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TCB Workshops Continue to Evolve as Successful Educational Program

Beckman Institute faculty member Klaus Schulten addresses students at a recent TCB workshop.

Participants and organizers of the recent Theoretical and Computational Biophysics (TCB) group workshops have been paving the way for the future of life sciences. Joining computational methods with traditional experimental methods, these researchers are working toward breakthroughs in fields including biochemistry, physics, and biomedicine, just to name few.

By Nancy Shen, Beckman Institute Intern. Published on December 07, 2010

Participants and organizers of the recent **Theoretical and Computational Biophysics** (TCB) group workshops have been paving the way for the future of life sciences. Joining computational methods with traditional experimental methods, these researchers are working toward breakthroughs in fields including biochemistry, physics, and biomedicine, just to name few.

The workshops were sponsored by the **NIH Center for Research Resources**, and TCB, the NIH Resource for Macromolecular Modeling and Bioinformatics, and were held Nov. 1-5 and Nov. 29-Dec. 3. TCB has a history of developing and implementing computational biophysics workshops that extends back to 2003. These workshops have taken place on the University of Illinois campus as well as in other national and international locations.

The **program** featured numerous high profile, well-qualified instructors. **Klaus Schulten** is Director of the TCB group, which is located at the Beckman Institute. Zan Luthey-Schulten, a William and Janet Lycan Professor of Chemistry at the University of Illinois, Emad Tajkhorshid, Associate Professor of Biochemistry, Biophysics, and Pharmacology at Illinois, and Chris Chipot, Research Director of the Centre National de la Recherche Scientifique at Nancy Université in France, helped instruct the students about the physical models and computational approaches.

James Gumbart, a postdoctoral associate with TCB, has worked at several workshops as a teaching assistant. He explained the goals of TCB. "Our group develops software for doing biomolecular simulations and visualization analysis. So in service of that goal, we train people in the use of our software and in general the use of tools in the field and how to approach such problems.

"What we can say the workshop program has really accomplished is the training of hundreds and hundreds of biomedical researchers in the United States."

In particular, these computational biophysics workshops investigate physical models and computational approaches utilized for the simulation of biological systems and the investigation of their function at an atomic level.

The course is structured around case studies focusing on the properties of membranes and membrane proteins, mechanisms of molecular motors, trafficking in the living cell through water and ion channels, and signaling pathways. Students were introduced to relevant physical concepts used in molecular modeling, molecular dynamics simulations on parallel computers, and steered molecular dynamics simulations.

The workshops are available to anyone who is interested in learning about the topic and encourage a wide range of participants from different backgrounds of academia. However, the workshops are designed and geared for graduate students and postdoctoral researchers who are studying the computational and/or biophysical fields, and for those who want to extend their research skills to include computational and theoretical expertise.

"One big component of these is it's both lectures and hands-on training," Gumbart said. "Generally, in the morning, they have lectures giving (the participants) the theory and a feel for what they are going to do and then in the afternoons they do hands-on training with the tutorials where they actually try out the software and learn how to apply it to different problems."

The hands-on computer labs in the afternoon allowed participating students a chance to set up and run simulations, and apply the knowledge that they learned in the morning theory-based workshops. Steven Wang, a Ph.D. student in Computational Chemistry and Biophysics from the University of Oklahoma, was one of the participants in the workshops.

"The motivation for me to come to the workshop is to learn the usage of VMD and NAMD, as well as what types of research projects these programs can be used for," Wang said. "I really enjoy the lectures given in this workshop. The hands-on tutorials are good, too."

The two types of software used for the workshops, VMD and NAMD, were created by Professor Schulten's group to help students learn computational simulation and modeling techniques. While NAMD is designed for simulations of large biomolecular systems, VMD is a visualization program that displays, animates, and analyzes large biomolecular systems using 3-D graphics. The two programs have more than 200,000 registered users and are used together by tens of thousands of researchers on a national and international level.

The lectures are given by researchers who have knowledge working with the theory, technique, and software. Over 700 pages of tutorials are available that have been written by those with personal experience working with computational simulations, NAMD, and VMD. At the same time, the same graduate students are present during the workshops to answer questions.

Various attendees come to the workshops hoping to have specific problems answered. The workshops help these participants apply the techniques that they have learned to their own research labs and educate other researchers as well. The tutorials are self-directed so that students can work at their own pace and focus on topics that deal with their own interests.

"There are many things that I learned during this week," Wang said. "As for the workshop's influence on me in the future, I would say I will definitely include more NAMD simulations in my next research project."

This seems to be a general trend.

According to Gumbart, recent students who came to the workshops have a fair share of understanding of the programs.

"In fact, what we're finding, more and more over the years, is that people have become more and more experienced coming in," he said. "Whereas a few years ago maybe people were all very new to the material or to simulations, now many of them have already done some and they're coming in and they want to know, (saying) 'okay, how can I take these tools and these ideas and apply them to my specific problem?'

"We're finding ourselves addressing more specific problems like that. It's great because we're really effectively jumpstarting a lot of different research projects of the participants."

The teaching assistants were given a chance to learn as well, Gumbart said. "It's amazing the problems people will find that you would never encounter on your own. You learn a lot in the sense that (you see) how people approach things differently and the stumbling blocks that they run into that perhaps you never thought about."

Gumbart said the workshops are a constant process of tweaking and refurbishing.

"The tutorials were really something new, and are something new; we're still developing new ones all the time for new features and tools, and updating them and that is a really massive undertaking," he said. "What we really like to see are people coming from labs that don't traditionally do computational work, experimental labs, saying 'Now we want to come and learn how we can integrate your tools and this approach into our work.' That synergy of combining our new methods with their work, I think, will lead to a lot of great new science."

In The Spotlight

Klaus J. Schulten

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