

Mingjun Zhang, *Mechanical, Aerospace, and Biomedical Engineering,* A nature-derived nanoparticle and nanofiber-based scaffold for enhancing chemical detection and imaging (Standoff detection and imaging of chemicals, Ali Passian)

*ORNL Laboratory Directed Research and Development (LDRD) project titles and principal investigators listed inside parentheses.

Today's scientists and engineers pursue a path of discovery and investigation that builds upon their own expertise while engaging in the cross-disciplinary collaborations so necessary to addressing today's critical issues. The working teams formed of JDRD- and LDRD-sponsored research constitute a source of on-the-job training for students as well as access to advanced computation and instrumentation, clearly fulfilling several of the Science Alliance's stated goals. From these relatively small grants at an exploratory level, researchers will go on to seek funding for larger and more ambitious projects.

Photo by Jack Rose

Joint Directed Research and Development

by Laura Buenning and Theresa Pepin

The Science Alliance has a history of support for research exploring new approaches to significant questions. In 2010-2011, the topics pursued by JDRD researchers have coalesced in a striking fashion under the headings of two such questions:

Can we GROW new and better sources of fuel?

Can we USE data to improve understanding and decision-making?

Extracting and consuming carbon from the earth is more and more fraught with seriously harmful consequences.

Can we GROW new and better solutions?

Lignocellulosic biomass—the technical phrase used for plant and plant-derived material—has enormous potential, not just as a sustainable feedstock for bioethanol, but also for other transportation fuels, chemical precursors for industrial products, and power production.[1] Furthermore, cellulosic ethanol can be made from a wide variety of plants, including switchgrass, leaves, and poplar chips, which can be grown on land that would otherwise be considered too poor for profitable crops.[2]

Still, ethanol—the first major instance of a widely produced, lignocellulosic biomass fuel—is a controversial commodity. First, there's the whole question of subsidies. And then, there's the uncertainty about ethanol's energy value versus its production costs. Meanwhile, owners of motorcycles, boats, lawn mowers, and weed eaters worry that smaller or older engines cannot be adapted to the new ethanol additives. Car and truck drivers doubt that lower prices at the pump will offset ethanol's decreased miles per gallon. Bloggers discuss the comparative energy gain or loss during production of ethanol versus gasoline. Others ask us to consider the food versus fuel dilemma before diverting farmland from food to biofuel production.

Amidst the debate, it's easy to overlook the basic motivation to explore plants as energy resources—to find renewable, alternative solutions to our increasing demand for oil and natural gas and in the process create a carbon-neutral economy.

Both UT and ORNL have strong programs exploring a biobased economy, including bioenergy, biofuel production and the development of new chemicals and materials from renewable biomass resources. In February 2011, the UT Institute of Agriculture opened a Bioenergy Science and Technology Laboratory in their new Center for Renewable Carbon (CRC). ORNL has managed the DOE BioEnergy Science Center (BESC) housed in the UT-ORNL Joint Institute for Biological Sciences since January 2008. The Science Alliance also creates opportunity for new UT-ORNL teams working in this important area of research.

Photo by Jack Rose

Growing Green

Most ethanol today comes from sugar, starch, and oil-seed based feedstocks. In the United States that means fermented corn kernels—but not the stalks and leaves.

"In theory, all biomass can be turned into syngas (synthesis gas)—a mixture of carbon monoxide and hydrogen," says JDRD team leader ***David Jenkins***. "Our trick is to turn the carbon monoxide and hydrogen into ethanol."

Currently, two major pathways for converting lignocellulosic biomass to ethanol exist: biochemical and thermochemical.[3]

A key challenge to thermochemical conversion of biomass-derived syngas is controlling the catalytic transformation so your process selects the product you want in sufficient quantities to make it worth the cost of production, Jenkins says.

Jenkins and postdoctoral associate Zheng Lu have paired with De-en Jiang and Sheng Dai of ORNL, whose LDRD project builds on a new process for synthesizing charged carbon films onto the inside surfaces of nanoporous zeolites. The carbon zeolites have precisely controlled pore sizes and the ion-exchange capability so important to tailoring active sites for catalytic processes. The materials undergo a multi-step process before the catalyst—rhodium nanoparticles—attaches itself to the carbon support inside the zeolite structure.

In contrast, the Jenkins group will simplify this catalyst-building process, pre-building atomic rhodium complexes with a single rhodium atom inside a ringed structure that holds it in place. These will be deposited individually inside the porous carbon zeolite structures.

Jenkins says, "The atomically positioned rhodium will be surrounded by carbon, which will be a strong electron donor, increasing the efficiency of the catalyst. The idea is that atomically positioned catalysts will have a much higher catalytic turnover than the larger nanoparticles [created in the multi-step process]."

Their goal is to improve ethanol production rates to exceed 30 percent. Current production rates yield less than 10 percent.

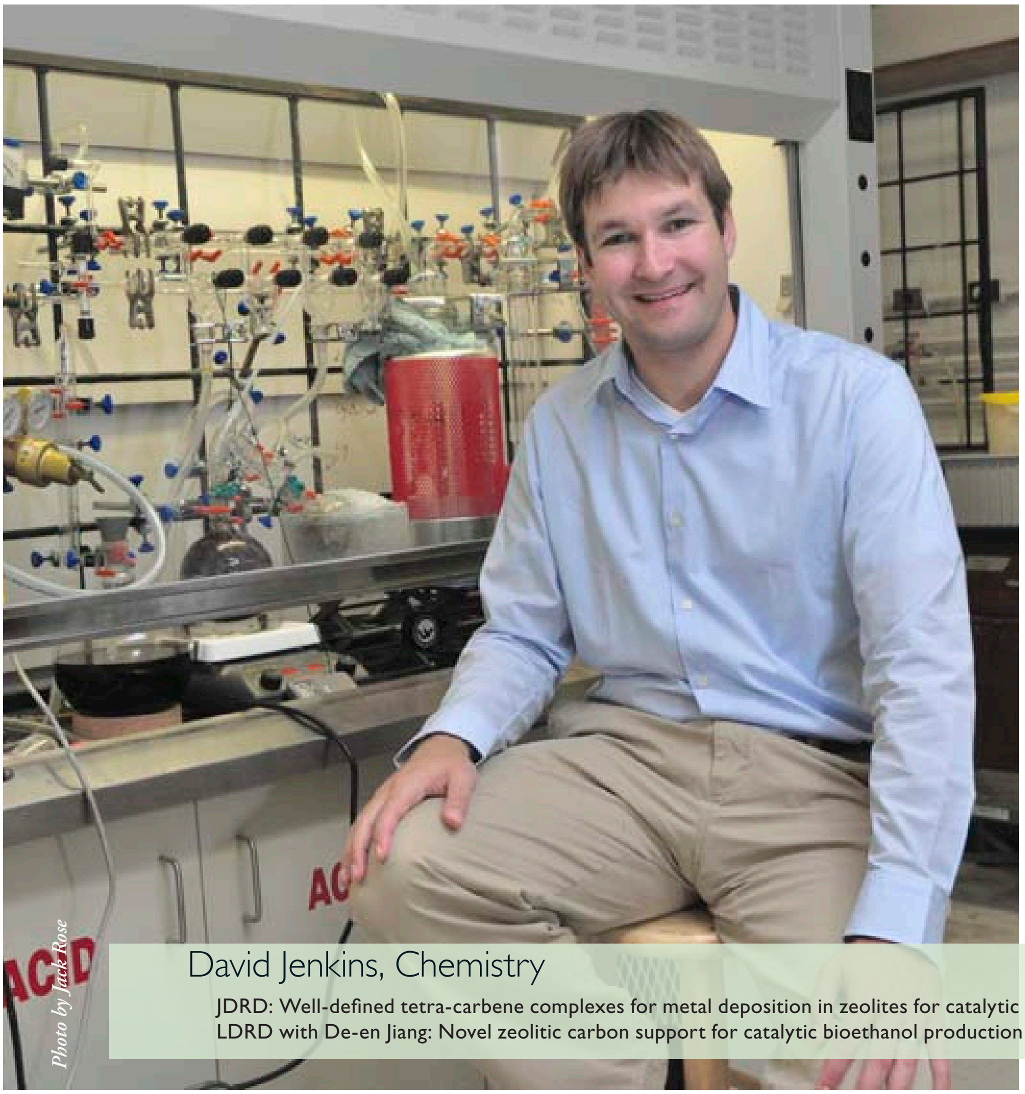
At that point, he says, it should be feasible for companies in the ethanol production game to consider the new materials for industrial application. ■

Qiang He, Civil and Environmental Engineering

JDRD: Lignocellulose bioconversion in anaerobic digestion, as a unique model
LDRD with David Graham: Harnessing nitrogen and sulfur cycles to develop microbial consortia for consolidated bioprocessing

Biofuel production from lignocellulose has the advantage of abundant and diverse raw material, but falls short when it comes to the intense pretreatment required to liberate the cellulose, composed of long chains of sugar molecules, from the lignin. Next, typically, hydrolysis exposes the cellulose to catalytic enzymes capable of breaking up the long strands into simple sugars. These feed the microorganisms used to ferment the sugar into ethanol. Both steps add additional expense and time to an already costly process.

JDRD project leader ***Qiang He*** with graduate student Si Chen, and David Graham, leader of the complementary LDRD project, take an approach called consolidated bioprocessing, or CBP, that merges hydrolysis and fermentation. The difficulty here is finding an ethanologenic bacterium capable of doing both reactions, while thriving on cellulosic feedstocks, in this research the energy crop switchgrass.



David Jenkins, Chemistry

JDRD: Well-defined tetra-carbene complexes for metal deposition in zeolites for catalytic alcohol production
LDRD with De-en Jiang: Novel zeolitic carbon support for catalytic bioethanol production

"Most CBP research focuses on creating a superbug, but it's hard to think you could pack everything into a single designer organism," He says.

He comes to this research via his interest in water quality and wastewater treatment. Initially curious about boosting biogas (methane) production from dairy manure, his research group set up six anaerobic digesters and studied what happened as they added increasing amounts of organic/nitrogen-rich poultry waste into the mix. Biogas production increased, as they had hoped, but even more fascinating, the team discovered a predominance of a different type of Archaea microorganism from the methanogens usually credited with methane production. Furthermore, the unchanging, robust anaerobic archaeal microbial community stabilized the co-digestion process.[4]

When He brought the data to Graham and his team of researchers with the DOE BioEnergy Science Center, they were immediately interested.

Feasibility tests already show the microbial consortia in the digesters work well to decompose plant biomass. Now it's up to the group to monitor digesters fed with pre-treated switchgrass to identify the microbial communities best suited to ethanol production. ■

Harsh conditions typify pretreatment of lignocellulosic biomass. Not only does the lignin have a death grip on the cellulose, numerous other physicochemical and compositional factors hinder the digestion process.[5] But, what if you could streamline bioconversion? What if you could develop techniques that make the biomass more immediately available to biochemical conversion and in the bargain increase the yield of sugars and other chemicals of value?

These questions drive JDRD team leader ***Gajanan Bhat*** and graduate student Vincent Kandagor, and their ORNL counterpart Ramesh Bhave's search for a recyclable, nanoporous membrane capable of withstanding pretreatments at moderately high temperatures and dilute acids or bases, while filtering out the sugars and other valuable components from the liquid biomass like a sieve.

"Bhave's team is developing the filter membrane," Bhat says. "Our challenge is to develop a coating that keeps the filter's surface free of debris and the nanopores open—prevents what we call fouling."

An expert in developing nonwoven fabrics, for filters in air and water purifiers and the like, Bhat says this project will use his skills in an entirely new way.

"The beauty of this coating material is, it does not attract fouling substances. Like the TEFLON in your skillet, it prevents things from attaching themselves to the filter. The key is to lay down a monolayer inside and out, without closing the pores." he says.

In the lab, Kandagor uses an airbrush technique to spray extremely low concentrations of an amber-translucent resin, Ulterm®, onto the surface of the filter material; he then analyzes scanning electron microscopic images and the performance of the coating material at high temperatures under caustic environmental conditions.

Bhat says coating thickness varies with concentration, the coating procedure they use, and other factors yet to be discovered. The JDRD study will look at two methods: dip and spray coating. ■

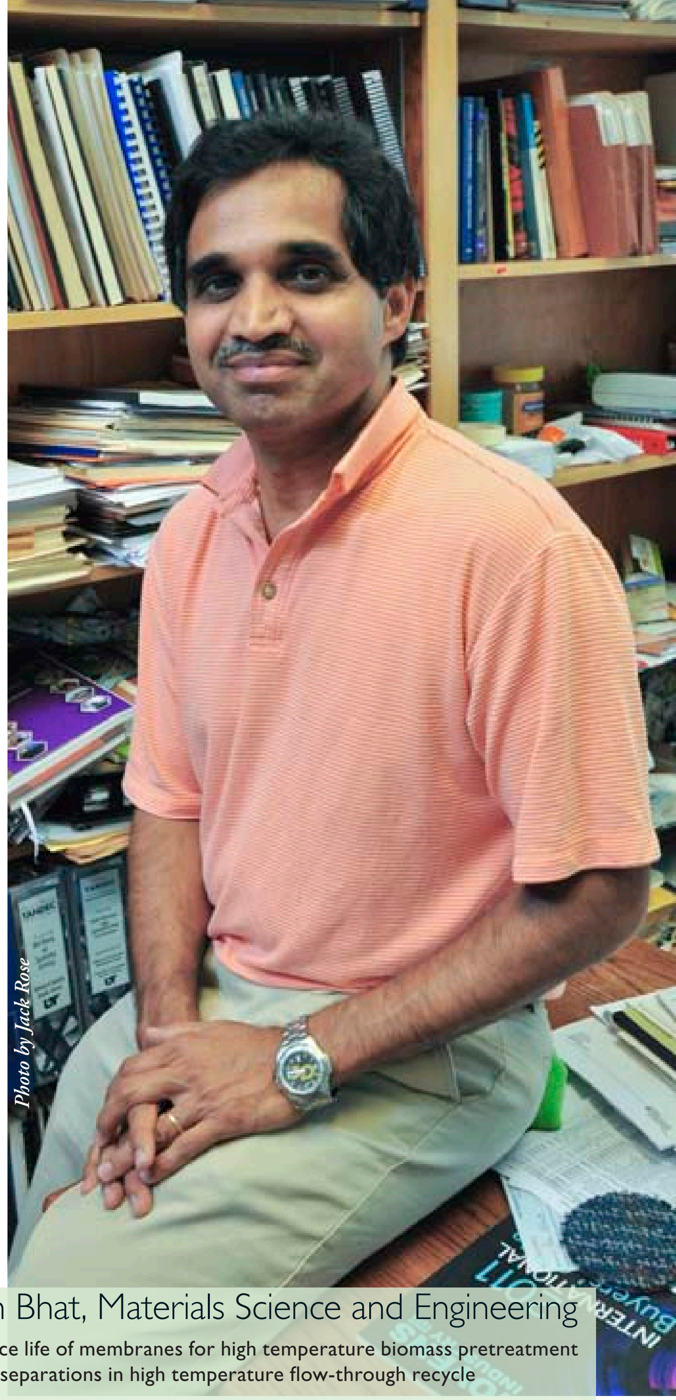


Photo by Jack Rose

Gajanan Bhat, Materials Science and Engineering

JDRD: Monolayer polymeric coatings to enhance the performance and service life of membranes for high temperature biomass pretreatment
LDRD with Ramesh Bhave: Nanoporous inorganic membranes for selective separations in high temperature flow-through recycle pretreatment of lignocellulosic biomass

Photos by laura buenning

Vincent Kandagor uses an airbrush technique to spray extremely low concentrations of an amber-translucent resin, Ultem®, onto the surface of an experimental filtering material that is being developed at ORNL for separating sugars and other valuable components from liquid biomass.

Photo by Jack Rose

Shane Foister, Chemistry

JDRD: Catalytic degradation of lignin to low molecular weight organics
LDRD with Wei Wang and Tommy Phelps: Biomass production and conversion for energy and materials

Cellulosic material from non-food crops—grass, leaves, wood—is an appealing alternative source for environmentally friendly, domestically produced biofuel.

But what to do with the vast quantities of lignin left over once the cellulose is removed? If biorefineries had a way to get high-value products from the lignin as well, biofuel economics would be even more attractive.

Found in most land-based plants, lignin surrounds and protects the cellulose, stiffens and supports plant structure, and forms stems that conduct food and water throughout the plant. JDRD project leader ***Shane Foister,*** postdoctoral assistant Ramez Elgammal, and the LDRD team led by Tommy Phelps and Wei Wang have joined forces to improve the value of lignitic waste, from the two cents-per-pound you can get as a heating fuel additive, to upwards of 40 cents-per-pound for transportation fuel components, and considerably higher for commodity chemical feedstocks.

Lignin's strong structure is chemically resistant to destruction. Composed of about four different building blocks, "what changes from plant to plant is the composition of the building blocks and the number of connections (bonds) the blocks have to each other," Foister says.

Some natural enzymes developed over billions of years are known to act on lignin and yield organic molecules useful for making highly valued products. But these would be prohibitively expensive. So, Foister's group took a lesson from nature and designed a non-precious metal catalyst modeled on enzymes that degrade biomass under mild conditions, using only oxygen or water.

"The real trick is to get a whole lot of really clean cellulose unsullied by metals that poison the enzymes used to convert it to ethanol. Current methods boil raw biomass in acid, which does get rid of the lignin, but also damages the cellulose.

"Our catalysts unzip the cellulose without destroying it," Foister says.

"But probably the most impressive part of this process is that the catalyst only turns the lignin into one or two products," Elgammal says. "Similar catalytic processes convert the lignin into 30 or more [products], which are impossible to separate."

"What we're working on is a value-added process," Foister says, pointing out that every chemical in his lab comes from non-renewable petroleum resources.

"Lignin could be another source of those molecules—only it's renewable because it grows." ■

The JDRD Program

Return on Investment

by Lynne Parker

The primary objective of the JDRD program is to foster new collaborations with ORNL that lead to new external funding for UT Knoxville. From 2006 (the first year of the JDRD program) to 2011, the program distributed nearly $3.6 million to UTK researchers, through 46 JDRD projects, averaging about $78,000 per project over two years. Now, five years into the program, sufficient time has elapsed to make it possible to evaluate how well the JDRD program achieves its main goal.

Accomplishments of the JDRD projects in terms of scientific and technical progress have been well documented each year, measured by peer-reviewed publications, student training, and popular press articles. However, we can also evaluate the program from a financial perspective, in terms of the funding return on investment. Specifically, we want to know: (1) Per JDRD dollar invested, how many dollars are generated in new external funding? And, (2) what is the financial impact of new collaborations between UTK faculty and ORNL researchers?

Of course, directly connecting an external research grant with a JDRD project can be challenging. In the easy cases, the work conducted in the project directly leads to a funded research proposal on the same topic. But in other cases, the project may lead to spin-off ideas that were not the direct focus of the JDRD research; nevertheless they contribute to proposals that otherwise might not have been successful. Or, the JDRD contribution might be one part of a much larger effort, funded down the road.

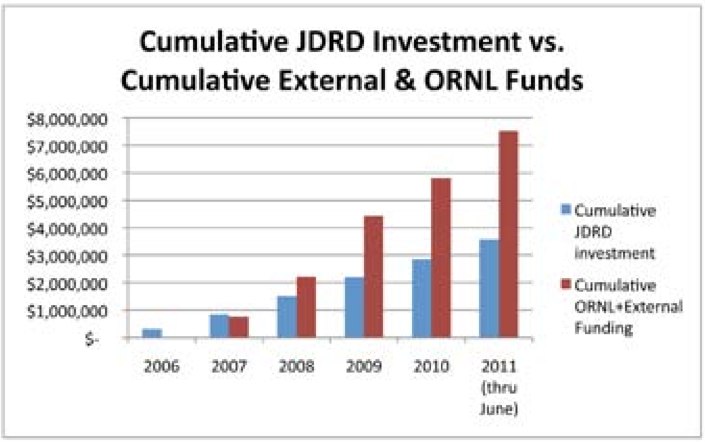


Figure 1. Cumulative JDRD funds invested versus the cumulative funds incoming from external and ORNL sources (Note that the external funding does not include ORNL funds.) A breakdown of the values in the graph is given in Table 1.

Year	Cumulative JDRD Investment	Cumulative External Funding*	Cumulative ORNL Funding
2006	$ 301,548	0	0
2007	$ 844,581	$ 293,999	$ 460,074
2008	$ 1,507,337	$ 1,038,419	$ 1,181,194
2009	$ 2,198,923	$ 2,727,778	$ 1,705,895
2010	$ 2,856,623	$ 3,410,425	$ 2,395,849
2011 (thru June)	$ 3,585,307	$ 3,726,729	$ 3,794,201

Table 1. Detailed funding values, as graphed in Figure 1. (*Note that external funding does not include funding from ORNL.)

Our Approach

So, how do we properly attribute external funding credit to JDRD projects? Our approach is to rely on the reporting of the JDRD principal investigators, including only those funded research proposals that were attributed by the principal investigator to the JDRD project. The actual funding amounts are then obtained from the UTK Office of Research database. In this category, only funds from non-ORNL sponsors are included.

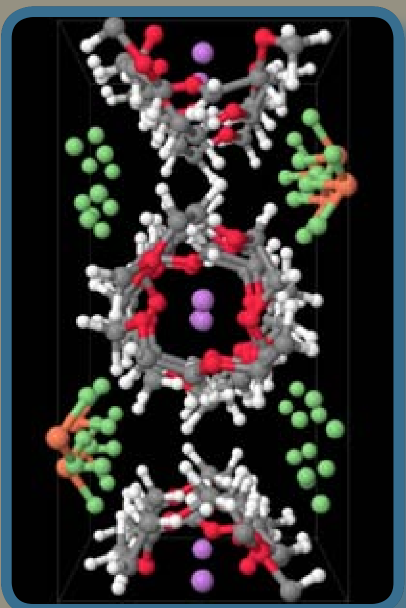
The second component of the JDRD objective is to foster new collaborations with ORNL researchers. By design at the time of the awards, very few of the JDRD recipients have had prior interactions with ORNL. Thus, a financial measure of success in generating collaboration with ORNL is new, project-related subcontracts from ORNL that bring funds into UTK. To measure this, we tallied the funds that JDRD project leaders received from ORNL (on any research topic) subsequent to their JDRD project award, as documented in the UTK Office of Research database.

Results: The results of this analysis are shown in the graph, which plots the cumulative JDRD investment since the beginning of the program, as well as the cumulative new funds from external sources and from ORNL. The accompanying table shows the breakdown of the cumulative new funds into external (non-ORNL) sources and ORNL sources. As this data shows, the amount of new research funds to UTK—over $7.5M – is more than double the amount invested by the JDRD program, balanced fairly equally between new external (non-ORNL) funding and ORNL funding. This data provides clear evidence of the positive financial impact the JDRD program has at UTK, as well as serving as an indicator of the high quality of research being funded.

In his recent book, *The Information*,[6] James Gleick states what became obvious only during the latter part of the second half of the 20th century: "We can see now that information is what our world runs on: the blood and the fuel, the vital principle."

But for most people, it is TMI—Too Much Information—and the data deluge of the Information Age continues to swell exponentially at the same time that our concern deepens at the immensity of the problems we confront. Still, where others see only difficulties, brilliant and enterprising scientists and engineers see treasure troves for their toolboxes, which can give us all hope for the future.

Photo by Jeff Slavin



Interpreting Data

Advancing technology generates massive amounts of information across time and space. How do we USE the data to build powerful tools for understanding and decision-making?

First-year and second-year JDRD awardees are hard at work to determine how to use both environmental and experimental data most effectively. Their research entails making sense of available data and going after new, essential data; selecting and testing optimal means to highlight and interpret data; and displaying those results in meaningful ways that can allow leaders and managers to make informed and critical decisions in time. In turn, a new spirit of knowledge sharing means that both the data and analytical tools can be used and improved upon by researchers all over the world.[7]

All JDRD research requires substantial computational resources. In this respect, UT and ORNL offer many distinct advantages in data management and discovery because of world-class expertise developed in the course of research applications on top-of-the-line supercomputers and scientific instrumentation. As a consequence, we can expect successful outcomes in these JDRD projects as well as a new generation of researchers skilled in applying advanced computational techniques to both their own research discipline and on collaborative, multidisciplinary teams. Their work promises to make a real difference in how we live our lives in the decades ahead.

Photo by Jack Rose

Left to right: graduate students Wei Lu (yellow shirt), Jun Liu (orange shirt), Qiang Yang (black shirt), and Ryan Overton (blue shirt), with the driving simulation car set up in Lee Han's laboratory. Appropriately, Wei Lu (of China's University of Science and Technology) has a last name that means "road"! His first name, "Wei," means "awesome," yielding the interesting English translation – "awesome road." (JDRD Ph.D. student, Jianjiang Yang, is not pictured here.)

Remember when we all wanted information in real-time? That is so old hat. Now we want to be able to know enough ahead of time in order to make decisions in a 10-minute window when disaster strikes or chaos threatens, or when we need to get emergency personnel in while we're getting evacuees out. Sounds like quite an audacious juggling act, doesn't it?

To get to that point, we have to meld a lot of simultaneous and heterogeneous data to develop and validate robust algorithms at scale—together with the learning, as ***Lee Han*** says, that comes from where "the rubber meets the road"—in order to actually project likely scenarios for a range of possible decisions and do so very quickly. Only then can we provide managers and decision makers with readily available, solid evidence in good time.

In traffic simulation, it is essential to preserve the sequential nature of the data. We all know what this means because we have intimate knowledge at an individual ("microscopic") level of driver-reaction times and behavior in stop-and-go driving and traffic jams. And

Photo by Jack Rose

Lee Han, Civil and Environmental Engineering

JDRD: Distributed computation framework for faster-than-real-time microscopic traffic simulation
LDRD with James Horey: Distributed computational framework for massive heterogeneous data fusion

we all can understand what a successful, overall system promises: safety; security in times of terrorist attacks, disasters, mass evacuations and major accidents; fuel savings; and emission reduction.

Massive heterogeneous real-time traffic data is required to build the foundation for a faster-than-real-time, random traffic simulation system. It must be some 1,000 times faster than the present state of the practice, and likely scenarios must be simulated at least 30 to 50 times each for validation. Soon, highway and on-board wireless sensors will add even more to the data mix and flood. Clearly, the scale and challenges of the required fusion of data and calculations—and the "sequential" constraint—is enormous.

Han and two doctoral students—one, Jianjiang Yang, with extensive background in transportation engineering, the other, Wei Lu, with training and expertise in computer science—will work with the computational scientists of the corresponding LDRD project led by James Horey. Together they will tackle this project by designing a new distributed programming model for optimizing traffic flow that can be tested in Han's large-scale microscopic traffic simulation system. ■

Even young scientists are old enough to recall days when mechanisms to capture and disseminate data based on space and time (spatio-temporal) were woefully inadequate to the task. Today, in contrast, the location-based data of GIS (geographic information system) is at everyone's fingertips. And temporal data is routinely collected over varying units of time in very large datasets.

But conventional "snapshot" GIS data are inadequate to the task of handling the huge datasets of temporal data, and so they do not perform adequately

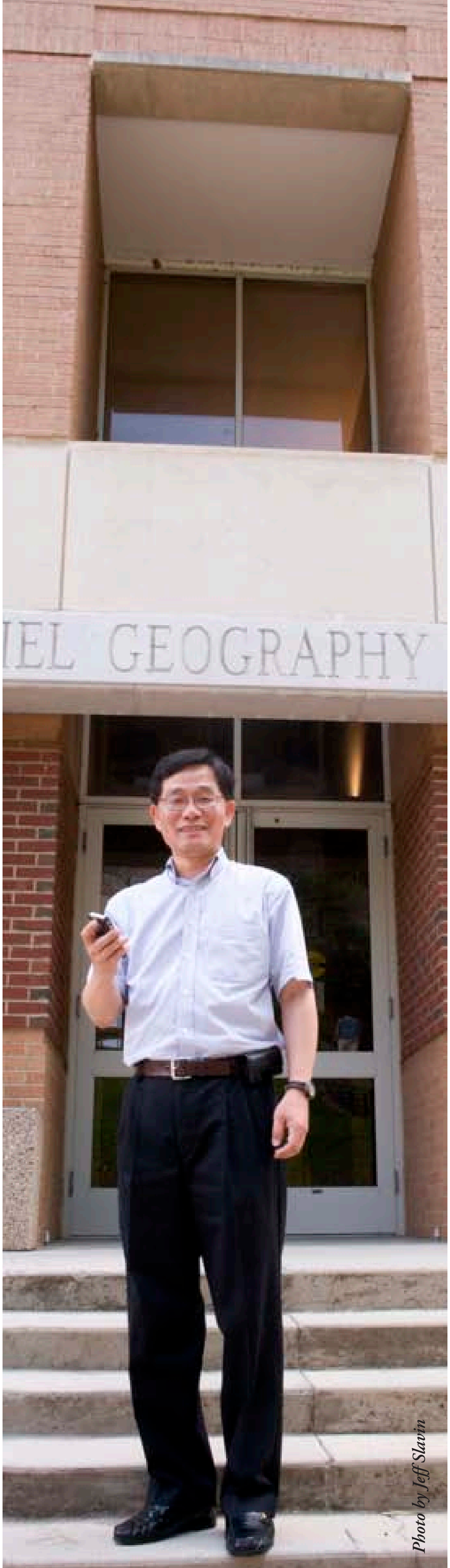


Photo by Jeff Slavin

for climate change research, which requires aggregation and integration of spatio-temporal data. Additionally, they do not afford the kind of tools for modeling and exploration of variations in attributes, parameters, and scales that are necessary to discover patterns of activity, relationships, and impact on elements in the environment. In order to determine actual effects—whether, for example, on water, or on vegetation—these capabilities are essential to evaluate results and inform good policy- and decision-making.

Shih-Lung Shaw has previously developed a space-time GIS through an NSF grant based on an innovative Temporal Dynamic Segmentation design. An operational prototype has been available on the Internet and accessed by hundreds of researchers around the world.

Although Shaw's design is capable of handling different types of data, it has not yet been applied to the highly diverse and very large datasets of climate change research. As they work to couple space-time GIS with climate informatics for climate change research, the JDRD and LDRD teams, including doctoral student Ziliang (Ray) Zhao, will also investigate options to enable spatio-temporal query, analysis, and visualization—representing point, line, polygon, and image data—of enormous databases via high-performance computing.

As LDRD team leader W. Christopher Lenhardt comments: "No small task!" ■

Shih-Lung Shaw, Geography

JDRD: Integration of space-time GIS with climate informatics for climate change research
LDRD with William Lenhardt: Enhancing climate impact integrated assessment for water through climate informatics

Qing Cao orders sensors, such as the one shown below, "off the shelf" for his JDRD project.

Not only are the tiny sensors easily available for purchase, they are also inexpensive and ubiquitous—all set to generate data almost anywhere in real-time.

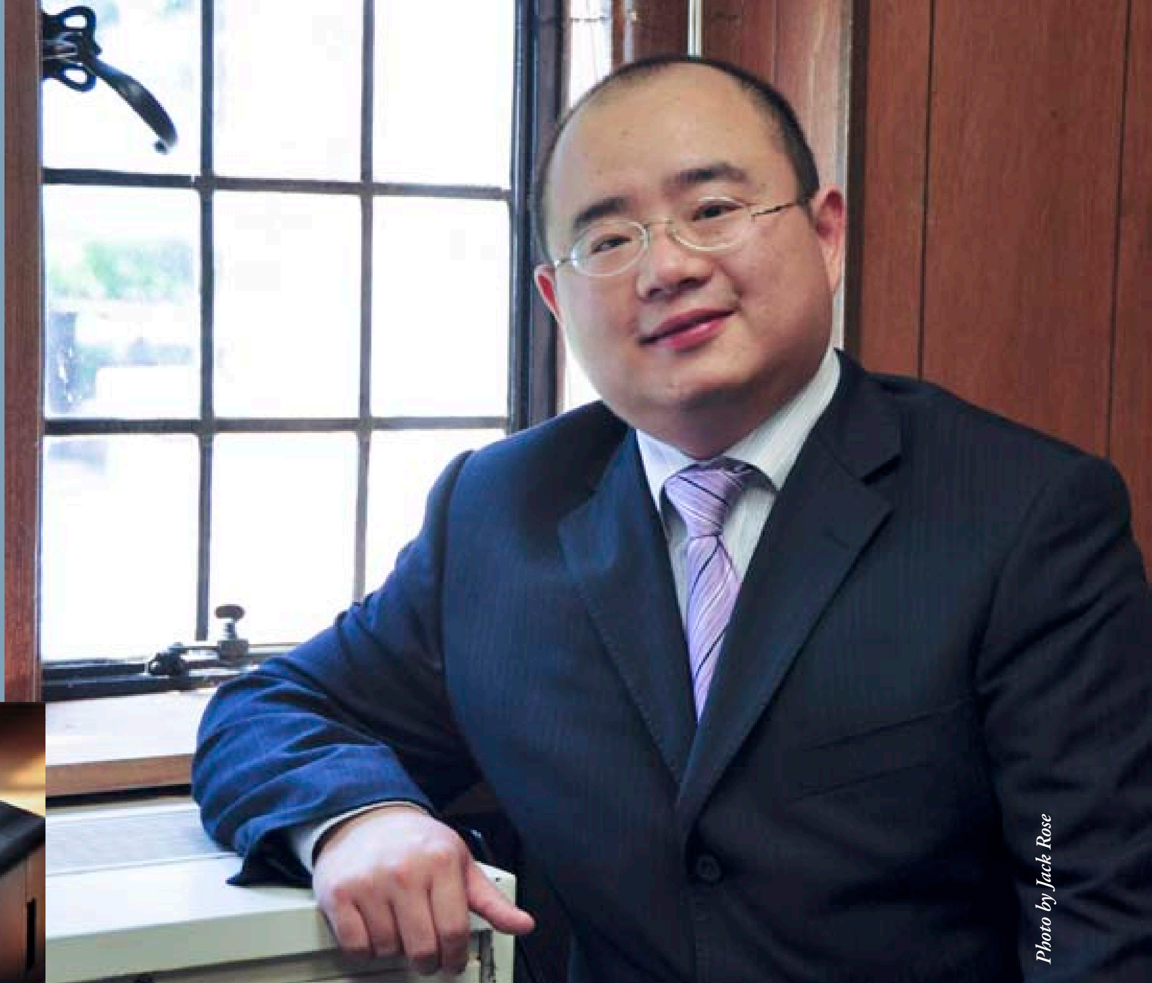


Photo by Jack Rose

Qing Cao, Electrical Engineering and Computer Science

JDRD: Distributed computation framework for massive heterogeneous data fusion: a location-centric approach
LDRD with James Horey: Distributed computational framework for massive heterogeneous data fusion

Walk into ***Qing Cao's*** UT Ferris Hall office and the first thing you notice are the Amazon.com equipment boxes. Instead of the more typical books, these contain sensors he's ordered "off the shelf" for his JDRD project. Recent progress on MEMS (microelectromechanical systems) has resulted in mass production and deployment of sensor networks, together with a number of new industry-led applications. Not only are the tiny sensors easily available for purchase, they are inexpensive and ubiquitous—all set to generate data almost anywhere in real-time. If one considers sensing devices in cell phones, alone, the potential for total yields of data is at a scale previously unimaginable.

But despite the mail order boxes, this is no kitchen-table operation. The centerpiece of the project is location-centric data fusion,[8] a comprehensive computational framework to specify, analyze, aggregate, and discover new relationships in streaming sensor data that involve location. Together with graduate students Kefa Lu and Yanjun Yao, Cao aims to build a distributed computational framework that develops and tests programming abstractions for a new class of location-aware applications. Enabled by the huge volumes of accessible, real-time data generated by networked sensors installed on numerous vehicles, these applications measure parameters, ranging from vehicle location to fuel efficiency.

As a result, it has become increasingly urgent to develop and assess tools and middleware that help make sense of such vast amounts of data (collected over months), optimize the data for useful applications, and allow individuals to exploit the data for their own use.

In similar fashion to the JDRD team, LDRD project leader James Horey and his computational scientists are engaged in design of a new distributed programming model to express spatio-temporal data fusion. Results from the complementary JDRD project will extend the LDRD to include additional techniques for location-based sensor networks, thereby greatly extending the number of applications that benefit from real-time data fusion. Both project leaders are interested in pursuing further research and funding in Cyber-Physical Systems (CPS), designated as an important emerging area of research by the National Science Foundation (NSF). ■

scientist who, in turn, has to learn what questions to ask.

Neutrons are uniquely suited for use in non-destructive imaging of a wide range of objects. Tomographic images yield cross-sectional views by reconstruction from two-dimensional radiographs. The JDRD research will advance the state of the art by introducing iterative[10] reconstruction. In year one, the JDRD team will modify in-house developed software to model neutron imaging geometry as well as dominant sources of signal "noise" and improve computational efficiency with Graphics Processing Units (GPUs). Their objective is substantial improvements in image quality together with a reduction in scan time.

Under the direction of Gregor, the JDRD team consists of graduate students Daniel Henderson and Jason Frank, and undergraduates Matt Johnson and Curtis Taylor. The corresponding LDRD team—providing high-quality data and a thorough understanding of the physics of neutron imaging—is led by Hassina Bilheux, instrument development scientist in the Neutron Scattering Science Division at ORNL.

Jens Gregor, Electrical Engineering and Computer Science

JDRD: Iterative image reconstruction for neutron tomography
LDRD with Hassina Bilheux: Neutron imaging of fluids within plant-soil-groundwater systems

With a tweak and a nod to the trademarked BASF slogan, ***Jens Gregor*** calls to mind: "I don't do the science of the study. I do things that make the science of the study better!"[9]

And indeed he does, in a substantial body of collaborative work with ORNL researchers for nearly a decade on a major NIH grant to develop a micro-SPECT/CT (Single Photon Emission Computed Tomography) system for small animal imaging. The current JDRD project builds upon many years of practical experience in x-ray CT along with a deep understanding of image reconstruction mathematics.

Gregor doesn't play it safe. He is a computational scientist who works with researchers who are experts in physics and in biology. That makes him, of necessity, a quick study in a minimum of three disciplines. It also affords his students the opportunity to acquire the kind of translational experience across subject fields that is in tremendous demand. More and more, the process of collaboration is one where experts from diverse scientific disciplines have to learn what to tell a collaborating computational

Interest in neutron imaging is on the rise within government funding agencies as well as in industry. Close to home, plans are underway to build a neutron imaging beam line called VENUS based on the SNS (Spallation Neutron Source), one of the premier research instrument facilities at ORNL. Follow-on work is projected in a number of domain science applications, including plant biology and soil analysis, materials science, energy, and national security. ■

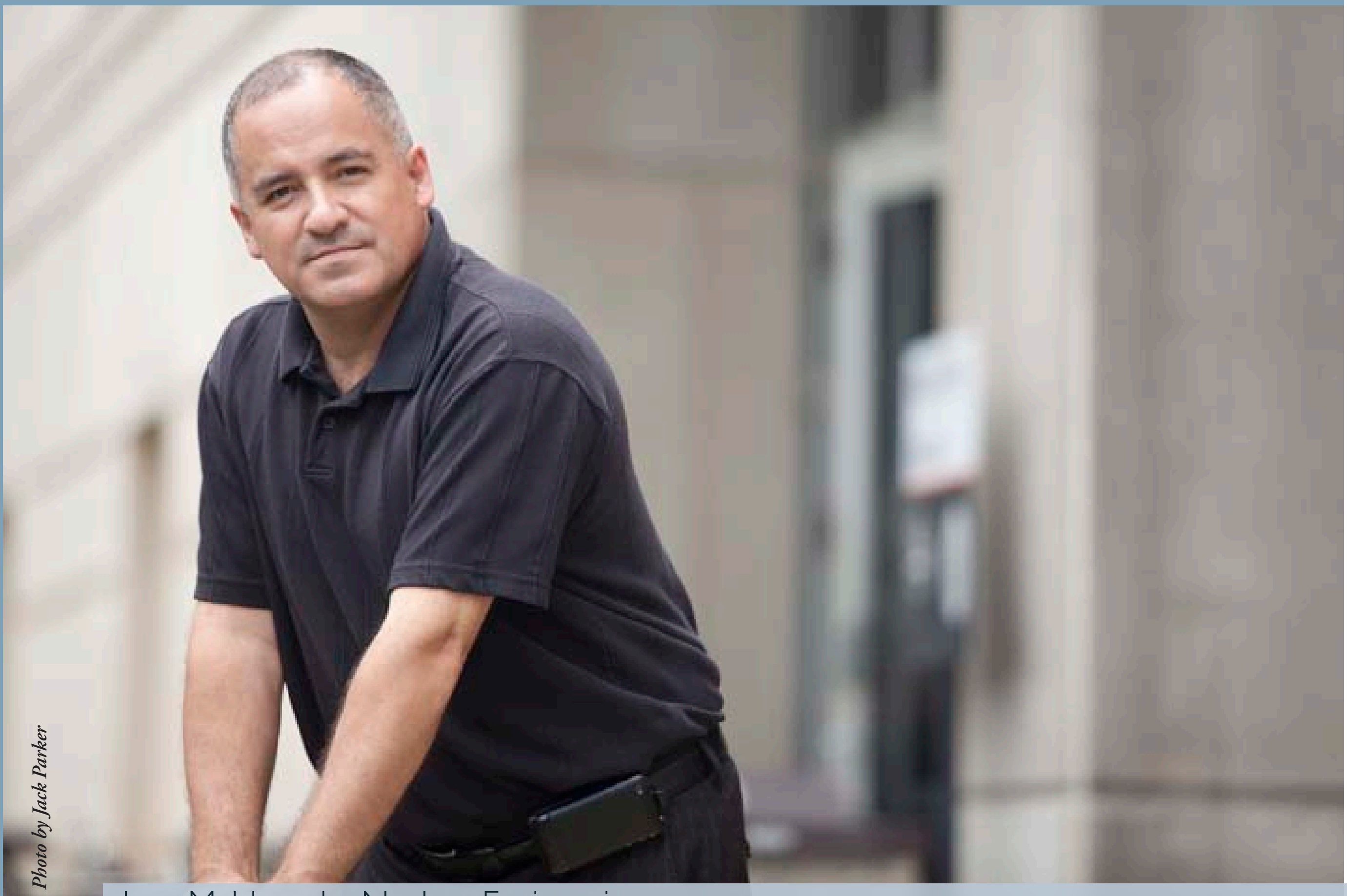


Photo by Jack Parker

Ivan Maldonado, Nuclear Engineering

JDRD/LDRD: Revolutionary radiation transport for next-generation predictive multi-physics modeling and simulation
LDRD with John Wagner

Nuclear power captures headlines only when there are nuclear accidents and emergencies. Otherwise, we all tend to hope they just keep working to provide the electricity we use every day. And they mostly do, despite the fact that existing power plants are old and the computational tools we have long used in their operations are also aged.

The fact of the matter is that much effort has been invested to develop advanced nuclear energy systems that offer significant improvements with respect to cost, safety, and sustainability. But, these newer designs will require robust computational tools and drastic (not incremental) improvements in modeling and simulation capabilities to predict and track the status and performance of every single nuclear fuel pin in the core of a reactor—before, during, and after operation. These methods will eventually make it possible to precisely determine the composition of each fuel pin. They also have important implications for the larger issue of nonproliferation of nuclear material by providing for inventory control and safeguards. The approach of this JDRD project exploits a unique solution developed by their partnering LDRD team, led by John Wagner of ORNL Design, Safety and Simulation Integration.

In its first year of funding the JDRD team, led by ***Ivan Maldonado*** with graduate students Brenden Mervin and Nicholas Sly, has developed a hybrid methodology that overcomes a major limitation of the conventional Monte Carlo approach (the code name Monte Carlo is due to the method's secret development by mathematicians during wartime) by distributing computational effort, and hence statistical precision, uniformly across the problem domain. Together with a new domain-decomposition algorithm, the researchers take advantage of the ORNL supercomputer Jaguar platform to construct a powerful and uniquely capable, Monte Carlo-based radiation transport package for high-performance reactor core simulations.

In its second year of funding, the teams will apply their methodology to large-scale, high-performance simulations of reactor designs. Several articles detailing accomplishments are in process as well as multi-year proposals for grant funding with ORNL and DOE. ■

The high volatility of the liquid electrolyte used in today's state-of-the-art lithium ion batteries for applications such as hybrid and all-electric vehicles makes safety engineering both difficult and expensive. A better class of high-energy storage devices—commonly called batteries—would be all solid state, based upon a robust, solid electrolyte, rechargeable, and inexpensive.

Together with LDRD researchers led by Nancy Dudney at ORNL's Materials Science and Technology Division, the JDRD team of ***Stephen Paddison*** and Brad Habenicht, a post doctoral researcher, is working to overcome current limitations by studying the option of replacing the liquid electrolyte with an efficient, solid lithium ion-conducting electrolyte. For their part, Paddison and Habenicht are examining composites developed in experiments by the LDRD group and simulating those materials and their interfaces at a molecular level. Their theoretical results are then used to guide further refinements of compositions and structures fabricated at ORNL.

The JDRD team has used the computationally-intensive simulation technique known as AIMD (Ab initio—meaning "from first principles"—Molecular Dynamics) to directly model what is happening at the molecular level between the lithium ions and the solid composites—polymer or inorganic electrolytes—produced in the LDRD experiments. While they have a substantial effect on the properties of a functioning storage device, interactions in the interfacial regions between different materials in the composites are complicated and not yet well understood.

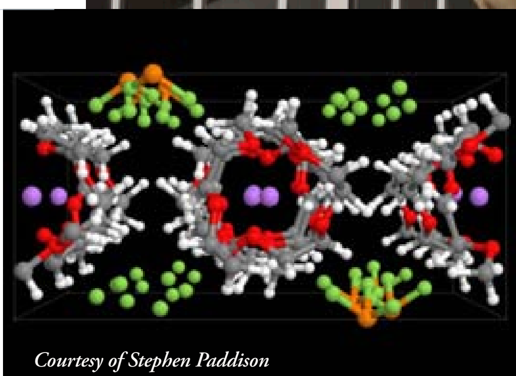


Image of PEO6:LiPF6 simulation cell. The PEO chains form coils around the lithium ions which shields them from the PF6- anions and provides a channel for lithium ion conduction. Carbon, fluorine, hydrogen, oxygen, lithium and phosphorus atoms are depicted in grey, green, white, red, purple, and orange, respectively.

Courtesy of Stephen Paddison

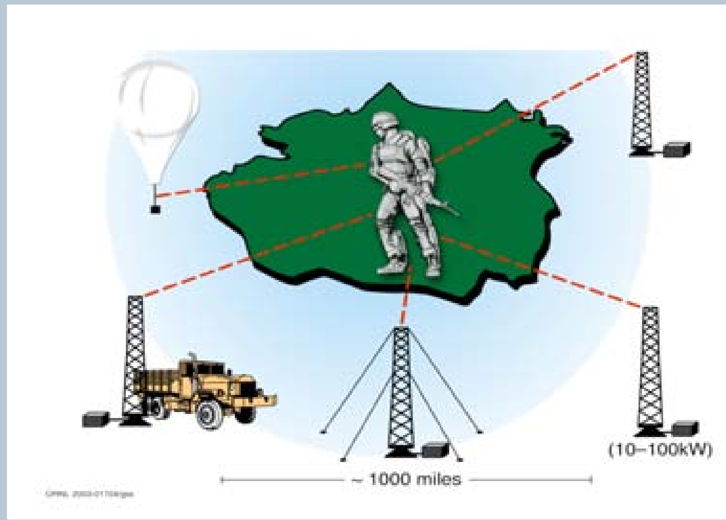
Photo by Jack Rose

Stephen Paddison, Chemical and Biomolecular Engineering

JDRD: Ab initio studies of Li+ mobility in solid polymer electrolytes
LDRD with Nancy Dudney: Tough electrolytes for batteries—composites inspired by nature

As a result of team discussions and the data from investigations in the first year of funding, the two teams have been able to focus on a new class of crystalline lithium ion-conducting polymers based on PEO—or poly(ethylene oxide). The second year will include AIMD simulations of the crystalline PEO, requiring 2.5 million CPU hours on the Teragrid Kraken Cray supercomputer. From the results of these simulations the teams expect to achieve an important development in the field of solid electrolytes that can be tested and correlated with experiment. ■

Photo by Jack Parker



Typical Theater Positioning System (TPS) deployment in a large operational area

TPS transmitters are typically, although not necessarily, deployed outside the main area of operations, to provide favorable angles of reception from the various transmitter locations. The TPS system provides useful two-dimensional location data; if special provisions are made to generate TPS transmissions at varying heights the system can produce 3-dimensional readings.

Paul Crilly and Seddik Djouadi, Electrical Engineering and Computer Science

JDRD/LDRD: Integrated navigation system for GPS-denied environments
LDRD with Stephen Smith

GPS (Global Positioning System) has rapidly permeated communication, information, and navigation infrastructure and applications worldwide. But it does not perform accurately in "GPS-denied" environments such as natural or urban canyons, mountainous terrain, underground, or deep inside large buildings. Worse, the faulty readings offer no clue that the location is inaccessible or the data is compromised by obstacles or obfuscated by intentional noise.

Technologies based upon low radio frequencies—such as TPS (Theater Positioning System), LORAN-C, and a low-cost, local INS (Inertial Navigation System)—promise to correct and augment the increasingly popular GPS. Now in their second year of JDRD funding, ***Paul Crilly*** and ***Seddik Djouadi*** continue to develop and test TRI-NAV, a triple-redundant, integrated navigation system with robust and efficient capabilities to substantially improve location precision, accuracy, and reliability in a multitude of commercial, consumer, and military applications.

Complementing the LDRD work undertaken by Stephen Smith at the ORNL Position, Navigation, and Timing Program, the JDRD team—including graduate students Xiao Ma, Zachary Crane, and Samir Sahyoun, and undergraduate research assistant Brian Doll—has succeeded in laying the foundation for comparing, correlating, and integrating data from both GPS and TPS systems. Results so far demonstrate that resolution location can be improved by a factor of at least five. Beyond the extensive mathematics involved, they have also made progress in mapping and simulations to account for errors in TPS due to the earth's curvature, terrain changes, and ground propagation effects.

In addition to preparing several IEEE journal articles and various conference papers, the team has already submitted an NSF proposal based on what they have achieved so far. Several agencies in the

Department of Defense have expressed interest in the project and a white paper has been submitted to the Computing Sciences Division of the U.S. Army Research Office. ■

It's not difficult to imagine a link between climate and energy consumption: warmer or cooler weather means increased cooling or heating of homes and public buildings; changes in precipitation affect available drinking water supplies not to mention irrigation and food-growing cycles. Less obvious, but no less serious, is the influence ground and atmospheric temperatures have on isoprene and other volatile organic compound (VOC) emissions and, as a result, the maximum daily average eight-hour (MDA8) ozone concentrations. Just how much climate change will influence future energy demand and risk-management policies is unknown?

These are the issues driving JDRD team leader ***Joshua Fu***, postdoctoral associate Yum Fat Lam, graduate student Yang Gao, and LDRD team leaders David Erickson (2010) and Steven Fernandez (2011). Fu is particularly interested in what happens on a regional scale, as compared to the global approach taken by many climate simulation models. Both types are computationally intense; Fu runs his simulations on UT's supercomputer, Kraken, managed by the National Institute for Computational Sciences, a part of the Joint Institute for Computational Sciences, and on Jaguar in ORNL's Leadership Computing Facility (OLCF), managed by the National Center for Computational Sciences.

In year one, Fu integrated regional and global models to simulate atmospheric concentrations over the continental U.S during 1999 – 2001 and 2049 – 2050, dividing the country into Midwest, Northeast, and Southeast regions. His simulations show climate change has a strong effect on air quality.

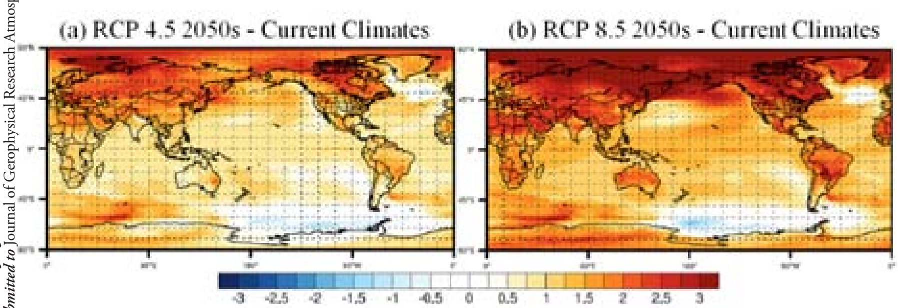
During the second year of the project, the team simulated two future climate scenarios for the entire planet from 1999 to 2099; representative concentration pathway (RCP), 4.5, moderate, and RCP 8.5, intense fossil fuel usage. Significant global temperature increases were observed in the 2050s on both scenarios, where mean temperatures are projected to increase 1.15 degrees and 1.72 degrees Celsius, respectively. Global mean duration of heat waves increased from 10 days in current climates to 17.9 and 24.3 days, respectively, by the 2050s.

The team is currently downscaling the model to study climate effects in the United States. ■


Photo by Jack Parker

Joshua Fu, Civil and Environmental Engineering

JDRD: Downscaling of global chemistry and climate predictions on energy demand: regional analysis and local impacts
LDRD with David Erickson in 2010: Climate change impacts on energy infrastructure; and with Steven Fernandez in 2011: Real-time simulation of power grid disruptions



Courtesy of Joshua Fu
Submitted to Journal of Gerophysical Research Atmospheres

Temperature differences between the projected future climates under representative concentration pathways (RCP) 4.5 and 8.5 in the 2050s verses current climates, at 2 meter intervals using the Community Earth System Model. Significant increases in global temperatures are observed in the 2050s on both scenarios where the mean temperatures are projected to increase globally 1.15 degree Celsius in RCP 4.5 and 1.72 in the RCP 8.5.

Photo by Jack Parker

Edmund (Ed) Perfect, Earth and Planetary Sciences

JDRD Neutron Imaging of Fluids in Rocks and Soils
LDRD with Hassina Z. Bilheux: Neutron Imaging of Fluids within Plant-Soil-Groundwater Systems

When it rains, water soaks down into the earth displacing CO_2 and other gases and liquids held in pores in the soil and rocks. Plant roots capture some of this moisture and transpire it back into the atmosphere. The remaining water moves downwards under the influence of gravity and is stored in underground reservoirs known as aquifers. Even deeper in the subsurface some of the pores are filled with hydrocarbons derived from fossil plants and animals creating oil and gas reservoirs.

Understanding air-water and gas-oil displacement in porous soils and bedrock has relevance for all sorts of environmental issues, including regulation of plant-water use, CO_2 sequestered in the soil or as a greenhouse gas in the atmosphere, extraction of oil and natural gas, and the movement of groundwater contaminants.

Theoretical simulations of a variety of fluids held or moving through heterogeneous Earth materials has improved substantially, says JDRD team leader ***Ed Perfect***, but validating these models with accurate data remains a major obstacle. Perfect and post-doctoral associate Chu-Lin Cheng, doctoral student Misun Kang, and LDRD team leader Hassina Bilheux have turned to non-invasive, non-destructive neutron imaging techniques to help supply the data they need.

Neutron imaging, with its high sensitivity to hydrogen and other light elements in pore fluids and root cells, allows scientists a look inside variably saturated rocks and soils. Both teams use the new CG-1 beam line tucked into the far corner of ORNL's High Flux Isotope Reactor's (HFIR) Cold Guide Hall. The two teams are closely aligned; the LDRD project focusing specifically on plant-soil-groundwater systems and the JDRD project on imaging and modeling drainage behavior in partially saturated soils and rocks.

In year two, Perfect's team will analyze the two- (radiography) and three-dimensional (tomography) neutron imaging data sets collected in year one and apply what they've learned to models depicting flow dynamics of water, brine, air, CO_2 and other fluids within plants, soils and rocks. ■

Inventors mimic nature to jump-start their ideas. Sometimes though, nature supplies the material itself, as in the case of bioadhesives, which technically speaking are natural polymeric glues. Lac bugs on trees in forests of India, for example, secret the resin shellac. Bioadhesives also have a wide range of medical applications, as orthopedic surgical glue, as the sticky surface on low-dose drug-delivery patches, or to attach cells to surfaces for laboratory cell and tissue cultures.

The carnivorous sundew plant, with its numerous species and a growing range from Alaska to New Zealand, produces one such gluey substance that stretches

Photo by Jack Parker

Mingjun Zhang, Mechanical, Aerospace, and Biomedical Engineering

JDRD: A Nature-derived nanopartical and nanofiber-based scaffold for enhancing chemical detection and imaging
LDRD Project with Ali Passian: Standoff detection and imaging of chemicals

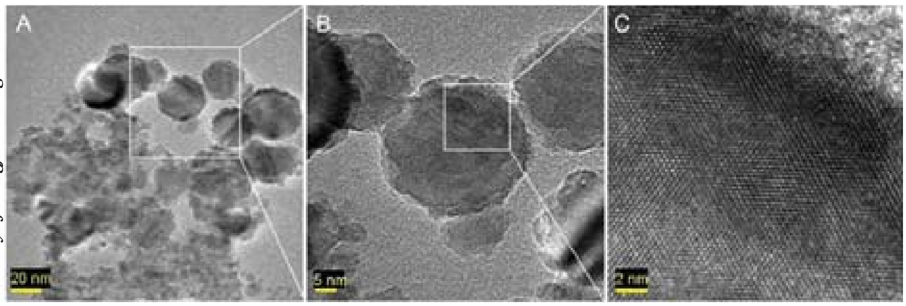
up to a meter long. The sundew uses it to capture insects.

JDRD team leader ***Mingjun Zhang***, postdoctoral associates Scott Lenaghan and Yuanyuan Li, eight undergraduate students, and LDRD team leader Ali Passian see great potential for sundew adhesive as a strong, easily identified nanoscaffold for anchoring the sensors used in signal detection and imaging systems. Passian's team will test the adhesive's usefulness for their new standoff chemical screening techniques. Standoff detection is done at distances that reduce the danger to humans or other vital resources.

During year one, Zhang's team isolated the nanoparticles and nanofiber scaffold responsible for sundew's adhesive and characterized its physical and chemical properties. In the process they also explored its potential for tissue engineering and other medical applications. The team experimented with three individual cell lines, growing them on a nanofiber network brushed onto a surface with a sticky sundew tentacle. They found the dried adhesive capable of promoting cell attachment and growth, maintaining its integrity when exposed to the harsh products of actively replicating cells. Their preliminary results support the nanomaterial's potential to help repair bone, nerve, and soft tissue injuries.

To advance their study, the JDRD team must develop a fabrication method to control the pattern of the dried adhesive scaffold. Further in-depth work on the adhesive's interaction and biocompatibility with neural and other stem cells will take the team into uncharted territory, where they will develop a method for testing sundew's nanoparticle toxicity—an area where no standard assays are currently available. ■

Courtesy of Mingjun Zhang



TEM images showing the crystalline structure of the nanoparticles. A) Agglomerations of nanoparticles with typical diameters around 35 nm (25 to 44 nm). B) The particle in the center of the image was 38 nm in diameter. C) Higher magnification demonstrating the crystalline structure of the previous nanoparticle.

UT-ORNL Partnerships

by Laura Buenning

Courtesy of UTK video and photography

Bring BIG SCIENCE to Tennessee

Main ORNL campus at night: an aerial evening view looking west ***(Courtesy of ORNL)***

Just 20 miles apart, The University of Tennessee and Oak Ridge National Laboratory have always shared a special relationship. After the war, ORNL shifted focus from weapons to research in medicine, biology, materials and physics, areas more in line with UT's curricula. Then as now, ORNL scientific staff members taught science and engineering courses as adjunct faculty at UT and university faculty worked as consultants and research collaborators at ORNL.

Over the years, joint research collaboration and programs have forged a solid bond between the university and national laboratory, strengthening the research agendas of both institutions. The first formal joint programs between the institutions were two UT graduate schools located at ORNL. One was the UT Graduate Program in Ecology; the other the UT-ORNL Graduate School of Biomedical Sciences, which opened initially in 1967; in the latter 1990s the focus and name changed to the UT-ORNL Graduate School of Genome Science and Technology. At that point the program moved to UT's Knoxville campus.[11]

The formal relationship grew in 1984 with the creation of the Science Alliance[12] and its inaugural joint venture, Tennessee's UT-ORNL Distinguished Scientist Program. That same year the Science Alliance began support for the UT-ORNL Joint Institute for Heavy Ion Research, the first of its kind to have a state-funded office and meeting facility on the ORNL reservation. Dedicated in 1984, JIHIR assists visiting scientists conducting research at the Holifield Radioactive Ion Beam Facility (until the 1990s known as the Holifield Heavy Ion Research Facility). JIHIR is the forerunner to the more recent UT-ORNL joint institutes for Advanced Materials (JIAM), Biological Sciences (JIBS), Computational Sciences (JICS), and Neutron Sciences (JINS). The Science Alliance had a part in the early development of all UT-ORNL joint institutes.

In 2000, the link with ORNL broadened when UT teamed up with respected technology giant Battelle to win the contract to manage the laboratory for the U.S. Department of Energy. Since then, the UT-Battelle partnership has invested $500 million in modernization of the ORNL campus.[13] The state of Tennessee also contributed significantly to the venture, including a $30 million investment for three new joint institute facilities, and additional matching funds to support high-level joint appointments in a new Governor's Chair Program. Much like the Distinguished Scientist Program, the Governor's Chair Program recruits exceptionally talented, internationally respected research scientists and engineers to joint appointments as tenured professors at UT and distinguished research staff at ORNL. The appointments include an ongoing discretionary research fund equal to twelve months' salary.

Courtesy of the UT-ORNL Joint Institute for Neutron Sciences

UT-ORNL Joint Institutes

On the surface, it seems like a simple idea: two or more organizations formally agree to join together to conduct business (or in this case research) in areas of common interest. By implication, they assume all have something to gain, if not always equally, enough so that both sides are strengthened by joining forces. The joint institute supplies a framework, the management, an environment conducive to collaboration, and the physical space where scientists and engineers can exchange ideas and work collectively to answer complex research questions.

Simple ideas, though, don't imply effortless execution. UT-ORNL Joint Institutes link two institutions with individual purposes, individual goals. As an institution of higher education, scientific research at UT leans toward creating teaching and learning experiences to increase basic understanding of scientific and engineering principles. ORNL's agenda is set by Department of Energy research and development goals and has a more practical, applied approach. These and other concerns are continually being addressed as the institutes grow and evolve.

Enter the state's first UT-ORNL joint institute

In the early 1980s, the ***UT-ORNL Joint Institute for Heavy Ion Research (JIHIR)*** set the stage for what was to come. Housed in two buildings at ORNL, one of which was constructed by the state of Tennessee, JIHIR helped usher in a new era of unique cooperation between a national laboratory, a state government, and the state's major research universities. Back in October 15, 1984, when UT, Vanderbilt University, and ORNL dedicated JIHIR's new facilities, the freedom to enter or leave the national laboratory reservation and the rules governing the use of its land were more restrictive. So, it was a major accomplishment to build a state-funded facility on national laboratory land.

Things changed dramatically in 2000 when UT-Battelle took over management of ORNL. UT-Battelle pumped $500 million in federal funding into modernization and improved access to the laboratory's sophisticated research instruments; Tennessee invested $32.1 million in three new joint institutes: Joint Institute for Computational Sciences, $10 million; Joint Institute for Biological Sciences, $11.6 million; and Joint Institute for Neutron Sciences, $10.5 million.[14]

This past December 3, 2010, when the ***UT-ORNL Joint Institute for Neutron Sciences (JINS)*** held its dedication ceremony with Governor Phil Bredesen as one of the speakers, it became the

The UT-ORNL Joint Institute for Neutron Sciences celebrates a landmark year—the first in its new building situated on the hill next door to the Spallation Neutron Source (SNS) and Center for Nanosphase Materials Sciences (CNMS).

fourth such institute to open doors on the ORNL campus. The ***UT-ORNL Joint Institute for Computational Sciences (JICS)*** dedicated its facility on May 21, 2004 and the ***UT-ORNL Joint Institute for Biological Sciences (JIBS)*** opened in November 2007. In addition, JICS recently opened an office on the UT campus and a fifth institute, the ***UT-ORNL Joint Institute for Advanced Materials (JIAM)***, will anchor UT's Cherokee Farm research facilities. JIAM building construction is scheduled to begin in 2011. The institute's Graduate Fellowship Program awarded six supplemental stipends in 2011. On September 2010, JIAM held a second seed project competition open to all materials researchers at UT and ORNL. Five of 15 proposals were selected for funding. Notable scientific contributions reported from the first-year seed project competition include the spatial mapping and spectroscopic analysis of plasmonic hotspots in metallic nanoparticles by Jon Camden's group in chemistry and a clarification of the mechanism behind graphene formation on metal surfaces by JIAM graduate fellow, Hua Chen, in physics. The seed program led to 13 external research proposals; two received funding, eight are pending. Finally, the state's investment in the JIBS building and equipment, and the Tennessee BioEnergy Initiative were central to UT and ORNL's early success in capturing $125 million in DOE support for the ORNL BioEnergy Science Center (BSEC), headquartered in the JIBS facility.

Work in progress

From the first, ***JINS Director Takeshi Egami*** has had something innovative in mind. Last fall, fresh from organizing a three-month workshop at the Kavil Institute of Theoretical Physics at the University of California, Santa Barbara, Egami put into play a mini-version of the type of seminar offered at the Kavil. Instead of the standard format, where a talk is followed by a few questions, Kavil's intense discussions can go on for hours. Participants go well beyond an initial understanding of the topic and interactions often lead to unusual, unforeseen collaborations. JINS seminars and workshops will follow this model.

UT and ORNL researchers in different fields often work independently, in part because they receive direct funding from, and report directly to, Washington D.C. Egami wants to change this research mode to one where scientists and engineers from all disciplines gather to exchange ideas, learn from each other, and possibly find collaborators in neutron scattering to add another dimension to their individual research projects.

UTK has developed a sizeable presence in neutron scattering, since Egami moved to UT to become a UT-ORNL Distinguished Scientist some eight years ago. "UT can play a good game," he says; because the neutron scattering field is smaller overall—say, in comparison with computer science—and new faculty, including Governor's Chairs Alexei Sokolov and Jeremy Smith, give UTK an edge.

The new, in-depth, JINS workshops and seminars will promote back and forth discussions between groups looking for common ground. The aim is to create new interdisciplinary projects. For this reason, building plans, which started out with only meeting rooms and offices, changed to include eight laboratories where interdisciplinary teams can carry out their research.

Recently, the institute started what has become a popular weekly coffee hour for people in nearby buildings to drop by. It's an occasion to converse with people you don't usually talk to, Egami says. These informal conversations can lead to new insights and new collaboration—perhaps spark an idea for a new way to look at an old problem.

Egami says the key to success is the involvement of strong people. "And we have a strong beginning in this with JINS." JINS will also capitalize on its close physical presence to the SNS, CNMS and HFIR, where neutron scattering and other materials experiments are done.

Courtesy of the UT-ORNL Joint Institute for Neutron Sciences

At JINS's dedication ceremony Governor Phil Bredesen, ORNL Director Thom Mason, and UT Interim President Jan Simek signed a framed, 1944 letter from E.O. Wollan of ORNL, which "could be considered the origin of neutron diffraction, leading eventually to the construction, six decades later, of the Spallation Neutron Source and JINS."

R*obert Harrison,* the new director of the ***UT-ORNL Joint Institute for Computational Sciences***, wants to bring clarity to the joint institute's mission.

JICS manages several joint faculty lines and researchers funded by ORNL projects (as well as some at UTK). It is home to the National Institute for Computational Sciences (NICS), which manages UT's Kraken, the world's fastest academic supercomputer. But, even though NICS is the institute's biggest project—and the research dollars associated with NCIS are equivalent and rising—Harrison says JICS has a broader role to play.

"UT is literally at the center of computational science in the U.S.," he says. The recent Top500 ratings place Kraken at number 11 in the world, the first time it's slipped out of the top 10 in four years of operation. Kraken and [the recently retired] Athena have provided 75 percent of the NSF's computational cycles—a huge accomplishment for UT.

Patricia Kovach, the new director, describes NICS as a "lean mean organization." Harrison says it's the smallest staffed supercomputer center, and yet by most metrics the most successful NSF has ever had.

Harrison says he wants JICS to play a primary role in advancing all aspects of computational science on the UT campus, from providing discretionary allocations of computer time, supporting graduate students as they start computational research, to providing training and contributing to the establishment of the curriculum in computational sciences—"essentially a catalytic role," he says. To do that, though, the joint institute needs a greater physical presence on the UT campus, where people can meet and interact.

"Some ten years ago, JICS was disengaged from the UTK life, as it was physically moved out to Oak Ridge. That 20-odd mile distance made a barrier that we need to consciously overcome," Harrison says.

Harrison began by opening a small JICS office on the UTK campus, which is already making a difference.

"UT has all the elements to be a top ranked institution in computational engineering. It's got visible, internationally strong research in this area: Jack Dongara in linear algebra and parallel computing, Joshua Fu on the climate side in civil engineering, David Keffer in chemical engineering Cynthia Peterson in biochemistry, Greg Peterson in electrical engineering. You can identify easily a dozen groups like this," he says.

Harrison says his long-term vision for JICS is to help cement UT's national presence in supercomputing.

"We have a clear mandate, to use JICS influence to advance the cause of computational science at UT; when we do that ORNL wins as well—and they recognize that."

Research by teams affiliated with the ***UT-ORNL Joint Institute For Heavy Ion Research*** found its way into the popular press again this year. JIHIR, the most mature of the joint institutes, has broadened its scope from the original exclusive focus on projects aligned with the ORNL Holifield Radioactive Ion Beam Facility (HRIBF) to include reaction and decay studies at other experimental facilities. The expanded focus includes work from other radioactive-ion beams, studies of relativistic and ultra-relativistic heavy ions, and a broadened emphasis on nuclear structure theory.

Tin-101

Experiments at the HRIBF revealed tin-101's unexpected reversal of ordering in the lowest energy states of the nucleus, a finding that appeared to violate the standard scenario offered by the nuclear shell model.

More than a half-century old, the shell model has become the blueprint for how nuclei—the heart of all atoms—are put together. Once the shell of the nucleus is full or "closed" it becomes much more difficult to add or subtract a proton or

Building construction on the Cherokee Farm Campus is scheduled to begin this year.

Courtesy of the UT-ORNL Joint Institute for Advanced Materials neutron. The neutrons and protons are depicted as moving in orbits, much like electrons in atoms, but their individual motion is modified by nuclear forces that tend to bind neutrons into pairs. If protons and neutrons within a closed shell are assembled in what are called "magic" numbers—2, 8, 20, 28, 50, 82, and 126—they bind the nucleus even further against decay. "Doubly magic" nuclei have magic numbers of both protons and neutrons. Tin-132, as JIHIR affiliate ***Kate Jones*** and her team reported last year, is one of the few observed "doubly-magic" isotopes.

Tin-101, which has a single neutron orbiting tin-100's closed shell of 50 protons and 50 neutrons, does not conform to the standard picture, found in nearby isotopes tin-103, 105, and 107. JIHIR-affiliated researchers ***Iain Darby*** and ***Robert Grzywacz*** found that the spin of the extra neutron determines the spin of the isotope, and that in its ground state the spin is opposite to that found in the other isotopes. They attribute this reversal to the strength of the pairing force between neutrons: the pairing force changes depending on the neutrons' orbits. The switch is unexpected because typically in territory around doubly magic nuclei, three-particle and single-particle systems have identical spin.[15]

Binding Energy in the Nucleus

Different combinations and arrangements bind an atomic nucleus together and store its energy inside. Approximately 3,000 kinds of nuclei are known to exist: 300 of these on Earth, the remainder in accelerators and the stars. Nuclear physicists speculate this number could double if coordinated experimental and computational methods prove successful, but many of these tiny systems are difficult to study, largely because they have such short lives before decaying.

Witek Nazarewicz, JIHIR affiliate, UTK physics and astronomy professor, and ORNL HRIBF scientific director, describes the basic structure of a nucleus as resembling a droplet of liquid with high density inside, a surface where the density drops, and an exterior where little density exists. The quantum behavior of protons and neutrons at its surface determines the energy of the nucleus and how it interacts with other nuclei.

"We need to know how the nuclear energy is generated," Nazarewicz says, but describing all the nuclei and possible reactions inside and among them is daunting. Density functional theory (DFT) is useful in determining the densities of protons and neutrons in nuclei, but computationally intense, given the number of parameters that must be taken into account.

"If we can determine the densities precisely, we can determine the binding energy—the energy stored in the nucleus," Nazarewicz says. But, describing all the nuclei and reactions among them require powerful new algorithms running on high-performance computers.

Combining novel algorithms with powerful computing resources at ORNL and Argonne National Laboratory, a team of collaborators bridged the gap between mathematical theory and an implementation designed for physicists and accelerated this discovery process . What used to take two years can now be done in two hours.[16, 17]

Proton Halo of Flourine-17

Most atomic nuclei are compact structures with defined, sharp borders. In certain exotic nuclei, however, weakly bound protons or neutrons will drift away from the core, creating a cloud that surrounds the central core like a halo. Halo nuclei appear at the limits of nuclear existence and being fragile and short-lived (lasting only a millisecond) are extremely difficult to study.

Thomas Papenbrock, and other JIHIR-affiliated collaborators have calculated the proton halo in fluorine-17—a daunting challenge in nuclear theory—with its 17 strongly interacting protons and neutrons and a weak binding state. Combining sophisticated mathematical methods with the supercomputing power of ORNL's Jaguar, the team reproduced the tiny separation energy of the halo and a computed binding energy (that which holds the nucleus together) that reflects experimental data.[18]

The Joint Institute for Advanced Materials is a UT-ORNL umbrella organization that fosters interdisciplinary research and education for the development of advanced materials.

As the cornerstone facility on the Cherokee Farm Campus, the JIAM building will be an interdisciplinary center of excellence for materials research and development.

Distinguished Scientists

Robert Hatcher
(July 1986)
UTK Department of Earth and Planetary Sciences

David Joy
(April 1987)
UTK departments of Biochemistry, and Cellular and Molecular Biology and Materials Science and Engineering
ORNL Materials Science and Technology Division

Georges Guiochon
(June 1987)
UTK Department of Chemistry

Joeseph Macek
(July 1988)
UTK Department of Physics and Astronomy
ORNL Physics Division

Jimmy Mays
(January 2002)
UTK Department of Chemistry
ORNL Chemical Sciences Division

Takeshi Egami
(June 2003)
UTK departments of Materials Science and Engineering and Physics and Astronomy
ORNL Materials Science and Technology Division

Elbio Dagotto
(June 2004)
Correlated Electron Theory Group, UTK Department of Physics and Astronomy
ORNL Materials Science and Technology Division


Photo by Jack Parker

Elbio Dagotto develops computational models and numerical techniques that predict how strongly correlated electronic materials will respond in the presence or absence of an electric or magnetic field.

Materials

Iron arsenide superconductors

A nanoscale or smaller object behaves differently from its larger-scaled counterpart.

Elbio Dagotto: nanoscale electronic behavior

Visualize a film, one-atom or one-molecule thick. Spread it out across a flat surface, with the atoms distributed individually like marbles on a tray. The film's increased surface area in relation to volume creates a different dynamic than you would expect to find in a three-dimensional material of the same substance, where the atoms surround each other. The film's electronic and atomic movements are confined (restrained) to the interior of the nanoscale surface—a fact that changes the material's mechanical, thermal, and catalytic characteristics. The reason is that electrons will collide with one another (i.e. interact with one another) more often in a low dimensional geometry, such as a surface or a wire, thus altering the properties of the material. Physicists use the phrase "strongly correlated electronic behavior" to describe this phenomenon.

Elbio Dagotto's research group studies transition metal oxides and the recently discovered iron arsenide (FeAs) materials, which become superconductors at temperatures as high as 55 Kelvin (that's -218 degrees Celsius; water freezes at 0 degrees Celsius). These materials, and others studied by Dagotto such as oxide superlattices, show promise for improved memory devices, solid-state batteries, and other energy-saving electronics.

Dagotto's group has modeled the interplay between electronic and magnetic properties in superconducting FeAs materials. At this tiny scale the physics becomes extremely complex.

Normally, electrons repel each other because of their similar charge. But when an electric voltage is applied to conventional superconductors operating at near absolute zero temperatures, the electrons pair-up and move through the material's crystal lattice without resistance. In theory the electrons coordinate their movement with vibrations (phonons) in the crystal lattice to overcome their repulsion to each other.

But, scientists think something else is at work in the higher temperature, superconducting iron arsenide because the vibrational mechanism isn't strong enough to make it superconducting.[19] This led Dagotto and others to propose that magnetism rather than atomic vibrations might provide the glue between electrons. His theoretical work this year supports this idea. ■

Takeshi Egami: dynamics of complex oxides and mechanical properties of liquids and glasses

Discovered some 25 years ago by Bednorz and Müller (Nobel Prize 1987), the microscopic mechanism underlying high-temperature superconductivity in copper oxide (cuprates) remains unknown. Strong electron correlation presents a formidable challenge both in theory and experiment. When Fe pnictides came on the superconducting scene in 2008 (FeAs being one of these), researchers were encouraged by their simpler structure and electronics. Nevertheless, varying magnetic structure and composition complicated the picture.

Neutron scattering is one of the few experimental tools sensitive to the nuclei of atoms and at the same time the magnetic interactions of their electrons. ***Takeshi Egami***'s group used neutron scattering to examine the iron pnictides and discovered they all share a common magnetic interaction in spite of apparent differences in magnetic structure; this magnetism strongly interacts with the lattice. Their results open a door to clarifying this phenomenon with a simpler, possibly more general, theory.

Elasticity and flow may not be what they seem.

Glasses and liquids

The atomic physics of liquids and glasses presents a similar problem in that little is understood about the underlying basic mechanisms of various properties. Egami's group used synchrotron X-ray scattering experiments and computer simulation to examine the atomic motion of flowing liquids and elasticity in metallic glasses—known for their mechanical strength.

The group found that in metallic glass elasticity is not what it seems. Under stress the glass deforms following Hook's law—the amount of change in shape (strain) is proportional to the stress. In a crystalline material this behavior is a natural consequence of elastic deformation of the lattice, which bends without changing the topology of the atomic structure—i.e. the connections among the atoms. But in glasses they found the topology changes under stress, including an exchange of atoms among neighbors. Still, because the amount of deformation is proportional to the stress, the deformation appears elastic, even when it is not.

Photo by Jack Parker

Takeshi Egami develops theoretical models and uses neutron and X-ray scattering experiments to understand the mechanical properties of liquids and glasses, and to seek the mechanism underlying high-temperature superconductivity.

With liquids the flow looks like a continuous process and so the details of atomic motion appear to be irrelevant because they are so random. But, atomic-level simulation proved this was not the case. Egami's group found the atomic-level flow of a liquid is always triggered by the collapse of the environment surrounding a randomly chosen atom, which causes relaxation of the atoms nearby. So, rather than being continuous, liquids flow through a series of discrete atomic processes. ■

Polymers

Jimmy Mays: synthesizing new polymers

DuPont™ Nafion® is the most widely used ion-exchange membrane inside fuel cells today; but in spite of some 30 years of study, we still don't understand how the material transmits protons—information that could help create more efficient membranes and fuel cells. We do know the material has fluorinated units and negatively charged sulfonic acid units in the polymer chain, but the debate about its internal structure continues.

Polymer scientists, ***Jimmy Mays*** among them, would like to understand how Nafion transports protons through the material, but they are thwarted by confusion about its morphology—namely how the fluoropolymer segments and sulfonic acid groups arrange themselves. Nafion structure is highly heterogeneous, with polymer chains of varying lengths and an unpredictable distribution of sulfonic acid groups along the chain. When dissolved the material aggregates into clumps. Even its molecular weight is in question. As a result, proton transport through the membrane remains a mystery.

So to begin to decypher the material's complex molecular arrangements, Mays's team synthesized polymer models that mimic Nafion's fluorinated and sulfonic acid units. Only these have diblock copolymers of uniform length and composition—meaning they are units with two distinct blocks bonded together. What they found was that when their materials self-assemble as solids they create structures opposite of the norm, where the majority component surrounds islands of the minority component. And, in watery solutions the copolymers also formed unique arrangements, including ribbon shaped structures and tapered rods. Simulations by Bobby Sumpter and co-workers at ORNL support the group's theory that these tapered rods and ribbons form because the polymer segregates into structures based on the sulfonation content of its individual chains. ■

Touted for their promise as a power source in future automobiles, safe, efficient hydrogen fuel cells, still have a way to go to live up to their "clean green" potential.

Jimmy Mays synthesizes new, precisely tailored polymer materials and examines their molecular architecture, composition, and blending capability to discover how the form and structure, including their nanostructural order, might be manipulated to create useful polymer materials.

Imaging: looking inside soft materials

David Joy: accurate microscopic and nanoscale imaging

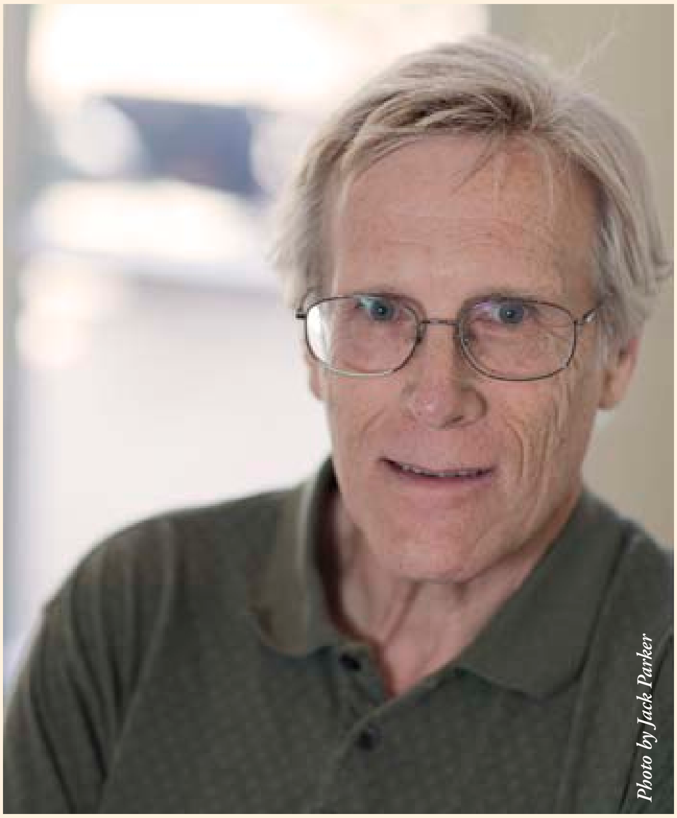
Although it is the flow of protons through the Nafion membrane that produces the desired electrical output, we still do not understand what happens to the ions and molecules iinside the material. ***David Joy*** and fellow team members Qianping He, David Keffer and Thomas Zawodzinski (Zawodinski is featured on page 38) have begun investigating the in-plane conductivity of the membrane, using an advanced imaging system they set up at the ORNL Center for Nanophase Materials Science. The team will correlate this information with physical attributes of the material and map the conduction pathways to see how the material's topography and thickness influence proton flow.

Soft material, especially biological material, cannot withstand the "heat" of high-energy scanning electron microscopes; but at the same time, precise nanoscale measurements are critical for setting standards and improving production in semiconductor and nanomanufacturing industries.[20]

"[One] promising option is . . . [to use] ion, rather than electron, beams," Joy says in "Protons, Ions, Electrons and the Future of the SEM."[21]

"As first pointed out by Levi-Setti more than thirty years ago, ions are much more massive than electrons and so their wavelength[s are] at least 50 to 100 [times] smaller than that of an electron of the same energy. Since scanning beam systems are always ultimately limited in performance by diffraction, reducing wavelength by such a large factor makes a substantial improvement in resolution a definite possibility."

Recently, Joy and long-time collaborator Philip Rack (JDRD project – 2007-08) created the first practical and detailed computer simulation of interactions among low energy helium ions, sample materials, and the secondary electrons that follow. Already highly successful, the program has proven useful for interpretation and prediction of ion images. ■



David Joy specializes in improving the accuracy and performance of electron and ion beam imaging and electron optical analysis. His team develops precise measuring techniques for imaging smaller and smaller materials, below the scale that most of today's instruments can measure.

Probing material with charged particles

Joseph Macek: electron vortices in simple atomic systems

The probabilities of finding electrons at given points in space are described mathematically in quantum mechanics. ***Joseph Macek*** relies on this theory to study what happens to simple, fragmented atomic systems when atoms collide.

In 2008, Macek's team began work with an experimental group from Frankfurt, Germany, which had data from electron

Joseph Macek's three-dimensional models show a proton punching its way into atomic hydrogen, creating vortices of electrons that encircle the atom and swirl like water being sucked down a drainpipe. His team's computations—now confirmed by experimental data—also show the electron movements are consistent with a hydrodynamic representation of quantum mechanics.

impact ionization (e,2e) experiments—a technique used to ionize and fragment sample molecules before analysis by mass spectrometry. The term e,2e is shorthand for what happens when electrons strike atoms, molecules, or larger solids and eject two electrons simultaneously. The German group's experimental studies probed correlations among these electrons and found circumstances where electrons were completely absent from the atomic system (a zero measurement). Computations by Macek's group related these instances of absent electrons to vortices in the underlying two-electron wave function. The German group's experimental confirmation of the vortices predicted by Macek's computations make this a significant textbook contribution to the description of basic quantum mechanics.

The evidence for atomic scale vortices in this context also has implications for control and manipulation of atomic processes, for example in the known velocity limits of charged particles used to probe atoms, molecules, and solid structures by fast electron beams. Early results from collaborative work between Macek's team and a group from ORNL show the ring vortices can be produced by short pulse excitation and ionization of atoms.

The team has also expanded their computational method to multi-electron species, to prove the vortices are not specific to single electron systems, alone. ■

The complexity of biological and chemical substances defies the most powerful analytical methods to separate and identify these mixtures of compounds.

Georges Guiochon is an expert in the art of separating components of complex samples with multidimensional chromatography. His team's extensive expertise improves the efficiency of chromatographic columns, optimizes conditions for maximum production of safe, effective pharmaceuticals at minimum cost, and studies the fundamentals of supercritical fluid chromatography.

Separating materials into basic components

Georges Guiochon: separation science

Chromatography involves injecting a plug of sample into a stream of solvent that percolates along a column packed with a suitable powder of porous particles. The sample components equilibrate between the solution and the surface of the particles allowing the molecules of the compound to stay adsorbed for a fraction of time, which delays their elution from the column. Each molecule's retention time depends upon its interaction with the solvent and the particle surfaces. If the system's solvent and solid are well chosen, the sample components will be separated and detected because they leave the column at slightly different times.

The fluid used to percolate a column can be gas, liquid, or what especially interests ***Georges Guiochon***'s group: supercritical fluid.

"Actually, a more accurate but less attractive name: 'nearly critical' fluid," Guiochon says.

Gas chromatography uses low-pressure fluids. Remarkably, certain fluids are liquid under high pressure but in intermediate ranges of temperature and pressure, their behavior is intermediate between those of gases and liquids. They remain nearly as good solvents as their liquid counterparts but have low viscosity and high diffusivity and are able to provide precise, reproducible results—a long-awaited feature in the chromatographic research community. Until recently supercritical chromatographs proved difficult to design, manufacture, and operate. But recent progress is opening the field for Guiochon's group to study the thermodynamics and kinetics of non-linear supercritical chromatography. The group has already discovered that the density of the fluid, more than its pressure, controls the characteristics of flow and solvent capacity. ■

Large faults, mountain chains, and continental crust

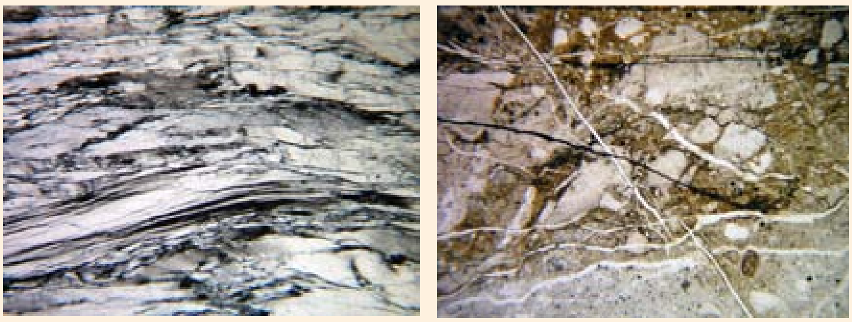
Robert Hatcher: structural geology and tectonics

Large faults in continental and oceanic crust help characterize the Earth's crust as a whole. For example the Brevard fault, a multiply reactivated fault traceable from Alabama to Virginia, and several large faults in the Georgia and Carolinas Piedmont, including one discovered by ***Bob Hatcher***'s graduate students during the late 1990s, have now been traced throughout the Carolinas and Georgia. While some of the faults have not reactivated, others nearby have, such as the Towaliga in Georgia, which formed 300 million years ago during the collision of Africa with North America. The Towaliga became inactive, and then reactivated some 200 million years ago as Africa and North America separated and the present-day Atlantic Ocean opened. The reactivation of Towaliga and its interaction with non-reactivated faults yield important data about large fault behavior in the deep crust, and addresses fundamental questions about why some faults reactivate (e.g., Towaliga and Brevard) while others located nearby do not.

Information gathered along deeply eroded ancient faults like the Brevard, Towaliga, and others helps Hatcher's team understand how modern active faults behave in the deep crust. Minerals present in rocks from different fault zones provide direct information about the pressure and temperature in the crust where a fault moved. Research by Hatcher's team has determined that some Appalachian faults moved at great depths under plastic (solid-state flow) conditions; whereas others nearby moved later, at shallower depths, then were reactivated after erosion thinned the crust to a thickness where fault movement involved both plastic and brittle (crushing) behavior. Brittle deformation on the Towaliga fault occurred between disconnected plastic segments joined by fractured and broken rock. The team also found that after first pulling straight apart, Africa rotated counterclockwise before resuming the pull-apart motion that opened the Atlantic.

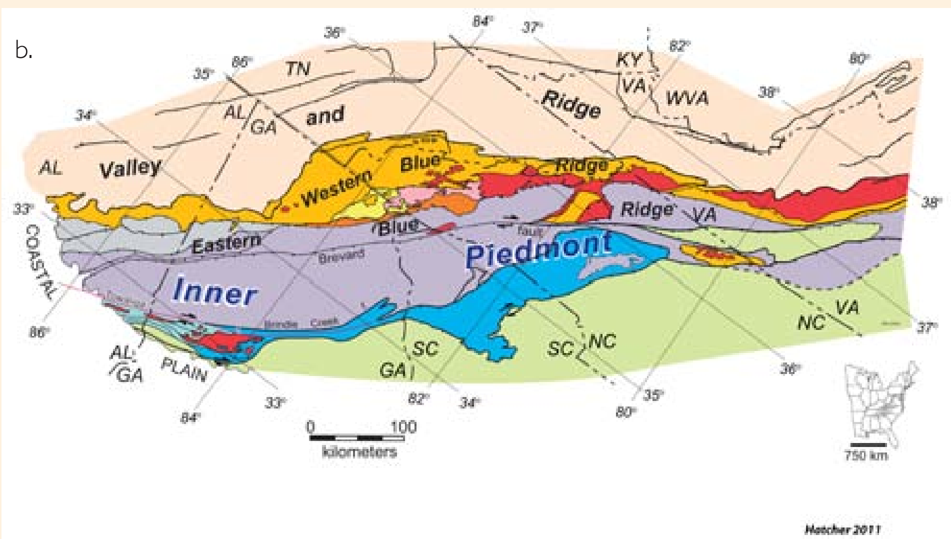
Hatcher's research into the prehistoric earthquake activity in the East Tennessee seismic zone continued during 2010-2011. Additional evidence of prehistoric earthquake activity has been found reconfirming that earthquakes of at least magnitude 6.5 shook this region in the prehistoric past. An important goal for Hatcher and his team is to determine how frequently large earthquakes occur here. ■

a.



(a) Photomicrographs (above) and hand specimens (below) of plastically (left, indicated by the flattened and drawn-out quartz grains) and brittlely (right, indicated by the multitude of fractures) deformed quartz-dominant rocks from the Towaliga fault in Georgia. They represent plastic deformation deep in the crust and brittle deformation in the shallow crust upon later reactivation of the fault. (b) Tectonic map of the southern Appalachians showing the locations of the large faults discussed here.

b.



A cornerstone of ***Bob Hatcher***'s research has been an attempt to understand the behavior of large faults. His team conducts intense, detailed field and laboratory studies of world-class southern Appalachian faults, comparing them with faults in other ancient and modern mountain chains.

Governor's Chairs

Jeremy Smith
(October 01, 2006)

UTK Biochemistry and Cellular and Molecular Biology Department

UT-ORNL Center for Molecular Biophysics;

ORNL Biosciences Division

Robert Williams
(April 29, 2009)

UT Health Science Center

Frank Loeffler
(May 01, 2010)

UTK departments of Microbiology and Civil and Environmental Engineering

ORNL Biosciences Division

Alexei Sokolov
(August 01, 2009)

UTK departments of Chemistry and Physics and Astronomy

ORNL Chemical Sciences Division

Yilu Liu
(August 01, 2009)

Power Information Technology Laboratory, UTK Electrical Engineering and Computer Science Department

ORNL Energy and Transportation Science Division

Tom Zawodzinski
(August 01, 2009)

Physical Chemistry of Materials Group, UTK Chemical and Biomolecular Engineering Department

ORNL Materials Science and Technology Division

William Weber
(May 01, 2010)

UTK Materials Science and Engineering

ORNL Nuclear Materials Science and Technology, Materials Science and Technology Division

Howard Hall
(May, 01, 2009)

UTK Nuclear Engineering Department

ORNL Global Nuclear Security Technology Division

Brian Wirth
(July 01, 2010)

UTK Nuclear Engineering Department

ORNL Consortium for Advanced Simulation of Light Water Reactors, Reactor and Nuclear Systems Division


Courtesy of Jeremy Smith


Courtesy of Rob Williams


Photo by Harrison Pang


Courtesy of Yilu Liu


Courtesy of the UTK College of Engineering


Courtesy of the UTK College of Engineering


Courtesy of the UTK College of Engineering


Courtesy of the UTK College of Engineering

Nuclear Security

Howard Hall

global nuclear security

Howard Hall is a member of an elite team of scientists, educators, law enforcement experts, policy advisors, and politicians assigned the task of protecting the U.S. from nuclear threats. He says global nuclear security comes down to two fundamental issues: opportunistic threats and arms-control negotiations.

With the explosion of computer technology, design secrecy is a thing of the past. So, controlling the material that could be used to make a nuclear weapon ranks number one in the rulebook of nuclear security. But, establishing realistic targets for securing weapon's grade nuclear material is not a simple exercise. It requires weighing the impacts of policy on other industries and organizations (such as the nuclear medical community) and the overall costs of removing or securing the material. Typically, Hall says, the 80/20 rule applies here: the first 80 percent being relatively inexpensive to secure; the other 20 percent extremely expensive. The trick is to figure out what quality and quantity of material is too low to pose a reasonable risk.

Hall also says it's "really, really dangerous" to assume an adversary is going to "think the way we think" or make decisions based on what we think is their capability. The key is to make sure we secure enough of the material so that no one can scrape together a sufficient amount to make a threat.[22] ■

Brian Wirth

computational nuclear engineering

Nuclear Regulatory Commission records[23] show the General Electric-designed nuclear reactors at Fukushima Daiichi are similar to several in the U.S. These went into operation in the early 1970s. They were designed to withstand a 7.0 earthquake and actually did function as designed immediately following the earthquake. It was the sequence of events, including the tsunami, which caused the subsequent problems with removing the radioactive decay-heat.[24]

The nation's aging nuclear reactors present Brian Wirth an unprecedented opportunity to examine the effects that decades of extreme temperatures and constant radiation have on specific reactor materials. Wirth's research group uses high-fidelity computer simulation to study the lifetime of nuclear reactor components and the physical processes responsible for material defects and degradation of reactor performance.

Wirth says the Fukushima Dai-ichi Unit 1 was originally scheduled for decommissioning at the end of March 2011, but recently received a 10-year license extension.

"Perhaps a lesson to heed from Japan is the cost of not acting," he says.[25]

"Ultimately, a pragmatic cost-benefit analysis of nuclear energy should be compared to similar cost-benefit analyses of other energy sources, where risks and costs associated with all energy sources are openly discussed, with a clear intention to reduce both the environmental

Howard Hall applies a background in nuclear chemistry to assess and find solutions for the nearly overwhelming challenges confronting nuclear security specialists. His research addresses questions of proliferation, detection, counter-proliferation, detection of and response to radiological or nuclear threats, radiochemistry, and nuclear forensics.

Brian Wirth investigates the performance of nuclear fuels and structural materials in nuclear environments. His research improves predictions about the longevity of nuclear reactor components.


Courtesy of Jeremy Smith

Jeremy Smith and the Center for Molecular Biophysics' team of UT professors and ORNL staff scientists combine experimental neutron scattering and large-scale computational simulation and modeling techniques to describe molecular structure and motion. Their research makes use of theoretical physics, quantum chemistry, statistical mechanics, computer science, supercomputing, catalytic chemistry, polymer science, biochemistry, and molecular biology.

impact and our reliance on politically unstable regions for energy."

In addition to identifying risks involved in aging nuclear reactor materials, Wirth's results can be applied to future development of high-performance, radiation-resistant materials for advanced nuclear fission and fusion energy power plants. ■

William Weber

radiation response of materials

When an electrically charged atom (ion) hits a solid, it both knocks the atoms about and transfers energy to the electrons. This second reaction is not well understood. Weber and Yanwen Zhang, a joint faculty associate professor who joined UTK in June 2010, developed an experimental approach to measure the energy lost to electrons in such collisions and its effect on material response. This is a vital step in understanding how material will respond to the effects of extreme radiation.

Energetic ions are the primary mode of energy dissipation from nuclear reactions and radioactive decay. So, understanding how the atoms in a material react is key to maintaining old and designing new nuclear reactors. Weber's team aspires to predict the performance of materials in nuclear reactors for 30 to 60 years. In the case of nuclear waste products, we may need to predict behavior over 10,000 or one million years, depending on what the Nuclear Regulatory Commission decides.

Weber and Zhang have been working with other faculty members and ORNL scientists to establish an advanced ion laboratory at UTK. It is scheduled to be operational at the beginning of 2012. ■


Courtesy of the UTK College of Engineering

William Weber studies the effect radiation and charged particles have on materials. Weber's team uses direct measurements of irradiated materials and powerful computational simulation to predict the long-term resilience of materials in extreme environments. Their work also examines defect-property relationships in ceramics and the use of ion- and electron-beam interactions to selectively engineer materials with desirable properties.

Molecular Biophysics and Dynamics of Soft Materials

Jeremy Smith

molecular biophysics

Neutrons give direct, simultaneous information on molecular structure and dynamics in a way that no other probe of matter can, Smith says. "This should help us design new materials in the energy sciences, and understand important topics in bioenergy and biology. For example, we recently demonstrated with neutrons how a cancer drug, methotrexate, softens the target it binds to. That is fundamental to understanding of how drugs work."[26]

Supercomputer simulations and modeling capability add a layer of complexity unavailable through molecular experiments alone. In one case, for example, Smith's team compared computer simulations of normal protein structures with mutant proteins from the rare but deadly neurodegenerative disease, Gerstmann-Sträussler-Scheinker (GSS) syndrome. This disease comes from a single mutation in a protein, which causes it to misfold, then accumulate and form amyloidal plaque in the brain. They found the GSS protein looks dramatically different from the normal protein and revealed how the shape was primed for plaque formation.[27]

Smith's team also turned the combined force of neutron scattering experiments and large-scale supercomputing simulation on lignin, the molecule complicating next-generation biofuels. Lignin, a major component of plant cell walls, aggregates into clumps that inhibit conversion of feedstocks into biofuel. The group's studies revealed the aggregates have a highly folded structure. The increased surface area creates more opportunity for capturing passing enzymes, which, in turn, reduces efficiency of the conversion.[28] ■

Photo by Harrison Pang

Alexei Sokolov studies molecular motion as the key to macroscopic properties of material. His team's interest is in the fundamental properties of soft materials—by definition materials that can change. They use various experimental techniques to learn about molecular movements in soft materials and develop basic principles, basic physics, basic understanding of nature that suggest how we might design material with unique properties.[29]

Alexei Sokolov

soft materials

Soft materials include liquids and glasses, colloids and liquid crystals, polymers and biological systems. Their applications span from energy (e.g. batteries and fuel cells), to lightweight materials to biotechnologies.

"The advantage of soft materials is that they are self-adapting, self-healing. They are smart." Alexei Sokolov says. You can change them; . . . They respond to any external force or field, or even a change in pH." Understanding this adaptation and self-organization is the key to design novel functional materials.

"If you understand the behavior of small molecules, you can apply it to complex systems," he says. Sokolov's group uses several experimental techniques to figure out how molecules move. These include various light scattering and dielectric spectroscopy techniques. Their most advanced tool, neutron scattering, provides critical information about molecular position and motion. Collaborations with researchers using computer simulations help to visualize the molecular motions.

Frank Loeffler explores microbial processes in soils, sediments, and groundwater. His team discovers new microbes and studies their properties, for example their ability to break down man-made pollution. He is an expert in using microbes to clean up contaminated sites, including impaired groundwater.

Sokolov's group works actively with chemists, biologists and engineers in developing novel materials for batteries and supercapacitors, for vaccines and tissue preservation, and other applications. ■

Microbiological Systems

Frank Loeffler

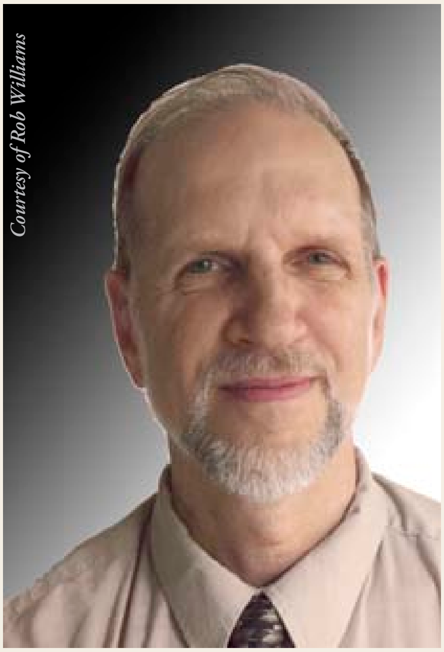
microbial processes

Frank Loeffler is one of the "good guys" in the fight to protect and restore environmental health amidst the pressures of an exploding human population. His team characterizes the intricate processes that enable naturally occurring bacteria to break down toxic contaminants, immobilize radioactive wastes, reduce greenhouse gas emissions; not to mention generate energy from waste materials.

"Of all the microbes out there, 99 percent have never been characterized, which means the undiscovered potential for innovative engineering and possibly medical applications is enormous," Loeffler says. "We can learn a lot from microbes and use them to produce things more efficiently without impacting the environment. There's a lot of promise in the microbial world for new biotechnological processes that clean up waste streams and produce new materials such as biodegradable plastics or generate energy. We have just scratched the surface."

Equally exciting are the new molecular and computational tools that allow his team to study this unexplored diversity and functionality (what the microbes can do) in much greater detail. The group's innovative discoveries form the basis for alliances with other researchers in microbiology, engineering, and industry, developing and testing molecular monitoring tools in real-world situations. UTK and ORNL's close proximity and strong cross-disciplinary base for doing fundamental research in environmental biotechnology give Loeffler's team a unique opportunity to develop their ideas.

"It's an exciting time [and place] to be a microbiologist," he says. ■



Courtesy of Rob Williams

Computational Genomics

Robert Williams

genetics and human health

Robert (Rob) Willliams says most studies to discover the role of genes in various diseases have relied on mutagenesis techniques pioneered at ORNL using the common house mouse. More recently, research has targeted single genes in genetically engineered mice, using the so-called "knock-out" technology, which inactivates a gene by replacing or disrupting it with an artificial piece of DNA.[31] Both methods disturb gene function. Scientists then study the mutant offspring to determine how this changes biological functions.

But, the single shot approach doesn't tell us enough about the most common and pervasive diseases, such as heart disease, neurodegeneration, and psychiatric disorders. Williams says these are usually caused by an accumulation of small detrimental effects to many normal genes, which for one reason or another don't work well together. Such complex and unfortunately common human diseases often correspond to an equivalent mouse trait or disease; even autism and schizophrenia have mouse models.

Robert Williams uses many different sets of identical mice (up to 100 sets) to study the genetics of diseases that range from high blood pressure to aging to impaired brain function. His group combines mouse resources with new, highly efficient DNA sequencing technology and sophisticated computational methods[30] to determine just how far we are likely to get with personalized human health care. Rob William's research group built the widely used, online Mouse Brain Library and GeneNetwork (www.genenetwork.org).

Through tricks of breeding, mice can be bred to be genetically identical, with identical genetic deficiencies—like human identical twins; except in this case it is possible to have hundreds of these identical mice. Williams's team studies the genetics of disease by cross breeding mice with specific, but different, ancestries (strains) and then comparing their offspring's risk of getting the disease. ■

Electrical Energy

Yilu Liu

smart-grid technology

Yilu Liu believes part of the solution to preventing large-scale power blackouts may lie in a powerful but low-cost technology housed in a small beige box called a Frequency Disturbance Recorder (FDR). Networked via the Internet, the FDR registers the electrical pulses moving through wires that connect power stations to business and homes.

At present, a frequency-monitoring network, or FNET, housed in UTK's Power Information Technology Laboratory monitors 80 FDRs placed around the country—a number Liu and her team will ultimately increase to 2,000, adding GridEye[32] units that connect a unique wide-area grid-monitoring network deployed by ORNL. The FDR measures subtle fluctuations in power supply 1,440 times per second. The unit's GPS receiver provides a timing signal—precise to the microsecond—while its algorithm detects and records fluctuations. The data is sent to servers at the Power Information Technology Laboratory where it is archived.

FNET enables a dramatic visualization of power fluctuations and disruptions on a map, with green indicating a system in stasis and flashing waves of red, orange, blue, and purple representing wildly fluctuating frequencies emanating outward from the source of the disturbance.

The work by Liu's team represents a critical segment of what will evolve into the brain of a smart grid. The project relies on UTK's Kraken and ORNL's Jaguar supercomputers to simulate, far more quickly than real-time, the potential ripple effect of disruptions to the power supply.[33] ■

Thomas Zawodzinski

electrical energy storage

A fuel cell is a device that takes in fuel and then converts the fuel's chemical energy into electrical energy. Batteries serve a similar purpose, but they store chemical energy in a closed system, converting and releasing it as electrical energy on demand. Rechargeable batteries use an external energy source to reverse the electrochemical reaction and return the battery to its prior state, ready, once again, to discharge electrical energy. These same oxidation-reduction reactions in a fuel cell are powered internally.

With industry pushing hard to put fuel cells in automobiles, Zawodzinski expects at least one company will release a fuel cell car by 2015, if not sooner. This is far and away the hardest application because of the relatively low cost of current automobile engines compared with any fuel cell powered car we can make today.

Tom Zawodzinski wants to make fuel cells more durable over the long term and ensure that they function properly at the high temperatures found inside the cell. His team works on methods to improve the basic mechanics of those all-important chemical reactions at the heart of fuel cell and battery storage technology. ■

Yilu Liu develops new and better ways to monitor and understand flow of electricity through the nation's power grid. Her group is working to devise a smarter electric grid that automatically resolves minor disruptions before they escalate to major blackouts.

Thomas (Tom) Zawodzinski explores the basic mechanics of elementary chemical processes occurring in the materials used in batteries and fuel cells. His team's work bridges the gap between fundamental fuel cell research and the practical ways to make the technology widely useful.

Collaborate AND Compete

by Theresa Pepin

We are what we repeatedly do. Excellence is not an act but a habit. – Aristotle

One of the best things about the enterprise of science is that it demands its practitioners to excel simultaneously in three related roles—learner, teacher and doer. Tested by setback, teased forward by hunch and lucky break, and tempered by painstaking work, the cycle of learner-teacher-doer is a powerful combination in the quest for enlightenment and innovation.

Genius is 1 percent inspiration and 99 percent perspiration. . . . Opportunity is missed by most people because it is dressed in overalls and looks like work. – Thomas Edison

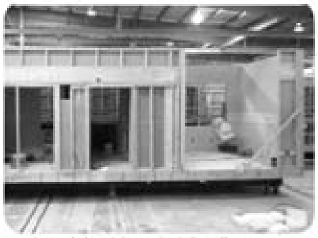
The Science Alliance goes beyond targeting brilliant research ideas to supporting the work of students and research leadership. In contrast to more traditional models, current scientific practices of collaboration and competition move forward much more quickly. They do so, at least in part, because they provide opportunities to present and, in turn, challenge interim research results through a critical peer review process, far in advance of the rigorous and time-consuming proofs required for scholarly publication.

If you don't make mistakes, you're not working on hard enough problems. And that's a big mistake – Frank Wilczek

Too often we think of the action verbs collaborate and compete in opposition to each other, but in scientific inquiry they are a natural pairing for learning, teaching and achieving. That is especially so because we learn at least as much from failure as from success. The Science Alliance contributes to several projects that promote this educational approach.

A New Norris House

off-site construction of modules



west module at 'marriage' wall

[insulating the west module] - The modular home builder worked in sync with the team of architecture students to design a home that would be compatible with its fabrication process. The installation of the modules was completed in one day, allowing on-site construction to proceed.

students and intern in discussion

finish materials in bedroom

installation of west module

installation of east module

'marriage' of east and west module

installation of dormer at west module

installation of insulation at north elevation

The [installation of the rain-screen facade] allowed students to synthesize aesthetics, building science, and the combination of off-site / on-site construction. the rain-screen allows the structure to breathe vapor properly while also shedding water and providing greater insulative properties to the wall assembly.

construction of rain-screen facade

completion of rain-screen at south facade

construction of special blocking at skylight

installation of high r-value insulation

installation of fixed window at east facade

This section of elements appeared on the presentation boards, submitted by the University of Tennessee School of Architecture and Norris community for a National Council of Architectural Registration Boards Prize. Subtitled "A Model for Integrated Project Delivery and Integrated Design Teams in the Academy that builds on the New Deal Legacy of the TVA," *A New Norris House* can be viewed on NCARB's website: http://www.ncarb.org/.

The project received one of five NCARB $7,500 prizes in 2011.

(Courtesy of A New Norris House *project)*

Collaborate

A New Norris House

It would be difficult to overstate the scale of the challenges undertaken by the Tennessee Valley Authority in the Depression years of the 20th century—taking on catastrophic flooding of agricultural land and population centers, enabling navigation of major regional waterways, and providing electricity for enormous areas of Appalachia previously without modern conveniences of any kind.

The small town of Norris, Tennessee, played an important part in that history when more than 500, 600-sq-ft homes were built from 1933 – 1936 based on a set of 12 designs. These incorporated the latest in construction techniques and are considered to be some of the most progressive home designs in America. The New Deal established Norris as one of the first planned, green belt communities in the U.S., including a vital community center and a network of walking paths. Today the town, home to 1,400 residents, is listed on the National Register of Historic Places and many of the original Norris Homes—most with some adaptation in the intervening 75 years—remain a valued part of the community.

At a compact 768 square feet, the New Norris House echoes the aspirations of the original cottages and land-use plan while seeking to work with the community to balance the best of the new and old in a way that is both sustainable and suitable for that particular community.

At the same time, it has afforded students, faculty, and professional practitioners the opportunity to learn how best to use new off-site fabrication techniques in a process of integrated project design/delivery (IPD) to arrive at a factory-built home that is prototypical but also site-specific. The work has involved confronting and resolving not only technological and scientific/engineering problems, but also the legal, social, and aesthetic issues that currently restrict green construction.

The award-winning result is an attractive, healthy, comfortable, affordable, energy-efficient, and environmentally responsible structure whose construction has taken students far beyond theory in a collaborative practice model. It bridges multiple disciplines, professions, trades, academe, and community. Now in its final phase, the project will continue to demonstrate the house to the public and evaluate its performance.

Visit www.thenewnorrishouse.com for more information.

Center for Intelligent Systems and Machine Learning

CISML
CENTER FOR INTELLIGENT SYSTEMS AND MACHINE LEARNING
THE UNIVERSITY of TENNESSEE UT COLLEGE of ENGINEERING

A new initiative for interdisciplinary research launched in late 2010, and led by Lynne Parker, of UTK Electrical Engineering and Computer Science and assistant director of the Science Alliance, CISML seeks to understand biological learning mechanisms and to design and develop computer-based systems that exhibit intelligent behavior, operate autonomously, and adapt to environmental changes.

CISML comprises six ORNL researchers from two divisions, ten UT faculty members from three colleges and five departments, and a talented pool of nearly 50 graduate students. Together they have produced in record time more than a half dozen proposal submissions and invitations to five separate federal agencies; this, in just the first half of 2011. Additionally, CISML has secured sponsorships from four private organizations as part of its industry affiliate program.

Visit http://cisml.utk.edu/ for more information.

Scalable Computing and Leading Edge Innovative Technologies

It will take truly collaborative and fully engaged interdisciplinary teams working fearlessly together to solve next-generation research questions. Given the vast quantities of data that can be collected with modern tools and techniques, and the exponential increase in high-performance computing power, a thorough grounding in computational science on the part of the multiple disciplines involved in today's research project teams is essential.

In 2010-2011 the Science Alliance continued support of the Integrative Graduate Education and Research Traineeship (IGERT) Scalable Computing and Leading Edge Innovative Technologies (SCALE-IT) program, which focuses on computational biology and the need to cultivate translational expertise of both computer scientists and biologists. Individuals from both fields come together into research projects from different cultures and methods of training in scientific inquiry.

To be successful in leading edge computational biology research, students must acquire a baseline of knowledge and skills beyond their own field's limits, and they must learn how to clearly explicate and teach others as their collaborative research programs develop. Two examples of skill sets that SCALE-IT students combined in successful student research projects include (1) graphics processing unit (GPU) computing, genetics, and informatics; and (2) ecosystem modeling, programming, and graph theory.

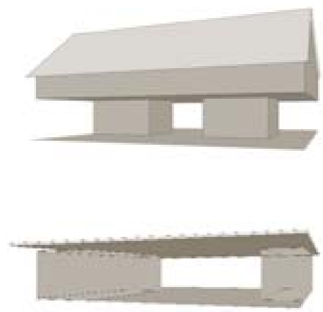
Significant outcomes of the program in 2011 also include the graduate course

"Introduction to Computer Programming for Scientists," which in its first semester attracted 19 students from 10 academic departments. It is expected that this course will soon become a regularly scheduled, cross-college offering. In turn, SCALE-IT computer science students have asked for a similar course to teach them biology. SCALE-IT biology students have responded by seeking funding to develop a bioinformatics lab course and class entitled "Introduction to Biology for Computer Scientists and Engineers."

Visit http://www.utk.edu/~scaleit for additional information on mentoring and outreach activities, publications, and accomplishments.


The UT Zero Energy House Prototype (above) was the first project completed by the UT Zero team. The house showcases innovations in building materials, solar energy, energy efficiency, and home design. The completed project serves as a platform for performance evaluation, material testing, and continued research.


Based on the success of UT Zero, the University of Tennessee formally established the Institute for Smart Structures in May 2010, a research center where academia, government research, and industry meet. The center is housed in UT's College of Architecture and Design and provides a platform for collaboration for faculty and researchers from the College of Architecture and Design, the College of Engineering, and Oak Ridge National Laboratory (ORNL). Living Light, UT's entry in the Solar Decathlon 2011 competition, is the institute's first project.

Inspired by the cantilever barns of southern Appalachia, Living Light's floor plan organizes support spaces into two cores, framing the open living space in between. The team created an energy-efficient living area connected spatially and visually to the landscape outside, using fixed aerogel panels on the north, moveable thermal shades on the south, and multi-pane glazing throughout with motorized shades and horizontal blinds sandwiched in between the panes. The house harvests the sun's energy using tubular photovoltaics that provide energy and shade for the home.
(Courtesy of the Living Light *project)*

Compete

Living Light

Enlisting academia, government research agencies, and industry partners in the disciplines of materials science, engineering, and architecture, the University of Tennessee's Institute for Smart Structures focuses on enabling technologies for sustainability, energy, health and safety, and economy, to solve immediate problems and to introduce revolutionary new concepts. From the time of the first UT Zero prototype in 2008, over 400 students have participated in this design-build-exhibit program.

In October the University of Tennessee will be one of 20 university teams from around the world competing on the National Mall in Washington D.C. in the 2011 U.S. Department of Energy's Solar Decathlon exhibit of energy-efficient solar-powered homes designed, built, and demonstrated by students. UT's entry is a cross-disciplinary, intercollegiate research and design project between the College of Architecture and Design, and College of Engineering, College of Business, College of Arts and Sciences, including the departments of Architecture, Electrical Engineering, Mechanical Engineering, Landscape Architecture, Interior Design, Graphic Design, and the Center for Entrepreneurship.

The inspired moniker of UT's 2011 Solar Decathlon net-zero-energy prototype is Living Light. The home integrates passive and active systems:

- Basic building design (siting, orientation, massing, and space planning);

Courtesy of the Tennessee Science Olympiad

- Passive design (daylighting, natural ventilation, cooling, and heat gain);
- High-performance building (efficient HVAC, active envelope, and building sensors); and
- Green power (decentralized and grid-tied systems such as solar and wind).

Taking historical cues from the cantilever barns of Southern Appalachia, the floor plan organizes spaces into two cores, framing the open living space in between and connecting to the landscape outside. The house optimizes electrical, mechanical, and architectural components for efficiency and includes an advanced control system to integrate complex systems with a simple user interface.

Following the national U.S. 2011 competition, Living Light may also exhibit in Madrid, Spain, if accepted for the European Solar Decathlon 2012 competition. Students are particularly looking forward to returning home and showcasing their prototype house on a tour of towns throughout Tennessee, where they will demonstrate energy-efficient technologies, sustainable design, and solar energy power generation to K-12 students and local communities. The tour and educational outreach builds upon Tennessee's long history of leadership in energy and "brings home" the value of solar and green technologies to its workforce and citizens.

Visit http://livinglightutk.com for more information.

Tennessee Science Olympiad and Tennessee Junior Science and Humanities Symposium

There is no question that universities in the United States of America are a beacon for exceptional students in science and engineering worldwide. Clearly, though, attracting and qualifying American students for higher education in the Science Technology Engineering, and Mathematics (STEM) disciplines of science, technology, engineering, and mathematics is a much harder sell. Our nation's future in the global economy depends on how well we can reverse current trends.

The Science Alliance has for several years contributed to two academic outreach programs as part of national and state initiatives to increase the number and caliber of students in STEM and to enrich science and mathematics education in our schools. The programs reinforce ongoing recruitment efforts and serve to give Tennessee's brightest young students the chance to get to know, first hand, about the exceptional reputation of the university's scientists and research facilities.

For full lists of sponsors and UT-ORNL staff researchers involved in these programs, visit the respective websites mentioned below.

Tennessee Science Olympiad

On April 2, 2011, UTK was host to 36 middle school and high school Olympiad teams with more than 800 participants. Held at the Knoxville campus since 1994, this state tournament brings winners from

A scientific and educational exhibit, staffed by representatives from research laboratories and STEM departments at UTK drew TJSHS students to view the exhibits and ask questions about research and educational programs at UTK and ORNL.

Jennifer Dye of Pope John Paul II High School in Nashville, TN received the 2011 Teacher Mentor Award.

seven regional Olympiads to compete for trophies and medals. The winning teams in each division receive travel support to advance on to the national competition.

First place winners this year were Montgomery Bell Academy (Nashville) in the high school division and Friendship Christian School (Lebanon) in the middle school division. Both advanced to the national tournament held at the University of Wisconsin, Madison, May 20-22, 2011, where they ranked 37 and 26, respectively, among the 60 teams.

Recent additions to the program include an upgrade of the website and development of workshops and handbooks for Olympiad coaches.

Visit http://tnscioly.utk.edu for more information.

Tennessee Junior Science and Humanities Symposium

Tennessee's 46th annual Junior Science and Humanities Symposium was held on February 24-25, 2011, with 37 students and 15 teachers representing 15 high schools. The event attracted five new Tennessee high schools this year from Shelby, Crockett, DeKalb, Knox, and Blount counties.

Fifteen students presented original research on a wide range of topics. Scholarships were awarded to the top three student presenters: Gloria D'Azevedo, senior at Oak Ridge High School, took first place; John Bollenbacher, junior at Webb School, took second place; and Bowei Deng, junior at White Station High School, took third place. Kevin Clavin of Pope John Paul II High School and Andrea Tipton of Cleveland High School earned honorable mentions in the competition.

All five award-winning students represented Tennessee at the National JSHS in San Diego, April 27-May 1, 2011, with the two top winners (D'Azevedo and Bollenbacher) competing against students from 48 states for additional scholarships. D'Azevedo won third place in the national competition and the opportunity to compete at the 2011 London International Youth Science Forum.

New this year was a teacher professional development workshop focused on mentoring student research led by Jennifer Dye, a noted high school teacher and author of *Investigating Science: A Guide to Conducting Independent High School Student Research* (Linus Publications, 2010). Also new was a scientific and educational exhibit staffed by representatives of research laboratories and STEM departments at UT Knoxville. Symposium attendees spent time visiting the exhibits and asking questions about the research and educational programs at UTK and ORNL.

Dye, of Pope John Paul II High School, also received the 2011 Teacher Mentor Award.

Visit http://jshs-tn.utk.edu for more information.

Grantseeking

All Science Alliance projects are expected to leverage the investment of their designated funding by UT-ORNL in follow-up competition for outside funding. In addition, since FY08 the Science Alliance has provided grant writing support for teams engaged in large, complex, and strategically important research proposals. In 2010-2011 professional contractor Jayne Dadmun worked with the Research Office director of proposal management to develop an Automatic Announcement Distribution System (AADS) for precise targeted funding for all UT faculty. Dadmun also helped with a web-based searches for faculty research interests, searching by research area to match specific funding or collaborating opportunities offered both by industry and funding agencies.

Professional contractors Carmen Trammell and Theresa Pepin assisted in proposal development for grants through the DOE, NSF, NIH and NEH amounting to $52.5M on behalf of researchers in nuclear engineering, materials science, psychology, industrial engineering, and solar energy. Not all of these will be awarded—and not all will result in unqualified success—but the ideas and work they entail are no less essential to future discovery and achievement.

It takes courage to grow up and turn out to be who you really are. – e.e. cummings

This annual report offers a summary of the intellectual endeavors of researchers in many different fields of science and engineering during Fiscal Year 2010-2011.

The Science Alliance acknowledges with pride and honor its mission to further the goals of students and scientific leaders at The University of Tennessee and Oak Ridge National Laboratory—some of the most compelling and productive people anywhere.

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UT-ORNL Joint Faculty

Appointee	ORNL Appointment in	Based at	Field	Appointment Title
Dagotto, Elbio	ORNL/MSTD	UTK/Physics	Materials	Distinguished Scientist/Professor
Egami, Takeshi	ORNL/MSTD	UTK/MSE	Materials	Distinguished Scientist/Professor
Joy, David	ORNL/MSTD	UTK/BCMB	Neutrons	Distinguished Scientist/Professor
Macek, Joseph	ORNL/PD	UTK/Physics	Atomic Physics	Distinguished Scientist/Professor
Mays, Jimmy	ORNL/CSD	UTK/Chemistry	Neutrons	Distinguished Scientist/Professor
Hall, Howard	ORNL/GNSD	UTK/Nuclear Engr	Nuclear	Governor's Chair
Liu, Yilu	ORNL/ETSD	UTK/EECS	Electrical	Governor's Chair
Loeffler, Frank	ORNL/Biosciences	UTK/Microbiology		Governor's Chair
Smith, Jeremy	ORNL/Biosciences	UTK/BCMB	Molecular Biophysics	Governor's Chair
Sokolov, Alexei	ORNL/CSD	UTK/Chemistry	Materials	Governor's Chair
Webber, William	ORNL/MSTD	UTK/MSE		Governor's Chair
Wirth, Brian	ORNL/CSMD	UTK/Nuclear Engr	NSTD	Governor's Chair
Zawodzinski, Thomas	ORNL/CSD	UTK/Chemistry	Materials	Governor's Chair

Name	Joint Appointment at	Based at	ORNL Contact	Field
Adhern, Shaun	UTK/EECS	ORNL/NCCS		
Banks, David	ORNL/NCCS	UTK/EECS	Ricky Kendall	Computing
Besmann, Theodore M	UTK/CIRE	ORNL/MSTD		
Bjornstad, David	UTK/Economics	ORNL/ESD		
Braiman, Vehuda	UTK/MABE	ORNL/CSMD		
Britton, Charles	UTK/EECS	ORNL/MSSE	Ted Fox	Detectors
Chen, Jin-Gui (Jay)	UTK/Plant Sci	ORNL/Biosciences		
Dadmun, Mark	ORNL/CSD	UTK/Chemistry	Mike Simonson	Neutron Scattering
Dai, Sheng	UTK/Chemistry	ORNL/CSD		
Datskos, Panos	UTK/CIRE	ORNL/MSSE		
Davison, Brian	UTKT/CIRE	ORNL/Biosciences		
de Almeida, Valmor F.	UTK/	ORNL/ETSD		
DePaoli, David W	UTK/Chemical	ORNL/ETSD		
Doktycz, Mitchel J.	UTK/CIRE	ORNL/Biosciences		Biosciences
Efremenko, Yuri	ORNL/PD	UTK/Physics	Glenn Young	Neutrons
Ericson, M. Nance	UTK/EECS	ORNL/MSSE	Ted Fox	
Fahey, Mark	UTK/IIE	ORNL/NCCS		
Ganguly, Auroop R.	UTK/IIE	ORNL/CSMD		
Gao, Yanfei	ORNL/MSTD	UTK/MSE	Thomas Schulthess	Materials
George, Easo	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Gleason, Shaun	UTK/CIRE	ORNL/MSSE		
Graham, David	UTK/Biosciences	ORNL/Biosciences		
Greene, David	UTK/ETSD	ORNL/ETSD		

Name	Joint Appointment at	Based at	ORNL Contact	Field
Greene, Geoffrey	ORNL/PD	UTK/Physics	Glenn Young	Neutrons
Grove, Robert E.	UTK/	ORNL/RNSD		
Harrison, Robert	UTK/Chemistry	ORNL/JICS	Jeff Nichols	Computing
Hauck, Cory D.	UTK/	ORNL/CSMD		
Hayes, Daniel J.	UTK/EEB	ORNL/ESD		
Hayward, Jason	ORNL/GNSTD	UTK/Nuclear Engr	James Rushton	
Hix, Ralph	UTK/Physics	ORNL/PD		
Jouline, Igor	UTK/Biology	ORNL/CSMD	Jeff Nichols	Comp. Biology
Kilbey, S. Michael	UTK/Chemistry	ORNL/CNMS	Linda Horton	
Klasky, Scott	UTK/EECS	ORNL/NCCS		
Maldonado, Ivan	ORNL/RNSD	UTK/Nuclear	James Rushton	
Mandrus, David	ORNL/MSTD	UTK/MSE		
Mench, Matthew	ORNL/ETSD	UTK/MABE		
Mezzacapa, Anthony	UTK/Physics	ORNL/PD		
Miller, William A.	UTK/ETSD	ORNL/ETSD		
Moreo, Adriana	ORNL/MSTD	UTK/PD	Peter Tortorelli	Materials
Morris, Jamie	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Narula, Chaitanya	UTK/CIRE	ORNL/MSTD		
Nichols, Trent L.	UTK/Grad School Med	ORNL/MSSE		
Norby, Richard J.	UTK/CIRE	ORNL/ESD		
Ostrouchov, George	UTK/CSMD	ORNL/CSMD		
Papenbrock, Thomas	ORNL/PD	UTK/PD	Glenn Young	Nuclear Physics
Paranthama, Parans	UTK/CIRE	ORNL/CSD		
Paul, Nathanael R.	UTK/EECS	ORNL/CSED		
Pennycook, Stephen J.	UTK/MSE	ORNL/MSTD		
Pharr, George M.	ORNL/MSTD	UTK/MSE	Steven Zinkle	Materials
Podar, Mircea	UTK/Microbiology	ORNL/Biosciences		Biosciences
Prowell, Stacy J.	UTK/EECS	ORNL/CSED		
Rack, Philip	ORNL/CNMS	UTK/MSE	Linda Horton	Materials
Rawn, Claudia	UTK/MSE	ORNL/MSTD	Steven Zinkle	Materials
Ray, William R.	UTK/MABE	ORNL/CSMD		
Read Jr., Kenneth F.	UTK/Physics	ORNL/PD	Glenn Young	Nuclear Physics
Sankaran, Ramanan	UTK/MABE	ONRL/NCCS		
Sayler, Gary	ORNL/JIBS	UTK/Biological Sci	Berry Berven	
Schadt, Christopher W.	UTK/Microbiology	ORNL/Biosciences		
Simpson, Michael	UTK/MSE	ORNL/CNMS	Linda Horton	
Simunovic, Srdjan	UTKL/CSMD	ORNL/CSMD		
Trinh, Cong	ORNL/Biosciences	UTK/Chemincal Engr		
Van Berkel, Gary	UTK/CIRE	ORNL/CSD		

Name	Joint Appointment at	Based at	ORNL Contact	Field
Vass, Arpad	UTK/Biosciences	ORNL/Biosciences		
Vazhkudai, Sudharshan	UTK/CSMD	ORNL/CSMD		
Wang, Fred	ORNL/ETSD	UTK/ETSD		
Wang, Shanfeng	ORNL/MSTD	UTK/MSE		
Weitering, Hanno	ORNL/MSTD	UTK/PD	John Wendelken	
Williams, Mark L.	UTK/CIRE	ORNL /RNSD		
Wilson, Bruce E	UTK/Enviro sci	ORNL/Enviro Sci		
Xiao, Kai	UTK/EECS	ORNL/CNMS		
Xing, Yulong	UTK/CSMD	ORNL/CSMD		
Zhang, Yanwen	UTK/MSE	ORNL/MSTD		

Key:

CIRE--Center for Interdisciplinary Research and Education
CNMS--Center for Nanophase Materials Sciences
CSD--Chemical Sciences Division
CSED--Computer Science and Engineering Division
CSMD--Computer Science and Mathematics Division
EEB--Ecology and Evolutionary Biology
EECS--Electrical Engineering and Computer Science
ESD--Environmental Sciences Division
ETSD--Energy and Transportation Science Division
GNSD--Global Nuclear Security Technology Division
IIE--Industrial and Information Engineering
ITSD--Information Technology Services Division
JIBS--Joint Institute for Biological Sciences
JICS--Joint Institute for Computational Sciences
MABE--Mechanical Aerospace and Biomedical Engineering
MSE--Materials Science and Engineering
MSSE--Measurement Science & Systems Engineering
MSTD--Materials Science and Technology Division
NCCS--National Center for Computational Sciences
NSSD--Neutron Scattering Science Division
PD--Physics Division
RNSD--Reactor and Nuclear Systems Division
ORNL--Oak Ridge National Laboratory
UTK--University of Tennessee Knoxville

Photo by Jack Rose

External Research Funds Awarded to UT-ORNL Distinguished Scientists in FY11

The table that follows lists the research funding brought in to The University of Tennessee from external sources by UT-ORNL Distinguished Scientists designated as principal investigators on the projects. These individuals also appear as investigators on many other funded research proposals, including large research grants awarded to Oak Ridge National Laboratory. A few examples of these are bulleted below.

- Elbio Dagotto is principal investigatorof an ORNL Field Work Proposal (FWP) with a budget of $1.7 million, which also supports R. Fishman, F. Reboredo, S. Okamoto, and joint faculty member A. Moreo. Dagotto also had a one-year ORNL subcontract of $126,381 to support three graduate students on a project entitled *Theoretical Studies of Model Hamiltonians*.

- Takeshi Egami was principal investigator on the $1.05 million ORNL FWP, *Atomistic Study of Bulk Metallic Glasses*, with J.R. Morris, E. George, D. Nicholson, and G.M. Stocks (08/01/04-07/31/11); and *Atomistic Mechanisms of Metal-Assisted Hydrogen Storage in Nanostructured Carbons* with N. Gallego, C. Contescu, and S. Pennycook.

- Georges Guiochon works with S. Dai of ORNL investigating the chromatographic properties of new silica and carbon adsorbents with hierarchical porosities and pore size distributions.

- David Joy works at both UTK and ORNL with UT-ORNL joint faculty member P. Rack on *Helium Ion Beam Imaging and Beam Induced Chemistry*; *Development of a Time of Flight Secondary Ion Mass Spectrometer* with B. Anderson, and P. Dodd of ORNL; and on an National Institutes of Health funded project, *Toxicity of Nanoparticles* with principal investigator M. Docktycz.

- Joseph Macek works on *Analysis of structure in low-energy ion-atom collisions* and on *Electron correlations in ion-atom collisions* with P. Krstic of ORNL and on *Benchmark calculations of atomic processes* with D. Schultz.

- Jimmy Mays is the ORNL Center for Nanophase Materials Sciences theme leader on Functional Polymer Architectures, one of three science themes in the center.

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 11 Expenditures
Dagotto	NSF-IMR-0716020	Correlated Electrons in Complex Oxides and Nanoscopic Systems	08/15/2007	07/31/2010	$ 408,000	$ 13,355
Dagotto	UT-B 4000099504	Theoretical Studies of Model Hamiltonians	09/29/2010	01/31/2012	$ 154,381	$ 79,340
Egami	UT-B 4000039517	Atomistic Study of Bulk Metallic Glasses	03/01/2005	12/31/2011	$ 642,164	$ 79,197
Egami	UT-B 4000039517	Atomistic Study of Bulk Metallic Glasses	03/01/2005	12/31/2011	$ 115,889	$ 47,180
Egami	UT-Battelle 4000039718	Atomistic Study of Bulk Metallic Glasses	03/14/2005	03/14/2012	$ 508,451	$ 189,783
Egami	UT-Battelle 4000071951	Atomistic Structure of Gold Nano-Particles	07/31/2008	07/30/2010	$ 76,148	$ 43,534
Egami	NSF DMR-0602876	Materials Research Network: Structure and Dynamics of Complex Ferroelectrics	07/01/2006	06/30/2011	$ 264,000	$ 4,169
Egami	DOE-DE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	05/31/2012	$ 1,980,000	$ 513,812

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 11 Expenditures
Egami	DOE-DE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States - Dept. Matching	09/01/2008	05/31/2012	$ 997,839	$ 101,323
Egami	DOE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States	09/01/2008	05/31/2012	$ 69,070	$ 63,797
Egami	DOE-FG02-08ER46528	Neutron Scattering Research Network for Epscor States - Dept. Matching	09/01/2008	05/31/2012	$ 23,340	
Egami	ARRA-Washington Univ WU-HT-10-51	Construction of the Parts for MRI-R2 Project	04/01/2010	03/31/2012	$ 146,046	$ 64,707
Egami	ARRA-Washington Univ WU-HT-10-51	Matching	04/01/2010	03/31/2011	$ 43,919	$ 21,855
Guiochon	DOE-DE-SC0001014	Separation of Highly Complex Mixtures by Two-Dimension Liquid Chromatography	07/15/2009	07/14/2012	$ 360,000	$ 85,582
Guiochon	NSF CHE-1108681	Fundamental Studies in Nonlinear Chromatography	06/01/2011	05/31/2012	$ 175,000	$ 11,283
Guiochon	Waters Technologies Corp 10-107	Studies in Supercritical Fluid Chromatography	08/10/2010	08/09/2012	$ 72,000	$ 69,508
Hatcher	USGS-G09AC00126	Detailed Geologic Mapping, Central Georgia inner Piedmont and Tennessee Valley and Ridge	04/30/2009	10/31/2010	$ 42,700	$ 13,457
Hatcher	USGS-G10AC00001	Conversion of Detailed Geologic Maps to ArcMap-Compatible Geospatial Databases: Part 2	10/20/2009	10/19/2010	$ 25,000	$ 10,512
Hatcher	USGS-G11AC20114	Detailed Geologic Mapping, Central Georgia Inner Piedmont	04/30/2011	04/29/2012	$ 11,244	$ 1,492
Joy	Electron Microscopy Facility	Unrestricted Research Support	04/11/1989	12/31/2047	$ 415,091	
Joy	Semicond. Res. Agency	Development of Analysis Software	03/01/2008	02/28/2011	$ 57,500	$ 312
Macek	DOE-DE-FG02-02ER15283-MACEK	Theory of Fragmentation and Rearrangement Process in ion-Atom Collisions	02/29/2008	02/28/2011	$ 375,000	$ 55,099
Macek	DOE-DE-FG02-02ER15283-MACEK	Theory of Fragmentation and Rearrangement Process in ion-Atom Collisions	03/01/2011	02/29/2012	$ 125,000	$ 48,893
Mays	Dow Chemical Co. - Jimmy Mays	Unrestricted Research Support	10/30/2002	12/31/2047	$ 35,000	$ 366
Mays	UT-B 4000076055	Plymer-Based Multicomponent Materials	11/20/2008	11/02/2011	$ 121,297	$ 38,033
Mays	NSF-DMR-0906893	Collaborative Research: Synthesis and Rheology of Strategically Designed Long-Chain-Branched Polymers	09/01/2009	08/31/2012	$ 120,000	$ 29,703

Principal Investigator	Project Name	Project Title	Start Date	End Date	Award Amount	FY 11 Expenditures
Mays	UT Research Foundation-Hydrocarbon-Mays	Hydrocarbon Based Membranes as Alternatiives to Nafion	10/01/2009	04/30/2011	67,224	27,100
Mays	UT Research Foundation-	Hydrocarbon Based Membranes as Alternatiives to Nafion - Matching	10/01/2009	04/30/2011		(3,125)
Mays	UT-B 400089712	Poly(cyclohexadiene)-Based Electrolytes for Batteries	01/26/2010	12/31/2010	24,500	22,249
Mays	UT-B 4000097974	Synthesis and Characterization of Novel Monomers	08/25/2010	02/17/2011	17,500	17,500
Mays	UT-B 4000103683	Polymer Based Multi-Component Materials	03/11/2011	09/30/2011	23,878	23,744
Mays	UT-B 4000105959	Fundamentals of Ionic Conductivity in Polymeric Materials for Energy Storage Applications: How to Decouple Ionic Motions from Segmental Dynamic	06/08/2011	09/30/2011	24,000	23,716
Mays	Army W911NF-10-1-0282	Acquisition of Instrumentation for Temperature Gradient Interaction Chromatogeraphy of Complex Polymers	07/01/2010	06/30/2011	105,778	105,013
Mays	Army W911NF-10-1-0297	Synthesis of Novel Hydrocarbon Soluble Multifunctional Anionic Initiators	07/15/2010	02/14/2012	180,000	70,095
Mays	Army W911NF-10-1-0374	Stimuli Responsive Self-Assembled Singl-Walled Carbon Nanotube Gels	08/10/2010	05/09/2011	50,000	47,198
Mays	NSF EPS-1004083	TN Solar Conversion and Storage Using Outreach, Research and Education (TN-SCORE	08/15/2010	07/31/2011	48,546	17,492
		Total External Funds			$ 7,905,505	$ 1,937,273
		Total Matching Funds ORNL			$ 992,119	$ 1,148,634

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