

# Software engineers lower the barriers for OSC clients

## Scientific Applications

Karen Tomko understands the challenges software developers face, having worked directly on development teams in the past. One of the main barriers is finding ways to make sure the applications that get developed are available and working in a given system.

Tomko, interim director of research and scientific applications manager at the Ohio Supercomputer Center, works to ensure the process is a smooth one for scientific applications developers as well as researchers who require help installing existing software packages.

“In working with research groups that use the system, you start to see how that can really hold them up,” Tomko said. “If they can’t get over that hurdle, it doesn’t matter if the hardware is up and running or how much hardware we have. They need their software to work to be able to utilize it.”

In recent years, the HPC community has increasingly recognized the importance of easing the process of allowing researchers and developers to get their software up and working.

“It’s becoming more acknowledged as a challenging aspect of maintaining these systems, and I think that’s because our user base has broadened, which means the number of software packages we need to maintain has gotten larger.”

### Default software upgrades

“What we have done this year is our first software refresh on the Oakley and Ruby Clusters. The Oakley Cluster was set up in 2012 and the default software toolset was basically a 2012 version. So we’re establishing all new updates for what the default software environment is for our users.

Our research scientists, who are mostly busy with the science aspects of their code, if they’re not thinking about these things, will use the default ones and they’re building on an older set of software. But there are changes. And it gets harder and harder to keep everything consistent if people are using older pieces of software. So updating them and making the updates the default encourages the users to move to the newer versions.

And, with that, they should see more robustness and reliability. They get a toolset that keeps up to date.

### Additional support, tools

We’ve added to the staff. That’s going to allow us to do more, some of it will be behind the scenes to make it easier to manage the software environment. And it gives us a little more capacity to work with specific research groups.

One of our main focus areas in this coming year is refining tools to track and understand software usage so we can make good decisions with respect to new purchases, what we should install and what we don’t need to maintain anymore.”



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### Top 10

Applications on the Oakley system for CY2014 are:

1. Gromacs
2. Matlab
3. Amber
4. Gaussian
5. OpenFOAM
6. Q-Chem
7. NAMD
8. Elk
9. VASP
10. LAMMPS