UC San Diego’s official launch of the Halicioğlu Data Science Institute (HDSI) in early March was welcomed by SDSC, which will house research labs and offices for HDSI’s senior staff and faculty in the Center’s East Building. “We’re pleased that SDSC will be home to many HDSI faculty and staff as this exciting new initiative gets underway,” said SDSC Director Michael Norman. “We look forward to SDSC being a hub of connectivity for data analytics and innovation for the entire UC San Diego campus.”

UC San Diego Chancellor Pradeep K. Khosla led the dedication event at SDSC’s auditorium on March 2, following last year’s announcement of a $75 million donation from UC San Diego Alumnus Taner Halicioğlu (hah-li-jyo-loo) to create such an institute.

“It just made sense to have the institute at SDSC because this place is all about data,” said Halicioğlu, who earned a bachelor’s degree in computer science at the UC San Diego in 1996 and interned at SDSC in 1995 and 1996. In remarks during the event, he noted that “data science has technically always existed, but I don’t think it really started to coalesce into an actual discipline until recently. I’m excited that we’ll hopefully be on the forefront of that.”

[Continued on Page 3]
The first quarter of 2018 has proved the adage that “change is constant.” I mean that in a positive way, because change often leads to new opportunities. Such a change occurred in March with the official dedication of the Halicioğlu Data Science Institute and the news that SDSC will be one of the homes for this new campus-wide initiative.

All of us welcome Taner Halicioğlu and the HDSI faculty and look forward to them leveraging SDSC’s expertise and resources in high-performance computing and data-enabled science. As a top research university, UC San Diego is leading the way in establishing data-enabled science as a key part of its curriculum, and SDSC’s reputation for computing-at-scale is foundational to achieving this goal.

When the time is right, SDSC will collaborate with HDSI to develop training opportunities for UC San Diego students and postdocs. We also expect that Comet will be used to advance HDSI research in data-intensive areas such as machine learning and artificial intelligence.

All of this dovetails with SDSC’s goal of increasing its own participation of undergraduate and graduate students in research activities as outlined in our recent campus review recommendations. There has been a series of discussions at the Executive Team level with selected staff about how to evolve SDSC’s own educational programs. There’s strong alignment within the group to extend our own Education, Outreach, and Training (EOT) program to involve more undergraduate/graduate students. More on this as discussions continue, so stay tuned.

Our featured SDSC Innovator is Kevin Coakley. Kevin's professional experience underscores how changes at the macro level of storage and computing opened new opportunities not only for him, but for SDSC. In this issue you’ll read about how Kevin’s job evolved from configuring just storage systems to storage/compute clusters designed to meet the specific needs of researchers.

Also, kudos to several SDSCers and affiliated researchers who were recently recognized by the Corporation for Education Network Initiatives in California (CENIC) for being innovators in networking applications. Recipients include SDSC Chief Data Science Officer Ilkay Altintas; John Graham (Qualcomm Institute, UC San Diego); and Frank Vernon (Scripps Institution of Oceanography), who now leads HPWREN after co-founding the network in 2000 with SDSC Research Scientist Hans Werner-Braun. Two other SDSCers – Network Architect Tom Hutton and Founding Director Sidney Karin – were honored by receiving CENIC’s Founders Circle Award which recognizes researchers who were instrumental in CENIC’s creation.

In short, advancing scientific discovery has always been about education and innovation, and recent events mean one thing for us: opportunities. By this, I mean opportunities to collaborate on both the campus and UC fronts, as well as through our mission of helping to develop advanced cyberinfrastructure on a national scale.

Michael L. Norman
SDSC Director
The gift from Halicioğlu, the first paid employee at Facebook, was the largest ever received from a UC San Diego alumnus. In addition to Facebook, Halicioğlu also worked at eBay and Blizzard Entertainment, and currently is a private investor as well as a lecturer in UC San Diego's Department of Computer Science and Engineering. HDSI will focus on cross-disciplinary studies involving computer science, cognitive science, mathematics, and other fields and be a campus-wide initiative.

The new institute has been collaborating with other research units at UC San Diego, including SDSC's Data Science Hub, where experts at SDSC and other parts of the university can apply their experience in building multi-disciplinary data science teams to help provide solutions to regional, national, and global challenges such as smart cities, precision medicine, advanced manufacturing, and data center automation. In addition to SDSC, the institute will have facilities in other campus locations including the Qualcomm Institute at Atkinson Hall.

CENIC Recognizes Technology Projects to Combat California Wildfires

Two UC San Diego projects involving SDSC – WIFIRE and the High Performance Wireless Research and Education Network (HPWREN) – have been selected as recipients of the Corporation for Education Network Initiatives in California (CENIC) 2018 Innovations in Networking Award for Experimental Applications. These awards recognize advances in IT and telecommunications technologies to help minimize potential damage caused by wildfires. CENIC, a nonprofit corporation formed in 1996 to provide high-performance, high-bandwidth networking services to California universities and research institutions, presented the awards at its annual conference, held this year March 5-7 in Monterey, California.

Project leaders being recognized include SDSC Chief Data Science Officer and WIFIRE PI Ilkay Altintas; John Graham (Qualcomm Institute, UC San Diego); and Frank Vernon (Scripps Institution of Oceanography), who now leads HPWREN which he co-founded with SDSC Research Scientist Hans Werner-Braun in 2000.

CENIC also honored technology leaders with a new Founders Circle Award to recognize researchers who were instrumental in creating the network. Among those recipients were SDSC Network Architect Tom Hutton; and SDSC's founding director, Sidney Karin. “Just as CENIC members today work collaboratively to shape and govern the organization, these leaders worked collaboratively to lay the groundwork necessary to launch the world-class research and education network used by millions of Californians,” said CENIC President and CEO Louis Fox.

Read more at <https://goo.gl/Kwnc78>
Compute Cluster Customizer: Meet Kevin Coakley

While Kevin’s current title is Senior Storage Systems Engineer, his role as part of SDSC’s IT Division has evolved to not only include storage but work with researchers at SDSC, across campus, and other UC schools to create purpose-built compute and storage platforms using open-source software. Kevin joined SDSC in 2013 after working as a programmer/analyst on campus at what was then called Academic Computing & Media Services. There he specialized in instructional IT, managed the Campus Learning Management System (LMS), and created the campus podcasting system. He joined UC San Diego full-time in 2003 after earning a degree here in Interdisciplinary Computing in the Arts. In 2014, he earned his Master of Advanced Study (MAS) degree in Architecture-based Systems Engineering.

Q: Can you briefly describe your role here at SDSC?
I spend most of my time working with PIs to create storage and compute platforms that meet their specific research needs. I use a standard set of tools, and usually start with a whiteboard sketch of black boxes, and analysis/exploration tools. Sometimes they have a specific software in mind, but if not I’ll research existing options that best meet their requirements.

Q: Can you give us some examples of platforms you have built?
I’d rather say that these platforms are a work in progress, as researchers’ needs evolve. One is the AWESOME platform being developed by SDSC Researcher Amarnath Gupta, with collaboration from researchers at UC San Diego, UC Irvine, and UCLA. That project focused on integrating research-intensive databases. Another is the MAS Data Science & Engineering program at the Jacobs School of Engineering. That required customized scripts to help students launch notebooks such as Jupyter, allowing them to install their specific course software. This too is a work in progress as researchers who teach often evolve their courses, so updates are needed on a routine basis.

Q: Your role at SDSC has evolved from data storage to also include research computing platforms. Can you give us some background?
The SDSC cloud storage system is based on OpenStack’s Swift object store, and also includes a compute facility based on Openstack Nova with Ceph. So being familiar with the cloud storage part, which is accessed via a web-based interface, isn’t that different from the compute side. The same technologies are used so it’s just a case of expanding the language. Deploying clusters essentially use configuration management tools that are programmatic. Working on storage-compute platforms instead of storage only means I get to learn new things and for me, that’s a lot of fun.

Q: How did you become interested in storage and compute clusters?
When I was five or six my mother bought me a Commodore 64 (an 8-bit home computer introduced in January 1982). When I got bored of playing the games on it, I started subscribing to magazines such as Jupyter, allowing them to install their specific course software. This too is a work in progress as researchers who teach often evolve their courses, so updates are needed on a routine basis.

Q: So when you’re not working on storage and computer platforms...
I try not to use the computer at home. I really need to get outside so I enjoy surfing when conditions are right, as well as biking.
SDSC Simulations Reveal How a Heart Drug Molecular Switch Is Turned On and Off

Armed with a robust computational approach that stretches the amount of time needed to capture the gyrations of proteins in their natural state, researchers have revealed for the first time intricate details about how a key molecular switch, implicated in a variety of medical conditions including heart disease, is turned on and off.

The study, published in the March 5 online edition of the *Proceedings of the National Academy of Sciences (PNAS)*, describes how the supercomputing power of SDSC’s Gordon, Comet, and other GPU clusters were used with improved accelerated molecular dynamics (aMD) or Gaussian aMD (GaMD) to simulate the merger of a G-protein “mimetic nanobody” to a G-protein-coupled receptor (GPCR), the largest and most diverse group of membrane receptors in animals, plants, fungi, and protozoa.

“This is the first molecular dynamics simulation for any GPCR-protein binding, a major advance since very few protein-protein binding simulations have been achieved due to the system’s complexity and slowly moving dynamics,” said Yinglong Miao, an assistant professor of Computational Biology and Molecular Biosciences at U. Kansas and the study’s lead author.

“Many of today’s heart drug medications act on M2 muscarinic acetylcholine receptors,” said J. Andrew McCammon, the Joseph E. Mayer Chair of Theoretical Chemistry and Distinguished Professor of Pharmacology, all at UC San Diego and a collaborator in the research. “However, many carry side effects, some of which are serious.”

The reason? The genetic sequence of the M2 mAChR’s primary ‘orthosteric’ binding site is found in least four other receptor types that are widely spread in the body, and when drugs accidently bind to these other receptors, unwanted and sometimes serious consequences can result.  

Read more at <https://goo.gl/DyYXmH>

Comet Aids Discovery of New, Inexpensive Material to Make LEDs

A team led by UC San Diego engineers used data mining and SDSC’s Comet supercomputer to discover a new phosphor material for white LEDs that is inexpensive and easy to make. As reported in the Feb. 19 issue of the journal *Joule*, the researchers built prototype white LED light bulbs using the new phosphor that exhibited better color quality than many commercial LEDs currently on the market. The new phosphor is made mostly of earth-abundant elements, can be made using industrial methods, and produces LEDs that render colors more vividly and accurately.

“Comet was especially well-suited for our project,” said Shyue Ping Ong, a nanoengineering professor at the UC San Diego Jacobs School of Engineering and lead principal investigator of the study. “By leveraging on our open-source high-throughput software infrastructure and Comet resources, we were able to compute the stability and photoluminescent properties of thousands of candidate materials within a matter of weeks, something which would have taken years to obtain experimentally.”  

Read more at <https://goo.gl/jJ7Q87>

**INNOVATIONS IN RESEARCH**
Some 15 San Diego-area high school students who interned as part of SDSC's Research Experience for High School Students or the Mentor Assistance Program presented research aimed at improving early diagnosis and treatment of a variety of ailments during the Third Annual Biomarkers International Conference held last February in San Diego.

Their research, displayed in posters and videos at the meeting, ran the gamut of potential new diagnostic and progression biomarkers for autism spectrum disorder, Parkinson's disease, diabetes, Alzheimer's disease, and several forms of cancer. Generally, biomarkers indicates a change in expression or state of a protein that correlates with the risk or progression of a disease, or with the susceptibility of the disease to a given treatment.

“We are pleased and proud of the participation of these young researchers in a national scientific conference of increasing importance to medical science,” said Valentina Kouznetsova, an associate research professor with the Moores Cancer Center and SDSC, who mentored the students in the biomarker program along with Igor Tsigelny, a research professor with the UC San Diego Department of Neurosciences and SDSC. “It's a rewarding experience for us to help these students gain traction toward a possible career in research.”

REHS Gearing Up for 2018

The Research Experience for High School Students (REHS) program, about to enter its ninth year, is part of the SDSC's student outreach program to help increase awareness of computational science and related fields of research to students in the San Diego region. The eight-week program, which runs from late June until mid-August, offers a wide variety of internships, from molecular dynamics research to learning how to communicate complex research results in a clear and compelling way. Students, mentored by SDSC's computational researchers and other staff, gain exposure to career options, hands-on computational experience, and work readiness skills.
San Diego County Invests in New UC San Diego Fire Detection Networking

The County of San Diego Board of Supervisors has approved an investment in technology developed at UC San Diego’s High-Performance Wireless Research and Education Network (HPWREN) and the Alert Wildfire network to improve the County’s fire detection and response capabilities. The County’s investment of just over $437,000 covers the addition of new cameras and a boost in the network speed of hazard detection technology developed by the university.

HPWREN and the Alert Wildfire network, operated by the Scripps Institution of Oceanography and SDSC, connect firefighters with real-time fire activity information across the San Diego County backcountry via a network of more than 60 fire stations using more than 160 cameras to provide on-demand time-lapse high-definition (HD) or better imagery to detect fire outbreaks and prevent them from reaching a catastrophic size. Fire officials have control of the cameras to monitor fires and triangulate on the location to better respond to fires at their earliest stages.

Read more at <https://goo.gl/QGLQeV>

UC San Diego, Japan’s AIST Extend Bilateral Memorandum of Understanding

UC San Diego and Japan’s National Institute of Advanced Industrial Science and Technology (AIST) have agreed to a new, broadened five-year pact to cooperate on research in the fields of computer science and technology, including artificial intelligence and other data-intensive domains. “We are building on a history of more than 15 years collaborating with AIST on specific projects,” said Phil Papadopoulos, SDSC’s chief technology officer, adding that the new pact expands the partnership to other units across UC San Diego. As part of the new agreement, signed in January, AIST and SDSC will share best practices on complementary systems such as SDSC’s Comet supercomputer and Japan’s ABCI hybrid computing cluster now under construction and scheduled to begin operations in fiscal 2018.

Read more at <https://goo.gl/94qGjK>
In 2013, SDSC launched a new high-performance computing program for UC San Diego researchers called the Triton Shared Computing Cluster (TSCC). Founded on the “condo computing” model, computer servers or “nodes” for the system are purchased by the research labs or groups using funds from grants or faculty startup packages, and the ongoing operating expenses of the system are shared by the university administration and participating groups.

By purchasing a few nodes, researchers can gain access to a medium-scale (200+ teraflops) supercomputer, a much larger resource than the typical research lab could afford on its own. Today, TSCC is supporting research across a wide variety of domains, including biology and life sciences, chemistry, climate, engineering, political and social sciences, and others. Spare capacity on TSCC is also available to industrial users at market rates, and the system currently supports industrial R&D in areas such as genomics and materials science.

As TSCC has grown, it has provided the opportunity to introduce and evaluate new technological innovations in computing. For example, in 2017 a grant was received under the National Science Foundation’s Campus Cyberinfrastructure (“CC*”) program called “Bioburst” (NSF Award #1659104). The Bioburst project is focused on introducing new technology to TSCC to support a growing bioinformatics workload. The award permitted the acquisition and integration of additional compute nodes; high-speed network switches (EDR Infiniband); an input/output (I/O) accelerator system; and a specialized bioinformatics accelerator using field programmable gate array (FPGA) technology. The new compute nodes and networking switches provide significant additional computing capacity for processing of bioinformatics analyses. The I/O accelerator is connected to the new compute nodes and supports high-performance data transfers specifically for biological data sets. The bioinformatics accelerator provides very rapid turnaround analyses of DNA and RNA samples, which might be needed in a clinical or precision medicine setting.

The TSCC program has permitted SDSC to deploy its capabilities in both integrating and operating production supercomputing systems as well as evaluating and acquiring the latest advanced computing technologies. Our SDSC Technology Partners Program provides industry with the ability to work with SDSC scientists and staff in these areas and others. Please contact us directly or visit our website for more information on how you can get involved.

Ron Hawkins
SDSC Director of Industry Relations