SCIENCE ALLIANCE



ANNUAL REPORT



THEC State Appropriations Request 2019-20

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The Science Alliance was established in 1984 to improve selected science programs at the University of Tennessee, Knoxville, and to increase collaboration between the university and Oak Ridge National Laboratory (ORNL).

The Science Alliance is composed of four divisions: the original three being Biological Sciences, Chemical Sciences, and Physical Sciences. A fourth division, Mathematics and Computer Science, was added in 1986.

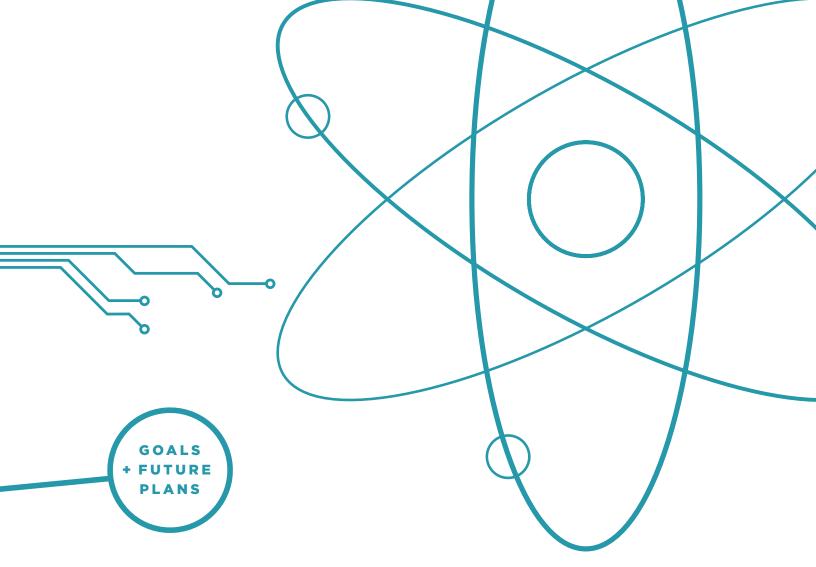
SCIENCE ALLIANCE OBJECTIVES

- Create a strong formal bond between UT and ORNL
- Hire joint UT-ORNL distinguished scientists
- Create joint UT-ORNL institutions
- Share resources and build areas of common strength at UT and ORNL as well as with industry and other institutions



- Provide incentives to attract and retain high-quality faculty
- Strengthen graduate and undergraduate opportunities
- Increase public and professional awareness of UT-ORNL partnerships





THE PRIMARY MISSION of the Science Alliance has always been to develop and support collaborations between the University of Tennessee and Oak Ridge National Laboratory.

With a solid foundation of decades spent working toward that end, the Science Alliance seeks to amplify that relationship with greater development and educational opportunities. Recent investments in the University-Industry

Demonstration Partnership and the Institute for Advanced Composites Manufacturing Innovation have laid the groundwork toward achieving this goal and will help guide the Science Alliance as it develops new cooperative models around stated strategic initiatives. These initiatives will translate into global scientific and economic impacts, intellectual capacity development and a prepared future workforce for Tennessee.

The Science Alliance will further advance these goals by deepening the collaborative relationships with ORNL via the Joint Directed Research Development (JDRD) program. An annual JDRD Symposium has been proposed to provide an opportunity for research teams to present their lab and university supported work. The Science Alliance will also maintain previous support of the FIRST Robotics Competition, an event designed to motivate high school students to become engaged in STEM fields in a collaborative environment. Additionally, graduate student support will continue to play an important role in the Science Alliance portfolio and emphasizing research connections with ORNL. The co-investment strategies that will support these initiatives will allow the Science Alliance to continue focusing on the joint development and acquisition of talented scientists and engineers as well as continuing to provide consistent graduate student support in arenas of global interest.

EXECUTIVE SUMMARY

The Science Alliance continues to be a crucial component in the continued growth of the partnership between the University of Tennessee, Knoxville, and Oak Ridge National Laboratory. Our researchers are collaborating on large initiatives in materials science, biomedical sciences, high-performance computing, and bioenergy science, to name a few.

This spring, a university-industry team led by UT researchers received a \$9.9 million grant from NASA. This project will provide breakthroughs that totally reshape the aviation industry, impacting the cost effectiveness, safety, and reliability of aviation. James Coder and Stephanie Termaath from the Department of Mechanical, Aerospace, and Biomedical Engineering will collaborate with researchers from five universities and two aviation companies toward this end.

Suresh Babu, the UT-Oak Ridge National Laboratory Governor's Chair for Advanced Manufacturing, won the university's first Multidisciplinary University Research Initiative (MURI) grant in 30 years. Babu will lead a team focusing on the properties, defects, and instabilities in advanced manufactured alloys. This research is of particular interest to the Navy.

Innovative ideas like these bring competitive faculty members and researchers and attract the highest-caliber students to our university. More than 146 graduate students received support through the Science Alliance in the past year. Many of them authored publications, presented their research at meetings or conferences, or worked on sponsored projects. These students are working in the nation's leading scientific laboratories and learning how to apply for funding, putting them ahead of their peers.

To ensure the success of future scientists and researchers, we must start reaching out to students earlier in their educational careers.

That is why the Science Alliance supports FIRST Robotics. The values espoused by FIRST support collaborative research, increased enrollment in higher education, and participation in STEM fields. You will read more about our investment in FIRST Robotics later in this report.

This report is not only a summary of the past year's efforts by our distinguished scientists, Joint Directed Research Development fellows, project leaders, and team members to advance the research enterprise here at UT and with our partners at ORNL, but also a glimpse into the future of research innovation in our nation.

ROBERT NOBLES

Interim Vice Chancellor for Research and Engagement





The floor of Thompson-Boling Arena becomes home to robotics teams from across the region.

Teams competed for less than three minutes to take home the title of Smoky Mountain Regional Champion. Robotics photos by Michael Messing

FIRST ROBOTICS

For Inspiration and Recognition of Science and Technology, or FIRST, was founded in 1989 as a nonprofit organization devoted to encouraging young people to participate in science and technology. FIRST's programmatic activities include Lego League, Lego League Jr., and Tech Challenge, but the organization is best known for its international robotics competition.

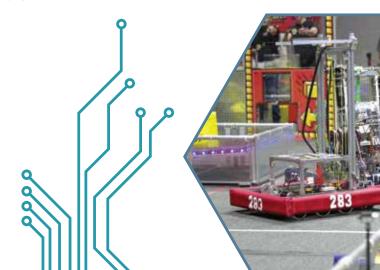
This year's participants were required to form alliances consisting of three teams. Titled "Destination: Deep Space," the 2018 FIRST Robotics Competition was sponsored by Boeing and required teams to design and construct robots capable of performing specific mechanical tasks.

Robots were required to operate autonomously from a set of programmed instructions for the first 15 seconds of the competition, leaving two minutes and 15 seconds for operator-controlled activity.

Over the course of three days, teams gathered in Knoxville to load in, register, and practice with their robots. On the final day, teams participated in a series of qualification and playoff matches, working with students from outside their team and, in the case of the winning alliance, outside their state.

The Robotics Competition is a perfect model of FIRST's core value of "gracious professionalism"—the notion that students can learn and compete with one another fiercely while treating one another with respect. In addition to nurturing the next generation of scientists, FIRST's practices and values engender the characteristics that make good collaborators.

Collaboration between researchers is the bedrock of the Science Alliance's programmatic activities. For the past three years the alliance has provided support to the Smoky Mountain Regional FIRST Robotics Competition as a means to foster the



future of collaboration in
East Tennessee and encourage
student participation in STEM
fields. In fact, about 75 percent of
FIRST robotics alumni are either
students or professionals in a STEM
field.

This year's winning group consisted of two teams from Tennessee—the Secret City Wildbots from Oak Ridge and the Robokomodos from Franklin—and a team from West Virginia. Of the 28 additional awards, 13 were secured by Tennessee teams, most of them from the greater Knoxville area.

The Science Alliance's activities encourage collaboration as a model for future innovation in research. The work of FIRST and the FIRST Robotics Competition, by laying the groundwork for a future generation of collaborators, is a natural fit with that model for innovation. Providing support to the FIRST organization helps offer a wealth of opportunities to young Tennessee students and contributes directly to the future of innovation and research.

The winning alliance of 2018 consisted of two teams from Tennessee and one from West Virginia.

Teams from different states and schools cheer each other on in the spirit of gracious professionalism.



DISTINGUISHED SCIENTISTS

The Science Alliance Distinguished Scientist Program supports high profile joint leadership in research areas where UT and ORNL share complementary strengths. It has been the anchor program of the Science Alliance since 1984.

Distinguished Scientists hold tenured professorship at UT; most also hold a Distinguished Scientist appointment at ORNL, nominally half time at each institution. Appointments include an ongoing discretionary research fund equal to twelve months' salary.

In the future, we intend to explore Distinguished Scientist positions that are co supported by endowments from our corporate research and development partners. This structure may allow us to amplify the investments made by the state and ORNL in areas of interest to our key tindustrial research and development partners.





ELBIO DAGOTTO Elbio Dagotto primar ily uses computational techniques to study transition metal oxides, oxide interfaces, and the recently discovered iron-base high tem perature superconductors. These materials, and others studied by his group, show promise for both technological applications and advancement of fundamental concepts in condensed matter physics. Dagotto has several active collaborations with ORNL scientists working with materials from manganese ox ides to iron-based high temperature superconductors. Additionally, he serves as principal investigator of a US Department of Energy field work proposal, Theoretical Studies of Complex Collective Phenomena, which secured a grant from the DOE that awarded \$1,992,999 over eigh teen months to ORNL.

TAKESHI ESAMI The physics of liquids is much less developed than the physics of solids. Takeshi Egami explores liquids and gases using computer simulation (including quantum mechanical calculations) and

neutron and synchrotron x-ray scattering experiments. Egami is currently participating in a number of active collaborations with ORNL scientists, including Department of Energy (DOE) projects whose fiscal year budgets total more than \$2.7 million. His work has been repeatedly highlighted by the DOE in the last year. Egami was recently named an Aris Phillips Lecturer by Yale University, the most prestigious award given by the department of mechanical engineering at Yale. Additionally, Egami has served as Editor for *Advances in Physics* from 2011 to the present and Divisional Associate Editor in Condensed Matter Physics for *Physical Review Letters*.





Michael McKinney, head of the Department of Earth and Planetary Sciences, presents Robert Hatcher with a plaque at a retirement event held in his

BOB HATCHER After 32 years of service Professor of Geology and Distinguished Scientist Robert D. Hatch er, Jr retired at the end of June, 2018.

Born in Madison, TN, Hatcher first came to the University of Tennessee, Knoxville in pursuit of his doctoral degree, after completing bachelor's and master's degrees in geology from Vanderbilt University. After completing his doctoral program in 1965 Hatcher left Knoxville for teaching positions at Clemson University, Florida State University, and the University of South Carolina. Twenty years later, in 1986, he was invited to return to Knoxville to join the University of Tennessee faculty.

"At first I said no," said Hatcher, speaking at a retirement event in his honor. "I didn't think you should teach where you went to school, but they convinced me to change my mind."

Fortunately for the university, he returned to his alma mater and became one of the earliest Distinguished Scientist appointees with the Science Alliance. Since that time, Hatcher has mentored 52 master's students and 17 doctoral students, and taught thousands of hours of classes. Over the course of his career, he has served in a variety of leadership roles within his field. He was president of the Geological Society of America from 1992 to 1993 and president of the American Geological Institute from 1995 to 1996. He was awarded the first ever Geological Society of America Distinguished Service Award. In 2014 he received the American Geosciences Institute's Legendary Geoscientist Medal.

"Every time I go to a conference, almost everyone I speak to asks if I know Bob Hatcher," said Michael McKinney, department head and professor in the Department of Earth and Planetary Sciences. "The further he got in his career, the more productive he seemed to get."

At the retirement celebration, McKinney presented Hatcher with a plaque commemorating his years of service to the university and the State of Tennessee. The department also gave Hatcher a large piece of Tennessee marble with a metal tag reading "In honor of a lifetime of major achievements, service, and contributions to science. With gratitude from thousands of colleagues and students whose lives you have touched."

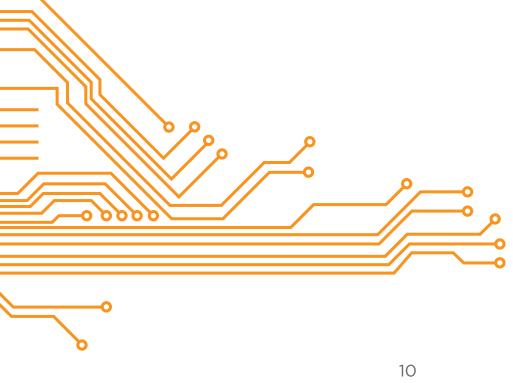
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FUNDING



PRIN INV.	PROJECT NAME	PROJECT TITLE	START DATE	END DATE	AWARD AMOUNT	FY 17 EXPEN DITURES
Dagotto	NSF-DMR- 1404375	Computational Studies of Multiorbital Model Hamiltonians for Iron-Based Superconductors in Quasi One-Dimensional Geometrics 09/01/14 08/31/17 435,000		435,000	150,650	
Dagotto	UT-B 4000159777	Study of multi-orbital Hubbard models for iron-based supercon- ductors and spin-orbit coupled transition metal oxides using the Density Matrix Renormalization Group technique	12/21/17	12/10/21	616,000	41,414
Egami	UT-B 4000126542 Egami	Dynamics of Biologically Relevant Model Membrane Systems	09/20/13	09/30/17	117,337	9,427
Egami	UT-B 4000149639 Egami	Viscosity of Aqueous Solution	08/23/16	07/31/18	144,217	33,306
Egami	UT-B 4000139883	Neutron Scattering Study of Disordered Materials Under pressure	06/16/15	07/31/19	177,718	52,730
Egami	UT-B 4000131427 Egami (Year 2)	Local Structure by Neutron Diffraction	07/01/15	10/01/17	278,712	51,019
Egami	Carnegie Inst of Was 4-10114-12 Egami	Study of Conducting Oxides Under pressure	03/01/16	07/31/17	162,606	13,395
Egami	UT-B 4000156221 Egami	Dynamics of Biologically Relevemt Model Membrane Systems	08/01/17	09/30/18	120,498	106,873
Egami	UT-B 4000160363 Egami	Atomistic Study of Bulk Metallic Glasses	04/01/18	03/31/19	50,000	117,240
Egami	UT-B 4000120790 Egami	Atomistic Study of Bulk Metallic Glasses	04/01/17	03/31/18	635,434	235,545

PRIN INV.	PROJECT Name	PROJECT TITLE	START Date	END Date	AWARD AMOUNT	FY 17 EXPEN DITURES
Hatcher	USGS G16AC00138- Hatcher	Geologic mapping of the Parksville 7.5-min quadrangle, & the kinematics of emplacement of larger horses along a major thrust fault, southeastern Tennessee	05/01/16	09/30/17	17,500	1,666
Mays	UT-B 4000152655	Designing the next generation high performance polymeric cathodes 01/19/17 09/30/18 47		47,186	26,690	
Mays	UT-B 4000153000	Scaled-up synthesis of deuterated isoprene	02/15/17 09/30/17 20,00		20,000	3,925
Mays	NOVA Chemicals Well-Defined Long	Well Defined Long Chain Branched Polythylene by Living Anionic Polymerization of 1,3-Butadiene & Hydrogenation	y Living of 10/19/16 05/31/18 170,012		170,012	24,063
Webster	NSF DMS- 1620280	Collaborative research: Mathematical methods for approximation & control of multi-dimensional parameterized systems	09/15/16	08/31/19	65,752	45,205





JOINT INSTITUTE FOR ADVANCED MATERIALS

The Joint Institute for Advanced Materials promotes interdisciplinary research and education related to developing new materials with superior properties, such as greater toughness and high-temperature strength, or those that can be tailored to support new technologies, such as pocket-sized supercomputers.

JOINT INSTITUTE FOR BIOLOGICAL SCIENCES

The Joint Institute for Biological Sciences supports interdisciplinary, crosscutting research that accelerates progress in complex bioenergy and bioenvironmental systems. It also aids access by UT-ORNL faculty, staff and students to state-of-the-art capability in genomic, transcriptomic, proteomic, and metabolomic analysis of biological and environmental systems.

The Joint Institute for Computations Sciences (JICS) advances scientific discovery and state-of-the-art engineering and computational modeling and simulation. JICS takes full advantage of the petascale and beyond computers in the DOE National Center for Computations Sciences and UT's National Institute for Computational Sciences.

JOINT INSTITUTE FOR NUCLEAR PHYSICS AND APPLICATIONS

The Joint Institute of Nuclear Physics and Applications links UT, ORNL and Vanderbilt University research to promote and support basic nuclear physics research and nuclear and radiological applications of common interest to the participants.

SHULL WOLLAN CENTER, A JOINT INSTITUTE FOR NEUTRON SCIENCES

The Shull Wollan Center promotes world-wide neutron scattering collaboration among researchers in biological and life sciences, energy sciences, polymer science, condensed matter physics, and computational sciences.

SCIENCE ALLIANCE

THE SCIENCE ALLIANCE IS A TENNESSEE CENTER OF EXCELLENCE.

established in 1984, and supported annually by the Tennessee General Assembly. The mission of the Science Alliance is to:

- Hire and support joint distinguished scientists of national note
- Create and support joint institutes
- Share resources
- Bring the University of Tennessee and Oak Ridge National Laboratory together to support technology transfer
- · Build areas of common strength
- · Provide incentives to attract and retain the highest quality faculty and students
- Strengthen educational opportunities
- · Grow government and industrial support of the shared research enterprise

Science Alliance funding is one critical way that the partnership between UT and ORNL is further advanced. Funds support a variety of significant investments in people and collaborations.

Much of our current collaborative research emphasizes strategic areas of importance to both organiza tions. Advanced manufacturing, advanced materials and materials science, neutron science, computa tional science, big data and data science, and bioinformatics are currently among the most prominent UT-ORNL collaborative areas receiving support.

The investment made by the state each year in this important collaboration is greatly appreciated and is instrumental in allowing the Science Alliance to provide a variety of opportunities to innovative and groundbreaking collaborations between people. Great science and discovery comes when people-to-people interactions are optimized, not unlike a chemical reaction. A reaction progresses because of interactions and these funds support those very activities. They hold a decisive role in leveraging the federal investments made at ORNL and UT in our areas of collaborative research and development.





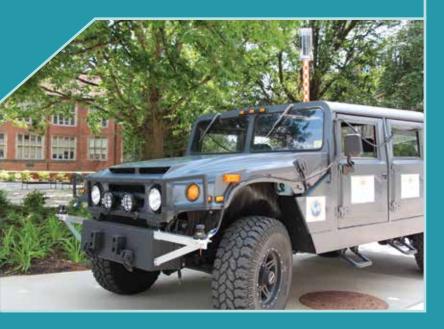
UT RESEARCH ADDRESSES CONNECTIVE VEHICLE TECH

Autonomous vehicles continue to gain steam as the technology improves. Google self-driving cars, for example, have traveled more than seven million miles and been in only about 11 accidents. Even then, the majority of these collisions were caused not by the autonomous vehicles but by other drivers around them.

"The Google driverless cars have been rear-ended multiple times, and not once was it the fault of the vehicle," said Subhadeep Chakraborty, associate professor of mechanical, aerospace, and biomedical engineering. "It was because someone came and rear-ended it. And why? The conjecture is that the car is driving too conservatively, too nicely, too safely, and other drivers aren't prepared to deal with that."

Self-driving cars are programmed to obey traffic rules and respond to situations based on those rules. Humans speed, follow too closely, and change lanes without signaling. This difference gives rise to a question: In a world moving toward more autono mous vehicles, how do they integrate with human drivers who don't always follow the rules? This is where Chakraborty's research into connective vehicle technology comes into play.

"The difference between connective vehicles and autonomous vehicles is that the autonomous vehicle is trying to mimic human driving behavior as best it can, and it fails sometimes. The idea behind connect ed vehicles is a little bit different. It asks how you can drive as a group so that it is best for everyone," said Chakraborty.



Connective vehicle technology works by allowing cars within a certain radius to communicate with each other and the city itself. In an ideal scenario, vehicles could travel through smart cities without ever need ing to stop at a red light. Communication between the vehicles and the streets or intersections would allow vehicles to adjust their speed to pass by and between one another without stopping.

"There are three main objectives with connective vehicles: safety, efficiency, and reducing congestion," said Chakraborty. These goals come with a number of complex research questions, including how much distance should be maintained between vehicles in intersections to prevent panic in the passengers.

His research team has been working with a donated Humvee outfitted with a series of sensors to feed data from the vehicle into a simulation. The resulting data will allow them to study and address the effects of the human element in connective vehicle technology

PROFESSOR DEVELOPING DEVICE TO ADMINISTER CANCER DRUG

A new device under development by a UT nuclear engineering professor will allow doctors to dispense accurate dosages of a drug made with actinium-225, an isotope that has been shown to be effective in treating myeloid leukemia. The device, brainchild of Assistant Professor Eric Lukosi and fabricated by master's student William Gerding, is currently in production. Once built, it will go through testing at ORNL.

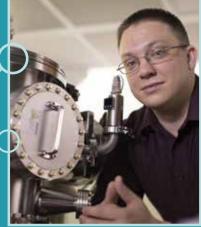
"We're slowly moving toward the demonstration of the device. It's been fabricated; now we just need to package it and make sure it works," Lukosi said. "This could help save lives."

Lukosi's device would act as a critical quality assurance mea sure, making sure that patients receive treatments exactly as recommended by their physicians.

Myeloid leukemia can spread quickly and affect lymph nodes, organs, and the central nervous system. Acute myeloid leukemia is found most often in adults over the age of 45 and is frequently fatal for patients 60 and older.

Actinium-225 is an isotope extracted from thorium-229, a waste byproduct of the fuel that was used for ORNL's Molten Salt Reactor Experiment in the 1960s. In 1994, ORNL began purifying thorium-229 in order to extract actin ium-225.

Since then, ORNL has sent approximately 900 shipments of actinium-225 to hospitals, clinics, and research institutions. The isotope has been studied as a treatment for cancer for a number of years and recently gained attention as a possible cure for myeloid leukemia.



As with many medical treat ments, particularly radiation ther apies, quality control issues that could jeopardize patient health are a concern. Support technologies play an important role in ensuring patient safety.

For example, modern insulin pumps assist in diabetes treatment by monitoring blood sugar levels so appropriate levels of insulin can be delivered to a patient throughout the day.

Actinium-based therapies could specifically benefit from support technology because current control methods can be time-consuming and costly.

"Right now, the method of finding out what is inside the sample requires an exter nal detector," Lukosi said. "There are a lot of factors that need to be taken into account to get an accurate measurement of the activity inside the sample."

Initially, Lukosi conceived of the device to use in spent nuclear fuel reprocessing. "There are a whole host of applications for this technology, including environmental sampling," he said.

JOINT DIRECTED RESEARCH DEVELOPMENT

The Joint Directed Research Development (JDRD) program offers an opportunity for collaborative research with ORNL.

A dual UT and ORNL venture, JDRD complements the Laboratory Directed Research Development (LDRD) program and ORNL Seed Money Fund. The LDRD is a US Department of Energy program that

encourages multi-program DOE laboratories such as ORNL to select a limited number of projects with the potential to position the lab for scientific and technical leadership in future national initiatives.

The ORNL Seed Money Fund provides a source of funding for innovative ideas that have the potential to enhance the laboratory's core scientific and technical competencies and provide a path for funding new approaches that fall within the distinctive capabilities of ORNL but outside the more focused research priorities of the existing major initiatives. The JDRD program identifies and supports corresponding areas of research at UT, and projects approved for the program have both a UT and ORNL component.

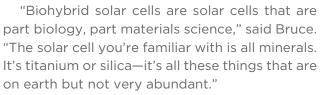
JDRD awards run for up to two calendar years. A progressive assessment at the end of year one determines if second year funding will be awarded, based on the partnership development research progress thus far.

Solar technology got its start in 1876, when the development of the first solar cell proved that light could be converted into electricity. Since then, solar cells have been used to power satellites, railroad crossings, and even vehicles and aircraft. As the technology has changed over time, so have its uses.

As with most technology, however, the future of solar power will certainly be dominated by the most cost-effective and energy-efficient developments. To meet these requirements, many researchers in the field have focused their efforts on testing more abundantly available new materials for the cells themselves.

BARRY BRUCH

Professor of Biochemical and Molecular Engineering Barry Bruce suggests trying a completely different approach to the problem: biohybrid solar cells.



Bruce turns to plants and photosynthesis as a possible alternative. He suggests that using photosynthetic components derived from biological materials could lead to less costly, more efficient solar cells.



"Photosynthesis is really the energy-driving metabolism for our planet, and most of the work in biofuels is really still photosynthesis," he said.

One of the major stumbling blocks on the path to biohybrid solar cells is the need to deal with fluctuating light levels. Photosynthesis requires sunlight and weather changes can greatly affect how much sun a solar cell actually gets, which could then affect its productivity.

Bruce's JDRD team plans to tackle this issue by studying how certain bacteria that depend on photosynthesis adjust to changing light conditions.

"This complex changes its architecture depending on whether we add high light or low light," he said. "This is very profound because we didn't understand that bacteria, which are considered to be more primitive, had the ability to adjust to alternating light levels."





JAMIII COBLE

In 2011 a massive tsunami struck Japan, resulting in nearly 16,000 confirmed deaths. On the heels of this natural disaster, the world bore

witness to a nuclear disaster that included three nuclear meltdowns at the Fukushima Daiichi plant. Since that time there has been an increased focus on accident-tolerant nuclear fuels. Jamie Coble, assistant professor of nuclear engineering and Southern Company Faculty Fellow, hopes to contribute critical data to the search for better fuels.

"One of the key problems we have, especially as we try to develop accident-tolerant fuels and new fuel forms, is knowing what's actually happening to the fuel while it's in the reactor," said Coble.

Currently, in order to study what's happening to a particular fuel, it is put in a test reactor, bombarded with radiation, and removed to measure any changes—a method that provides limited data.

of protein complexes in a

in solar cells. •

specific strain of cyanobacteria. He hopes the results will serve as a guidepost for solving the light variability problem

"What we'd really rather do is measure what's happening while the fuel is in the reactor, but that's very challenging to do for a number of reasons," said Coble. "It's a high-radiation, high-temperature environment. It's also very tight. There's not a lot of space to put in big bulky sensors."

Her JDRD work attempts to address these difficulties by developing a sensor capable of surviving such extreme conditions while being small enough to fit inside the reactor. Coble's sensor, once constructed, will fit around the fuel rod and measure any dimensional changes that occur as a result of irradiation.

"Our hope is that we can identify a sensor material that is radiation resistant and heat tolerant so that our sensor won't change dimensions while it's in the reactor," said Coble.

Her team is working with simulations to test a variety of existing materials. Once potential materials have been identified, Coble plans to build the sensor and conduct testing without radiation.

"Our goal for the first year is to see if we can actually measure a change in a metal tube," she said. "We want to be able to say that our simulations match what we'd expect to see in the real world."

plays a crucial role in international trade as

the most cost-effective mode of transport for

goods. It is estimated that approximately 95 percent of US foreign trade occurs via the water.

As a result, underwater threat detection con-

tinues to be an important area of study for both

Monitoring for underwater threats, however, is

a complex problem with a large number of vari-

ables. Even the noise generated by devices used

economy,

military and commercial applications.

of what's really going on.

In an increasingly global

maritime transport



James Coder, assistant professor of mechanical, aerospace and biomedical engineering, wants to find a better way.

"Basically, we want to do better simulations of how fluids like water flow," he said. "Right now we have equations that describe and define how it happens, but they're very general because they apply to air the same as water."

According to Coder, to be applied to water these equations often have to be approximated.



to perform the monitoring has to be accounted for. Current methods for filtering out these variables often involve making approximations and may not give the most accurate representation



The result is often missing information, usually in acoustics or thermodynamics—properties inherently important to the understanding of how water flows.

Coder's JDRD team is working to create better simulations of these flows by developing a new way to address the equations, approximations, and missing information.

"This project is trying to approach the physics of the problem in a way that allows for some modern numerical analysis," he said. "We're also looking at some different ways of expressing the equations that may be effective at capturing thermodynamics."

Coder's work has possible applications in a variety of fields beyond threat detection, including energy and even biomedical opportunities. "Water is so prevalent in our lives. If we could simulate that better, we could get a better grasp of the physics with fewer approximations," he said.

Robert Wilson, senior research and development staff member at ORNL, is serving as Coder's collaborator. Wilson is currently working on developing next-generation underwater threat detection devices with support from the US Office of Naval Research.

MARK

For generations, the human brain has served as a source of inspiration for artists and scientists alike. Composed of neurons, blood vessels, and glial

cells, the brain governs all the functions of a human body. Millions of individual pieces come together to make a person who they are, all in a relatively small package using a minimal amount of energy. Unsurprisingly, the brain has become a model for a relatively new area of computational science.

Neuromorphic computing is an approach to computation based on the model of the human brain with widespread potential applications, from medicine to autonomous vehicle development. In order to have such far-reaching effects, neuromorphic computing has to be both efficient and scalable.

Mark Dean, interim dean of the Tickle College of Engineering and Fisher Distinguished Professor of Electrical Engineering and Computer Science, hopes to address these requirements with his JDRD work.

From the outside, neuromorphic computing systems look like any other computer, according to Dean. They might even have chips like traditional computers. The content of those chips, however, makes new computational skills possible.

"On the chip you might see artificial neurons and synapses built from traditional digital logic, but you might also see new forms of devices," he said. "This means of storing information allows them to be used like synaptic elements."

Dean suggests this way of storing and transferring information could affect the very functionality of such computing systems, allowing them to learn and improve over time.

"Right now, computers are pretty static. You program them to do something and that's all they do," he said. "Neuromorphic computing would be more flexible than that. It would be able to deal with variations in information and come up with a set of insights that traditional computers just couldn't do."

His team is currently working to develop low-power interconnects for neuromorphic elements to support the work of his LDRD partner Raphael Pooser, Quantum Sensing Team lead at ORNL. Dean's goal is to show that neuromorphic elements can be connected in a way that will maximize efficiency without losing functionality.

"Our expectation is that we will demonstrate how neuromorphic components can be connected together in an efficient way that minimizes power consumption and optimizes scale," he said. "We're hoping to show that it can be done and done well."





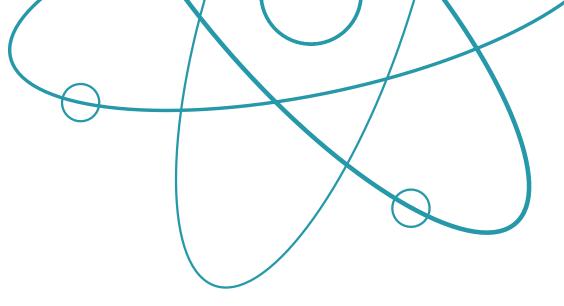
The adoption of new technology into society does not happen all at once. Take cars, for instance. Initially only a few consumers owned the Model T. Now automobiles are ubiquitous, with 95 percent of American households owning at least one. There was, however, a time when both cars and horse-drawn wagons existed on the road simultaneously, creating a series of unique challenges for drivers and pedestrians alike.

Similar challenges occur with more recent major technological changes. With his JDRD project, Professor of Electrical Engineering and Computer Science Seddik Djouadi hopes to address the challenges happening right now in renewable energy.

"Renewable energy

and the penetration of renewable energy sources into the modern grid require power converters that interface with the current devices in the power grid," said Djouadi. "But these sources of renewable energy—like solar energy and wind turbines—are variable, meaning the power throughput is variable."

According to Djouadi, this variability can cause instability and inconsistent performance in the power grid, which is designed to handle a steady flow of electricity. His solution is to design better controllers for the power converters that integrate renewable energy into the grid.



"It's basically designing a switching control so if there's a disturbance in the system it triggers a mechanism that can ensure the safe operation of the power grid," said Djouadi. "These energy sources introduce variability in frequency and voltage and improved controllers will help maintain consistency in both these areas."

Diouadi and his team hope the design will encourage further integration and use of renewable energy sources.

"From my perspective, this kind of control design will show people in industry that we have the capability to achieve this type of performance," said doctoral student Yichen Zhang, who is working on Djouadi's team.

"From the industrial point of view, they may think this design will cost a lot for them-to change from their traditional controller—but the duty of our research is to let them know this can be done."

At the conclusion of their first year, Djouadi and his team hope to have developed some successful algorithms and made advances in designing their proposed controller. •

been employed to successfully trace the sources of infection. Thus far, they have been used mostly in Salmonella outbreaks, but Jeremiah Johnson, assistant professor of microbiology, hopes to extend their capability to trace other bacteria.

> "Something that's actually starting to happen nationally, in terms of public health, is that they're moving away from more archaic genomic analyses and actually mandating that all state public health departments start using whole genome sequencing," he said.

Specifically with regard to food-borne illness outbreaks, these techniques have

DNA testing and whole genome sequencing have become increasingly important tools in the arsenal of public health professionals.

This is where his team steps in. While many health departments are acquiring the equipment necessary to conduct this kind of sequencing, they are lacking the in-house expertise needed to conduct the work. Johnson's team possesses the bioinformatics experience required to analyze the genomes of the subject bacteria—in this case, *Campylobacter*.

Campylobacter was recently identified by the CDC as a serious threat to public health, as it is becoming increasingly resistant to antibiotics. It also takes significantly less of the bacterium to make a person sick than other bacteria in the past.

"With *Campylobacter*, it only takes a few hundred bacterial cells to make a person sick," said Johnson. Another hurdle with *Campylobacter* is how rapidly the bacteria mutate and evolve, making some older genomic techniques ineffective.

In the first year of support, Johnson's team focused on acquiring *Campylobacter* samples from a variety of sources.

The cooperative effort saw contributions from UT's College of Veterinary Medicine and the US Food and Drug Administration. Team members also ventured out into other areas of East Tennessee to collect additional samples for sequencing.

"We've collected samples from area farmer's markets and grocery stores. We've done local waterways, including the Tennessee River and the Hiwassee River. We've also done animals around here, like sheep, pigs, cows, and some birds," said Johnson.

In the second year of the project, the team is hoping to establish proof of concept by running a transmission study with Johnson's ORNL partner, computational biologist Dan Jacobson. The goal, based on a genomic sequencing conducted on the front end, is to see if the ORNL collaborators can identify the original strain of *Campylobacter* once it's passed through this transmission study.



Machine learning algorithms allow a computer to learn and make predictions based on existing data. Machine learning is already in use in the everyday lives of many. Netflix, for example, uses machine learning algorithms to make recommendations based on the viewing habits of its approximately 125 million subscribers.

Machine learning is becoming more widespread in a variety of arenas, including health care and finance. Steven Johnston, assistant professor of physics and astronomy, thinks it can also be applied to physics.

STEVEN JOHNSTON

Johnston works
with quantum Monte
Carlo simulations. These
simulations work by taking
a configuration or set of
parameters and proposing a
random change over and over again in the search
for the best arrangement.



"The difficulty is that deciding whether or not you accept that proposed change is incredibly expensive computationally," he said. "We need to find a way to do this cheaper and faster."

Johnston's JDRD team is working with machine learning to train a computer using a neural network to guess whether a proposed change is going to be accepted. His team has run some benchmark tests that show the machine learning algorithms capable of completing calculations at a significantly faster rate than other methods.

"The neural network approach can do in about six hours what used to take five or six days. The idea is now that we can do it faster, we can make the problem bigger and use the same computing time as before," said Johnston.

He hopes to have completely benchmarked an algorithm by the end of the funding year, determining how well it performs against a conventional algorithm. He also plans to carry out at least one comparative study to confirm that both conventional and machine learning algorithms produce the same results.

Johnston's ORNL collaborator, Markus Eisenbach of the Center for Computational Sciences, is using the same machine learning techniques to tackle a different set of algorithms. The work of both teams could contribute meaningfully to the future use of machine learning in physics.



MAIK LANG

Demand for nuclear power has increased steadily since the first commercial nuclear power station came online in the 1950s. Nuclear energy is now

responsible for approximately 11 percent of all power generated in the world. Due to this growing popularity, greater emphasis has been put on areas of research relating to the generation of

nuclear power, specifically the materials used in and around reactors, and the waste those materials generate.

Safe disposal of nuclear waste is of primary concern, given its potential effects on the environment and surrounding communities should a leak occur. One of the methods used to combat this possibility is vitrification—the conversion of waste into a stable glass.

The glass serves as a safe containment method for the spent fuel over hundreds of thousands of years. However, the effects of radiation, one of the key drivers of microstructural evolution of these types of glass, are not fully understood. This is where Maik Lang, associate professor of nuclear engineering and Pietro F. Pasqua Fellow, and his JDRD team come in.

The goal of Lang's JDRD project is to develop an understanding of the structure of these glasses using ORNL's Spallation Neutron Source (SNS) and Integrated Computational Environment-Modeling and Analysis for Neutrons, or ICE-MAN. In its second year, Lang's team has pivoted to focus their modeling efforts on the nuclear fuel itself.

"In the renewal, we shifted away from glasses to nuclear fuel materials," he said. "The overall goal is still to understand the glass structure, but we think we first have to understand defect formation in crystalline materials. Once we have a good handle on that, we can move on to the more complicated glass system, which is an aperiodic material."

Lang's team is working alongside ORNL's Anibal Ramirez-Cuesta, Chemical Spectroscopy Group leader, and Matt Tucker, Diffraction Group leader, to further develop the ICE-MAN platform as well as making use of it to decode their data. In turn, Lang's data is serving as a test bed for the platform itself, setting the stage for future collaborations.

Since the earliest days of farming, ensuring adequate food production to consistently feed a population has been the primary goal. This goal has not changed in the thousands of years since plant cultivation began, although the mechanisms of achieving it have evolved considerably. Irrigation, pesticides, automated machinery—all these advancements have arisen from the need to produce enough food to keep pace with the growing numbers of humans on the planet.

In recent years, this drive has shifted toward the plants themselves. Genetically modified seeds designed to withstand drought and blight have become commonplace. Sarah Lebeis, assistant professor of microbiology, believes the next advances will be made by studying plant microbiomes, specifically the effects of certain bacteria on those microbiomes.

SARAH Lebeis

"One thing we've found is that the more we look at which microbes associate with plants, we find these bacteria over and over again.

They can be pathogens or they can promote growth of the plants," she said.

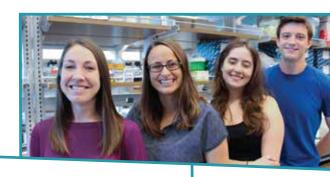
Some agricultural companies have seized on the idea that plants can be helped with the introduction of so-called good microbes and have begun marketing products designed to do just that. Lebeis describes these products as plant probiotics and emphasizes that they are not always effective.

"It's really exciting that people are trying to find these ultimate microbes that can change the way plants grow, but they're not always going to work. When they don't work, we want to know why they don't work," she said.

She believes *Streptomyces*, a particularly large genus of bacteria, is playing a role in determining which microbes are allowed into a plant. Lebeis suggests that, in addition to keeping out harmful microbes, the *Streptomyces* may also be preventing some beneficial microbes from entering the plant's system.

Lebeis's ORNL collaborator, Daniel Jacobson, chief scientist for computational systems biology, has provided her team with a large data set to serve as the basis of her JDRD work. By the end of the year she hopes to have compiled a list of microbes that either work with or are repelled by *Streptomyces*.

"We want to see who they influence, who they let in and who they don't. The JDRD will help us generate a giant list of hypotheses, which we're so excited about," said Lebeis.



JIAN LIU

Rush-hour traffic is part of life in most metropolitan areas in the US.

The presence of large numbers of people traveling in the same general direction at the same time is bound to result in congestion and frustration. Picture that same rush hour during the summer. Air conditioners crank as heat ripples off the blacktop and,

inevitably, somewhere along the way a car is pulled to the side of the road, steam pouring from under the hood.

Overheating is an issue for much of the technology that defines modern life. Cars, computers, mobile phones—all are subject to the effects of too much heat. As technology continues to speed up and devices get smaller, this heat problem compounds as internal parts shrink and move closer together.

Jian Liu, assistant professor of physics and astronomy, is working to address this issue with his JDRD project. It all starts with an electron.

Transistors, the building block of modern electronics and technology, work by moving an electron back and forth across an interface. This switching action can be sped up by decreasing the distance the electron has to travel through the interface, letting the device operate faster. This is where heat can become a problem.

"When the electron travels, it generates heat because it interacts with other atoms. The electron is trying to go and at some point it's going to hit an atom, causing the atom to vibrate," said Liu. "Basically, you're transferring the energy from the electron to the atom and that's how it generates heat."

Because heat has the ability to affect device performance, its management is an important factor in technology development. Liu's team hopes to find a way to predict how heat is moved within a device, laying the groundwork for more effectively controlling how and where heat is transported out of the device.

"If you can control heat transport, you can have an electronic device that works faster. Then you can maybe pack your devices into a more confined area and make sure there's no hot spot," said Liu.

His JDRD team is working to build a prototype that will use the same interface for both electron and heat movement. Once complete, the prototype will be given to Lucas Lindsay, materials research scientist at ORNL, for experimental testing and comparison with computational predictions. The teams hope to have generated preliminary data by the end of the funding year.

Salt is a complicated molecule. It can make bland food more palatable and even melt hazardous ice on roads. However, the same salt that makes roads safer for driving, if not removed promptly, can cause major issues for the vehicles that drive through it. Over time, brine kicked up from the road onto the car can corrode and rust the metal parts, ruining engines and destroying paint jobs.

The same can be said for the metals within molten salt reactors and concentrating solar power plants. Molten salt reactors are a type of nuclear reactor using salts as either a coolant or fuel, and concentrating solar power plants use liquid salts as a heat transfer and storage medium. A major area of research involves the effectiveness of different materials within the reactors, especially those coming into contact with salts.







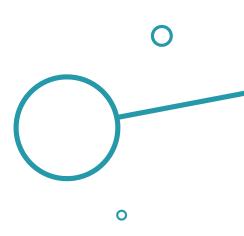
Claudia Rawn, associate professor of materials science and director of the Center for Materials Processing, and her JDRD team are investigating the effects of these salts on chromium-containing alloys in conjunction with Stephen Raiman, research associate in corrosion science at ORNL.

"Our colleagues at Oak Ridge are studying the chromium in structural materials that are in contact with molten salts in places including concentrated solar or nuclear reactors," said Rawn. "The molten salt is in contact with different structural components and there is concern about the chromium leaching out into the salt."

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Rawn's team plans to complement the work at ORNL by using X-ray diffraction to study the effects of these salts on structural materials that contain chromium. Raiman's team will be investigating the interactions between molten salts and chromium in structural alloys, while Rawn will look at the salt itself.

In order to take an atomic look at the salts. Rawn's team will use the recently established diffraction facility at the UT-ORNL Joint Institute for Advanced Materials. She hopes their work will provide an important piece of the molten salt-chromium interaction puzzle and serve as a stepping stone to future collaborations. •



Human history is divided into time periods

based largely around the types of tools or technology being employed. The Iron Age was characterized by the increased use of iron weapons and tools, edging out the previously used bronze.

This iron, however, wasn't simply iron. It was iron heated with carbon, marking the start of a new era when humans realized that metal alloys could perform better than single metals.

Alloys are the result of mixing two or more metallic elements together with the goal of creating more desirable attributes such as rust or heat resistance.

SHUNGHA

The search for better alloys continues into the present, as scientists chase super alloys for use in a variety of technologies. Seungha Shin, assistant professor of mechanical, aerospace, and biomedical engineering, is on the hunt for one such alloy.



"We are studying super alloys, which can have high stress and heat resistance," he said. "To achieve high-efficiency vehicles or airplanes, we need some lightweight materials. Normally light metals are not that good at high temperatures, so we need to develop some new materials."

If sufficiently heat- and stress-resistant materials can be developed and used to build engines, vehicles can become more fuel efficient simply by virtue of being lighter. Shin's team is working to create such an alloy with aluminum, focusing their work on its thermal transport properties.

Shin's LDRD partner Amit Shyam, research scientist at ORNL, is also studying the effects of microstructures on alloy properties. Shin's team contributes a much-needed level of expertise in thermal transport properties to their shared goal.

Shin hopes to conclude the project with a deeper working relationship with his ORNL partner and enough useful data to secure more funding from external sources. •

team have partnered with Dale Pelletier, senior staff scientist in the Biosciences Division at ORNL. Pelletier is studying the microbial community within sphagnum, or peat bogs. Sphagnum is responsible for approximately 20 percent of the carbon storage on the planet.

"It acts as such a good carbon sink because the sphagnum plants themselves change the chemistry of the system so that typical microbes do not grow very well. As a result they don't break down the carbon, so as the sphagnum dies the carbon builds up," said Wilhelm.

To study these viruses further, Wilhelm and his

His team is investigating what could be controlling the existing microbes in the peat bogs other than chemistry. He believes the answer is viruses.

Doctoral student Helena Pound is currently working with bioinformatics to determine how prevalent these viruses are. Her work will include snapshots as well as work over time, which should provide a better picture of how the viruses operate.

"I believe in 10 to 15 years, we will realize viruses are just as important as microbes," said Wilhelm. "When we then build models of how these microbial systems work, we'll have to start to account for the viral community."

STEVE WILLIEUS LINI

Microbes affect everything from the human body to the decomposition of plant and animal waste in the environment. The health and habits of these organisms can have a huge impact on every facet of life. Steven

Wilhelm, professor of microbiology, believes viruses hold similar importance.

"The world as we know it now is really a microbial planet. Microbes are the interface of our daily lives and how the world works," he said. "They recycle nutrients, they play important roles in carbon fixation and photosynthesis—and these microbes are all susceptible to viruses."

Viruses are incredibly abundant: hundreds of thousands of them can exist in a puddle. According to Wilhelm, they're also quite fragile, meaning they must reproduce quickly to maintain such a large population.

STUDENT SUPPORT

Integral to the charter of the Science Alliance is this principle: Science Alliance funding will be used to "provide incentives to attract and retain the highest quality students and strengthen the educational opportunities for both UT and ORNL."

Consequently, each year a portion of the Science

Alliance's funding is distributed directly to two colleges

within the university with the express purpose of supporting graduate and undergraduate education and research. As a result, many students have had occasion to add significantly

to the foundation of their future careers through direct support provided by Science Alliance projects.

ALI YOUSEFZADI, doctoral student working the Seungha Shin, is in his second year of support on a Science Alliance supported JDRD project. Yousefzadi's work with Shin has included conducting analyses using machine learning techniques. He has authored two publications currently under review, serving as first author on one.

Mark Dean's student, **AARON YOUNG**, began his work with Dean in 2016. His current research focuses on the architecture and design of neuromorphic computing, the subject of Dean's JDRD project. Young's doctoral work with Dean will place him at the forefront of an emerging area of research.

SABRINA SCHWERZLER has benefitted from Claudia Rawn's JDRD work by gaining familiarity with several new laboratory techniques. Schwerzler has also established professional relationships with several ORNL researchers as a result of her work with Rawn.

Maik Lang's JDRD supported student, **WILLIAM CURETON**, actually began his work with Lang as an undergraduate. After graduation, he continued his work with Lang's team as a graduate student. His time on the project has allowed him to work on the Spallation Neutron Source at ORNL.

JIAN LIU has both a graduate and undergraduate student on his JDRD team. Physics doctoral student Junyi Yang has been tasked with leading the project; invaluable experience for any researcher. Kyle Noordhoek is a double-major undergraduate student working in both physics and chemistry. His work with Shin has allowed him to leverage his chemistry knowledge while gaining cross-disciplinary skills in physics beyond his class curriculum.

Many Science Alliance funded students are actively collaborating with ORNL scientists. They have earned additional funding for their work from a variety of sources, including the U.S. Department of Energy, the National Science Foundation, the National Nuclear Security Administration and the Army Young Investigator Program. The contributions made by these scholars to each supported project ensure the University of Tennessee, as well as the State of Tennessee, a substantial foothold in the future of the nation's scientific community.



PUERTO RICO STUDENTS CONTINUE WORK WITH SCIENCE ALLIANCE SUPPORT

In September 2017, Puerto Rico fell victim to two separate hurricanes, leaving the island in a state of emergency with thousands dead and millions without power. At the beginning of the month, Hurricane Irma, then a Category 5 storm thought to be the most powerful Atlantic hurricane on record, swept by just north of the island after devastating the Caribbean.

Puerto Rico was still recovering from the destruction and loss of power left in Irma's wake when Hurricane Maria struck. Maria, another Category 5 storm, is thought to be the worst natural disaster to strike the region since 2004. Arriving just two weeks after Irma, the storm caused major flooding and destroyed entire sections of the island. In addition to the catastrophic damage and loss of life, higher education in Puerto Rico was greatly impacted. Much of the island was subject to extended power outages. Roads and other infrastructure were destroyed, and many students were forced to look elsewhere to continue their education.

The University of Tennessee, Knoxville, with funding from the Science Alliance, become home to a group of these students thanks to the efforts of Terry Hazen, UT-Oak Ridge National Laboratory Governor's Chair for Environmental Biotechnology. Hazen was once a faculty member at the University of Puerto Rico, Rio Piedra, the students' home institution.

"I have a lot of good memories of my time there, and I maintain a strong connection to the university," said Hazen. A former postdoctoral student of Hazen's, Gary Toranzo-Soria, is a faculty member at the University of Puerto Rico, and Hazen reached out to him in the aftermath of the storm.

"It took more than a week, but I finally got in touch with him by cell phone and told him I was more than happy to help in any way I could," said Hazen. Less than six months later, a group of students arrived in Knoxville to continue their academic careers.

Science Alliance funding provided housing for the students as they worked to get back on track. Much of the work the students had already completed was lost in the storm, as research in biology and microbiology often requires a steady power supply. Relocating to the University of Tennessee allowed these students to stay on path to completing their research and earning their degrees.



STUDENT FUNDING

DEPART MENT	TOTAL SUPPORT	TYPE OF SUPPORT	# OF STUDENTS	HIGHLIGHTS
Biology	305,315	GTA/GRA	38	Supported students have produced 28 publications and 14 posters and presentations. They have affiliations, either via mentors or directly, with multiple divisions at ORNL, including the Spallation Neutron Source, the Biosciences Division, and the Center for Molecular Biophysics.
Chemistry	106,692	GTA/GRA	25	Nine publications have been produced by supported students. Nearly all students have affiliations with ORNL via faculty members or advisors. Some students have received additional support from NSF, NIH and the DOE.
Earth & Planetary Sciences	40,975	GTA/GRA	8	Half of supported students have ORNL affiliation in one of a number of areas, including the Neutron Data Analysis and Visualization Division and Climate Change Science Institue. They have produced 3 publications, 15 presentations and one student has been awarded an Exxon Mobile Fellowship.
Electrical Engineering & Computer Sciences	93,396	GTA/GRA	13	Students have been first authors on 4 of the 9 total publications produced by the group. They have affilations with DoD, NSF and the USDA.
Geography	10,100	GTA/GRA	3	All supported students have an ORNL affiliation in the Geographic Information Science and Technology Group, the Populations Distribution and Dynamics Team, or the Center for Transportation Analysis. They have produced one publication and two presentations.
Math	92,000	GTA/GRA	33	Three publications and five presentations have been produced by supported students. Six of these students have an ORNL affiliation via a joint faculty member, Distinguished Scientist Clayton Webster or another faculty member.
Physics	222,500	GTA	25	Approximately two thirds of supported students are affiliated with ORNL via advisors or joint faculty members. Students are working with the Division of Neutron Sciences, the Center of Nanophase Material Science, the Material Science and Technology Division, and the Physics Division.
Psychology	19,000	GTA/GRA	1	The supported student has authored three publications. His work focuses on behavioral science regarding the effect of opiods.

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ELBIO DAGOTTO

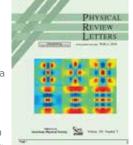
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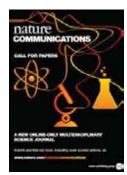
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Graduate students receiving Science Alliance support authored more than 50 publications and presented more than 30 posters.



Compressed

Sensing

Current JDRD teams have a total of 9 publications currently under review as a result of Science Alliance funded work.

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