# FROM THE DIRECTOR

Welcome to the second issue of *PSC Science Highlights.*

I'm honored to follow in the footsteps of Michael Levine and Ralph Roskies, whose vision created PSC and then sustained it for more than three decades. Through their leadership and with the continuing support of PSC's outstanding staff, PSC is known for its commitment to science and to users. I look forward to building on the remarkable foundation Mike and Ralph established, both continuing PSC's excellence in leadership computing and folding in emerging fields, such as artificial intelligence, as we've already begun with Bridges. I also look forward to working even more closely with both Carnegie Mellon University and the University of Pittsburgh.

I'm happy to announce that Bridges successfully passed its first operational review, earning high marks in user satisfaction and scientific achievement. Bridges now supports more than 1,000 projects and 4,000 users.

Researchers nationwide are using Bridges for research, collaboration and education. To give examples of the latter, Carnegie Mellon's Deep Reinforcement Learning course last spring made the system available to about 200 students. At a higher educational level, the 2017 Jelinek Summer Workshop on Speech and Language Technology (JSALT) consisted of a two-week summer school followed by a six-week workshop, bringing together about 60 experts from around the world to learn how to leverage Bridges in their own work.

You can read more about research enabled by Bridges in this issue. I'd also like to share an update on a story in our last (Spring 2017) issue, about the AI program *Libratus*, which ran on Bridges. *Libratus* made history in artificial intelligence by defeating some of the best poker players in the world at heads up, no-limit Texas Hold'em. A further refinement of Libratus, named Lengpudashi, or "Cold Poker Master,"reinforced the value of strategic reasoning at an exhibition in China. Strategic Machine Inc. has licensed *Libratus* to target a broad set of applications such as business strategy, cybersecurity and medical treatment planning, demonstrating transition from AI research to commercialization.

Up to 10 percent of Bridges' capacity is available to industry to foster discovery and innovation. In addition to making the system available to researchers across the country for academic research under the usual XSEDE allocation system, we are aggressively pursuing avenues by which Bridges can advance the private sector under these discretionary allocations.

We're amplifying our focus in two timely and vital areas. PSC's new Artificial Intelligence and Big DataGroup, led by Paola Buitrago, addresses the convergence of HPC, AI and Big Data for Bridges and beyond. The new AI & BD Group will keep PSC at the forefront of the rapidly evolving and increasingly ubiquitous of AI, spanning hardware, software, algorithms, research, education and industrial outreach. Our Computational Biology Group, led by Phil Blood (who is also principal investigator for PSC's Anton 2 project), now encompasses Biomedical Applications and Public Health Applications, to enable a unified strategy across the life sciences. Significantly, PSC, with CMU and Pitt, was recently awarded $4.8 million by NIH to establish an archive for confocal fluorescence microscopy brain data.

Finally, I would like to acknowledge all our funders, especially the NSF, the NIH and the Commonwealth of Pennsylvania. I'd also like to thank our staff for the superlative work that made all these successes happen.

Nicholas A. Nystrom

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Interim Director

PITTSBURGH SUPERCOMPUTING CENTER

## About PSC

PITTSBURGH SUPERCOMPUTING CENTER provides university, government and industrial researchers with access to several of the most powerful systems for high performance computing, communications and data storage and handling available to scientists and engineers nationwide for unclassified research. PSC advances the state of the art in high performance computing, communications and data analytics and offers a flexible environment for solving the largest and most challenging problems in computational science.

Pittsburgh Supercomputing Center is a joint effort of Carnegie Mellon University and the University of Pittsburgh. It was established in 1986 and is supported by several federal agencies, the Commonwealth of Pennsylvania and private industry.

## Computing Resources

**Bridges** – a uniquely capable resource for empowering new research communities and bringing together HPC and Big Data. Bridges is designed to support familiar, convenient software and environments for both traditional and non-traditional HPC users.
**Anton 2** – a special-purpose supercomputer for biomedical simulation designed and constructed by D. E. Shaw (DESRES). A successor to Anton, Anton 2 is a 128-node system, made available to PSC by DESRES without cost for non-commercial research use by U.S. universities and other not-for-profit institutions. It is hosted by PSC with support from the National Institute of General Medical Sciences.
**BioU** – a bioinformatics educational resource funded by the NIH.
**Olympus** – a flexible, multiple-use compute cluster dedicated to research in the MIDAS community.


## Thanks for your Support

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D. E. Shaw Research
The Buhl Foundation
Bill and Melinda Gates Foundation
The Grable Foundation
UNICEF
USAID


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PITTSBURGH SUPERCOMPUTING CENTER
# SCIENCE HIGHLIGHTS
FALL 2017

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FEATURE

# THE BEST THING SINCE SLICED BREAD?

## ZEBRAFISH STUDY REVEALS FIRST FINE STRUCTURE OF A COMPLETE VERTEBRATE BRAIN

### WHY IT'S IMPORTANT

Every thought, every feeling, every sensation—and every behavioral illness—ultimately depends on how our brains work. Despite decades of stunning advances in imaging the brain and measuring its activity, though, we still don't understand how even a simple vertebrate brain works.

Enter the zebrafish larva. Small and transparent—yet able to swim freely and even hunt small prey—these baby fish have long been studied by researchers to understand how their tiny brains generate behaviors. David Hildebrand, working in the laboratories of Florian Engert and Jeff Lichtman at Harvard University, took this work a step farther, creating electron microscopic images of the zebrafish brain cut into tens of thousands of slices. With the help of co-author PSC's Art Wetzel, they led an international collaboration that used these images to reconstruct specific nerve cells that spanned nearly the entire larval zebrafish brain. The hope is that this kind of thorough "nano-scale" imaging will make it possible to extract the brain's complete "wiring diagram." While this work has only just begun, it may eventually shed new light on past studies of zebrafish behavior—and point the way toward a better understanding of more complex brains, such as ours.

### HOW PSC HELPED

To generate image datasets containing all the nerve cells in the zebrafish brain and their many intricate connections, then-graduate-student Hildebrand had to dig deeper than the previous studies. Using a technique developed by Lichtman's laboratory, he cut the front quarter of the zebrafish larva—a total length of 1 millimeter, or about 4 hundredths of an inch—into more than 18,000 slices. Then he used an electron microscope to get images of these slices. The slices, though, are inevitably imperfect, with some varying in thickness and having tears and other defects. To recombine the distorted images to reconstruct the brain in three dimensions, Hildebrand needed advanced automated image registration techniques.

To "un-distort" these images, Wetzel used SWiFT (Signal Whitening image Fourier Transform), software he developed as part of PSC's involvement in the National Center for Multiscale Modeling of Biological Systems. SWiFT gave the scientists the ability to handle distortions and defects stemming from tissue variations, compression of slices and image distortions caused by the electron microscope's inner workings. Thanks to Wetzel's work, fewer than 1 percent of Hildebrand's slices could not be used in the analysis.

Some 12,500 of the slices contained parts of the brain. The scientists examined these in more detail, collecting a massive 4,900 gigabytes of data in the process—enough to fill five to 10 high-end laptops. They fully or partially traced the path of about 2,500 nerve cells and their axons—the long tails the cells use to connect with other nerve cells. The investigators were able to follow 805 of these nerve cellsover the entire length of their axons through the brain.

One early finding is that certain nerve fibers on one side (left or right) of the fish brain have twin fibers on the other side. The organization of axons within these nerves on each side followed nearly mirror-image paths. While the scientists don't know exactly what this means yet, they suspect it may have something to do with a pre-programmed brain development process. This could also be an important clue for a number of inborn behaviors fish follow. It isn't yet clear whether nerve cells in the human brain, which develops slowly and changes greatly throughout life, will have the same degree of left/right symmetry. The collaborators published their initial findings in the prestigious journal *Nature* in May 2017.

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HIGHLIGHTS

### A Picture is Worth a Thousand...Dollars?

It's not hard to believe that when you advertise a property, a good picture will help you sell or rent it. What isn't so clear is what factors make for a good picture and how much each of these factors contributes to the bottom line. Using PSC's Bridges, researchers at the Tepper School of Business at Carnegie Mellon have created a computer program that identifies these elements and shows how to present a photo for the best sales impact.

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### Synergistic Voyage

Since the science fiction novel *Fantastic Voyage*—and before—people have been fascinated with the idea of shrinking our tools so we could carry out miniature tasks with extreme precision. While the field has some way to go, PSC helped Carnegie Mellon University researchers rewrite their software for simulating microrobots, enabling them to move the program to the supercomputing environment and helping them test many more ideas than possible by creating physical robots to test every idea in the lab.

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### Inner Space

Experiments can detect chemical changes on a scale as short as about a thousandth of a second. Most supercomputers can only simulate complex biomolecules for as long as a few millionths of a second. Scientists at the University of California, San Diego used the D.E. Shaw Research Anton supercomputer at PSC to understand what happens in that thousand-fold gap, between the snippets we understand from computer simulations to the longer responses we see when a protein, say, encounters a drug.

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### The Future is STEM

The future of employment is increasingly STEM-related. To prepare its students for higher-paying, computationally-savvy jobs in science and industry, the North Carolina School of Science and Mathematics has obtained time on the XSEDE-allocated Bridges supercomputer at PSC for its high-school chemistry students.

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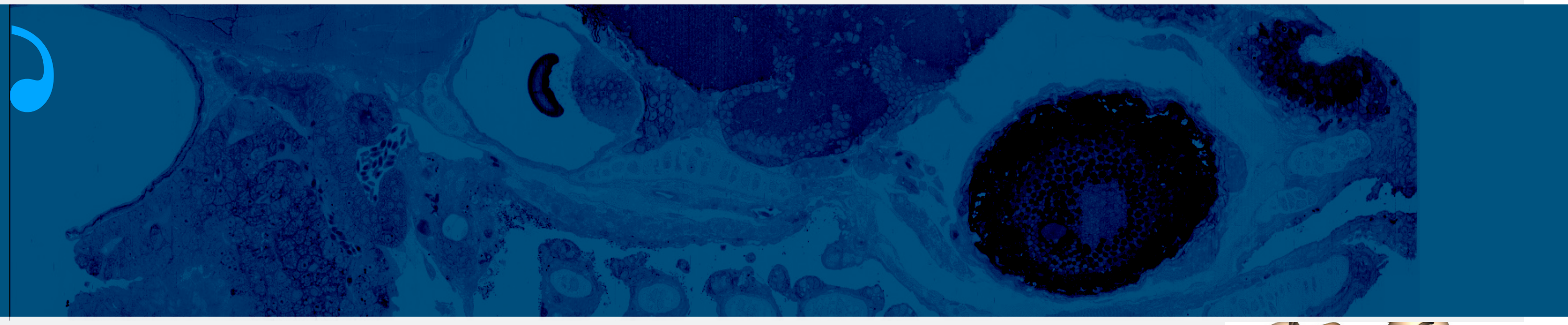
**"Our goal [was] to develop techniques that allow researchers to examine the morphology and circuit connectivity of any neuron in the brain of a larval zebrafish at about five days after fertilization. This is when interesting zebrafish behaviors such as hunting emerge, giving us the opportunity to ask how circuits of neurons parse incoming information from the environment to generate useful behavioral outputs."—David Hildebrand, Harvard University**



### Choice Works

Less than half of children and adults under age 65 get vaccinated for influenza. Researchers at PSC, the University of Pittsburgh and Soongsil University in the Republic of Korea used PSC supercomputers to simulate the effects of offering different types of vaccination—the familiar injected vaccine or two types of "needle sparing" vaccines. Their results suggest such a choice would reduce flu cases and make vaccination more cost effective.

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### Blue Acres?

Commercial abalone "aquaculture"—farming the shellfish in enclosures—has exploded over the past decade, becoming a $100-million global industry. Understanding the DNA of the abalone is key to improving and expanding its aquaculture for California producers. That's why scientists at Iowa State University and the National Oceanic and Atmospheric Administration worked with PSC experts to "assemble" the DNA sequences of several species of abalone on the Bridges supercomputer.

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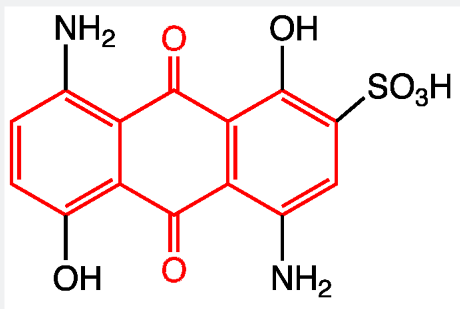


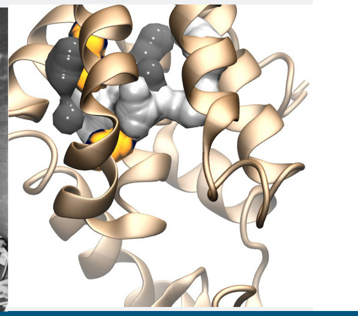

### NEWS BRIEFS

- PSC Interns Advance AI, Cybersecurity, System Administration
- Bridges-Powered Research Wins PEARC17 Award
- Early Successes on Anton 2
- WVU Awarded $1 Million Grant from NSF for New HPC Cluster at PSC

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