FROM THE DIRECTOR

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

PSC's 32nd year of operations is off to an exceptional start, with multiple important initiatives in motion and some exciting new ones imminent. Those initiatives build on PSC's leadership in converging high-performance computing (HPC), artificial intelligence (AI), and Big Data (BD) to enable discovery and accelerate innovation. This convergence lets researchers easily scale data analytics, modeling, and simulation to tackle challenges vital to science and society.

AI strategically cross-cuts PSC's activities. We will soon launch an innovative initatiative to bring cutting-edge AI solutions to research, education, and in academia and industry (watch our website and social media!). On Bridges, our flagship system funded by the National Science Foundation (NSF), 114 projects center on AI, and many others are beginning to include AI in their workflows, for example, to detect formation of storm clouds in large-scale weather data. Bridges is also being used extensively by university courses. Significantly, 260 students are using Bridges for CMU course *Deep Reinforcment Learning and Control*, illustrating both the fantastic energy around AI and Bridges' outstanding impact on education.

Bridges is entering its third year of production. Its first two years have been outstanding. To date, Bridges has served 1,239 projects and 6,316 users, including numerous communities and applications that have not traditionally used high-performance computing. Bridges recently enabled breakthroughs in, for example, understanding glioblastoma (a form of brain cancer) through deep learning, applying machine learning to develop new materials for energy applications including the first iron-bismuth compound, and revealing genetic changes induced by time spent in space in the NASA Twins Study. An innovative use of Big Data can be seen in our featured article, in which a Univerity of Pittsburgh team used Bridges as a cloud to advance our understanding of traumatic brain injury (TBI).

The innovative Anton 2 molecular dynamics modeling system, hosted at PSC thanks to D. E. Shaw Research and operational funding by the National Institutes of Health (NIH), continues to provide stunning simulations of long-time-scale molecular interactions. Anton 2 continues to illuminate the sub-microscopic world of medically relevant molecules, for example, powering a University of Delaware study of maturation—and the development of virulence—in HIV, the AIDS virus. A project headed by the National Institute of Standards and Technology used Anton 2 to unlock puzzles about the protein tubulin—the cell's "Lego brick"—with possible applications in chemotherapy side effects, cancer, and brain development. And there's an exciting avenue of research that pairs Anton's longer time scales with Bridges' capacity for large-scale molecular modeling to create longer simulations of larger, medically-important systems.

Our News Briefs section describes other advances made possible by PSC. The stunning poker victory last year of the Libratus AI, developed at CMU and run on Bridges, earned "Best Paper" at the prestigious NIPS 2017 conference and appeared in a much-anticipated article in *Science*. PSC, CMU, and Pitt joined to build a Brain Data Repository, part of the federal BRAIN Initiative. We were recognized for our Public Health Application Group's flu vaccine research with a 2017 Innovation Excellence Award from the Hyperion Research User Forum Steering Committee. And HPCwire's annual awards included five awards to PSC—a best-ever showing for any single site—including awards for data analytics, work on the CRISPR gene-splicing technology (shared with the UCSD and SDSC), energy research (shared with Texas A&M and TACC), Libratus's poker victory, and outstanding leadership in HPC.

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

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Interim Director

Carnegie Mellon University | PSC | University of Pittsburgh

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, 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

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The National Science Foundation
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The U. S. Department of Energy
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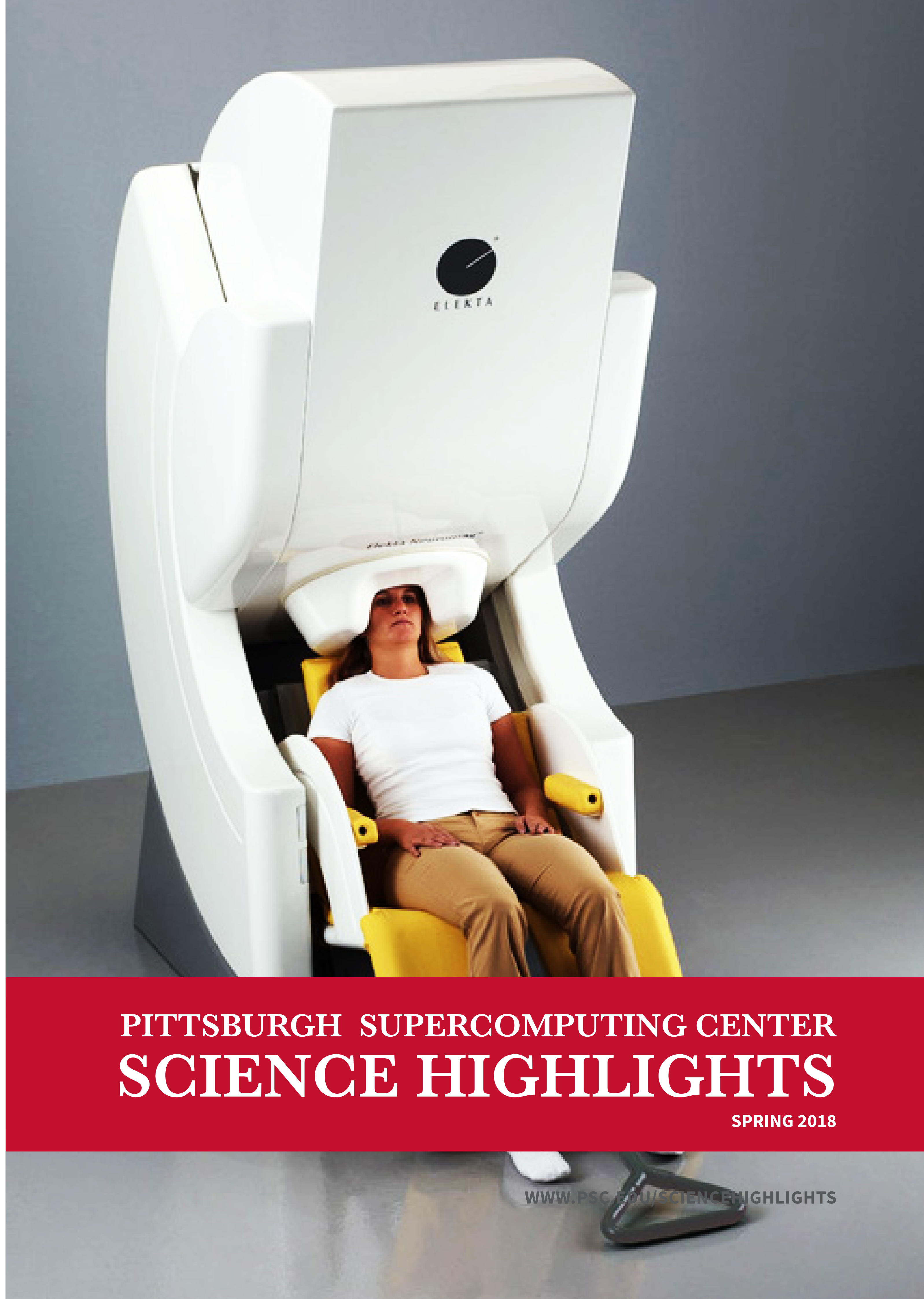
D. E. Shaw Research
Bill and Melinda Gates Foundation
The Grable Foundation
University of Pittsburgh
USAID

On the cover: The magnetoencephalographic (MEG) scanner. University of Pittsburgh researchers are using PSC's Bridges to produce very high-resolution functional MEG brain images that show promise in identifying and guiding research into traumatic brain injury.

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 also contribute to PSC's nonprofit, academic mission at https://www. psc.edu/donate.



PITTSBURGH SUPERCOMPUTING CENTER
SCIENCE HIGHLIGHTS
SPRING 2018

WWW.PSC.EDU/SCIENCEHIGHLIGHTS

FEATURE

HEAD INJURY IN THE CLOUD

USING "CLOUD"-BASED "BACKFILL CYCLES" ON BRIDGES ENABLES VERY HIGH RESOLUTION FUNCTIONAL BRAIN IMAGING

WHY IT'S IMPORTANT

From children's playing fields to professional stadiums to battlefields, doctors are more and more worried about brain trauma that lurks after a seemingly minor concussion. Kids and adults may walk off the field and suffer from headaches, difficulty thinking, memory problems, attention deficits and mood swings for weeks, months or longer. A key problem in finding better ways to diagnose and treat concussion is that imaging studies show no abnormalities in more than 80 percent of TBI patients. For most, doctors don't know whether the imaging methods aren't sensitive enough or even whether there is any structural damage to detect.

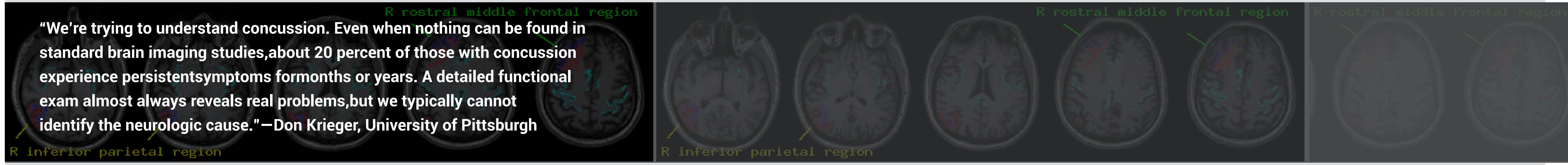
Don Krieger is part of a team of clinician-researchers at the University of Pittsburgh who are studying TBI. They produce very high resolution functional brain images from magnetoencephalographic (MEG) recordings usinga powerful new method called "referee consensus processing."MEG measures the magnetic fields caused by cooperative nerve-cellactivity. The technologyis noninvasive, silent and safe. But it's also computationally expensive, requiring supercomputers to generate images.

HOW PSC AND XSEDE HELPED

To carry out their computations the Pitt team used the Open Science Grid (OSG). OSG is a loosely coupled supercomputing resource composed of compute cycles donated by government laboratory and academic computing centers throughout the Americas. Using the OSG reduced the time required for the calculations from many decades to one to two years. To reduce that time further, they turned to two additional systems that work very efficiently with the referee consensus solver the Pitt scientists had developed: PSC's Bridges and Comet, at the San Diego Supercomputer Center (SDSC). Employing "backfill" and other unused cycles on the two supercomputers made more computing time available, did not impact other researchers using the same machines, and required only a few changes in the Pitt team's software. PSC's Anirban Jana and Derek Simmel and SDSC's Mahidhar Tatineni helped the team make these minor adjustments in just a few days. The work was supported by grants from XSEDE, the NSF network of supercomputing sites that includes both PSC and SDSC, and with continuing support from OSG operations and University of Southern California Viterbi School of Engineering's Mats Rynge.

Krieger and his colleagues analyzed MEG data from 64 volunteers with persistent symptoms of TBI, most of whom were combat veterans. They compared the scans with MEG data from 414 individuals who were similar to the TBI volunteers other than not having TBI symptoms. This second group of scans had been collected by the Cambridge (UK) Centre for Ageing and Neuroscience (CamCAN). The latter served as "controls," providing the researchers with recordings from asymptomatic people to compare with the volunteers' recordings. Together, Bridges and Comet reduced the computational time for the critical CamCAN control recordings from anestimated 20 months to seven. With the results from the CamCAN cohort, scientists have a picture with unprecedented resolution of patterns of cooperative neural activity from brains that are unaffected by TBI. Comparing these results with those from symptomatic patients will help the scientists identify the mechanisms which cause symptoms in TBI. It may also help them find better treatments.

WWW.PSC.EDU/BRAINTBI



"We're trying to understand concussion. Even when nothing can be found in standard brain imaging studies,about 20 percent of those with concussion experience persistentsymptoms formonths or years. A detailed functional exam almost always reveals real problems,but we typically cannot identify the neurologic cause."—Don Krieger, University of Pittsburgh

HIGHLIGHTS

Locked, not Loaded

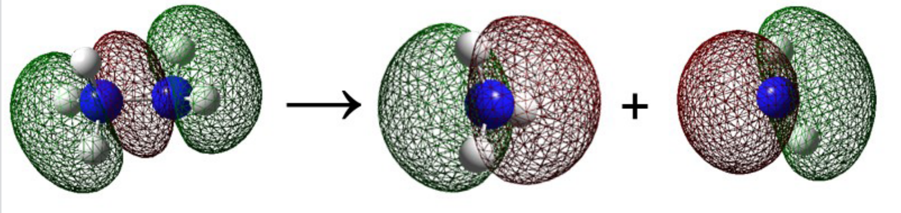
Though AIDS survival is up and new cases are down, the HIV virus is still a major cause of sickness and death. Juan Perilla of the University of Delaware and his colleagues used the Anton 2 system at the Pittsburgh Supercomputing Centerto understand better how HIV"matures" to its active state. They found that a class of anti-AIDS drugs may work by locking the virus in its immature form, suggesting a route toward new treatments.

WWW.PSC.EDU/LOCKEDLOADED

You Break it, You Understand It

The U.S. Air Force would like to detect remotelywhenbad guys have fired a rocket. They'd also like, in an emergency, to seed the atmosphere to damp down communicationdisruptions fromsolar flares. To better understand the very different chemicals involved in these two problems, quantum chemist Peter B. Armentrout and his team at the University of Utah turned to the XSEDE supercomputersBridges at PSC and Comet atSan Diego Supercomputer Center.

WWW.PSC.EDU/QUANTUMCHEM



$$N_2H_5^+(^1A') \longrightarrow NH_3^+(^2A_2'') + NH_2(^2A_1)$$

Above: The bond between the two nitrogen atoms in hydrazine rocket fuel broke to produce fragments that weren'tat the lowest possible energy level. While the result was a little surprising, a comparison with the theory via Bridges helped explain it.

Snapping into Place

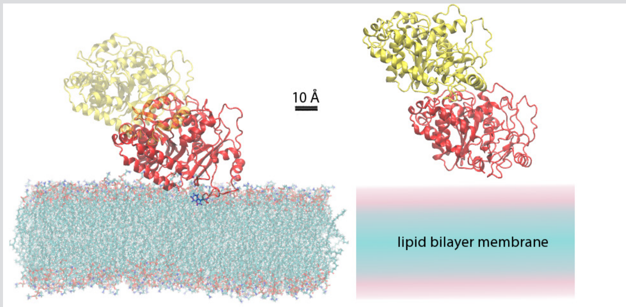
Tubulin proteins are the cell's "Lego bricks," connecting with themselves into tubular structures that help give living cells shape and stiffness. But the protein may also play a role in energy generation by the cell's mitochondria, with individual tubulin "bricks" sticking to the surface of mitochondria by a poorly understood mechanism. Scientists at the National Institute of Standards and Technology and elsewhere used the Anton 2 system hosted at PSC to unravel how tubulin snaps into place—offering clues to phenomena as different as chemotherapy side effects, cancer, and brain development.

WWW.PSC.EDU/TUBULIN

Finding the Balance

The biggest causes of death in developed countries—heart disease, cancer, chronic organ failure—are complex conditions that may be best treated by long-term management rather than attempting to "cure" them. Researchers at the University of Pittsburgh have used the Bridges supercomputer at the Pittsburgh Supercomputing Center to mine a massive database of medical records to optimize preventive doctor visits for individual patients with chronic kidney disease.

WWW.PSC.EDU/KIDNEY



NEWS BRIEFS

- CMU Group Describes "Superhuman"Poker AI in *Science*
- CMU, PSC and Pitt to Build Brain Data Repository
- PSC-Led Flu Vaccine Research Wins International Award
- PSC Wins a Record Five HPCwire Readers', Editors' Choice Awards HPC Cluster at PSC

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/NEWSBRIEFS18