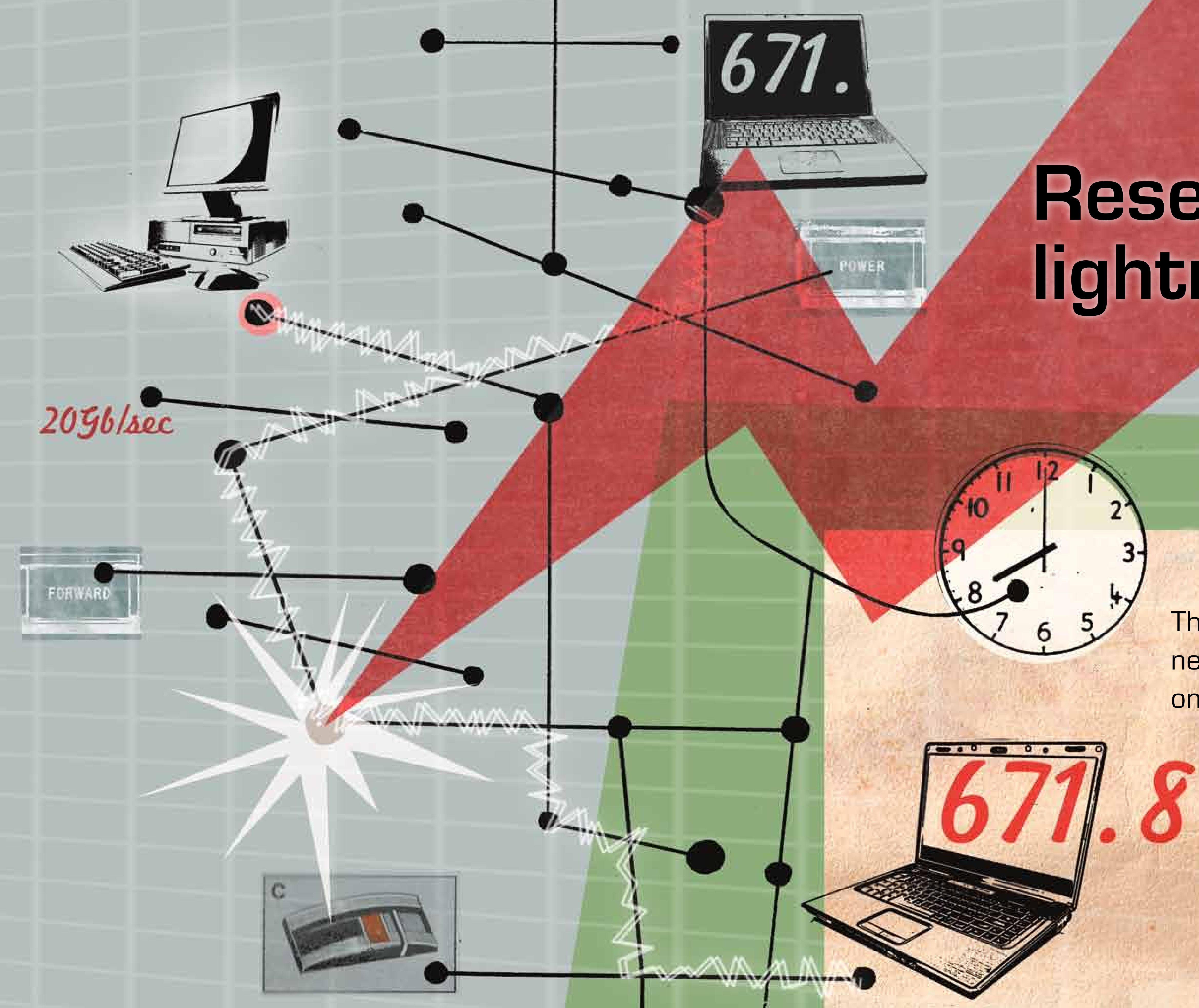

Research at lightning speed

The supercomputing power of the new MUGrid is amping up research on campus and beyond.

By Nicole Sweeney Etter

Now work that would have taken a year takes just a day or two.

Marquette researchers are tackling ambitious projects with potential for enormous societal impact: They're developing new drugs for diseases such as tuberculosis, trying to reduce radiation risk for women undergoing CT scans and studying the impact of multinational corporations around the world. But these projects wouldn't even be possible — at least in their current form — without the supercomputing power of the new MUGrid.

With a $560,000 grant from the National Science Foundation, Marquette recently installed a computer cluster that has the capacity of up to 1,000 desktop computers. It also connected more than 550 individual computers across campus, creating the first high-performance campus-wide computing network in southeast Wisconsin. Led by Dr. Craig Struble, an associate professor of computer science, this resource is already boosting exponentially the efficiency of researchers on campus and off. Nearly 70 researchers, including some from the Medical College of Wisconsin, have signed on as users, and the MUGrid has even helped a company as far away as Thailand.

Dr. Craig Struble

Struble hopes it's just the first step to even more computing power. Eventually, he'd like to see Marquette's grid linked to others. "We're a small school, but we have some people who have really big computing needs, and it's going to continue to grow," he says.

The need goes beyond Marquette: In 2010, the Milwaukee Institute released a report, "A Case for High-Performance Computing Investment in Southeast Wisconsin," that cited the area's higher-than-average rate of technology-intensive jobs. The institute thinks cyberinfrastructure is key to the area's economic growth, and Struble agrees. "We realize that this is a long-term direction [in which] science and engineering and other disciplines like economics are heading," he says.

The MUGrid works by using software that harnesses idle computer resources across campus, particularly student lab computers overnight. Researchers can then tap that campuswide power from their own desktops. "Rather than have our resources sit idle, we'd rather have people using them to do good science and good research," Struble says.

Here is a glimpse at how the MUGrid is already making an impact.

Developing new drugs

Doctoral student Terry Neumann didn't come to Marquette intending to fall in love with high-performance computing. But after working for four years in the lab of Dr. Daniel Sem, an associate professor of chemistry, Neumann is hooked. He recently was one of just 50 students worldwide invited to a prestigious workshop in Italy to learn more about TeraGrid, the National Science Foundation's computing network made up of hundreds of thousands of cores.

Sem's lab focuses on drug targets for tuberculosis and schizophrenia, but he also works with collaborators on drug targets for heart disease, cancer and diabetes. The Thailand-based Thai Natural Products also recently turned to Sem's lab to screen plant compounds.

It's computer-intensive work. "We screen drug-like chemicals against proteins to see if we can identify chemicals that will bind and thus lead us down a drug discovery path," Neumann explains.

Each protein is screened against the lab's collection of 10,000 chemicals. On a single-core machine, it would take 440 days to complete a single protein test. Now that work can be done in as little as 12 hours.

"We've kind of developed this niche in the community because we can test a lot of compounds very quickly," Neumann says.

But it has only whet Neumann's appetite. He and Sem will next use the TeraGrid to test 1 million compounds. And that's only a fraction of what's available in a commercial database.

"Right now, 13 million chemicals is out of our reach," Neumann says, "but it's in our dreams."

Lowering cancer risk

Dr. Taly Gilat-Schmidt, an assistant professor of biomedical engineering, wants to make women safer. Gilat-Schmidt studies medical imaging systems and is particularly interested in the radiation exposure caused by CT scans. Radiation can elevate one's cancer risk, and a recent study found that women have a higher risk of developing cancer from radiation, partly because breast tissue is highly radiosensitive.

Dr. Taly Gilat-Schmidt

"Any time you get radiation, there's a risk. If you could reduce radiation and preserve image quality, that would be a good thing," she says.

Gilat-Schmidt's two-year study, which is supported by the Food and Drug Administration, aims to quantify the radiation reduction — and assess image quality — of different methods. "It's very difficult to measure how much radiation is deposited inside the body during a scan," she says. "It would require some sort of sensor in the body. So we have these models instead, and with the simulations we can accurately estimate how much radiation is deposited in every organ."

The work involves tracking billions of X-ray photons. "Without the grid, we couldn't do these simulations," she says. Now work that would have taken her a year takes just a day or two.

One early outcome is a small database that calculates the radiation levels for an average patient at various scanning perimeters — so the information will be available to researchers who don't have a resource like the MUGrid.

Gilat-Schmidt also uses the grid for projects that aim to improve cardiac scans and single photon emission computed tomography scans.

Already improving patient care

Dr. Christopher Butson is an assistant professor of neurology and neurosurgery at the Medical College of Wisconsin and an adjunct professor in Marquette's Department of Biomedical Engineering. His MCW lab studies therapeutic and diagnostic deep brain stimulation, a technique most often used with Parkinson's patients. The research involves a combination of human experiments and computational modeling — and that's why he turned to the MUGrid. "It allows our experiments to be a lot more interactive," he says. "We can have an answer in a couple of hours and actually iterate several times a day."

Dr. Christopher Butson

Butson is trying to better understand therapeutic deep brain stimulation. "When it works, everybody's happy, and when it doesn't, we don't know why and we have few tools to examine why it doesn't work," Butson explains. One challenge is that existing imaging techniques can't show what's happening in the brain during stimulation. So Butson uses the MUGrid to run thousands or tens of thousands of neuron models to see how stimulation affects a patient's individual neurons.

"These computations allow us to predict and see things that we would not otherwise be able to see," he says. There's also a lot of variability in how brain stimulation is used, and Butson's computer models can help physicians decide where to place the electrode and how much stimulation to use.

Butson also works with a Marquette graduate student to use the grid to study transcranial magnetic stimulation, a non-invasive technique that comes with the same unknowns as deep brain stimulation.

The MUGrid's ability to produce results in just a few hours is a huge benefit to patients, Butson says. But to speed physician decision-making even further, he'd love to get the processing time down to an hour or even seconds.