

# Computational Biophysics Workshop Popular

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Researchers and students who attend the “Hands-On Workshop on Computational Biophysics” get more than just a five-day training session on molecular simulation techniques.

Presented by the Beckman Institute’s [Theoretical and Computational Biophysics](#) group, the workshop is seen as a way to introduce a new generation of researchers to the incredible potential of computer simulations. The training sessions are part of the group’s mission under a grant from the National Institutes of Health, but there is a greater good, according to Klaus Schulten, TCBG director.

“We also do it because there is an important cause,” Schulten said. “Biomedicine, the life sciences and their medical applications are changing character dramatically today through the use of the computer. ... In short, one can see soon a day in which the typical life scientist and medical researcher spends about half the time in front of the computer.”

The training program started with a workshop for 90 students on the University of Illinois campus last year, and has gone global with sessions in Australia this past summer. The group has downsized the workshop to a more workable number of students, and will continue the sessions both here and at locations on the West and East coasts.

This past week, 21 participants got an introduction to the potential of biological computer simulations during a five-day workshop held at the Beckman Institute. Putting on the workshops is a lot of work, according to the group’s associate director, Emad Tajkhorshid, but he said the benefits are many.

“You really feel like you have contributed to the field and promoted research in general,” Tajkhorshid said. “So it’s a lot work but definitely worth it.”

And there’s another benefit that can’t be measured, he said. “After every workshop we feel like we have 20 more friends.”

Some of the participants at the most recent workshop, which was sponsored by the National Center for Supercomputing Applications, were graduate and postdoctoral students, while others were researchers from industry and government. There are many more applicants than the workshops can accommodate, thanks to the reputation the University of Illinois and TCBG have in the area of computer simulations.

“This field is developing dramatically,” said Schulten, who is one of the workshop instructors, along with group member Zaida Luthey-Schulten and Tajkhorshid.

“So there is an enormous demand for systematic instruction,” Schulten added. “Our group is really one of the leaders in the field of computational biology and many people come here to learn the particular techniques we pioneered at Illinois. Our university is one of the leading institutions in the country in computational science engineering.”

The workshop’s introduction says its purpose is to “explore physical models and computational approaches used for the simulation of biological systems and the investigation of their function at an atomic level.”

The course instructors use case studies that focus on such things as the properties of membranes and membrane proteins, molecular mechanisms, water and ion channels, and signaling pathways. There are theory sessions in the morning, followed by the ‘hands-on’ part of the workshop, where students run their own simulations, using the case studies, and sometimes even their own research models.

The training program boasts 21 laptop computers, paid for by the University of Illinois, that contain all the

applications needed to run the simulations. The TCB group has developed its own program over the years, called Visual Molecular Dynamics, for simulating molecular structures. Students are taught the finer points of that program, as well as a parallel dynamics code program called NAMD, at the workshop.

“The programs that our group develops, that are used by over 40,000 life scientists a day, and these powerful laptops, make this a wonderful training experience,” Schulten said. “As you know, in all walks of life, it is much better to learn something by doing than in a passive way.”

There are a wide variety of reasons why people take the workshop. Some are already proficient in certain types of computer simulations, but want to improve their knowledge of molecular modeling. Some of the students come from more theoretical backgrounds, but are finding the simulations complement their research.

“We think that computational methodologies and modeling studies have reached a mature level,” Tajkhorshid. “Now many groups that might be experimentally oriented want to integrate theoretical calculation and computational modeling into their research. It’s a very powerful tool, and can be complemented very nicely to experiments. You can do experiments and calculation at the same time.”

Workshop participant Rene Nome, a graduate student in chemistry at the University of Chicago, thinks the training program will prove helpful in his research.

“I come from the experimental side,” he said. “I think it’s going to provide a much more complete picture at the end of the day. It’s extremely helpful in trying to understand the meaning of what is going on.”

Ole Huilster Olsen came from Copenhagen, Denmark, where he works for Novo Nordisk. He liked the hands-on approach of the workshop.

“What I really liked is the emphasis on the case studies,” he said. “I’m looking forward to going back home and trying things out.”

Soumya Partnaik works at the Air Force Research Laboratory in Dayton, Ohio, as a materials scientist. The types of simulations done at the workshop are something new for her but she said the techniques she has learned extend her own research.

“Once you learn how to do it, you can create your own script,” she said. “You can do a lot more with that, so it is really a big service to the community.

“It’s been easy to use and I’m really impressed with all the stuff one can do with it.”

All three students were impressed with the quality of the workshop.

“They had wonderful tutorials,” Partnaik. “We had a lot of support from the faculty and the students with the group.”

“It’s an extremely friendly environment,” Olsen said. “They encourage you to keep in contact with the group. And they’re extremely smart.”

“It’s an intellectually very stimulating group, all the way from the students to Klaus,” Nome said. “When they spoke, you could feel the excitement about their own projects. It’s inspiring.”

That’s exactly the kind of response the group is hoping for.

“(The workshop) is part of our mission and an NIH-funded resource, but it’s also based very much on the goodwill and excitement for teaching of the faculty involved,” Schulten said. “It’s a great example of showing that university faculty really care very much about training and teaching to the degree that, when totally new forms of training are necessary, they do it completely voluntarily.”

This most recent workshop was for students from out of state, but future ones are planned on campus for in-state students. Schulten expects it to grow into a regular course offering at the University someday. But for now, the

workshops will concentrate on spreading the special knowledge TCBG has in the field through the workshops.

“People come here to the mecca of computational science engineering, and it’s a place where computational biology is very well-known and very visible,” Schulten said. “They want to learn the secrets of the trade from us.

“We want to be sure that the next generation can better cope with the challenges ahead. It really shows that the modern professor is not just a selfish researcher, but he and she always feel very much like teachers and are concerned about giving the next generation the best possible opportunity.”