EDITOR'S NOTE Our biannual science magazine "People.Science.Collaboration." has changed. Our new "PSC Science Highlights" is an all-electronic magazine (e-magazine) available at www.psc.edu/sciencehighlights. This electronic format will make it easier for you to find the article you are interested in reading.

The document you are holding is a printed summary of what's contained in our e-magazine, including a feature article, pointers to other articles highlighted here, news briefs and our computing resources.

LETTER FROM THE DIRECTORS

Welcome to the new PSC Science Highlights!

This first issue of our new format highlights a number of success stories in our ongoing mission to enable and support computationally dependent research in traditional and emerging fields, including the life sciences, public health, networking; to educate the next generation of researchers in using high-performance computing and big data systems (HPC); and to architect and deploy novel HPC systems.

The last year saw major developments in our HPC systems, furthering our efforts to better serve existing and new HPC users. The NSF-funded Phase-2 completion build of our Bridges system, accomplished on time and within budget, gives the heterogeneous, uniquely flexible Bridges increased speed, memory and storage. Quite independently, D.E. Shaw Research (DESRES) replaced its Anton system at PSC by an Anton 2 which supports much longer simulation times of much larger molecules. The only such machine publicly available to biomedical scientists carrying out non-commercial research, its operational funding comes from the NIH.

Our featured article is an artificial intelligence (AI) story made possible by Bridges: For the first time, an AI program has beaten the world's best humans at an "incomplete information" game: in this case, "heads-up, no-limit Texas hold'em" poker. Libratus, a creation of researchers at the Carnegie Mellon School of Computer Science, used roughly 80 percent of Bridges' powerful capacity to decisively defeat four of the world's best specialists in this form of poker. The victory carries major relevance to optimizing solutions to important, real-world problems such as cybersecurity, antiterror operations, business negotiations and even medicine.

We also report on the use of Bridges in a study of the factors that affect feasibility of electric power storage for commercial users. In addition to providing details on Anton 2, we describe a study performed on the earlier Anton system exploring the dependence of protein molecule functionality on their proper folding. The potential application range of this work includes cancer and degenerative brain diseases.

Our News Briefs section covers additional achievements by our Biomedical Applications Group, our STEM education efforts and research by our Public Health Group and our Network Applications Group. An important collaboration with the popular Galaxy framework and scientific gateway at Penn State is making Bridges available to genomics researchers and other scientists using Galaxy.

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

Michael Levine and Ralph Roskies

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.
Greenfield – a Data Exacell research system funded by the NSF.
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 Global Fund
UNICEF
USAID

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FEATURE

NO TELLING

PSC'S BRIDGES POWERS ARTIFICIAL INTELLIGENCE THAT BEAT POKER'S BEST PROS

WHY IT'S IMPORTANT

While computers have beaten human champions at a number of games—like checkers, chess or Go—these games offer *perfect information*. No information is hidden from the contestants and they have limited ability to deceive each other. Poker, on the other hand, is an *imperfect information* game. Unlike in chess, in an imperfect information game the opponent's hand is secret, and he or she is trying to mislead. Imperfect information games are like many real-world problems, including cybersecurity, terror defense, negotiation—even cancer treatment, because the tumor is actively evading both the patient's immune system and any treatments. Tuomas Sandholm of Carnegie Mellon University and his PhD student Noam Brown have created a series of artificial intelligence programs (AIs) capable of optimizing how to play essentially any imperfect information game. The scientists wanted to find out whether the AI's strategic reasoning had finally reached the point at which humans couldn't beat it, even under imperfect information. To find out, they took on the world's best specialists at heads-up, no-limit Texas hold'em poker—a benchmark game in which hidden information and deception are paramount. The AI would have to learn how to deceive—and how to win despite deception. In 2015, the team's earlier AI, called Claudico, narrowly lost to top human players.

HOW PSC HELPED

Heads-up, no-limit Texas hold'em has 10^{161} possible situations—more than there are atoms in the known Universe, and far more than any computer can directly calculate. To master the game, the scientists' new AI, called Libratus, had to find the optimal way to simplify the game to be computable and how to bluff in ways that tricked some of the most expert human players into holding, and folding, when they shouldn't. For their January 2017 "Brains vs. AI" rematch with the pros, they turned to PSC's Bridges system, using about 600 of Bridges' compute nodes. This raw power gave Libratus the capacity to plot each move in real time—and reformulate its strategy each night, even as the four human experts—Dong Kim, Jason Les, Jimmy Chou and Daniel McAulay—were doing the same to try to expose any weaknesses in the AI.

In the end, Libratus scored a resounding victory, beating the pros by more than $1.7 million in chips at the Rivers Casino in Pittsburgh. The scientists calculate that an outcome this lopsided or larger was only 0.5 percent likely to happen just by chance. The win marked the first time that an AI had beaten the world's best players at a game that had emerged over the years as the leading benchmark for solving imperfect-information games. This paves the way for AIs to help transform how humans approach real-life problems in security, negotiation and medicine.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/NOTELLING

SCIENCE HIGHLIGHTS

MORE POWER TO US

If everyone used electricity at a constant rate, generating power would be simple. But spikes in use lead to under-utilized power and ultimately increased costs. Scientists used PSC's Bridges and former Greenfield systems to understand the economic and engineering challenges of "behind the meter" battery storage.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/MOREPOWER

ANTON 2 SUPERCOMPUTER OPERATIONAL AT PSC

Anton 2, a specialized supercomputer developed by D. E. Shaw Research that simulates the motions of biomolecules, has replaced the original Anton 1 system previously at PSC. The new machine, operationally supported through a grant from the National Institutes of Health, enables life scientists to simulate much larger biomolecules for longer timescales than was previously feasible.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/ANTON2

GUT CHECK

While diabetes poses many life- and limb-threatening problems, it also causes serious changes and problems in the digestive tract. A study using PSC's Bridges system sifted through the DNA of thousands of microbe species in the healthy and diabetic intestines to learn how to help reduce digestive symptoms—and maybe even slow the course of the disease.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/GUTCHECK

HOOKED UP

A common way for proteins to hold themselves together is with *disulfide bridges*. But scientists don't completely understand why some proteins need them to "hook up" their structure. Researchers used the DESRES Anton system hosted at PSC to discover the critical role disulfides play in holding together MCoTI-II, a natural pesticide that would fall apart without disulfide bridges.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/HOOKEDUP

PHASE 2 OF BRIDGES APPROVED

The National Science Foundation has approved the Phase 2 upgrade of the new Bridges supercomputer it funded at PSC. The enhanced system offers more speed, memory and data storage for investigators who have used supercomputers and those in fields that never before needed them.

WWW.PSC.EDU/SCIENCEHIGHLIGHTS/**PHASE2**

BRIEFS

News Briefs

- PSC Projects win HPCwire Awards for Best Data-Intensive System, High-Performance Data Analytics
- More Intensive Programs Needed to Make Bioinformatics Available to Minority Students
- DANCES Project Reaches Benchmark for "Opening Up" Network Connections for Better Diagnosis, Repair
- Galaxy Science Gateway Now Offering Seamless Access to PSC's Bridges for Largest RNA Assemblies

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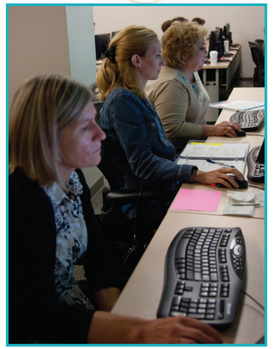

"We didn't actually look at any data, just the rules of the game ... It was like practicing by shadow boxing and then stepping into the ring with Mike Tyson." —Tuomas Sandholm, Carnegie Mellon University