

Lab Lucks Out

Rick Kendall is a self-proclaimed computer geek, but he's not too concerned about his "geeky" image. It's paid off. He laughed all the way to the R&D 100 Awards banquet in September. He received one of the prestigious awards for his contribution to the development of the Molecular Science Software Suite, called MS³ for short.

MS³ was developed as part of the construction of the Environmental Molecular Sciences Laboratory at Pacific Northwest National Laboratory, where Kendall worked for over nine years. But we've got him now! Kendall joined the Lab's Scalable Computing Lab staff in early September.

MS³ was created at PNNL to help solve DOE's grand challenge molecular science problems relevant to DOE's environmental restoration and waste management missions. The suite is a highly efficient and portable parallel computational chemistry package that provides solutions which are scalable with respect to chemical system size as well as the size of the computational resource.

"The suite consists of three tools," says Kendall, whose background is in theoretical and computational chemistry. "NWChem is a full-fledged computational chemistry software package, which was designed from the get-go to work on massively parallel supercomputers. It has electronic structure and molecular dynamics capabilities."

Other components of MS³ include the Extensible Computational Chemistry Environment and Parsoft Tools. Kendall explains that ECCE is a graphical user interface to computational chemistry codes, and Parsoft Tools is a set of tools used to develop parallel application codes.



Rick Kendall

Kendall says he's glad to be at Ames Lab and the SCL for a number of reasons. "I wanted to look into cluster computing in general, and here I'll have more opportunity to set my own research direction. I'm looking forward to that. And the staff here is very dedicated — that's another thing that attracted me to Ames Lab."

In addition to the pluses the Lab offers, Kendall and his wife, Angie, an analytical chemist, are excited about living closer to Angie's home turf. She grew up in Cedar Falls, where her parents still live. "We're very happy that our young sons, Phillip and Zachary, will be closer to their grandparents," says Kendall.

Kendall notes that he comes from the application developer's side of cluster computing while many others in the field are looking at it from the computer science side. "We need to learn how to work together so we can maximize the performance of cluster computing but in a very usable way," he says. "That bridge, that combination of talent — computational science and computer science — merging those things is something that takes a lot of work, focus and commitment on the part of the people involved. The trick is learning to speak the same language." ■

~ Saren Johnston