

CAMPUS NEWS

Learning about protein structures at Pitman workshop



Rich Karalus (red shirt), building-facilities manager for UB's Clinical and Translational Research Center, and Jeanette Sperhac, scientific programmer for the Center for Computational Research, lead workshop participants on a tour of CTRC. Photo: Center for Computational Research

By CHARLOTTE HSU
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One student, from Williamsville East High School, liked learning about the process that scientists use to figure out the shape of proteins. Another, from Springville, had her first experience programming computers. And a third, from Clarence High School, thought it was exciting to get a behind the scenes look at high-tech research tools like the genome-sequencers in UB's New York State Center of Excellence in Bioinformatics and Life Sciences.

All three students spent two weeks at UB in late June and early July as part of the Eric Pitman Annual Summer Workshop in Computational Science.

The event honors Eric Pitman, son of College of Arts and Sciences Dean E. Bruce Pitman. Eric Pitman, a curious young man who loved learning new things, was a freshman at St. Joseph's Collegiate Institute when he died after a brief illness in 2007.

UB's Center for Computational Research (CCR) runs the workshop, planning hands-on projects and tours of research facilities that give students the chance to learn programming and explore the intersection between computing and the life sciences.

This year's theme was protein structures: how scientists determine proteins' shape, why this information matters and how computers expedite this kind of research.

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Jeanette Sperhac,
scientific programmer
Center for
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Research

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them process massive amounts of data,” said CCR scientific programmer Jeanette Sperhac, who served as the workshop’s lead instructor. “They learn how to take a data set, slice into it, think about the statistics, make plots, and visualize the data and understand what’s in there. Our hope is to expose students to new ways of thinking of things, both on the computation side and on the science side.”

This year, 11 high school students participated, most from Western New York.

On July 5, they presented what they learned to an audience of faculty members, parents and at least one grandparent who gathered in the Zebro Room at the Roswell Park Center for Genetics and Pharmacology. The lights dimmed and the students came to the front of the room, taking turns showing slides and discussing the knowledge they had gained.

“This is a very talented and inspiring group of young people,” Sperhac said, introducing the young programmers.

The first team to present, “Protein,” told listeners that proteins are large, critically important molecules consisting of strings of biological compounds called amino acids.

In humans and other living organisms, proteins play a role in vital tasks like DNA replication, and mutations and other flaws can lead to disease. Proteins also can be used to treat various disorders, replacing faulty proteins in the body or binding to various molecules to block unwanted processes from taking place.

Knowing the 3-dimensional shape that different proteins take is crucial to understanding how they can cause and treat disease, and in their talks, Protein members and fellow students explained that this process is complicated.

First, the presenters said, researchers must mix the proteins into various chemical cocktails. When these cocktail solutions become supersaturated, protein molecules may start to form crystals, whose structure scientists then can analyze using a technique called X-ray crystallography.

Crystallizing proteins is a very challenging process—part science and part art.

During the two-week workshop at the Center of Excellence, the students used the programming language R to analyze huge data sets from protein crystallization experiments conducted by crystallographers at the Hauptman Woodward Medical Research Institute across the street.

Among other results, the students found that crystallization is extremely hard to achieve. In the experiments they examined, proteins crystallized just over 1.5 percent of the time, and less than 25 percent of chemical cocktails were successful at crystallizing any proteins at all.

One student told the audience that a great takeaway lesson from the workshop was “how to look at data and analyze it, and what it’s really trying to tell us.”

Tom Furlani, UB interim associate vice president for information technology (CIO) and CCR director, told parents that he hoped students would leave with a heightened sense of the incredible role that technology plays in science.

CCR, in collaboration with Bruce Pitman, has been holding a summer workshop since 1999, and the field of computing has changed dramatically in that time, Furlani said. Today, it’s possible to complete in a single hour calculations that would have taken 24 years to compute back in 1984, he said.

Besides Furlani and Sperhac, researchers from the UB Center of Excellence in Bioinformatics and Life Sciences, UB Clinical and Translational Research Center, Hauptman Woodward Medical Research Institute and Roswell Park Cancer Institute contributed to the workshop, as well as other scientists from CCR.

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