

Canada's Biggest Calculator

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A University of Alberta professor has **harnessed the power of 4,000 computers across the country to condense 20 years worth of computing work into 48 hours.**

Dr. Paul Lu, a professor in the Department of Computing Science, spearheaded the Trellis Project, a national effort to help medical research projects at the University of Calgary and Toronto's Hospital for Sick Children. The 48-hour project, staged Sept. 15 - 17, created a virtual supercomputer spanning many different universities, with the combined power to tackle problems that would otherwise be too large for one research group or institution.

In this case, the Trellis Project helped a University of Calgary research project headed by Dr. Peter Tieleman. He and his research team are trying to understand the way a protein folds on itself. Proper folding is essential for a protein's function. Misfolding can lead to disorders such as Alzheimer's and "mad cow" diseases.

Tieleman's team is studying an important step in the folding process, in which parts of the protein form the final structure of the entire protein. To study this process, they use detailed mathematical models that describe how the atoms in the protein interact. Computer simulations trace the motions of tens of thousands of atoms according to these models, showing in "real time" how a protein might fold.

The Trellis Project also aided a second study at Toronto's Hospital for Sick Children, which is examining the way protons are transported

across biological membranes. The phenomenon is considered one of the most important chemical reactions in life. The physical basis for this reaction is difficult to characterize – a high level of molecular detail is required to understand how proton transport arises, and how it is coupled to other reactions.

Lu said that in both cases, researchers are working on basic research questions. But he and his colleagues are learning a lot about such enormous computing projects.

"There are other research groups around the world who are much better known than we are, who are doing this kind of work. We've made some fundamental design decisions that are different and the consequence is that I can get all these systems across the country working together a lot easier than they can."

That edge gave Lu the ability to add more clusters of computers to the project in mid-stream.

"There was one cluster of computers that was literally being moved from one building to another, and they got in touch with us and said, 'OK, we want to be part of this.' And in about 30 minutes of real work we were able to include that cluster."

At the project's peak, Lu had more than 4,000 computers at 19 universities, three research institutions and six high-performance computing consortia working together.

He's as impressed with that achievement as he is with what he calls the "social infrastructure" assembled for the project.

"Our biggest supporters are Computing and Network Services here on campus, and WestGrid (a western Canadian grid computing consortium),

and we got really strong support from Quebec and Atlantic Canada."

One centre in Atlantic Canada suffered a power failure during the project so team members there shut down auxiliary power to other operations and brought in portable fans to keep their computers cool and running.

In November 2002, the Trellis Project set a Canadian milestone when it completed 3.5 years worth of computation in a single day, studying the fundamental properties of chiral molecules, using the first Canadian Internetworked Scientific Supercomputer (CISS) with 1,376 computers at 16 different partner universities. This is the third such project Lu has piloted.

Lu says it is his goal to make such efforts routine. When will that happen?

"It's my job to make that happen but it is years away," he said. Lu added that he's confident WestGrid, "will be able to do what I've just done in a few months," but on a smaller scale.

But before that happens, Lu will take a well-deserved rest. The Trellis Project was labour-intensive, with Lu acting as a sort of babysitter over all the different computing systems involved.

"I don't even want to think about how many e-mails were sent back and forth over the past few days," he said. "I'm taking Ibuprofen for my hands."

Source: University of Alberta

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