Department of Scientific Computing

Spring 2015

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Huang studies molecule movements

Dr. Chen Huang joined Scientific Computing (SC) in August 2014 as our newest assistant professor of computational science. Huang arrived at SC following three years as a postdoctoral research associate in the Theoretical Division at Los Alamos National Laboratory. At Los Alamos, his research focused on developing theoretical methods to elucidate long timescale dynamics in materials. During his Ph.D. study, Huang worked on the quantum mechanics embedding theory, which aims to obtain highly accurate electronic properties of molecules and materials. Using this embedding theory, Huang and coworkers successfully uncovered the complicated oxidation process of aluminum surfaces, which has puzzled the scientific and industrial communities for decades.

Huang received the Bachelor of Science in Physics from Tsinghua University in Beijing in 2003, then spent one year in China working as a software engineer.

"After I graduated, I worked in Hefei City, my home town, at a small local database company. I wrote code to connect website pages with databases. My job was to deliver a platform to the customers – which were mainly electricity companies – to help them understand how much money they could earn by feeding (selling) their electricity to users, what the most profitable lines were, and what the potential gross profit of the electric supply would be."

Later, Huang was accepted by Princeton University, and came to the United States in 2004 to begin his doctoral study in physics. When he first arrived at Princeton, he focused on experimental physics. Within a few years, however, Huang became more and more interested in computational science, and decided to work with Professor Emily Carter, a leading researcher in computational quantum chemistry.

"Initially, I tried to do experimental physics. In my third year, I found that I want to work in the field of computational science. I am very interested in employing computer models to understand materials properties. I was lucky, since Prof. Carter just moved from UCLA to Princeton. The atmosphere in the physics department was very fluid, and I was free to choose an advisor from an external department who was actually a chemist."

Huang spent the next four years in Carter's group; his Ph.D. thesis focused on developing multi-scale quantum mechanics methods to solve non-trivial electronic properties of materials. Upon graduation, he learned of

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Professor Meyer-Baese to develop system for detecting challenging breast cancers

IMPROVING DIAGNOSIS AND PROGNOSIS OF BREAST CANCER has been the subject of ongoing research for SC Professor Anke Meyer-Baese. Recently she received a coveted and prestigious award from the European Union's Horizon 2020 Research and Innovation Framework Programme under its Global Fellowships category to continue her cutting edge cancer research.

Along with Dr. Ignacio Alvarez Illan of the University of Granada, Meyer-Baese plans to develop a novel automated diagnosis system that supports the radiologist in the breast cancer diagnosis by using Dynamic Contrast Enhance-Magnetic Resonance Imaging (DCE-MRI), a method which uses a contrast agent to enhance tumor images for a better, more accurate comparison between healthy cell tissue and active cancer tissue. By including critical components such as motion compensation and segmentation and diagnosis of tumors, Meyer-Baese expects to improve the radiological work-flow diagnosis of breast cancer, an EU research priority.

The main goal and overall objective of this project is to develop computer aided diagnosis (CAD) methods and image processing techniques to improve diagnostic accuracy and efficiency of cancer-related breast lesions. Non-mass-enhancing lesions exhibit a heterogeneous appearance in breast MRI with high variations in kinetic characteristics and typical morphological parameters, and have a specificity and sensitivity much lower than mass-enhancing lesions. For this reason, new segmentation algorithms and kinetic parameters can be potentially used as an alternative to the methods for mass enhanced lesions. To develop and implement CAD methods and image processing techniques, the project has basic, strategic, and applied research objectives: i) develop non-rigid registration and segmentation techniques to incorporate spatial variations in temporal enhancement; ii) develop kinetic feature descriptors to quantify significant differences between the benign and malignant lesions; and iii) develop and validate algorithms, interfaces and software implementation for real applications of CAD of breast cancer.

The funding for Meyer-Baese's research is provided by Horizon 2020, a six-year research and innovation program with nearly €80 billion ($90 billion U.S.) to focus on three priorities: excellent science, industrial leadership, and societal challenges. The initiative is designed to secure Europe's global competitiveness, create world class science, and dissolve barriers to innovation and collaboration between the public and private sectors. Horizon 2020 provides research support for broad challenges such as health, demographic change and wellbeing; food security, sustainable agriculture, sustainable forestry, and water research; climate action; and secure, clean and efficient energy.

For more, go to http://ec.europa.eu/programmes/horizon2020.

Professor Anke Meyer-Baese

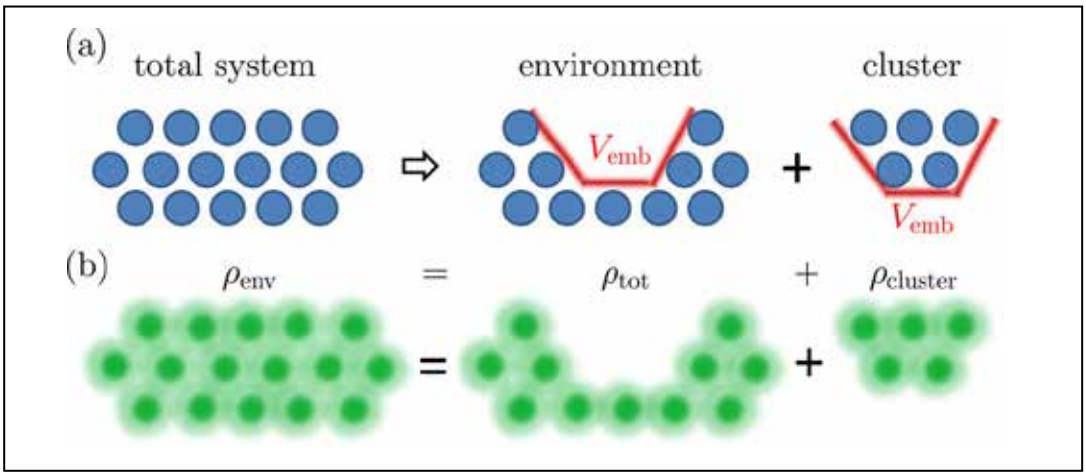

Figure 1. (a) Schematic view of density-functional embedding theory: a bulk system is partitioned into a (possibly periodic) bulk environment and a finite-sized cluster. Their interaction is mediated by an embedding potential, Vemb (red). (b) The embedding potential is chosen such that the sum of the electron densities of cluster, ρcluster, and environment, ρenv, reproduces the total electron density, ρtot, which is calculated in advance.

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an opening in Dr. Arthur Voter's group at Los Alamos National Laboratory.

"Dr. Voter is an expert in the field of molecular dynamics, a field I knew nothing about. In Carter's group, I worked in the field of quantum chemistry. I studied electronic properties of materials, all of which were static properties. It seemed risky to change my research field, but it turned out to be a great idea to work with Dr. Voter. In order to model materials realistically, we need to combine different methods. If I only know how to calculate static properties of materials, there's no way for me to expand my research field. I was fortunate to join this very interdisciplinary department."

Huang accepted the postdoc position to work with Dr. Voter and moved to New Mexico in 2011. There he contributed to the development of the accelerated molecular dynamics (AMD) method, a promising approach to study long timescale dynamics in materials. His work aimed at bridging the timescale gap between experiments and computer simulations, in order to provide an effective way to predict striking kinetic processes in materials.

"It is important to understand the response of the materials to changes in external parameters. Such insight is critical if we want to precisely fabricate materials at the nanoscale. However, it is very challenging to experimentally monitor these kinetic processes in materials in real time. This makes the computer modeling of kinetic processes very important. I was fortunate to spend three years working with Dr. Voter in that field."

Now Huang has settled into his new position as an assistant professor in SC, and has given considerable thought to his research path for the

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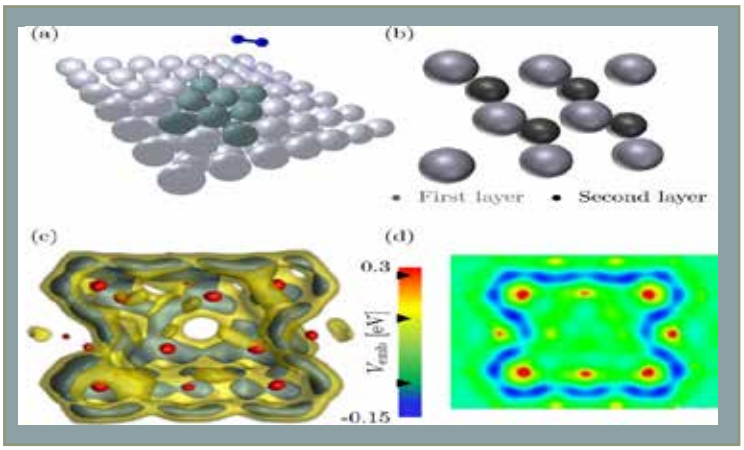
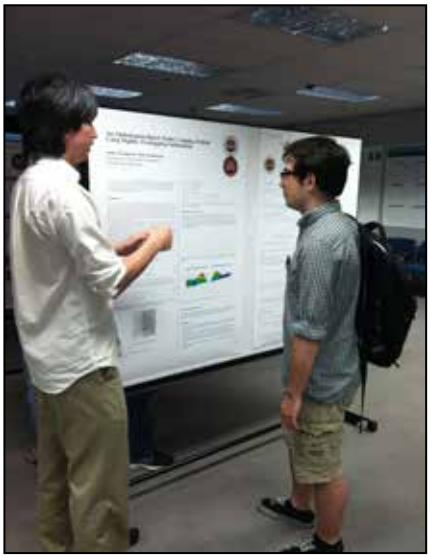


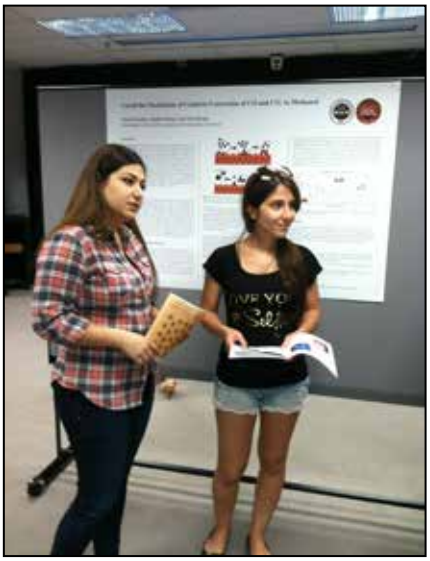
Figure at left.
(a) Aluminum (111) surface and approaching oxygen molecule (blue). A possible selection of atoms for a bridge-site cluster is shaded. (b) Bridge-site aluminum cluster [see shaded atoms in panel a] consisting of 12 atoms (eight in the first and four in the second layer). (c) Equipotential surface plot of the embedding potential for the bridge cluster in panel b. Black triangles in the color bar mark the contour values drawn. (d) 2D cut of the embedding potential shown in c along the first atomic layer.

Student research shines at Computational Xposition

Scientific Computing holds annual Spring Term Computational Research Xposition

At Xpo 2015, more than 30 undergraduate and graduate students presented research results at the poster session. Faculty members supported the work of their individual students and viewed the research from other faculty laboratories. Students, faculty and invited guests had many opportunities to make connections with SC faculty, graduate students, alumni and other attendees at the reception and throughout the half-day event.





Xposition attendees and presenters eat and display resesarch posters.

Smith elected VP of national student association

NBGSA announces newest slate of officers

SC grad student Aria Smith was elected to serve as the new Vice President of Administrative Affairs for the National Black Graduate Student Association (NBGSA) in April. Smith, who has been at Scientific Computing for two years, has been an active participant in Florida State University's local BGSA chapter since 2013. FSU has the only affiliate chapter in the state of Florida. Smith has served as social chair and historian for FSU BGSA. She was instrumental in the recent national conference, having served as a member of the conference organizing committee and presenting a poster entitled, 'fMRI Data Analysis Techniques in Substance Abuse Conditions: A nicotine-addiction study.' Smith was elected to the national organization along with fellow FSU students Kenneth Johnson, an English graduate student and Genevieve Bell, a doctoral student in neuroscience. In addition to her administrative duties, Smith will recruit members and assist affiliate chapters at colleges and universities in the southeast region of the U.S.

"As VP, I plan to strengthen the communication between the Executive Board and the Leadership Team. The FSU chapter will host a Memorial Day celebration at the FSU Reservation this summer; this will be the final event until the fall semester. We will use the remainder of the summer to prepare for the upcoming semester which includes the new graduate student organizational fair, our general body meetings, and social and community service events," said Smith.

The National Black Graduate Student Association is a non-profit interdisciplinary organization that was founded in 1989 to provide an opportunity for students all over the United States the chance to participate in presentations, professional workshops, and roundtable discussions. The organization has over 100,000 members and is the largest interdisciplinary graduate student organization. Smith will serve as vice president from June 1, 2015 – May 31, 2016.

For more information on memberships, NBGSA students, chapters, alumni, state and academic representatives, and national and regional conferences, go to the NBGSA national and FSU websites at http://www.nbgsa.org. https://studentgroups.fsu.edu/organization/BGSA
For more information on the department, go to sc.fsu.edu.

Xu selected for AARMS summer school

Feifei Xu departs in the coming weeks to study mathematics in Halifax, Nova Scotia. Xu was accepted to the Atlantic Association for Research in the Mathematical Sciences (AARMS) Summer School in Differential Equations and Numerical Analysis. The prestigious school and workshop series will be held at Dalhousie University in Halifax, Nova Scotia July 6 – 31. The AARMS Summer School invites highly regarded faculty from around the world to teach graduate level courses and workshops in mathematics.

Xu registered for two of the available courses, Topics in reaction-diffusion systems: theory and applications, led by Michael Ward and Juncheng Wei from the University of British Columbia, and Structure-preserving discretization of differential equations taught by Elena Celledoni and Brynijulf Owren from the Norwegian University of Science and Technology. "Last year in Bejing I took the course on singularly perturbed problems, which is also provided as a course in AARMS, so now I am doing these two courses. I think this is a good opportunity for me to learn more." Xu said.

"I am interested in these workshops because I came here with a certain mathematics background, especially numerical methods, to do research. My research is computationally based; I study things with my research such as adaptive refinement and multiscale modeling so I can solve discontinuous solutions. In reality, these problems involves cracks, deformations or fractures - things like that. Because traditional numerical tools focus on smooth or continuous solutions, they don't know how to treat discontinuous solutions accurately so we use modified or hybrid methods to solve these problems."

> "I hope to learn more and to get more powerful tools to solve the problems in our research."

"I hope to learn more and to get more powerful tools to solve the problems in my research."

Xu is excited about visiting Canada and this learning opportunity. "In Tallahassee, there are very few people working on my research topic. Generally, my research is based on nonlocal problems. Working on this topic gives me the opportunity to look outside and work and study outside. Research doesn't have national boundaries so we can do research everywhere as long as we have common interests," said Xu.

Each course consists of five 90-minute lectures each week. Participants receive grades and certificates after successfully completing courses.

For more information, go to https://aarms.math.ca/summer/

For more on the Department of Scientific Computing, go to sc.fsu.edu.

Graduate students accept internship offers

SC doctoral student Lukas Bystricky accepted a six month research internship at the Centre National d'Etudes Spatiales (CNES) in Toulouse, France. Bystricky will work with Silvia Salas Solano on BASILES (BAncs SImulateurs et Logiciels d'Etude de Satellite), a program designed to standardize all the various kinds of simulations required for satellite operation. "My job will be to improve on the satellite orbit module as there have been some discrepancies between their current model and actual observations," Bystricky said. CNES is the government agency responsible for shaping and implementing France's space policy in Europe. The CNES complex in Toulouse is the largest space center in Europe. Bystricky will be in Toulouse from mid-June through December. Toulouse is located in the southern France close to the border with Spain. Working with Dr. Janet Peterson and Dr. Sachin Shanbhag, Bystricky's work at Florida State has focused on porous media flow for material engineering applications.

James Cheung and Nick Lopez having lunch with Sandia mentors

Ryan Learn returns to Lawrence Livermore National Laboratory to work with Richard Sacks on the complex, high level problem of frequency conversion of broadband beams. In discussing the project, Sacks said, "The Virtual Beamline (VBL) computer code is the laboratory's premier tool for simulating laser operation and performance, including day-to-day setup and operation of the NIF laser and design optimization of new advanced laser architectures. There is an active program to continue to add features and laser physics modeling capability to this code. One of the highest current priorities is to add an explicit broadband simulation mode, in which beam objects may exist alternatively in either temporal or spectral representations. Ryan will work with me to help address a particularly challenging and interesting aspect of this task: frequency conversion of broadband beams." Learn leaves for California in June.

For his summer internship at Sandia National Laboratories, James Cheung will work on a protein folding problem, where a continuous water electrostatic model is coupled with a discrete amino acid chain model. Former Scientific Computing postdoctoral associate Mauro Perego and Pavel Bochev, a computational mathematician, will be Cheung's advisors for the project.

Other students with summer placements are Rui Gu, who is interning at Datamaxx, a software company local to Tallahassee; Nick Lopez who is at Sandia National Laboratories and is working with Mark Taylor, the chief computational scientist for Accelerated Climate Modeling for Energy; and Nathan Crock, who has accepted a summer position at the Max Planck Florida Institute for Neuroscience.

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The department's mission is to be the focal point of science and computation at Florida State University. Max Gunzburger is the Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies are available by calling 850.644.0196. This publication is available in an alternative format on request.

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coming years. "There are two emerging topics that I want to study - fuel cells and heterogeneous catalysis." The key to improve the catalysts used in the industry is to determine their parameters accurately. Most conventional electronic structure methods fail to give reliable numbers. Using the embedding theory developed in his group, Huang aims to obtain these key parameters with unprecedented accuracy, in order to achieve the predictive design of catalysts.

Currently Huang, his graduate student Maliheh Shaban Tameh, and his postdoctoral research associate Dr. Albert Dearden are working on unveiling the true mechanism of the catalytic conversion of carbon dioxide/carbon monoxide gases to methanol. Methanol is a major building block for synthesizing many other chemicals, and is of great importance in the industry.

"Methanol synthesis is a very typical and important industrial process that has been around for many years. However the catalyst used in methanol synthesis hasn't evolved much since the old times. We still use a mixture of copper, zinc oxide, and alumina as the catalysts to produce methanol from carbon sources, such as coal and natural gases." By nailing down the detailed catalytic conversion process, Huang and coworkers are trying to design more efficient catalysts for methanol synthesis, which would greatly benefit the chemical industry.

> "It is important to understand the response of the materials to changes in external parameters. Such insight is critical if we want to precisely fabricate materials at the nanoscale."

To see more about Chen Huang, go to
https://sites.google.com/site/huangfsu/home
The Department of Scientific Computing is online; check us out on Facebook or send us a Tweet.

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