## GATEWAYS GAZETTE

San Diego Supercomputer Center

SC16 Edition

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# Supercomputing for All!

### SDSC Leads New Science Gateways Collaboration

- Join us in Booth 1801 Monday evening for a Science Gateways Community Celebration
- Meet the Science Gateways Community Institute Team Tuesday Morning
- Learn More About "The Internet of Things"
   & Comet's New Virtual Clusters Wednesday
   Afternoon
- "Wow! Learn This Now!" Lightning Tutorials Tuesday & Wednesday Afternoons
- Full SC16 SDSC Booth Schedule on Back

### What is a science gateway?

It's a community-developed set of tools, applications, data services, and collections integrated through a web-based portal or suite of applications. Such gateways provide scientists access to many tools used in cutting-edge research – everything from supercomputers to seismic shake tables, sky surveys, telescopes, remote sensors, and more – and connect often diverse resources in easily accessible ways that save researchers and institutions time and money.

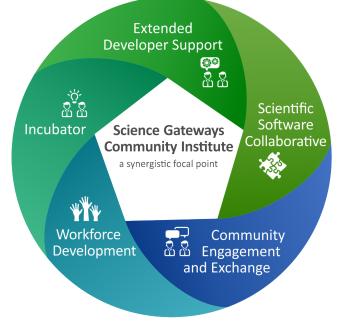
(Salt Lake City) Before long, many more researchers from many more science domains will have unfettered access to some of the nation's most capable supercomputers to help them accelerate discovery. How? Through web-based science gateways.

Thanks to a five-year, \$15 million grant from the National Science Foundation (NSF) earlier this year, the San Diego Supercomputer Center (SDSC) at UC San Diego is leading a multi-partner collaboration to establish a Science Gateways Community Institute (SGCI). Its goal is to develop a suite of highly functional, sustainable science gateways that address the needs of researchers across the entire spectrum of NSF directorates. The collaboration is funded via NSF award number ACI-1547611.

"The Institute's mission is to increase the number, ease of use, and effective application of gateways for the greater research and engineering community, resulting in broader gateway use and more widespread engagement in science by professionals, citizen scientists, students, and more," said Nancy Wilkins-Diehr, SDSC associate director and principal investigator for the project.

#### **Democratizing Supercomputers**

"This novel collaboration will go a long way in democratizing access to supercomputers such as our own *Comet* resource," said SDSC Director Michael Norman. "In fact, *Comet* and our data-intensive *Gordon* supercomputers together accounted for 86%



of gateway jobs on XSEDE resources during the past year. NSF's XSEDE (Extreme Science and Engineering Discovery Environment) is the most advanced collection of integrated digital resources and services in the world."

"Gateways foster collaborations and the exchange of ideas among researchers and can provide broader access to resources sometimes unavailable to those who are not at leading research institutions," said Wilkins-Diehr

### Science Gateways Community Institute Partners

- > Elizabeth City State University in North Carolina
- Indiana University
- University of Notre Dame
- Purdue University
- ➤ The Texas Advanced Computing Center (TACC) at the University of Texas, Austin
- University of Michigan at Ann Arbor



Nancy Wilkins-Diehr is co-PI of the NSF-funded Extreme Science and Engineering Discovery Environment (XSEDE) program. "In XSEDE, we have observed tremendous growth in terms of the number of gateway users, the number of processing hours used on HPC resources and the number of published research papers using gateways in the last couple of years," she said. "We see the services offered by the Science Gateways Community Institute dovetailing nicely with those offered by XSEDE. In the XSEDE Extended Collaborative Support (ECSS) program, our primary focus is supporting developers of existing gateways with their back-end connections to XSEDE resources."

### Gateways exist via the XSEDE program for numerous science domains

- Anthropology
- Biochemistry
- Earth Sciences
- Particle Physics
- Materials Research
- Seismology
- Astronomy
- Computational Chemistry
- Environmental Sciences
- Nanotechnology
- Neurosciences
- •...and more!



https://www.xsede.org/gateways-listing

### SDSC and Science Gateways

SDSC has a proven track record in leading the creation of science gateways. One of the most popular ones is the CIPRES (CyberInfrastructure for Phylogenetic RESearch) gateway, a web-based portal developed by SDSC researchers that lets scientists explore evolutionary relationships between species. In 2015, the NSF and the UK's Biotechnology and Biological Sciences Research Council awarded funding for a new Neuroscience Gateways project led by SDSC. That

project, which is contributing to the national BRAIN initiative, is a collaboration between UC San Diego, Yale University, and University College London. The OpenTopography gateway provides easy access to earth science-oriented, high-resolution topographical data and processing tools for a broad spectrum of research communities. The project is a collaboration between UC San Diego, Arizona State University, and UNAVCO





### San Diego Supercomputer Center | SC16 Schedule

SDSC Booth 1801 (Gateways Bar and Café)
Salt Palace Convention Center, Salt Lake City, Utah

All presentations at SDSC Booth 1801 except where otherwise noted

MONDAY, NOVEMBER 14	
7:00 – 9:00P	EXHIBITION OPENING GALA -
Reception Sponsored by Dell EMC and Intel	Science Gateways Community Institute Kickoff Celebration Craft beers served
	TUESDAY, NOVEMBER 15
10:30 – 11:30a	Craft coffees and pastries served
Presentations Sponsored by	WELCOME BY SDSC DIRECTOR MICHAEL NORMAN
Dell EMC and Intel	Science Gateways Community Institute Panel Discussion Lead by: Nancy Wilkins-Diehr, Associate Director, SDSC; co-PI, XSEDE; PI, SGCI
	Participants: John Towns, Executive Director for Science and Technology, NCSA; PI, XSEDE Maytal Dahan, Scientific Software Collaborative, TACC Sandra Gesing, SGCI Campus Engagement, Notre Dame Linda Hayden, SGCI Workforce Development, Elizabeth City State University Marlon Pierce, SGCI Extended Developer Support, Indiana University Michael Zentner, SGCI Incubator, Purdue University
	SDSC Science Gateways Overview: CIPRES, NSG-R Gateway Amit Majumdar, Division Director, Data Enabled Scientific Computing, SDSC Wayne Pfeiffer, Distinguished Scientist, SDSC
1:30 – 3:00p Sponsored by Aeon	GATEWAYS TO LEARNING: "WOW! LEARN THIS NOW!" (LIGHTNING TUTORIALS)
	*** WIN ONE OF 16 RASPBERRY PI 3s! ***
	Multi-threaded and Out-of-core Programming in Python Andrea Zonca, HPC Applications Specialist, SDSC
	Machine Learning: Face Recognition Robert Sinkovits, Director, Scientific Computing Applications, SDSC
	KMeans Clustering of Weather Data Ilkay Altintas, Chief Data Science Officer, SDSC
3:00 - 6:00p	MEET & GREETS - Craft beers served
Sponsored by Aeon 4:00 – 5:00p	Pacific Research Platform High-Speed Large Data Transfer Demonstration Tom DeFanti, Research Scientist, Calit2, UC San Diego - PRP Data Experiment John Graham, Senior Development Engineer, Pacific Research Platform
4:00 – 5:00p	National Data Service Meet & Greet Christine Kirkpatrick, Executive Director, NDS; Division Director, IT Systems & Service, SDSC
	WEDNESDAY, NOVEMBER 16
10:30 – 11:30a	Craft coffees and pastries served  Panel Discussion: Data Science for Life Sciences Research & the Public Good Moderated by: Michael Norman, SDSC Director  Ilkay Altintas, Chief Data Science Officer, SDSC - WIFIRE, MetroInsight
	Tom DeFanti, Research Scientist, Calit2, UC San Diego - PRP Data Experiment Geoffrey Fox, Distinguished Professor, Intelligent Systems Engineering Chair, Indiana University - Streaming Data Glen Otero, Solution Architect, Life Sciences & HPC, Dell – Life Science Computing Architectures
	Robert Sinkovits, Director, Scientific Computing Applications, SDSC
	Versatile HPC: Comet Virtual Clusters for the Long Tail of Science Michael Norman, SDSC Director Phil Papadopoulos, Chief Technology Officer, SDSC Frank Würthwein, Lead, High-Throughput Computing, SDSC; Executive Director, Open
1:30 – 3:00p	Science Grid  GATEWAYS TO LEARNING: "WOW! LEARN THIS NOW!"
Sponsored by Aeon	(LIGHTNING TUTORIALS)  *** WIN ONE OF 16 RASPBERRY PI 3s! ***
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	Machine Learning: Face Recognition Robert Sinkovits, Director, Scientific Computing Applications, SDSC
	KMeans Clustering of Weather Data Ilkay Altintas, Chief Data Science Officer, SDSC
3:00p [NCSA Booth 2501]	National Data Service (NDS) Meet & Greet Christine Kirkpatrick, Executive Director, NDS; Division Director, IT Systems & Service, SDSC
3:00 – 6:00p	MEET & GREETS - Craft beers served
Sponsored by Aeon 4:00 – 5:00p	Pacific Research Platform High-Speed Large Data Transfer Demonstration Tom DeFanti, Research Scientist, Calit2, UC San Diego - PRP Data Experiment John Graham, Senior Development Engineer, Pacific Research Platform
4:00 – 5:00p	WBDIH/BD Hub Meet & Greet Christine Kirkpatrick, Deputy Director, West Big Data Innovation Hub; Division Director, IT Systems & Services, SDSC
	THURSDAY, NOVEMBER 17
40.00	MEET & GREETS- Craft coffees and pastries served
10:00a – 2:00p	THEET & GREET'S CRUIT CONJUGES WITH PUSITIES SERVED

Special thanks to:













### LIGHTNING TUTORIALS

Tuesday & Wednesday
1:30 – 3:30 pm
SDSC Booth 1801

Participants will automatically be entered to

WIN one of 16 RASPBERRY PI 3s!
All participants receive a 16 GB THUMB DRIVE!

Sign up soon – seating is limited

SDSC's resident experts will be conducting a series of lightning tutorials Tuesday and Wednesday afternoon on several topics designed to increase your HPC IQ!

Mini courses include:

#### Multi-threaded and Out-of-core Programming in Python

Tutorial on processing data larger than memory (out-of-core computing) and using multiple cores (multi-threading) in Python using dask.

#### **Machine Learning: Face Recognition**

Demonstration using Python and the Computer Vision library OpenCV to detect faces in images.

### KMeans Clustering of Weather Data

Tutorial on loading tabular weather data with pandas, computing statistics, plotting and running KMeans clustering with scikit-learn.

Participants will receive a 16G thumb drive with the mini courses loaded. At the end of each course there will be two drawings to win a Raspberry PI 3 featuring a 1.2GHz 64-bit quad-core ARMv8 CPU, 802.11n Wireless LAN, Bluetooth 4.1, and Bluetooth Low Energy (BLE).

Tutorial sign-ups begin on Tuesday morning. Seating is limited to eight workstations per tutorial, but everyone is welcome to participate. Participants may sign up for more than one tutorial.

Use your QR code reader to learn more about SDSC's Science Gateways...



Science Gateways ScienceGateways.org sciencegateways.org



CIPRES Gateway
CI for Phylogenetic Research
www.phylo.org



NSG-R Gateway
Neuroscience Gateway
www.nsgportal.org



OpenTopography Gateway
Topographical data and processing tools
www.opentopography.org



SGCI Press Release Science Gateways Community Institute goo.gl/xuAw3S