Comet Simulations Provide Preview of Solar Eclipse

On August 21, 2017, a total eclipse of the Sun was visible across much of the U.S., tracing a 70-mile-wide band across 14 states. Several weeks earlier, a team from Predictive Science Inc. (PSI), based in San Diego, created a large-scale simulation of the solar event using massive supercomputers including SDSC’s Comet. The simulations are among the largest the research group has performed, using 65 million grid points to provide greater accuracy and realism.

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For a brief moment, the recent total eclipse of the sun last month diverted our collective eyes and minds from more worldly and sometimes tragic news to glimpse a rare moment of celestial alignment by two of this planet's nearest neighbors. As an astrophysicist and director of SDSC, I was particularly excited about some of the incredible simulations our Comet supercomputer helped to create in advance of this historic happening, as highlighted on Page 1 of this issue.

As many of you already know, Comet’s large roster of researchers has been reporting major advances and discoveries that are dramatically altering and increasing our understanding of a myriad of long-held questions – from the nanoscopic world of the human genome to the massive geological cleavages that trigger earth-shattering quakes and torrential volcanoes. SDSC is on the vanguard of this new era of research, something we call "computational convergence", a bridge that's connecting advanced computation with large-scale data management and expertise.

Toward that end, SDSC has been working with our UC San Diego colleagues to further leverage computational convergence to broaden our collaborations with the university’s faculty, staff, and students. This effort includes expanding our role in campus’ IT Services (ITS) as well as the new Halicioglu Institute of Data Science (HIDS) that will be formally announced soon. More details to come as we progress on those fronts.

This summer also brought about some staff changes at SDSC. Nieves Rankin, our Chief Administrative Officer, has joined the Division of Social Sciences as Assistant Dean. We thank Nieves for the tremendous work she has done for us during the last three years. I’m also pleased to report that Samuel ‘Fritz’ Leader will succeed Nieves beginning later this month, before moving into the role full-time on November 1. Fritz’s 12 years of experience at UC San Diego includes positions in Core Bio Services, Health Sciences, and the Financial Analysis Office, plus his strong IT background, makes him well qualified to help lead SDSC in leveraging greater integration across campus.

Karen Flammer had been splitting her time between being SDSC’s EOT Director and Interim Director of the Center for Digital Learning at UC San Diego, the latter position becoming permanent this month. Bob Sinkovits has been named Interim Director of EOT and a search for a permanent director will start soon. Bob will continue his role as Director of the Scientific Computing Applications group. Please join me in wishing Karen success in her new endeavors, while welcoming Bob to his expanded role.

More news and features inside this issue of SDSC Innovators!

Michael L. Norman
SDSC Director
Ilkay Recognized by ACM
SDSC Chief Data Science Officer
Ilkay Altintas has been named the inaugural winner of the Association for Computing Machinery (ACM) Emerging Woman Leader in Technical Computing Award. Presented by the ACM’s Special Interest Group on High-Performance Computing, or SIGHPC, the biennial award is unique in recognizing mid-career women in the technical and high-performance computing communities.

SIGHPC is the first international group within a major professional society that is devoted exclusively to the needs of students, faculty, researchers, and practitioners in high-performance computing. The award will be presented at the SC17 conference that takes place November 12-17 in Denver, Co.

Altintas was recognized “for research leadership that makes distributed scientific and technical computing applications more reusable, scalable, and reproducible,” according to SIGHPC. She was named SDSC’s first-ever Chief Data Science Officer in August 2015.

“Ilkay has an impressive history of leading research and development of application-oriented computational data science solutions for many scientific domains, as exemplified by the award-winning WIFIRE project,” said SDSC Director Michael Norman. “Her expertise means that SDSC is well-positioned to create data platforms that include ‘big data’ applications that are scalable and extensible for numerous computing and analytical needs.”

With over 100 journal articles and conference papers, Altintas’ work has been applied to computations in bioinformatics, geoinformatics, high-energy physics, multi-scale biomedical science, computational drug discovery, smart manufacturing, hazard management, and smart cities. She also is a co-founding developer of Kepler, a widely-used tool that enables research teams to build and run workflows, and to share computational models across a broad range of scientific and engineering disciplines.

SDSC’s ‘Sherlock’ Launches Secure, Compliant Cloud Services in Amazon Web Services
SDSC’s Health Cyberinfrastructure (CI) Division has deployed its secure and compliant Cloud solution, Sherlock Cloud, in Amazon Web Services (AWS). This solution addresses the gap that currently exists in infrastructure-level compliance offered by public cloud platforms with a comprehensive, managed compliance capability offered by Sherlock Cloud, giving customers the option of buying services on premise (@SDSC) or in the Cloud (@AWS). With this new capability SDSC becomes one of the few academic institutions to offer secure, compliant, managed services through a Hybrid Cloud leveraging both a private Cloud (@SDSC) and a public Cloud platform (@AWS). “Public Clouds only offer basic compliance at the infrastructure level, and significant effort, both in terms of technical resources and capital, needs to be invested to build additional services to make the environment fully compliant,” said Sandeep Chandra, Executive Director of Sherlock Cloud. “Sherlock Cloud addresses this need while providing its customers with the ultimate compliant solution.”

Read more at https://goo.gl/1s5m6i

Comet Helps Break the “Millisecond Barrier” for Complex Biological Simulations
Using a novel molecular dynamics method capable of capturing the motion of gyrating proteins at time intervals up to one thousand times greater than previous efforts, a team led by UC San Diego researchers has identified for the first time the myriad structural changes that activate and drive CRISPR-Cas9, the innovative gene-splicing technology that’s transforming the field of genetic engineering. The researchers once again returned to Comet to perform CRISPR-Cas9 simulations at the lengthened time-scale. “In particular, we wanted to design a system that doesn’t cause ‘off-target’ effects or non-selective cleavage of DNA sequences, that can now create unwanted collateral damage,” said J. Andrew McCammon, the Joseph E. Mayer Chair of Theoretical Chemistry at UC San Diego, a Howard Hughes Medical Institute Investigator, and principal investigator of the study, published in the June 26 early edition of the Proceedings of the National Academy of Sciences (PNAS).

Read more at https://goo.gl/fHKKJy
OK, Michele Strong’s official title is really Research Administrator / Supervisor, but most researchers at SDSC know her as the one who makes their lives much easier by helping them navigate through the often convoluted process of submitting proposals. Michele moved to SDSC from the Scripps Institution of Oceanography 15 years ago. Prior to that she was an interpreter for the deaf in the San Diego Unified School District, as well as an accountant for small businesses.

Q: You play a vital role here at SDSC by managing the submission of a wide range of sponsored projects, including major grants such as multi-year funding from the National Science Foundation to develop and operate our Comet supercomputer. Can you briefly describe what other kinds of contract and grant proposals come through your department?

Strong: SDSC receives funding from multiple sources. We work with the National Institutes of Health, the Department of Energy, Department of Defense, NASA, plus various foundations and donors, as well as private donors. Types of funding include contracts, grants, cooperative agreements, service agreements, and gifts.
Q: On average, how many contracts and grants does your department manage per year?
Strong: Between 100 and 140 a year.

Q: I understand that your department also is responsible for post-award administration. What does that entail?
Strong: We ensure that the agency regulations and the Office of Management Budget’s Uniform Guidance policy are correctly applied to our contract and grant funding. We also ensure that Principal Investigators (PIs) of various grants don’t overspend!

Q: Sounds like you’re never not busy! There also must be dozens of deadlines that you have to keep track of. Can you share one or two examples of how the submission process became a close call but worked out well in the end?
Strong: I have to say that some of our PIs like to make our lives exciting by cutting it pretty close from time to time. One in particular was for a non-profit that had a deadline of 10 p.m. The campus’ Office of Contract and Grant Administration gave me permission to submit on their behalf so I stayed until the deadline to submit. It was about 10 minutes before the deadline—I had all the docs uploaded and just then the PI called and asked to make "a small change." We had a very bad phone connection and I could not understand what was being requested. I began to panic—I have never missed a deadline—and was almost in tears. Realizing this, the PI said “Michele, please do not cry—it's OK to submit as is.” Or at least that is what I think he said, and we submitted it with two minutes to spare.

Q: What background or previous experience do you think is essential for the responsibilities you currently have?
Strong: One must have a good knowledge of agency guidelines, be proficient in Excel, and have an understanding of cost accounting standards. One must also be able to multi-task and be very flexible. Oh, and a good sense of humor helps!

Q: What brought you to SDSC?
Strong: I was working at Scripps Institution of Oceanography with Alma Palazzolo and she came to SDSC. There was a job opening and she asked me to apply. I’m so happy I did!

Q: What sage advice do you have for any researcher or research team submitting a proposal?
Strong: Submit proposals early! If one submits their proposals a few days prior to the deadline, we and our contract office have a chance to review for any errors or omissions. For the post-award process, it really helps to keep your fund manager informed of any large purchases or any changes to the budget.

Q: What do you do outside the office for relaxation and fun? And are deadlines involved?
Strong: Ha! I have to admit that I’m pretty much early to every party, movie, or other event with some kind of deadline. My favorite thing to do is to read. As a child I used to hide in the closet to read, while I was supposed to be doing chores. I love dancing, singing, and eating! Once I joined a choir and learned the entire Messiah and sang it at various cathedrals in San Diego. So much fun! I had to just pretend to sing the trills! Someday, I’d like to be in a play—perhaps ‘Fiddler on the Roof’ as Yente?

“I have to say that some of our PIs like to make our lives exciting by cutting it pretty close from time to time.”
Researchers also used NASA’s Pleiades supercomputer, as well as Stampede2 at the Texas Advanced Computing Center. “Advanced computational resources are crucial to developing detailed physical models of the solar corona and solar wind,” said Jon Linker, president and senior research scientist of PSI. Once completed, the researchers’ computer simulations were converted into scientific visualizations that approximate what the human eye might see during the solar eclipse. Making predictions about the appearance of the corona during an eclipse is a way to test complex, three-dimensional computational models of the sun against visible reality.

(Left) Visualization of the three-dimensional (3D) magnetic field of the sun’s corona for the August 21, 2017 total solar eclipse. By tracing magnetic field lines at extremely high resolution, we can calculate a 3D map of the so-called magnetic squashing factor—a scientific measure designed to indicate the presence of complex structuring in the magnetic field. We then integrate the map along the line-of-sight, with special weightings to create a composite that resembles solar eclipse images. This is intended to highlight the inherent complexity of the Sun’s magnetic field and its connection to visible emission from the solar corona.

(Right) The top image shows a digital processing of the polarized brightness using a “Wavelet” filter to bring out the details in the image. The bottom image shows traces of selected magnetic field lines from the model. It also shows the intensity of the radial component of the photospheric magnetic field, with the brightest colors showing the location of active regions (strong magnetic fields). Images courtesy of Predictive Science Inc.
SDSC recently graduated its 2017 Summer Institute group representing 31 institutions from around the U.S. with 40 participants selected from four times as many applications. The annual week-long workshop, first offered in the mid-1990s, offers introductory to intermediate topics on high-performance computing and data science. The program allows attendees to perform hands-on exercises on SDSC’s Comet supercomputer, and includes plenary sessions covering essential skills including data management, running jobs on SDSC resources, and various techniques for turning data into meaningful and usable knowledge. The program continued to evolve, keeping pace with changes in computational and data science. The latest sessions covered new topics such as Machine Learning at Scale, distributed programming in Python, cluster computing with Spark, and CUDA programming.

Participants represent a broad range of scientific fields: mathematics, marine and atmospheric sciences, physics, chemistry, astronomy, computer science, pharmaceutical sciences, ecology, biomedical, economics, as well as mechanical, chemical, electrical, and aerospace engineering. “An integral part of the Summer Institute is the informal opportunities attendees have to interact among themselves and with SDSC’s experts,” said Andrea Zonca, a Computational Scientist at SDSC and Director of Summer Institute 2017. “They have opportunities to discuss specifics about their research, understand how to directly apply high-performance computing skills to their domain, and get a broader view of the data science and supercomputing world.” Kudos go to Andrea Zonca for leading this year’s program, and to Susan Rathbun and Cindy Wong for making the event run so smoothly.

Event information is available at http://si17.sdsc.edu

2017 Research Experience for High School Students Wraps Up

SDSC’s eighth-annual Research Experience for High School Students (REHS) summer program concluded in early August with another packed house as students displayed their posters and videos following the eight-week internship. Some 66 students—accepted from more than 200 applications—were paired with a team of 16 SDSC mentors to gain experience in an ongoing research project or computationally-centric subject.

As before, a wide range of internships were offered, from studying molecular makeups of diseases and disorders such as cancer and autism, memory analysis of high-performance computing applications, multi-scale simulations in chemistry and biophysics, and even a course designed for students to learn how to communicate the complexities of advanced research to a layperson audience.

“Coming into the program, I knew I wanted to study and work in STEM, and this program just enhanced that desire,” said Holly Murphy, who participated in the Science Communications internship by developing and directing a short video highlighting the SuAVE (Survey Analysis via Visual Exploration) data analysis and sharing project led by Ilya Zaslavsky, director of SDSC’s Spatial Information Systems Laboratory and also an REHS mentor. “The most important thing I learned was how to work with others on a project that was a combination of my own ideas and my mentor’s ideas,” said Murphy. Her video can be viewed at: https://youtu.be/s5OvBZ-UAF4

“REHS was an invaluable experience because my mentors taught me how to meet and exceed high standards, while making research enjoyable and exciting,” said Sidney Lenz, a recent graduate of Mission Vista High School who worked with SDSC Research Scientist Igor Tsigelny and Valentina Kouznetsova, an Associate Research Professor with the Moores Cancer Center, to identify metabolic signatures of glioblastoma subtypes.
The end of summer is always a good time for reflection, looking back on a busy year and thinking about how we want to shape things in the months ahead. For SDSC’s industrial program, it’s been a busy year on multiple fronts including the Internet of Things (IoT), smart manufacturing, machine learning and artificial intelligence, life sciences computing, and all things data-enabled.

SDSC researchers have been contributing their expertise to the development of smart manufacturing technologies and systems. In late 2016, the Smart Manufacturing Leadership Coalition (SMLC) received an award from the Department of Energy for the Clean Energy Smart Manufacturing Innovation Institute (CESMII), a $140 million, five-year public-private partnership and part of a national network of Manufacturing Innovation Institutes that has been ramping up in 2017. The SyGMA Lab, established in 2016, is making advancements in signal processing and event analysis on the basis of data obtained from Smart Grids, a realization of the IoT. In 2017, the SyGMA Lab augmented its capabilities through installation of a real-time microgrid simulation system provided by RTDS Technologies and an equipment donation provided by SEL, Inc.

Technological advances in DNA sequencing and cryo-electron microscopy are generating vast amounts of data that help enable research discoveries crucial to understanding illnesses and developing personalized medical treatments. In late 2016, SDSC, with funding from Dell and Intel under the Dell “Centers for Innovation” program, carried out a project to characterize the performance and identify optimization opportunities for key bioinformatics applications on high-performance computing systems. The project was finalized in early 2017 and the team is making plans for a follow-on effort.

A key aspect of SDSC’s industrial programs has always been to provide a neutral forum where companies can come together to explore emerging technology topics of mutual interest. In December 2016, SDSC held the inaugural “Data West” conference, providing a discussion-oriented forum on emerging business opportunities in data geared toward senior thought leaders and decision-makers. Based on the success of that forum we are planning a second Data West conference in December 2017 and by all indications it will be a well-attended and exciting event.

Looking forward, we’re always thinking about ways to improve our program and add more value for our industrial partners. We’ve been working on a revamped partners program with new features and new opportunities for collaboration with SDSC scientists and researchers. Stay tuned to our website and these pages for more details. We hope to see you at Data West in December!

Ron Hawkins
SDSC Director of Industry Relations