An Automotive Project with Global Impact

Creating a collaborative network to improve on automotive design is the purpose of students from Tecnológico de Monterrey (Mexico), coming together with students from Clemson University, to form an initiative to innovate the automotive industry. Dr. Hugo Sanabria of Clemson Physics and Astronomy is one of the principal collaborators on the project.

This has been made possible thanks to the “100,000 Strong in the Americas” grant, which is an initiative by the United States government to strengthen the competitiveness of higher education in the western hemisphere, and whose funds were provided by Exxon Mobil.

The Department of Automotive Design at Tec Monterrey, together with the Departments of Mechanical Engineering and Physics and Astronomy at Clemson, were awarded the funds. After a careful selection process, the first stage on the program started on May 23, 2016 at Clemson.

Having received these funds has a great impact for a major in automotive design engineering and for all students at Tec Monterrey, because it opens a great door for collaborative projects with an international focus on the automotive industry,” remarked Dr. Luis Fernando Rodriguez, director of the program at Tec Monterrey. The project, which focuses on structural failures of truck brakes, will include laboratory tests in order to provide possible solutions to the discovered errors.

This work was recently presented to the U.S. Consul for Education, Press, and Culture, in Monterrey, Jeffrey T. Lodermeir, who recognized the need of such collaborations between both countries.

The first stay at Clemson lasted four weeks, and the second stage of the project continued at Tec Monterrey, where the students completed the program on July 15th.

Adapted from June 23, 2016 Panorama article by Luis Mario García (Continued on page 3)
A Message from the Department Chair

It has been a very active summer and fall semester for our department. It is hard to believe that I have been in this position just over one year. We had a very successful graduate recruiting season, with thirteen new teaching assistants who arrived for the fall semester. It was also gratifying that several of our top-rated applicants accepted our offers. And we are about to do it all over again and hope we are just as successful. The Department had a very successful search for a new atmospheric physics faculty member last spring, and Dr. Xian Lu joined the faculty in August. Her expertise is in atmospheric physics modeling. Currently, we have three open faculty searches that are ongoing. The areas are: astrophysics (planet formation), experimental condensed matter physics and experimental atmospheric physics. The astrophysics position search is complete, and we have an extremely strong slate of candidates from which to choose.

Clemson University was recently designated a Carnegie R1 Research Institution. This has helped in both our graduate student and faculty recruiting. Of upcoming interest this year will be the activities surrounding the solar eclipse in August, 2017, all of which will be highlighted in our spring newsletter.

The strength of our department is in its students, faculty and staff. One very important component to department success is our relationship with our alumni and former faculty and staff. If there are ways that I may do this better then, I would appreciate your ideas. Your financial support of our department is crucial as we continue to grow, as well. Funds for undergraduate scholarships and awards and for faculty recruiting efforts are essential to our success. One of the very exciting events that happened this summer was the formation of the new College of Science (COS) and our integration into this new college. Our very own Dr. Mark Leising is serving as its founding Interim Dean. We all look forward to the challenges and the opportunities that this coming year will bring to our department and the new college.

Dr. Terry Tritt, Interim Chair
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There are several ways to donate. You may send a check to the Clemson University Foundation, P.O. Box 1889, Clemson, SC 29633. Checks should be made payable to the Clemson University Foundation with Physics and Astronomy specified on the memo line. Alternately, you may visit the Clemson website: http://www.clemson.edu/giving/how/ and make a secure electronic donation. Again, please specify that the donation go the Physics & Astronomy Department and indicate to which project you would like to donate.

Thank you, as always, for your continued support of the Department. You may contact the Annual Giving Office at (864) 656-5896, should you have any questions regarding your donations. If you have other questions you may contact the Department directly at (864) 656-3416.
Dark matter, the mysterious substance that constitutes most of the material universe, remains as elusive as ever. Although experiments on the ground and in space have yet to find a trace of dark matter, the results are helping scientists rule out some of the many theoretical possibilities. Three studies published earlier this year, using six or more years of data from NASA's Fermi Gamma-ray Space Telescope, have broadened the mission's dark matter hunt using some novel approaches.

“We've looked for the usual suspects in the usual places and found no solid signals, so we've started searching in some creative new ways,” said Julie McEnery, Fermi project scientist at NASA's Goddard Space Flight Center in Greenbelt, Maryland. "With these results, Fermi has excluded more candidates, has shown that dark matter can contribute to only a small part of the gamma-ray background beyond our galaxy, the Milky Way, and has produced strong limits for dark matter particles in the second-largest galaxy orbiting it.”

Among the new studies, the most exotic scenario investigated is the possibility that dark matter might consist of hypothetical particles called axions or other particles with similar properties. An intriguing aspect of axion-like particles is their ability to convert into gamma rays and back again when they interact with strong magnetic fields. These conversions would leave behind characteristic traces, like gaps or steps, in the spectrum of a bright gamma-ray source.

Manuel Meyer at Stockholm University led a study to search for these effects in the gamma rays from NGC 1275, the central galaxy of the Perseus galaxy cluster, located about 240 million light-years away.
High-energy emissions from NGC 1275 are thought to be associated with a supermassive black hole at its center. Like all galaxy clusters, the Perseus cluster is filled with hot gas threaded with magnetic fields, which would enable the switch between gamma rays and axion-like particles. This means some of the gamma rays coming from NGC 1275 could convert into axions - and potentially back again - as they make their way to us. Meyer's team collected observations from Fermi's Large Area Telescope (LAT) and searched for predicted distortions in the gamma-ray signal. The findings, published April 20, 2016 in Physical Review Letters, exclude a small range of axion-like particles that could have comprised about 4 percent of dark matter. "While we don't yet know what dark matter is, our results show we can probe axion-like models and provide the strongest constraints to date for certain masses," Meyer said. "Remarkably, we reached a sensitivity we thought would only be possible in a dedicated laboratory experiment, which is quite a testament to Fermi."

Another broad class of dark matter candidates are called Weakly Interacting Massive Particles (WIMPs). In some versions, colliding WIMPs either mutually annihilate or produce an intermediate, quickly decaying particle. Both scenarios result in gamma rays that can be detected by the LAT.

Regina Caputo at the University of California, Santa Cruz, sought these signals from the Small Magellanic Cloud (SMC), which is located about 200,000 light-years away and is the second-largest of the small satellite galaxies orbiting the Milky Way. Part of the SMC's appeal for a dark matter search is that it lies comparatively close to us and its gamma-ray emission from conventional sources, like star formation and pulsars, is well understood.

Most importantly, astronomers have high-precision measurements of the SMC's rotation curve, which shows how its rotational speed changes with distance from its center and indicates how much dark matter is present. In a paper published in Physical Review D on March 22, 2016, Caputo and her colleagues modeled the dark matter content of the SMC, showing it possessed enough to produce detectable signals for two WIMP types. "The LAT definitely sees gamma rays from the SMC, but we can explain them all through conventional sources," Caputo said. "No signal from dark matter annihilation was found to be statistically significant."

A study led by Marco Ajello at Clemson University and Mattia Di Mauro at the SLAC National Accelerator Laboratory took the search in a different direction. Instead of looking at specific astronomical targets, the team used more than 6.5 years of LAT data to analyze the background glow of gamma rays seen all over the sky. The nature of this light, called the extragalactic gamma-ray background (EGB) has been debated since it was first measured by NASA's Small Astronomy Satellite 2 in the early 1970s. Fermi has shown that much of this light arises from unresolved gamma-ray sources, particularly galaxies called blazars, which are powered by material falling toward gigantic black holes. Blazars constitute more than half of the total gamma-ray sources seen by Fermi, and they make up an even greater share in a new LAT catalog of the highest-energy gamma rays.

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Some models predict that EGB gamma rays could arise from distant interactions of dark matter particles, such as the annihilation or decay of WIMPs. In a detailed analysis of high-energy EGB gamma rays, published April 14, 2016 in Physical Review Letters, Ajello and his team show that blazars and other discrete sources can account for nearly all of this emission.

https://www.sciencedaily.com/releases/2016/08/160812160422.htm

Clemson Biophysicist to Continue Work on Molecular Modeling

Clemson biophysicist, Dr. Emil Alexov, was awarded $1.42M by the National Institutes of Health to continue the work on developing methods and software for modeling various processes in molecular biophysics. The work builds upon the previous research project on enhancing DelPhi capabilities to calculate electrostatic field and energies of biological macromolecules as proteins, DNAs and RNAs. Altogether the lab has received $3.7M in NIH funding to provide the biophysical community with tools to model electrostatics and the effects of disease-causing mutations and to assess the role of ion concentration of protein binding and folding.

The first one is to enable DelPhi to model large macromolecular assemblages as molecular machineries, neurons and cellular compartments. This is a very important development, since, to understand how cells function, one should model not just a single macromolecule, but many macromolecules as they interact and form large macromolecular assemblages. This is how individual macromolecules get involved in the complex interactions in the cell to dynamically form networks and pathways that are essential for normal cell function. Modeling such large systems with dimensions typically over 1000 Angstroms is not an easy task and requires computer code optimization.

To address this challenge, computational expert Dr. Marcin Ziolkowski, together with Dr. Zhe Jia and Dr. Lin Li of Clemson, will develop modern code architecture that allows the computation to be distributed over different CPUs and GPUs. This will represent a major breakthrough and will make DelPhi the only software capable of modeling extremely large macromolecular assemblages.

In many cases the structure of the abovementioned large macromolecular assemblages is not available, but typically researchers can take a picture via various experimental techniques, for example, using Cryo-EM. In the new funding period, the team will further develop Protein-Nano-Object-Integrator (ProNOI) to converts such images into a 3D object made of pseudo atoms. This is crucial to modeling these objects, since almost all tools in computational biophysics deal with the atomistic depiction of the object.

Another essential component of the new development is to enable DelPhi to model other quantities different from electrostatics. These include (but are not limited to) temperature, flux, and heat. While electrostatics is one of the major forces in molecular biophysics, many other reactions and forces are involved in the complex function of the cell. These include the flux of ions across various membranes, temperature distribution across different cellular compartments, and heat transfer due to various reactions.

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In particular, one wants to know how much energy should be radiated into a tumor in order to kill most of the cancer cells, but not to affect healthy tissue. In combination with ProNOI capabilities and new code development to allow various differential equations to be solved via DelPhi, the team is aiming to provide the biomedical community with a tool that (given the photograph of a tumor the radiation therapist) will be able to estimate the amount of radiation and the size of the radiation spot that most effectively will treat the tumor.

In addition to this medical application, the team believes that the new development will address fundamental large-scale biological questions. For example, they, in collaboration with Dr. Joshua Alper, applied DelPhi to model the motion of transport molecules (kinesin and dynein) along microtubules. The microtubules are very large objects and cannot be modeled with standard biomolecular packages. The team showed that electrostatics is the dominant force controlling kinesin directionality. They also showed that electrostatics provides guiding funnel for kinesin and dynein binding. This allows the long legs of dynein to adjust their position as dynein walks along the microtubule.

The team is very excited and is working hard to deliver the planned development. It is anticipated that the work will be completed by 2020, and the biophysical community will be given a powerful tool to address the challenges of modeling cellular processes, with applications for basic science and medicine.

**Symposium for the Introduction to Research in Physics and Astronomy 2016**

On August 15, 2016, this year's annual Symposium for the Introduction to Research in Physics and Astronomy (SIRPA) was held at Clemson’s Watt Innovation Center and featured keynote speaker, Dr. Mildred Dresselhaus, professor of physics emerita at the Massachusetts Institute of Technology. Dr. Dresselhaus has been called the “Queen of Carbon” for her pioneering work in carbon, carbon nanotubes and graphene and has earned many awards in her field. She also was postdoc advisor to Clemson professor Dr. Aparao Rao and has collaborated with Dr. Rao for almost twenty-five years.

During this symposium physics graduate students and faculty members highlighted the Department’s research activities through poster presentations and brief talks. The winners for their presentations are as follow:

The “Best Talk” award went to Sai Sunil Mallineni, Graphene: a novel 2D material for use in transparent flexible electrodes an triboelectric generators.

The “Best Poster” award was a tie between Fengjiao Liu for his work on Electron and Phonon Transport in SnSe 2D Nanoplates and Amy Gall for her poster on the Contribution of the 1s2l3l’ Dielectronic Recombination in Li-Like Ar to the Hypothesized Dark Matter Related Faint Feature in Galaxy Clusters.
Imperfection could be the key to more perfect energy storage, according to a team of researchers at Clemson University’s Nanomaterials Center near Pendleton.

Capacitors complement batteries in computers and other devices. They release electricity faster than batteries to get devices up and running, because batteries rely on chemical reactions to release electricity. But capacitors can’t match the batteries when it comes to storage.

Led by physics professors Apparao Rao and Ramakrishna Podila, and funded by a National Science Foundation grant, the team at Clemson has improved the amount of electricity that can be stored in carbon-based supercapacitors up to 500 percent.

The storage breakthrough came, more or less, by poking holes in the surface of microscopically thin carbon graphene sheets used inside capacitors. According to doctoral candidate Jingyi Zhu, the holes are made by replacing some of the carbon atoms on the outside layers of graphene with nitrogen atoms. That, in turn, creates gaps for more electrons to burrow deeper inside the graphene.

Their work suggests that cars that run on electricity could have lighter, more efficient energy storage that allows for greater range, and homes with solar cells could better store the free energy generated for nights and cloudy days — and rely less and less on burning coal or natural gas or other fossil fuels. Making clean energy a reality means integrating solar cells with energy storage devices, according to Podila, to mitigate the fluctuations associated with photovoltaics due to weather.

“For instance, the output power may be significantly low on a cloudy day when sun is blocked,” he said. “Energy storage devices, such as batteries and supercapacitors, can be used as buffers and smooth out the fluctuations by jumping in at an appropriate time when the solar panels are producing low power.”

Graphene-based capacitors are much cleaner and lighter than batteries that rely on chemicals such as lithium. Graphene is both strong and malleable enough to be fashioned into bodies for cars, or trucks, or buses, said Zhu, and those graphene bodies would be capable of storing the energy needed to run such vehicles.

Clemson Area Transit and Clemson University recently landed a federal grant to buy up to a dozen electric buses. Those buses will charge up at the CAT garage, but this supercapacitor technology could turn up in future additions to the bus fleet. In fact, Rao and Zhu said, some public transport systems in China already rely on electric buses with supercapacitors that charge up station-to-station.

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The researchers are still trying to determine how to configure these imperfections to best store energy, but they are already talking to private partners about next steps. Rao, who runs the Nanomaterials Center, said the technology could start turning up in industry within a few years.

The team – Rao, Podila, Zhu, Anthony Childress, Mehmet Karakaya, Sushmita Dandeliya, Anurag Srivastava and Ye Lin – published their findings over the summer in Advanced Materials.

International Students Learn Astrophysical Modeling from Clemson Professor’s Network Tools

From August 19 through August 26, 2016 the 3rd Astrophysical Nuclear Reaction Network School was held in Schmitten, Germany. The focus of the school was the understanding and application of nuclear reaction networks to astrophysical models for systems such as novae, x-ray bursts (rp-process) and neutron star mergers (r-process). The reaction network employed was the public NucNet Tools developed and published by Dr. Bradley Meyer of Clemson University.

The school’s target group was a diverse, international group of graduate students and postdocs with an interest in astrophysical reaction networks. Participants were typically astrophysics students interested in including nucleosynthesis into their models or in interpreting observations, or nuclear physics students interested in exploring nuclear physics sensitivities in astrophysical models.

The Network School emphasized group work and practical training with Meyer’s suite of codes. The practical work was complemented by a series of lectures on numerical techniques, reaction rate formalism and the underlying nuclear physics, astrophysical applications, and observations.

Previous network schools have been hosted at Notre Dame University (2005) and at Abtei Frauenworth, Germany (2011).

At the end of the school, students had the code installed on their computers, knew how to run it, understood how it works, and were able to interpret results.

This school was sponsored by the Nuclear Astrophysics Virtual Institute (NAVI) and the Joint Institute for Nuclear Astrophysics - Center for the Evolution of the Elements (JINA-CEE).

Workshop group describes the results of their study of beta-decay half lives and r-process nucleosynthesis, computed with NucNet Tools.

For more information on the opportunities offered by NAVI and JINA-CEE, please visit http://jinaweb.org. To access Dr. Meyer’s code, see: https://sourceforge.net/p/nucnet-tools/home/Home/.
Clemson Scientists Receive $1.8M Grant to Combat Type 2 Diabetes

By Jim Melvin, College of Science Media Release, September 15, 2016

A pair of Clemson University scientists is using high-tech computer modeling and experimental validation techniques to unveil the intricate molecular causes of adult-onset diabetes, one of the world’s most widespread, damaging and costly diseases. Increased incidences of obesity, poor diet and lack of physical activity have contributed to a disturbing rise in the number of people afflicted with adult-onset diabetes. Clinically known as Type 2 diabetes, the disease affects tens of millions in the United States and hundreds of millions across the globe.

In an ongoing effort to find higher-quality therapeutic treatments, Clemson researchers Feng Ding and Weiguo Cao recently received a collaborative $1.8 million grant from the National Institutes of Health to attain a deeper understanding of how a peptide protein co-secreted with insulin in the pancreas is associated with beta cell death and subsequent insulin deficiencies. The primary function of beta cells is to produce and store insulin, a hormone that regulates the amount of glucose in the blood. “We use computer modeling to understand the molecular mechanisms in the pancreas where insulin is produced and then we make predictions based off the models,” said Ding, an assistant professor of biophysics in the College of Science who is the principal investigator of the grant.

“After that, we employ biophysical and biochemical methods to validate our predictions. Finally, we will be able to design therapeutic approaches based on what we’ve learned. This combined computational and experimental approach can improve research efficiency and significantly shorten the discovery cycle.”

In people who are not diabetic, the peptide hormone called islet amyloid polypeptide (IAPP) helps to regulate blood-sugar levels and also slows emptying of the stomach, the latter of which plays a crucial role in how much and how often we feel the need to eat. Proteins such as IAPP (also known as amylin) are composed of a coiled chain of amino acids. For those who have prediabetes or Type 2 diabetes, it is hypothesized that the entanglement of uncoiled amylin, promoted by overproduction of insulin and amylin due to insulin resistance in the pre-diabetic stage, creates a toxic environment that kills beta cells and leads to full-blown diabetes.

“In our bodies, proteins are the workhorses. And in order for these proteins to function, they need to fold into a particular shape,” said Cao, a professor of biochemistry in the College of Science who is a collaborative investigator for the grant. “If they unfold, they stretch into long chains that tend to stick together. And once many of them stick together, they become what is called an aggregate, which interferes with the biological processes within the pancreas and causes beta cells to function abnormally and eventually die.”

Ding’s simulations generate large amounts of data, most of which is produced and analyzed via the Palmetto Cluster, Clemson University’s highly regarded supercomputer. With these computational models, Ding and Cao will investigate anti-aggregation approaches from three novel directions:

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First, they will study how the internal mechanisms of healthy individuals are able to maintain their effectiveness and prevent IAPP aggregation.

Then they will examine how naturally occurring plant-based molecules that are known to regulate biological processes can play a role in inhibiting IAPP aggregation. Finally, they will design new microscopic materials that can aid in the inhibition of IAPP aggregation and also transport medicines between and within cells with vastly improved efficiency.

“How do healthy individuals — many of whom are overweight — naturally prevent these proteins from aggregating? From this, we can learn the mechanisms. Then we can design therapeutics to mimic or promote these mechanisms,” Ding said. “The second topic is to look at how the small molecules, the naturally occurring polyphenols, help prevent aggregation. From this, we can design better inhibitors. The third topic is engineering nanosized objects that can be used as drug carriers and also increase the efficacy of the drug.”

A slew of other diseases, including Alzheimer’s, Huntington’s, Lou Gehrig’s and Parkinson’s, might also be caused by similar forms of protein aggregation. For instance, people with Type 2 diabetes have much higher incidences of Alzheimer’s than occur in the general population. So the results of Ding and Cao’s research could potentially produce a menagerie of treatments.

“All these aggregation diseases look similar in that the molecular damage is caused by either the elongated protein fibrils or intermediate smaller aggregates that have become stuck together,” Ding said. “So this indicates that there might be an underlying commonality. In fact, some people are starting to call Alzheimer’s ‘Type 3 diabetes.’”

Clemson Recognized at International Thermoelectrics Conference

Dr. Jian He’s former Ph.D. student Dale Hitchcock (currently senior staff scientist at Savannah River National Lab) and current undergraduate Andrew Shore conducted inelastic neutron scattering experiments at Oak Ridge National Lab earlier this year.

The results were included in a poster presented at International Conference on Thermoelectrics, in Wuhan China. The poster was selected as one of twenty outstanding posters from over 400 submissions. He’s current Ph.D. student Yufei Liu (pictured at right) accepted the award at the conference banquet on behalf of the team.
Clemson University will host a conference on the future of integrative structural biology in April, 2017. One of the focuses of the conference will be to address the grand challenge for structural biologists to build a complete molecular atlas of the cell. Rather than the mere acquisition and accumulation of high-resolution structural data from any one of multiple biochemical, biophysical and computational approaches, the complete molecular atlas of the cell will require “integrative structural biology” approaches that rely on data from multiple methodologies. Because cells are comprised of complex, dynamic macromolecular machines, it is critical that this atlas incorporates data from both high-resolution static and dynamic methods.

This one-day workshop will serve as a platform to discuss the future of integrative methods in the field of structural biology. Three sessions of talks with invited and contributed speakers, a poster session, and a round-table discussion will cover topics in i) electron microscopy, ii) label-based methods, iii) scattering methods, and iv) computational approaches.

The local workshop organizers are Dr. Joshua Alper (alper@clemson.edu) and Dr. Hugo Sanabria (hsanabr@clemson.edu), and the sponsors are ORAU (Oak Ridge Associated Universities), Clemson’s Eukaryotic Pathogens Innovation Center (EPIC), and Clemson’s College of Sciences, Department of Chemistry, Department of Genetics and Biochemistry, and Department of Physics and Astronomy. For more information on the workshop, please contact the organizers listed above.

Graduate Student Awarded NSF Career Development Supplement Grant

Dr. Feng Ding’s graduate student, Bo Wang, has received a Career Development Supplement Grant from the National Science Foundation in the amount of $9,000.

Wang joined Clemson in 2012, working for Dr. Ding’s Lab—Structure, Dynamics, and Functions of Biomolecules and Molecular Complexes. Bo’s projects include soft condensed matter, nanoparticle-protein interactions, and protein aggregations. Bo has published four research papers in the area of nano-bio interface, and protein aggregation inhibition by nanoparticles.

The Ding Lab’s current research focus is multiscale modeling of biomolecules and molecular complexes. Experimental characterization of biological systems is often hindered by the limited ability to cover a wide range of time and length scales, associated with many biological processes. Multiscale modeling, which innovatively combines atomic and coarse-grained simulations, provides a unique opportunity to bridge the gaps of time and length scales between experimental observation and underlying molecular systems. Wang’s efforts have contributed to this research.

The Department’s sympathies are extended to the family of Carroll Garvin Hughes III, Clemson physics class of 1958, of Brevard, North Carolina, who passed away on Tuesday, October 11, 2016.

Dr. Lin Li has been promoted to research assistant professor at Clemson.

Dr. Chuan Li and Tugba Kucukkal, former postdocs of Dr. Emil Alexov have been promoted to assistant professors at the Westchester campus of the University of Pennsylvania and Gaulladet University, respectively. Shaolei Teng (former student of Dr. Alexov) has been hired as an assistant professor at Howard University.

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