Researchers Have Partners at the NCCS

The Scientific Computing Group works with users to make sure they get the most from ORNL's next-generation supercomputers.

The Scientific Computing Group

Researchers using Oak Ridge National Laboratory's (ORNL's) world-class supercomputers and other high-performance computing resources have a group of full-time advocates on-site, dedicated to making a daunting task practicable.

These research scientists, visualization specialists, and work-flow experts belong to the National Center for Computational Sciences (NCCS) Scientific Computing Group (SCG). The group helps users take full advantage of the center's unique, next-generation systems to advance the boundaries of knowledge.

At its core is a group of liaisons to the research projects. The liaisons are experts in their fields—chemistry, physics, astrophysics, mathematics, numerical analysis, computer science—but they are also experts in designing code and optimizing it for the NCCS systems.

The challenge faced by researchers using these computers is formidable because the computers are indeed unique. With more than 5,000 dual-core processors, the center's Jaguar system is the nation's most powerful computer for open scientific research, while the center's Phoenix computer is the most powerful vector system in the country, boasting more than 1,000 custom vector processors.

Some applications must be reworked, an especially big challenge for code that dates back years or even decades, while others must be written from scratch. And all use a number of processors that until recently was unheard-of in a single system.

"Scalability is the hardest thing to solve," said Ricky Kendall, the group's leader. "Some codes are not scalable, while retrofitted codes sometimes don't work as well as they ought. Every domain (scientific discipline) has codes that are ported, some that are retrofitted, and some that are written from scratch."

The SCG also gives users a voice in the internal workings of the NCCS, making certain their needs and desires are represented. "Within the day-to-day operation of the facility, we are the user's voice," Kendall noted.

SCG liaisons work with the research teams at a variety of levels, from full-fledged partners in developing code to more informal troubleshooting consultants. Their contribution is appreciated by users.

The SCG's Trey White, for instance, has been the center's liaison with the Climate-Science Computational End Station Development and Grand Challenge Team, a cutting-edge climate change model.

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"Trey's been instrumental in being a bridge between our science and development teams and the computational resources," said Lawrence Buja of the National Center for Atmospheric Research, based in Boulder, Colorado. "He's been critical in getting us going and running there."

John Drake, an ORNL scientist working on the project, agrees. "Trey has really helped manage the code optimization," Drake said. "He's really joined the climate group in learning the project and the code. He's had to gain a pretty in-depth knowledge of the algorithms, and that's been very helpful. You have to know where to look in the code to debug it."

The SCG's Mark Fahey has been liaison to the High-Fidelity Numerical Simulations of Turbulent Combustion, a project that promotes the development of combustion models. According to principal investigator Jacqueline Chen, Fahey has been instrumental in helping the group scale, optimize, and port its code.

"He knows the computing side of things," Chen said, "and we know the combustion science. Bringing the two together has been really helpful in getting the combustion science done."

Fahey also gets kudos for help he's provided to General Atomics, a San-Diego-based company, in running its GYRO code for simulating plasma microturbulence in a fusion reactor.

"Mark Fahey of ORNL has been a crucial person in this effort," principal investigator Jeff Candy said in an interview with *HPCwire*, "especially for code optimization. He sees things we sometimes don't. I have nothing but great things to say about him."

End-to-End

A new set of challenges arises once the programs are running: Researchers must analyze, organize, and transfer an enormous quantity of data. The SCG's End-to-End task works to streamline the work flow for system users so that their time is not eaten up by slow and repetitive chores.

"We have to understand the way they work," said task lead Scott Klasky. "We're not trying to revolutionize the way they work; we're trying to make it less painful."

The goal is to automate tasks such as monitoring the system, analyzing results, and moving the data to their final destination. Ultimately, said Klasky, the center is working toward a dashboard application to give researchers all the information they need day to day on a single screen.

Visualization

Once users have completed their runs, specialists in the SCG's Visualization task help them make sense of the sometimes overwhelming amount of information they generate.

"Humans are visual animals," said task lead Sean Ahern. "We help people understand a tremendous amount of data by transforming it into images or movies."

This mission is exemplified by the EVEREST Powerwall at the NCCS. EVEREST, which stands for "Exploratory Visualization Environment for Research in Science and Technology," is a 30-foot-wide, 8-foot-tall tiled display that can show 35 million pixels of information. It provides a unique opportunity to view more data and to view them in larger groups.

Members of the Visualization task use both open-source and commercial software, choosing packages that are both flexible and able to accommodate large amounts of data.

The group has made its presence felt most in areas such as materials science, astrophysics, and climate and fusion science. While not all users seek visualization services, Ahern suspects more and more will as the amount of information being generated grows exponentially.

And while the visualizations themselves can be beautiful, Ahern stressed that beauty is not the goal. "The purpose of visualization is insight, not pictures," he said. "We want the scientists to have a better understanding of the simulations they run. We help them have 'now-I-get-it' moments."

Taking advantage of the SCG

Any NCCS project with a large allocation on the center's systems is given a liaison with whom to work. The liaison is carefully selected to provide the best fit for a project's specific scientific and computing needs. Once the relationship is established, the liaison will work as closely as possible with the project to ensure its success.

Ultimately, said Kendall, the liaisons and all members of the SCG work toward producing the best science possible by following a simple motto: Whatever It Takes.

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