

## FROM THE INTERIM DIRECTOR

Welcome to the Fall 2018 issue of *PSC Science Highlights*!

We continue our ongoing project to make PSC ever more relevant, agile and tuned to the needs of the scientific community. The past six months have seen us reorganize to better exploit our strengths and continue to lead in the HPC community.

Recognizing the vast strategic importance of artificial intelligence (AI) to science and society, we've created a new Artificial Intelligence & Big Data Group, directed by Paola Buitrago. This group will strengthen our AI environment for users; develop and disseminate best practices; enable and drive research; provide education and training; and foster collaboration. One important thrust of this work is to strengthen computational partnerships with regional corporate entities. We've already played a key role in significant progress in AI made by researchers at the Carnegie Mellon School of Computer Science—see the brief in this issue on the paper in the prestigious journal *Science* describing their Libratus AI's 2017 victory over some of the world's best poker players. A more recent accomplishment was in the Big Data field. This issue includes a feature article on our role in providing GPU capability to the IceCube Neutrino Observatory, supporting the recent first detection of cosmic neutrinos by that facility. We also announce a new Big Data collaboration, with Fermilab's CMS detector at the Large Hadron Collider.

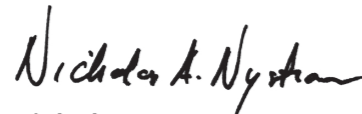
To unify our research efforts and strategic planning in computational biology and public health, we've launched a new Computational Biology Group. The senior director of the new group, Phil Blood, will oversee PSC's Biomedical Applications and Public Health Applications Groups. One major recent development in this sphere, also covered in this issue, was a collaboration with Pitt to create a Brain Image Library, led by Alex Ropelewski. This confocal fluorescence microscopic data library will give researchers easy, searchable access to petabytes of unique data. It is funded by National Institute of Mental Health as part of the federal BRAIN initiative. On the public health side, you can also read about how, with colleagues at Johns Hopkins, we released the HERMES public-health supply-chain modeling software for public use in April.

We have world-class teams of researchers in the above fields. We also remain a facility providing HPC systems to U.S. researchers (at no cost to them, it bears repeating). Thanks to a supplemental award from NSF, we are greatly enhancing PSC's NSF-funded Bridges system with "Bridges GPU-AI," a new resource configured to balance singular capability and substantial capacity. You can read more about this new resource in this issue.

Keeping PSC's systems humming is the responsibility of Jason Sommerfield, who has been appointed director of our Facilities Technology Group. The group currently manages Bridges, Anton 2, Olympus, the Brain Image Library and integration and support for hardware infrastructure for groups at CMU, Pitt and other institutions.

Finally, we maintain our award-winning STEM education efforts. Thanks to a grant from Microsoft, we're continuing our GCode program to offer young women, particularly from under-represented communities, the opportunity to experience coding and think about it as a career path. Our ongoing program of HPC workshops for researchers and computing professionals continues as well.

We would like to thank our sponsors, especially NSF, NIH, and the Commonwealth of Pennsylvania. We'd also like to thank our staff for the superlative work that made all these successes possible.



Nicholas A. Nystrom  
Interim Director

Carnegie Mellon University



University of Pittsburgh

### About PSC

PITTSBURGH SUPERCOMPUTING CENTER (PSC) unites the most advanced computing technologies with multidisciplinary expertise and data to drive discovery for the benefit of society.

A joint effort of Carnegie Mellon University and the University of Pittsburgh, PSC creates and provides advanced computing ecosystems and solutions scalable to the greatest challenges. It engages in transformative, collaborative, cross-disciplinary research. It provides and supports education for academia, industry and the wider community. It promotes the transformative contribution of advanced computing to people's lives. And it engages with business and industry to drive economic and workforce development.

PSC 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, AI 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

PSC gratefully acknowledges significant support from the following:

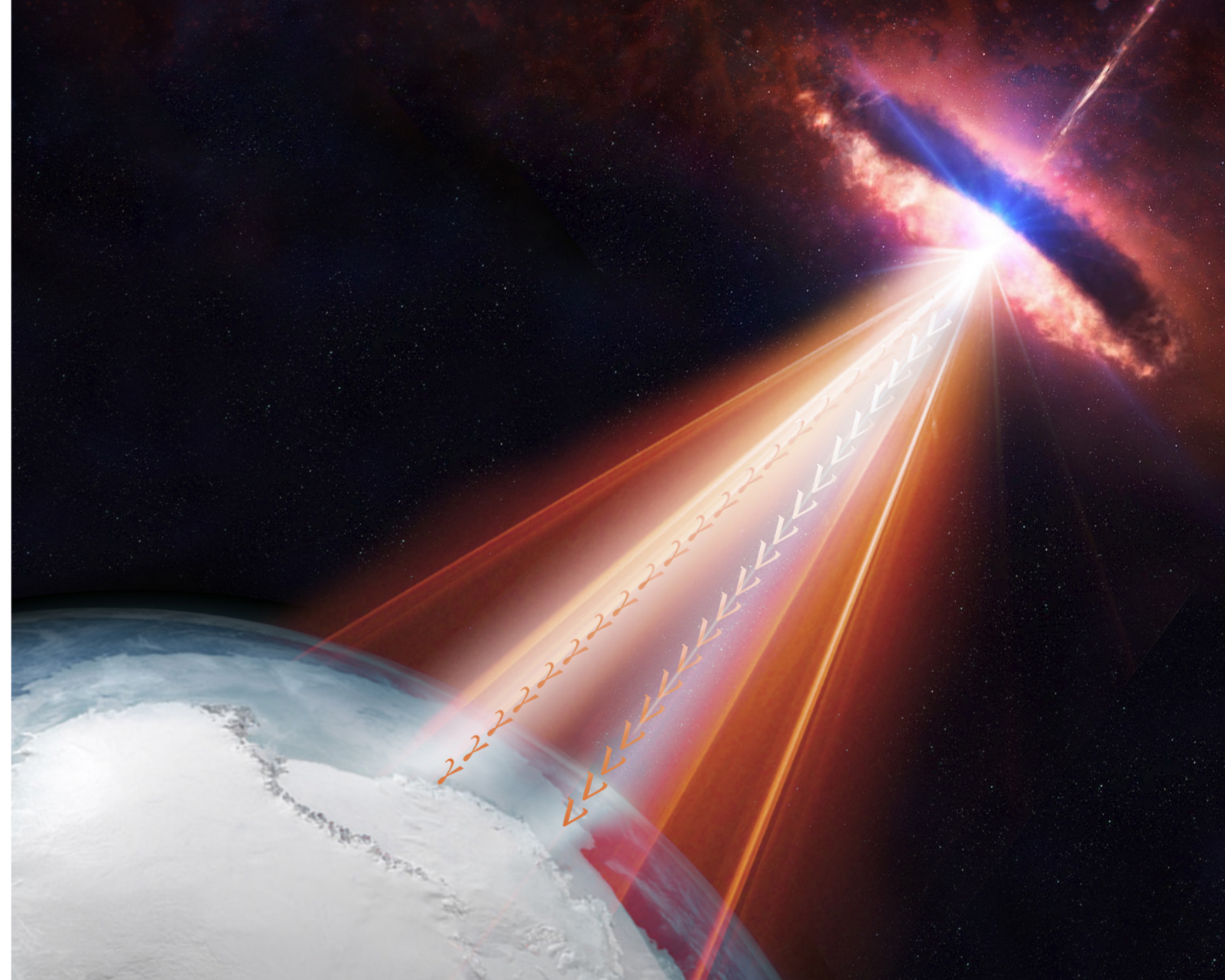
The National Science Foundation  
The National Institutes of Health  
The U. S. Department of Defense  
The Commonwealth of Pennsylvania  
D. E. Shaw Research

Bill and Melinda Gates Foundation  
The Grable Foundation  
Microsoft  
University of Pittsburgh  
USAID

**On the cover:** Blazars are a type of active galaxy with one of its jets pointing toward us. In this artistic rendering, a blazar emits both neutrinos and gamma rays that could be detected by the IceCube Neutrino Observatory as well as by other telescopes on Earth and in space.

**Feedback:** We would like to hear any feedback you have, on our work or this new publication. You can send any comments or suggestions via our feedback page at <https://www.psc.edu/feedback>. You can contribute to PSC's nonprofit, academic mission at <https://www.psc.edu/donate>.

# PUTTING NEUTRINOS ON ICE



## PITTSBURGH SUPERCOMPUTING CENTER SCIENCE HIGHLIGHTS

FALL 2018

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# PUTTING NEUTRINOS ON ICE

IDENTIFICATION OF COSMIC-RAY SOURCE BY ICECUBE NEUTRINO OBSERVATORY DEPENDED ON GLOBAL COLLABORATION, PSC'S BRIDGES

Four billion years ago—before the first life had developed on Earth—a massive black hole shot a proton out at nearly the speed of light. A result of this cosmic catapult was the creation of a neutrino, a strange, tiny particle lighter than any other known type of matter.

Fast forward—way forward—to 45.5 million years ago. Early primates and elephants had just appeared on Earth. The Antarctic continent had started collecting an ice sheet. Eventually Antarctica would capture 61 percent of the fresh water on Earth, creating an ice mass of continental scale.

Thanks to PSC's Bridges system and expert help from PSC staff, scientists running the IceCube Neutrino Observatory in Antarctica and their international partners have used these distant events as a tool to answer a hundred-year-old scientific mystery: Where do cosmic rays come from?

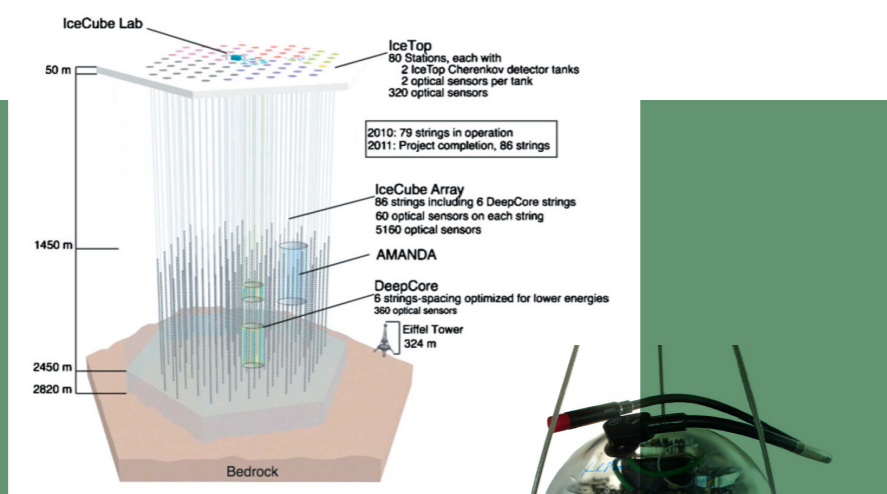
"The reason IceCube was envisioned and built was to try and understand the origin of cosmic rays," says Gonzalo Merino, computing facilities manager for the Wisconsin IceCube Particle Astrophysics Center at the University of Wisconsin-Madison.

First identified in 1912, cosmic rays have puzzled scientists. The higher in the atmosphere you go, the more of them you can measure. The Earth's thin shell of air, scientists came to realize, was protecting us from potentially harmful radiation that filled space. Today, the existence of cosmic rays remains a big concern in human space travel, posing a potential risk to astronauts. The concern is particularly high for long-term trips, such as to Mars.

"These particles that get to the Earth have an energy that is completely crazy," Merino adds. "Orders of magnitude higher than anything we can produce with accelerators like the LHC," the most powerful proton-smasher built by humans.

But where were cosmic rays coming from? FIND OUT AT [WWW.PSC.EDU/NEUTRINOS](http://WWW.PSC.EDU/NEUTRINOS)

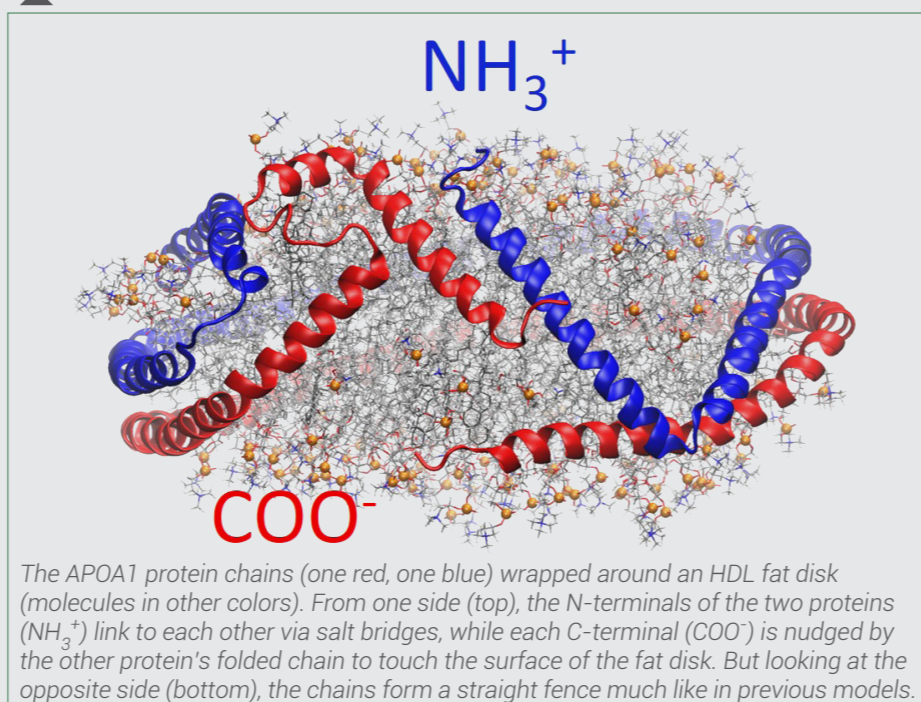
IceCube detector schematic: Detector by NASA-VERVE—IceCube Science Team—Francis Halzen, Department of Physics, University of Wisconsin



## "Sticky and Loose Ends" Shed Light on Heart Health

Until recently, scientists couldn't agree how the protein APOA1 holds together the "good cholesterol" that protects us from heart disease. Scientists from the National Heart, Lung, and Blood Institute led a collaboration that used the D.E. Shaw Research Anton 2 supercomputer hosted at PSC to discover how the two APOA1 protein chains wrap around a disk of HDL fat, locking themselves in place via their "sticky ends" and nudging aside their "loose ends." The finding will help doctors understand how the body regulates cholesterol and may point to better heart-disease treatments.

[WWW.PSC.EDU/LOOSEENDS](http://WWW.PSC.EDU/LOOSEENDS)



## When Winds Get Rough

Rough winds are an issue for generating electricity from wind power. They can cause early failure of turbine components that limit the method's monetary bottom line. Researchers formerly at Penn State University, working with real wind-turbine data from GE Global Research and with the help of PSC experts, used high-performance computers at PSC and its partners in XSEDE to simulate the windloads driving a 1.5-MW GE wind turbine. They discovered three different types of non-steady changes. In particular, a set of strong, sub-second changes in forces they found may contribute to early failure of bearings. Their results offer the possibility of better wind-turbine component design that extends component lifetimes and improves economic feasibility for wind power.

[WWW.PSC.EDU/ROUGHWIND](http://WWW.PSC.EDU/ROUGHWIND)

## Function Follows Form

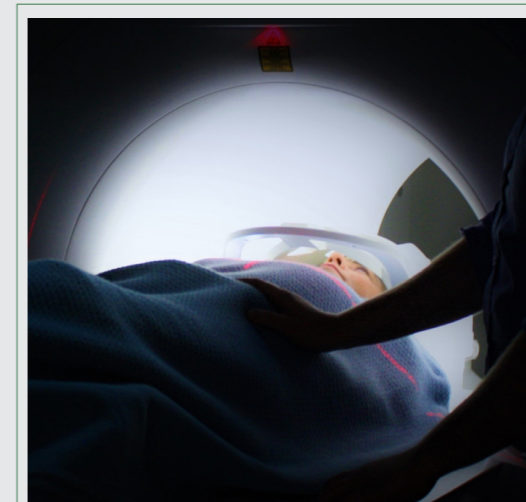
When a nerve cell passes a message to its neighbors, it must do so via chemicals sent across the synapse—a small space between the cells. Early researchers studied a synapse called the frog neuromuscular junction (NMJ) because it is large and easy to work with. But its differing organization and behavior compared with mammalian synapses led many scientists to dismiss it as not relevant to human biology. A team from the University of Pittsburgh and PSC performed simulations on the Bridges supercomputer and parallel lab experiments on the frog and mouse NMJ. They showed that, when reorganized into the same geometric pattern as in the mouse, the components of the frog NMJ act like those in the mouse. Lessons from the work are already being used to design candidate drugs to treat human neuromuscular diseases.

[WWW.PSC.EDU/FUNCTIONFORM](http://WWW.PSC.EDU/FUNCTIONFORM)

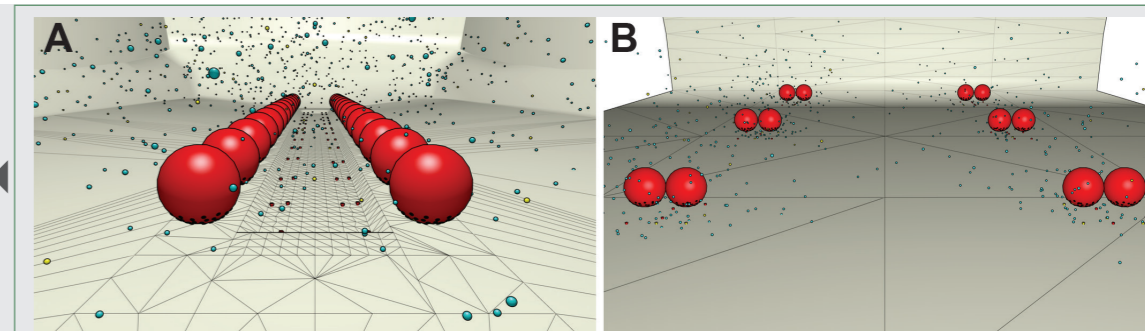
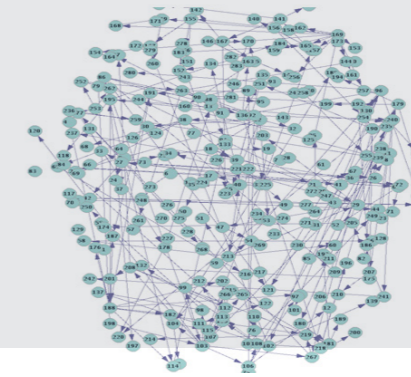
## Testing the Footing

The movement of white blood cells to fight infections and the spread of cancer cells both rely on the same natural process. The cell reaches out to a new surface with a lamellipodium—a kind of tiny foot that tests the surface like we'd test ice before stepping onto it. As part of a multi-institutional collaboration, a team from the University of Chicago simulated how the lamellipodium works, using PSC's Bridges supercomputer in concert with laboratory experiments. Their virtual cells duplicated their lab findings perfectly, showing how integrin and fibronectin—two proteins scientists had previously not expected to play a role—tug on the surface before the cell commits to moving onto it. The discovery points to possible ways for doctors to encourage good cell movement and discourage bad cell movement.

[WWW.PSC.EDU/TESTINGTHEFOOTING](http://WWW.PSC.EDU/TESTINGTHEFOOTING)



Below: A sample of the causal connections in an analysis of the human cortex, using the fGES method on an fMRI BOLD time series of 51,000 voxels. The voxels are 2 cubic millimeters wide.



View from the inside of a nerve cell. The synapse and the muscle cell are not pictured, but would be below the nerve cell's cell membrane, at the bottom. In the frog NMJ (A), neurotransmitter-containing packets (vesicles) waiting to be dumped into the synapse are arranged in two rows. (Vesicles are in red, calcium channels below the vesicles are small red dots, and the calcium ions diffusing in the nerve terminal are represented as small blue or yellow dots.) In the mouse (B), the vesicles are organized in clusters that each contain two vesicles. Simulations on Bridges showed that the frog system, when rearranged in clusters like the mouse, began to behave like the mouse NMJ.

## World's Tiniest Test Tubes in Alzheimer's Protein Simulation

The progressive memory loss of Alzheimer's disease is devastating. Doctors have known for more than 100 years that plaques of clumped-together protein form in the brains of people with Alzheimer's. But they aren't completely sure whether the clumps *cause* Alzheimer's or are a *consequence* of the disease. Using a series of PSC systems, Paul Axelsen and fellow scientists at the University of Pennsylvania have undertaken computer simulations of plaque-forming beta amyloid molecules inside reverse micelles, the tiniest test tubes in the world. Their results offer insights into beta amyloid and why it clumps that can offer targets both for further investigation and possible drug therapies.



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## Finding Cause

Functional magnetic resonance imaging (fMRI) measures brain activity as it happens. But on the surface, it's hard to tell whether activity in one part of the brain is caused by activity in another, or whether their apparent relationship is a coincidence. Scientists in Carnegie Mellon University's Department of Philosophy are trying to identify *causal relationships* in fMRI brain scans using a new set of statistical tools run on the Bridges system at PSC.

[WWW.PSC.EDU/FINDINGCAUSE](http://WWW.PSC.EDU/FINDINGCAUSE)