SYNERGY

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A Sea of Possibilities

Blue Waters is a brand new supercomputer housed at NSCA at the University of Illinois. Beckman Institute researcher Klaus Schulten used Blue Waters to create a map of the HIV capsid, detailing 64 million atoms.

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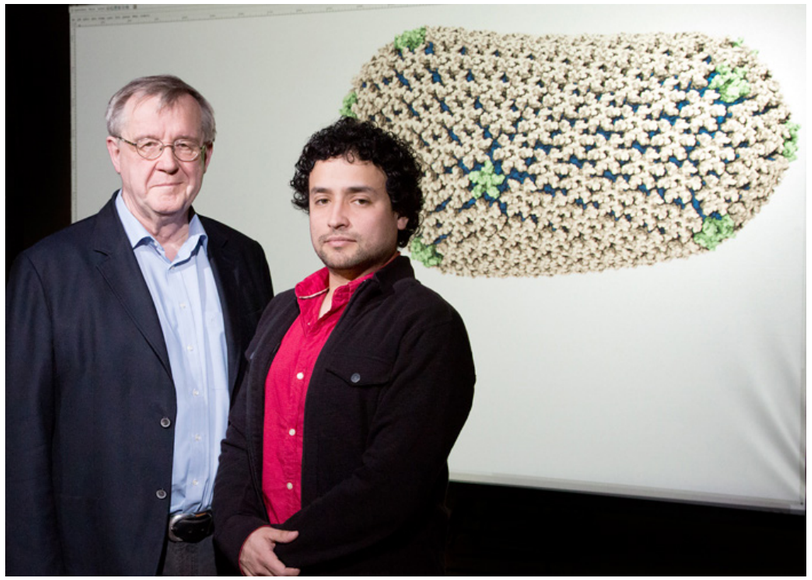
Blue Waters: Sea of Possibilities

For Beckman faculty member Klaus Schulten, Blue Waters has opened up a sea of possibilities. The recently launched Blue Waters supercomputer is one of the most powerful systems in the world, offering sustained performance of one petaflop (that is, a quadrillion mathematical operations per second) on a range of scientific and engineering codes, and offers more than 25 PB (25 million gigabytes) of usable storage.

Schulten's Theoretical and Computational Biophysics Group was one of three chosen to participate in the Blue Waters acceptance test phase, helping to benchmark the supercomputer's performance using its molecular dynamics program NAMD on a structure with 100 million atoms. It was also one of just a few groups chosen to use and test the machine while construction was being completed. Schulten's group had been preparing for the launch of Blue Waters since 2007, when plans for the machine were first announced, making sure that NAMD would be ready to take on the challenge of petascale computing. And this preparation paid off, because just as Blue Waters was coming online, Schulten's colleagues at the University of Pittsburgh approached him with an irresistible problem: could he help them to solve the structure of the HIV capsid?

"We were challenged with describing an extremely large structure. It was a total coincidence that it happened at the very moment when Blue Waters was available," said Schulten. "Five years ago, this breakthrough simulation of the HIV virus wouldn't have happened. At that time, the biggest computer could only handle a million atom simulation." Together with the experimental collaborators at Pittsburgh, Schulten's group was able to construct a full model of the HIV capsid, atom by atom—64 million atoms in total, to simulate on Blue Waters.



Beckman faculty member Klaus Schulten and postdoctoral researcher Juan Perilla and their collegues have determined the precise chemical structure of the HIV capsid, a protein shell that protects the virus' genetic material and is key to its virulence.

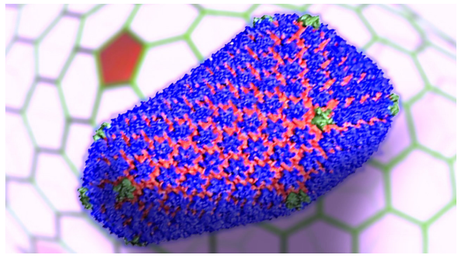
"The work of constructing the overall capsid to match the diverse experimental data can only be done through computer simulation using a methodology we have developed called Molecular Dynamic Flexible Fitting (MDFF)," Schulten said. "You basically simulate the physical characteristics and behavior of large biological molecules, but you also incorporate the experimental data into the simulation so that the model actually drives itself toward agreement with the data."

Possessing a chemically detailed structure of the HIV capsid allows researchers to further investigate how it functions, with implications for pharmacological interventions to disrupt that function.

"This was truly a project using the Beckman approach," said Schulten. "The Beckman Institute is for advanced science and *technology*. For this project we had scientists working with technologists, engineers working with researchers, and computer scientists working with scientists. What we have achieved here would have been impossible to achieve without the combined work of researchers in many diverse areas."

Schulten eagerly looks forward to tapping the power of Blue Waters again in the future, with plans to use it to simulate, among other systems, another virus—this one 200 million atoms in size. "This computer is opening the door for a new era of cell biology," says Schulten. "We are able to examine large molecular structures that couldn't be handled before."

A video about Klaus Schulten's research on the HIV capsid can be found on the Beckman YouTube channel: youtube.com/beckmaninstitute.



Schulten is not the only Beckman researcher who uses the power of Blue Waters to facilitate advances in research. Five other Beckman faculty members are also using Blue Waters on research projects.

Aleksei Aksimentiev's project, entitled "Molecular Mechanism of DNA Exchange," examines the repair of double-stranded DNA breakage in order to determine the molecular mechanism of the process—how one DNA strand is transferred from one DNA molecule to another.

Narayana Aluru is using Blue Waters to perform high-accuracy calculations of the electronic structure of two condensed matter systems of interest: water adsorbed on graphene and hexagonal boron nitride (h-BN) surfaces.

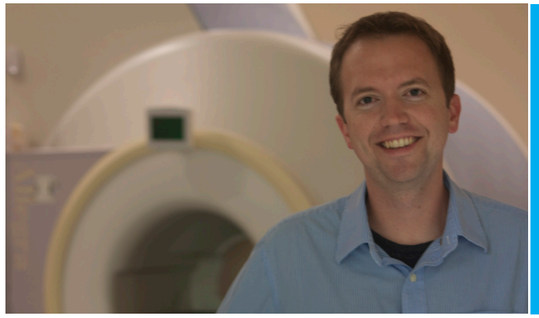
"We are now tackling some unique problems that would not be possible without Blue Waters," said Aluru. His project, "Quantum Monte Carlo Calculations of Water-Graphene and Water-h-BN Interfaces," will provide unique insights to those attempting to develop effective models of the electron correlation in these materials.

Thomas S. Huang is harnessing the power of Blue Waters to create a distributed learning framework for Heterogenous Networks (HN) using Asynchronous Stochastic Gradient Descent (ASGD), which scales up to thousands of computers. His project is titled "Feature Learning by Large-Scale Heterogeneous Networks with Application to Face Verification."

"Researchers in machine learning and pattern recognition have found recently that using many-layer neural networks can often achieve superior results in important visual and speech recognition tasks, when large-scale training samples are used," said Huang. "A major challenge is the huge computational requirements. Blue Waters is a powerful tool to help us to face and conquer this challenge."

Zaida Luthey-Schulten's project, "C. Crescentus Cell Division Using Our In-House Lattice Microbe Simulation Program," focuses on the dynamics and spatial heterogeneity of key regulators of chromosomal replication and cell-cycle timing. Blue Waters will be used to perform stochastic simulations of the reaction models on the whole cell level. Her second project, "Interactions between Ribosomal Signatures and 5′ and Central Domain of the Ribosomal Small Subunit Using NAMD 2.9 Accelerated by GPUs," looks at the assembly of the pre-30S ribosomal complex. In this instance, Blue Waters will provide molecular dynamics simulations of the ribosomal assembly process.

Quantum mechanical effects play an essential role in chemical and biological processes. **Nancy Makri**'s group has developed a rigorous but practical quantum-classical path integral (QCPI) methodology, in which a small quantum mechanical system is treated by full quantum mechanics while the effects of the environment are captured via classical trajectories. Implementation of the project, "Quantum-Classical Path Integral Simulation of Proton and Electron Transfer," on Blue Waters allows for the simulation of multiple proton transfer along water chains and in biological channels and of bridged electron transfer with unprecedented accuracy.



Beckman New Hire Profile:

Curtis Johnson

Degree: Ph.D., Mechanical Engineering, 2013
Then: Graduate Fellow at Beckman
Now: Research Scientist, Biomedical Imaging Center

Curtis Johnson was a great Beckman graduate fellow. He was so great that when he received his Ph.D. from the University of Illinois in mechanical engineering in June, he got a job in July—at Beckman. After working for six years under Beckman researchers John Georgiadis and Brad Sutton, he became well-versed in not only mechanical engineering, but also magnetic resonance imaging (MRI) and, more specifically, magnetic resonance elastography (MRE). With this expertise, he was able to land a position as research scientist in the Biomedical Imaging Center (BIC).

"I was a long-time user of the BIC as an MRI engineer, and my graduate fellowship was a natural extension of that," Johnson said. "I have always felt part of the family here, so when I graduated, the opportunity came along at Beckman to continue what I was working on, but also help with other projects that as a user, I wasn't necessarily involved in. It's a great position, and I'm really excited."

One of the groundbreaking projects Johnson will be working on is research in MRE, which is a noninvasive medical imaging technique that measures the mechanical properties, such as stiffness, of soft tissues using MRI. Knowing the stiffness of tissues can lead to more accurate diagnosis and care of many diseases, as pathological tissues are often harder or softer than the surrounding normal tissue. Currently, MRE is being used in liver imaging in the medical field and is being done with a high degree of accuracy so that it is now replacing biopsies.

"It's pretty revolutionary that biopsies, a tried and true method for testing the liver, are being replaced by MRE," Johnson said. "Because of this success, we're looking at diseases of the brain now, including tumors. Knowing how stiff brain tumors are before surgery can improve outcomes and ensure the surgery is as noninvasive and short as possible. Brain tumors will take less time to remove if doctors know it's a softer tissue before they start surgery. Otherwise, they have to plan for a harder tumor, and the surgery may be unnecessarily long or invasive."

The MRE scan to test for brain tumors is much like an MRI, but instead of the patient lying completely still (a requirement of most MRIs), researchers actually shake the patient's brain.

"The movement is totally controlled and synchronized. If you move but we know how you're moving, we can measure that. Through this motion measurement, we can then calculate tissue stiffness," Johnson said.

This advanced research is possible thanks to the expertise and resources available at Beckman.

"My research leveraged the resources and expertise we have here at Beckman for creating really high-quality images very quickly. In doing that, we were able to create a technique that is really cutting-edge for the field," Johnson said. "Many sites don't have the expertise or resources that we do, and, with that, we're able to develop new approaches so that we can in turn collaborate with researchers throughout the world. What I'm doing as an extension of this research is moving this process from the lab to something that everyone can use, like making the software easy to use, testing on complex populations, and looking for different diseases."

> **The beauty of MRIs is that scientists can walk in and say, "Can I do this?" or "Can I measure this?" and it won't be a crazy question or an impossible task. We say "Yeah, sure. We can probably figure that out."**
>
> Curtis Johnson

MRE is a function of the MRI, which is a tool to accomplish many different tasks for a variety of experiments, Johnson said. He will be working with the MRI to create many different scans, like MRE.

"We set up protocols, so if a researcher comes to us to do new research, we help solve his or her problems initially and along the way. People can come to us with all sorts of propositions, and we write code to make that happen," Johnson said. "The physics of MRI allow for a lot of flexibility. In the scope of MRI, there are a number of different contrast agents. We write code for pulse sequences that make the scanner do different scans to see various parts of the brain and the body. The beauty of MRIs is that scientists can walk in and say, 'Can I do this?' or 'Can I measure this?' and it won't be a crazy question or an impossible task. We say 'Yeah, sure. We can probably figure that out.' Someone just needs to ask the question."

Tackling these projects will be Johnson's main objective in his new job, and he is up for the challenge.

"It's exciting because I've always been part of the team, yet it's really different. Despite the fact that I've been here a long time, there's new stuff I'm encountering already that I get to be involved in. I like being involved in a wide range of projects," Johnson said.

Get inside the minds of scientists at the Chambana Science Café

Joe Toscano is going above and beyond the call of duty as a postdoctoral fellow at the Beckman Institute. His primary job as a postdoc is to conduct leading-edge research for three years at one of the top interdisciplinary research facilities worldwide. But Toscano decided to bring a little bit more to the University of Illinois campus.

While completing his graduate studies at the University of Iowa, Toscano attended a Science Café in Iowa City, an informal gathering that brings scientists out of their labs to public areas to talk about their work and answer questions. Science cafés are a grassroots movement in the United States that have drawn inspiration from Café Scientifique, a network based in the United Kingdom.

The café in Iowa City was enjoyable and was a good addition to the cultural community, Toscano says, so shortly after arriving in Champaign-Urbana, he and a fellow Illinois postdoc (Jessica Love) decided to organize one for this community.

"Science cafés are meant to make science approachable to the general public. Oftentimes, many people feel like science is hard to understand. Most of what non-scientists know is that we conduct research and then tell them about what we find, but they don't find out about how we do it or how it really works," Toscano said.

"So we want scientists to come out to a nonacademic setting, like a coffeehouse, and have a discussion about their work and what they do. There is always lively and thought-provoking discussion, and we have a broad audience."

Cafés encourage conversation, debate, interaction, and dialogue between the scientists and the public. Past presenters have even included interactive projects, such as oragami with a mathematician.

After a successful year, Toscano will continue this program for the 2013-14 school year and is excited about the four researchers who will present this semester: Bryan White from the Institute for Genomic Biology, Preethi Jyothi and Abhi Singharoy from the Beckman Institute, and Jana Diesner from the Graduate School of Library and Information Science.

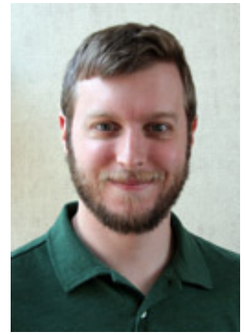
The Science Cafés occur the first Wednesday of every month, starting September 4, at 5:30 p.m. at the Champaign Public Library in Robenson Pavilion Room C. For more information, visit its Facebook page at facebook.com/ChambanaScienceCafe.

The Lineup

Sept. 4, Bryan White
Oct. 2, Preethi Jyothi
Nov. 6, Abhi Singharoy
Dec. 4, Jana Diesner

5 facts about Joe

1. Beckman Postdoctoral Fellow since August 2011
2. Received his Ph.D. in 2011 from the University of Iowa
3. Originally from Rochester, NY
4. Hobbies include astrophotography and brewing beer
5. He and his wife are expecting a baby in August



Why he came to Beckman

"Beckman is an ideal postdoc opportunity. Not only are there many people here who I can collaborate with, but there is also a high level of independence and flexibility to choose what you work on."

His research

"I work on language processing and am specifically interested in speech recognition. How do we understand speech, and how do we learn to understand it? Humans are very good at this. The first time you meet someone, you are able to communicate with them almost instantaneously, learning their voice and the characteristics that differentiate it from other voices you've heard. Computer systems aren't able to do this nearly as effectively. By figuring out how humans recognize speech, we can hopefully make computer systems better at it, too. We're also interested in understanding how speech perception is affected by hearing loss so we can develop ways to improve devices like hearing aids and cochlear implants."

What I did on my summer vacation

Summer generally means a break from the usual routine—perhaps a beach vacation or at least time away from the office or classroom. The Beckman Institute hosts a number of students who want a change from their regular routine and an opportunity to engage in scientific pursuits. This year Rohit Bhargava's Chemical Imaging and Structures Laboratory is hosting a number of students.

This fall, **William "Joey" Smith** will be starting his sophomore year at Columbia University in New York, where he plans to go into biomechanics or biomedical engineering, with the goal of getting his M.D./Ph.D.

"When I was a senior at Uni (University Laboratory High School in Urbana), Sarah Holton gave a speech about the breast cancer research going on at Beckman, and she mentioned that they hire students over the summer," Smith explained. "When she was finished speaking, I told her I would be interested and I met with Professor (Rohit) Bhargava, who got me involved in the project."

Last summer, Smith worked at Beckman with Matt Schulmerich on a project looking at Raman spectroscopy of breast cancer tissue. The project not only provided him with new skills, but gave him an opportunity to do research in an actual working lab.

"Joey was involved in collecting Raman spectra from tissue biopsies with a prototype Raman instrument designed for collecting large spot dark-field Raman spectroscopy," said Schulmerich. "Joey collected measurements from more than 100 biopsy sections and showed great enthusiasm in both collecting and analyzing the data. He quickly became familiar with the software written in-house for collecting and processing it."

The experience was so rewarding to Smith that about midway through his freshman year at Columbia, he contacted Bhargava about opportunities for this summer. Smith will be working with Matt Kole on a project quantifying the lipid and protein content from sunflower oil specimens.

"This summer's project will be focused on building spectroscopy instrumentation as opposed to operating it," said Kole. "This will involve learning about the design and evaluation of mechanical components for handling specimens as well as writing software for controlling the different parts of the instrument."

The learning experience works on many levels for Smith. "Dr. Bhargava's lab is very friendly," he said. "Everyone in lab 3420, where I work, has given me good advice about undergraduate studies and tips about research.

"This is a good opportunity to work on stuff that interests me. I'm getting good exposure to biomedical engineering. Biomedical imaging has helped me learn more about biomedical systems and engineering."

Shachi Mittal has just completed her bachelor's degree in biochemical engineering and biotechnology at the Indian Institute of Technology. She worked this summer at the Beckman Institute as a scholar in the Khorana program, which promotes scientific cooperation between the U.S. and India.

Mittal's research interests lie in chemometrics, the science of extracting information from chemical systems by data-driven means. At Beckman, she has been working with David Mayerich, a postdoctoral researcher in computer engineering, who is developing Chemical Imaging and Structures Laboratory (CISL) Automated Pathology Packet, a software that can classify infrared images of tissue biopsies.

"The goal is for the software to classify all types of cancers, so that the software can be used as a cancer detection method," said Mittal.

"Basically, current clinical disease diagnosis (say, for cancer) is done in a hospital by using a series of chemical stains," explained Mayerich.

"However, this method is non-quantitative, lacks repeatability, and destroys the tissue sample. The system we propose takes a single tissue biopsy and images it under mid-infrared radiation. This allows us to quantitatively extract chemical information that can be used to accurately classify cell types, which will allow us to accomplish the same task as current clinical techniques while preserving the tissue and providing repeatable results.

"We've already done most of the prototyping in the lab, so Shachi and others are building the software and putting it to more general use on different tissue types."

Mittal's work at Beckman is exposing her not only to how research actually happens, but how it is done in the United States.

"I applied for this program because I thought the internship would make me realize my weaknesses and strengths in research areas," said Mittal. "I am getting to actually analyze things, to know what aptitude I have for research.

"Working at Beckman has shown me that people are open to questions: the environment is such that you feel like asking questions. I am invited to seminars and meetings, and I am not at the same intellectual level as some other people, but they are willing to explain things."

Photo by Charlie Yu

Mittal also believes that the connectivity between the facilities at Beckman and labs throughout the building is exciting.

"I visited the Microscopy Suite, and they showed me the instruments there, and the instruments that they had built to meet a researcher's needs," she said. "Everyone in the building has knowledge about what everyone else is doing and [the facilities] cater to the labs. All the floors are interdependent and there are relationships between the labs."

When Mittal completes her two-month stay at Beckman, she'll return to India to pursue her master's in biochemical engineering and biotechnology. She would like to pursue a Ph.D., and, if fate allows it, she may even return to the States one day to work in research.

"There are more opportunities in industry here in my field," said Mittal. "If I stay in India, I will probably prefer academia, but if I stay in United States after my graduate studies, I would also like to explore industrial research for some years before getting into academia."

> **Working at Beckman has shown me people are open to [answering] questions, and the environment is such that you feel like asking questions.**
>
> **Shachi Mittal**

Max Li and **David Bergvelt**, senior students from Uni High, are assisting Mayerich and Shachi in writing the software package.

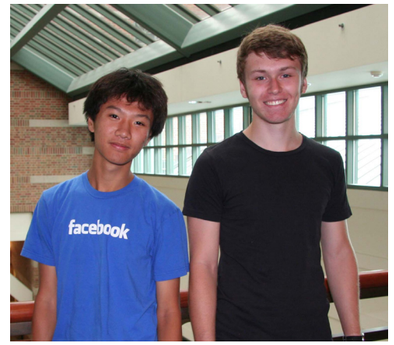
The school's ISTEM program placed them at the Beckman for a few weeks for school credit. "We both liked what we were doing here so much that we kept on going," said Bergvelt.

Li enjoys the diversity of the environment he has encountered at Beckman.

"I enjoy the fact that we are working with so many people from other fields, like biology and chemistry, not just programmers or computer scientists," said Li.

Someday they believe that the software they are helping to write will be used in a hospital, Bergvelt explained, but the immediate use is in labs by researchers.

"By having us here at Beckman along with the researchers, we're helping to bridge the gap between researchers and programmers," said Bergvelt.



From left, Joey Smith, Shachi Mittal, Max Li, David Bergvelt, and Mallory Schroeder.

"I'm glad that we've had this opportunity," said Bergvelt, who was planning to go into the engineering field, but because of this experience is becoming more interested in computer science. "It's nice to get this kind of exposure to research and programming."

Li plans to study mechanical engineering with a goal of working in the aerospace field.

Mallory Schroeder has just completed her freshman year at the University of Illinois. Her summer experience has helped her decide on a course of study.

"Toward the end of spring semester I decided to find a research lab that matched my interests and hopefully stay on campus for summer break," said Schroeder. "After exploring several labs and talking to a few professors I decided the Chemical Imaging and Structures Laboratory at Beckman best suited my interests and personal academic goals.

"I was trying to decide between the two bioengineering tracks of cell and tissue, and imaging and sensing, and I've since settled on cell and tissue, so [working in] Dr. Bhargava's lab was perfect."

Schroeder hopes to pursue her M.D./Ph.D. after she completes her undergraduate degree. She's met several graduate students in the lab who are in the program.

"I'm working with Mark Gryka, who is starting his first year of graduate school," said Schroeder. "I'm assisting him with his projects with tissue phantoms, Raman tomography, and a high-throughput breast cancer screening microfluidic device, which interests me the most. The low cost of microfluidics, little reagent use, and quick turnaround for results make it ideal for drug screening (as well as tons of other applications)."

Along with the other students, Schroeder thinks the early foray into the world of research won't be her last.

"The cleverness of some current microfluidic devices really sparks my imagination and desire to make my own," said Schroeder. "I'm planning on continuing research throughout my years as an undergraduate."

The new scientists on the block

Four of the six 2013 postdoctoral fellows settled in this summer and are laying the groundwork for exciting new research.

Nathan Medeiros-Ward

Before he walked through the doors, Nathan Medeiros-Ward had already had a close connection with Beckman Institute. He first heard about it through his advisor at the University of Utah, David Strayer, who previously worked under Art Kramer, director of Beckman. "So in a way," Medeiros-Ward said with a laugh, "Art is my academic grandfather."

Now, Medeiros-Ward has joined the coveted group of postdoc fellows at Beckman and is able to do what his advisor did: work collaboratively with Kramer and other top researchers in a leading-edge interdisciplinary research facility.

Medeiros-Ward completed his Ph.D. at the University of Utah in the spring and began his fellowship shortly after. Only a few months into his research, he's already fostering many collaborative studies with four researchers—Kramer, Aron Barbey, Alejandro Lleras, and Dan Simons.

"Beckman offers something that a lot of other postdoc opportunities do not," said Medeiros-Ward. "Normally in postdocs, you only work with one professor, in one lab, with their specific techniques. What is unique about Beckman is that it's very interdisciplinary. To get to work with several different collaborators is quite exciting. In addition, it was really easy in grad school to forget about methods and applications outside of my specific area. Beckman encourages breaking traditional boundaries and collaborating across the disciplines."

His research focuses on learning more about multitasking and knowing how shifting and dividing attention are similar and different in various laboratory and real-world contexts, as well as whether or not these abilities can be trained.

"I'm looking at many aspects of multitasking," said Medeiros-Ward. "I'm asking questions like, "If you were really good at switching between tasks, would you be good at doing two tasks at the same time? And then, how is that mapped out in the brain? Or can we train people to multitask? Would it be possible to teach people how to shift and divide attention?"

Although his research is just beginning, Medeiros-Ward has hit the ground running at Beckman, a sure sign of his future success.

Nathan Medeiros-Ward, left.
Abhi Singharoy, below.

Renee Sadowski, above.
Kelly Wiggins, right.

Abhi Singharoy

If anyone understands how much he can accomplish at Beckman, it is Abhi Singharoy. His work in the next three years, in collaboration with full-time Beckman researcher Klaus Schulten, will be to bridge x-ray crystallography and molecular dynamics simulations (MD), "two very distinct yet complementary fields" to create a program that will accurately determine all-atom structures of hitherto unresolved or poorly resolved biological systems, a feat that can redefine the field of low resolution x-ray crystallography, said Singharoy. His interest for these fields started as a graduate student.

"In theoretical chemistry at Indiana University I was fortunate enough to receive an education in two modern fields, biophysics of viruses and multiscale simulation," Singharoy said. "I caught great interest and love for these interdisciplinary areas that combine the physical sciences, the life sciences, and computational science."

X-ray crystallography is a process that uses x-rays to diffract on crystals in order to determine atomic and molecular structure. MD is a computer simulation on the physical movements of atoms and molecules based on Newton's equations of motion for a system of interacting particles. Putting these two processes together by using MD to derive crystal structures is what Singharoy has coined as xMDFF, which is in part based on the highly successful method for structure determination called Molecular Dynamics Flexible Fitting (MDFF).

"I am working with Beckman researchers to extend MDFF to interpret low-resolution structural information from x-ray crystallography experiments in terms of all-atom models," Singharoy said. "Professor Schulten has developed the revolutionary MDFF method for structure analysis that I would like to extend from electron microscopy to low resolution x-ray scattering structure determination (xMDFF)."

With this new technology, Singharoy will focus his immediate efforts on investigating transport across cell membranes. His long-term goal is to create new materials, like new or safer vaccines, by determining their atom-level structure.

It is clear Singharoy has very specific plans to carry out in his time here, and thanks to the researchers and world-class capabilities at Beckman, he is sure to make ground-breaking discoveries.

> **Beckman offers something that a lot of other postdoc opportunities do not. Beckman encourages breaking traditional boundaries and collaborating across the disciplines.**
>
> Nathan Medeiros-Ward

Renee Sadowski

Finding a passion, and then taking the appropriate steps to excel at it is the key to any career. Renee Sadowski knows that she has a knack for toxicology and neurotoxicology, which both study the adverse effects of chemicals on living organisms.

After completing her Ph.D. in neuroscience at the University of Illinois, she wanted to continue her work as a postdoctoral fellow.

"I decided to work at Beckman because the opportunities provided by the postdoctoral fellowship and collaborative environment," Sadowski said. "Through the training grant in toxicology that I received in my last few years of graduate school, I became interested in neurotoxicology because of its high relevance to human health.

"I am working with Susuan Schantz, who has current data that suggests that early exposure to PCBs in rodents can result in increased seizures in response to loud noise. I am also working with Daniel Llano, who has published studies using the flavoprotein autoflourescence technique. This technique measures the activation in a brain region in response to electrical stimulation of another brain area."

In her current study, she will be combining the knowledge and expertise of Schantz and Llano to measure differences in activation of the auditory cortex and hippocampus by use of the flavoprotein technique in adulthood after developmental exposure to PCBs.

"This project contributes to my research goals, which are to continue training in neurotoxicology while also employing techniques that have not been previously applied to the field," Sadowski said.

Her long-term goals are to keep getting better at what she loves: "a career in academia where I can continue to characterize the neural basis of how toxicants contribute to increased susceptibility to developmental and adult neurological disorders."

Kelly Wiggins

Though she is only a month into her fellowship, Kelly Wiggins has big plans. Wiggins has teamed up with Scott White, Nancy Sottos, and Jeff Moore of the Autonomous Materials Systems (AMS) Group to work on the next generation of self-healing materials.

AMS has created materials that can autonomously heal cracks, and now they are looking to not just repair damage, but to regenerate the material after catastrophic damage occurs.

"Right now, they've figured out how to heal damage that's the equivalent of a cut in your skin, but moving forward, we're looking at how to regenerate materials. The idea is to create a material that responds to severe damage by regrowing new material. For example, if you shot the material with a bullet, it could actually refill that bullet hole and become a solid, usable material again," Wiggins said. "Coming in with a chemistry background, I'm able to suggest new approaches on how to make this happen."

Wiggins completed her Ph.D. in chemistry at the University of Texas at Austin. She discovered Beckman through her graduate advisor, Chris Bielawski. As an undergraduate, Bielawski was advised by Moore, who is the principal chemist in AMS. Wiggins knew her research interests and goals acutely matched Moore's. This led her to a fellowship where she is not only able to continue her research in chemistry, but also cross disciplines and learn about engineering and materials science.

"I love [the diversity of] Beckman," Wiggins said. "I'm looking forward to working with both materials and aerospace engineers instead of just chemists and learning how we can combine our individual technical expertise to solve complex problems. Sometimes we become a bit too focused on our own division or even our own subdivision in science. To see the bigger picture and understand the needs of not only our own field but other areas of science, we need to bridge those disciplines, which is why Beckman is a perfect place to conduct research."

For Wiggins, the opportunity to apply her Ph.D. to conduct research will be one of the most rewarding aspects of her fellowship. "A lot of my research as a grad student was fundamental, and the work here can be more application-based. It's great to apply my chemistry research to creating new materials," said Wiggins.

Rotary International Group Study Exchange

Beckman senior research programmer Kirby Vandivort went on the trip of a lifetime to spend a month in Italy to learn about vocational practices, experience the culture, and, of course, indulge in homemade Italian pizza.

Kirby Vandivort, a senior research programmer with Klaus Schulten's Theoretical and Computational Biophysics Group, participated in a Rotary International Group Study Exchange in northwestern Italy from mid-May to mid-June.

Rotary International is an association of business and professional leaders who provide humanitarian service, promote high ethical standards in all vocations, and help build goodwill and peace in the world. The organization sponsors the Rotary International Group Study Exchange (GSE) program, which provides travel grants for teams of young professionals to exchange visits between paired areas in different countries. For four to six weeks, team members study the host country's institutions and ways of life, observe their own vocations as practiced abroad, and exchange ideas.

After a rigorous selection process, Vandivort was chosen to a part of a four-person team to travel to Italy for a month.

"I had heard about these trips from a Rotary member for years. But because of my work here at Beckman with renewals and proposals, it was impossible for me to even think about being gone for a month," Vandivort said. "This year, however, we were in between critical time periods, so I applied for the exchange and I was accepted."

"It seemed like an amazing opportunity" he said. "I had never been to Europe, and I really wanted to go to learn about the culture. Most of the trips I have gone on were related to scenery and cool places to visit, so I made the decision to truly immerse myself in the culture on this trip."

Top: Vandivort visited the Milan Cathedral in Milan, Italy. The Gothic cathedral took nearly six centuries to complete.

Bottom: Vandivort at the Department of Agriculture learning about the European Union.

The host Rotary district arranges the entire schedule for the visitors, from where they eat to where they sleep. The basic biographies of the Rotary team were sent to the district supervisors, and, from there, the supervisors selected places in the area that were aligned with the visitor's interests and vocational practices. Vandivort had the opportunity to share information about his vocation as well as the Beckman Institute with many Italian researchers.

Some of the places Vandivort visited included: Proplast, a consortium of European plastic manufacturing companies; an alternative energy lab producing ethanol from waste biomass; the Mario Boella Research Institute in Torino; and the Italian Institute of Technology in Genova, where he met with Walter Rocchia, an Italian researcher who uses the VMD Molecular Visualization software written and distributed by Schulten's group.

"It was really neat to see our software being used," Vandivort said. "It's not a surprise that we have users overseas, but I was impressed that the local Rotary members had looked into my biography well enough to see that connection."

Vandivort also learned about other aspects of Italian life and culture through visits to historical sites and governmental agencies. From all these experiences, he gained a greater understanding of the Italian culture, and believes this kind of experience makes the world a smaller, more accepting place.

"The highlight of the trip for me was a deeper appreciation for how similar we are as human beings," he said. "Minor cultural differences aside, people can be passionate about their families, their research, their country, and their food no matter where they are in the world."

HONORS & AWARDS

Bhargava Recognized with 2013 Craver Award

The Coblentz Society has chosen Rohit Bhargava, a member in the Bioimaging Science and Technology Group, as the recipient of the 2013 Craver Award in recognition of his work in the area of spectral chemical imaging, including the development of the fundamental theory and modeling of Raman and infrared chemical imaging.

Bhargava and Group Receive FACSS Innovation Award

Rohit Bhargava received the 2012 Federation of Analytical Chemistry and Spectroscopy Societies (FACSS) Innovation Award, which showcases the newest and most creative science debuted orally at a FACSS organized conference. Bhargava's presentation was "Advancing Infrared Microscopy Instrumentation by Theory and Computation."

King Named Nano-CEMMS Director

William P. King has been named director of the National Science Foundation (NSF)-funded Center for Nanoscale Chemical-Electrical-Mechanical Manufacturing (Nano-CEMMS). King's research focuses on nanoscale thermal and mechanical measurements, engineering of nanomechanical devices, nanomanufacturing, and nanometrology.

Lewis Recognized by Materials Research Society (MRS)

Jennifer Lewis of the Autonomous Materials Group has been recognized by the MRS for her "pioneering contributions in the design of viscoelastic inks composed of colloidal, polymeric, and organometallic building blocks and their directed assembly into planar and 3D functional architectures."

Nahrstedt Honored by IEEE Computer Society

The IEEE Computer Society honored 14 prominent technologists at its annual awards dinner in June, including Klara Nahrstedt, from the Image Formation and Processing Group. Nahrstedt's award citation reads, "For pioneering contributions to end-to-end quality of service and resource management in wired and wireless networks."

White Receives Humboldt Research Award

Scott R. White, head of the Autonomous Materials Systems Group, has been chosen to receive the prestigious Humboldt Research Award honoring a lifetime of research achievements. Recipients of this award are "academics whose fundamental discoveries, new theories, or insights have had a significant impact on their own discipline and beyond and who are expected to continue producing cutting-edge academic achievements in future."

Liang Invested as Woeltge Professor

Zhi-Pei Liang, of the Bioimaging Science and Technology Group, was invested as a Franklin W. Woeltge Professor of Electrical and Computer Engineering. Being invested with a professorship is one of the highest honors a faculty member can receive.

Bashir to Head Illinois' Dept. of Bioengineering

Rashid Bashir, a Beckman affiliate faculty member in the 3D Micro- and Nanosystems Group, has been chosen to head the Department of Bioengineering, beginning August 16.

Cangellaris Named Dean of Engineering

Andreas C. Cangellaris, Beckman faculty member in the Computational Multiscale Nanosystems Group in the Molecular and Electronic Nanostructures theme, has been named dean of the College of Engineering.

Arnold and Mabel Beckman and former U of I president Stan Ikenberry, 1988.

Check out Beckman's Throwback Thursdays every week on Facebook and Twitter. And keep us up-to-date on your research and activites at Beckman by using #beckmaninst.

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