

Science Gateways : An Overview

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What is a Science Gateway

- 1. an online community space for science and engineering research and education.*
- 2. a Web-based resource for accessing data, software, computing services, and equipment specific to the needs of a science or engineering discipline.*



Catalyzes and democratizes science research for scientists and students

Gateways for many different fields

GATEWAY (357)	Computational Anatomy	Neuroscience Biology	Visit Portal
SOFTWARE (55)			Visit Portal
SGCI AFFILIATE (5)			Visit Portal
SGCI CLIENT (25)			Visit Portal
USED IN CLASSROOM (29)			Visit Portal
PHYSICAL (172)			Visit Portal
Chemistry (39)			Visit Portal
Physics (25)			Visit Portal
Earth Sciences (97)			Visit Portal
Space Science (29)			Visit Portal
LIFE (152)			Visit Portal
Biology (137)			Visit Portal
SOCIAL (70)			Visit Portal
Anthropology (4)			Visit Portal
Archaeology (4)			Visit Portal
Demography (1)			Visit Portal
Geography (3)			Visit Portal
History (4)			Visit Portal
Linguistics (5)			Visit Portal
Pedagogy (1)			Visit Portal

Links: catalog.sciencegateways.org

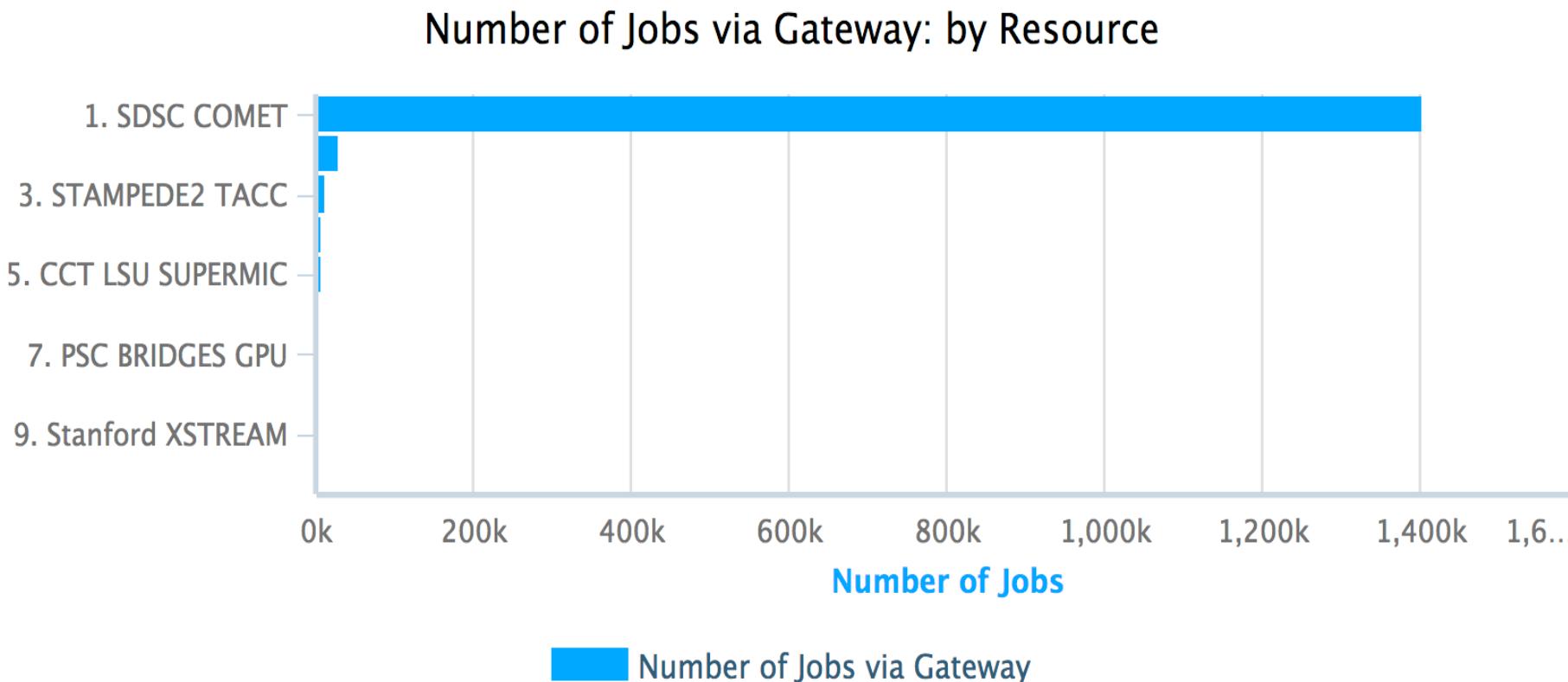
<https://www.xsede.org/ecosystem/science-gateways>

Some common features

- **Easy web-based user interface.**
 - Upload input files/models
 - Download output results
 - Some provide post processing/viz
- **Software/scientific applications already installed optimally on computing resources at the backend**
- **HPC resources - available via XSEDE (Extreme Science and Engineering Discovery Environment)**
- **Gateway team writes annual allocation proposal**

SDSC leads in hosting science gateways

//Jobs by Resource/Number of Jobs via Gateway



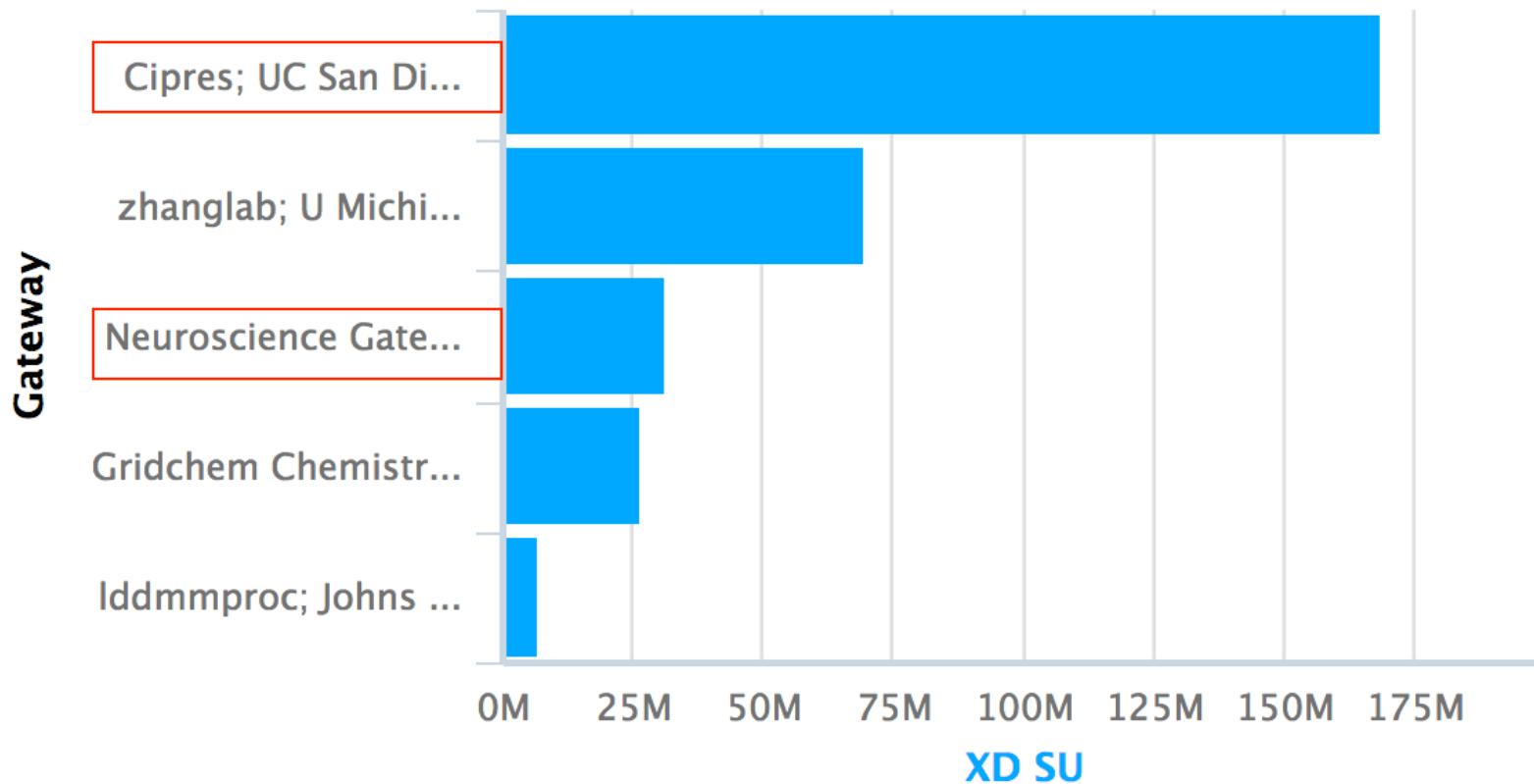
XDMOD – July 2017 – July 2018

SDSC leads in developing science gateways

Total XD SUs Charged by Gateway (Top 5)



Service Provider = SDSC



XDMOD - July 2017 - July 2018

Gateways are changing the way science is conducted in so many ways

nature International weekly journal of science

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Archive > Volume 530 > Issue 7588 > Letters > Article

NATURE | LETTER

日本語要約

New deep-sea species of *Xenoturbella* and the position of *Xenacoelomorpha*

Greg W. Rouse, Nerida G. Wilson, Jose I. Carvajal & Robert C. Vrijenhoek

Affiliations | Contributions | Corresponding author

Nature 530, 94–97 (04 February 2016) | doi:10.1038/nature16545

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nature microbiology

Letter | OPEN | Published: 11 April 2016

A new view of the tree of life

Laura A. Hug, Brett J. Baker, Karthik Anantharaman, Christopher T. Brown, Alex J. Castelle, Cristina N. Butterfield, Alex W. Hernsdorf, Yuki Amano, Kotaro Ise, Yo



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NSF 14-044

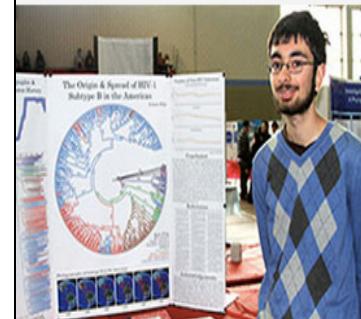
Dear Colleague Letter: BRAIN EAGERs to Enable Innovative Neurotechnologies to Reveal the Functional and Emergent Properties of Neural Circuits Underlying Behavior and Cognition

Date: March 7, 2014

This Dear Colleague Letter is aimed at identifying opportunities to leverage and synthesize technological and conceptual innovation across disciplines and scales to accelerate progress toward an integrated understanding of neural circuits in behavior and cognition, or more simply “catching circuits in action”. The neuroscience research community and specialists in other areas including, but not limited to genetics, physiology, synthetic biology, engineering, physics, mathematics, statistics, behavior and cognition are encouraged to work across disciplines to develop new approaches and neurotechnology focused at understanding the properties of circuits that underlie behavior and/or cognition in any organism. Projects that take advantage of existing DBI investments in informatics, computing and other infrastructure, such as the Neuroscience Gateway, in novel ways are also eligible.

Budding Scientist Wins State Fair Prize Using CIPRES Science Gateway

10th Grader Creates Timeline, Map of How HIV Spread



Neuroscience Gateway

NSG Team:

*Amit Majumdar, Subha Sivagnanam, Kenneth Yoshimoto (SDSC)
Ted Carnevale (Yale school of medicine)*

HPC Challenges for Computational Neuroscience

- Modeling projects start “small” and many are forced to stay “small”
- Rapid growth in development of complex neuronal network models, parameter sweep estimations, data processing etc. require HPC
- Not all neuroscientists, in the world, have access to large scale HPC
- **Barriers of entry to HPC**
 - Write peer-reviewed proposals for computer time
 - Understand HPC machines, policies, complex OS/software
 - Install and benchmark complex tools on HPC resources
 - Figuring out data transfer, management, storage issues

The Neuroscience Gateway (NSG)

The NSG provides simple and secure access through portal and programmatic services, to run neuroscience related software and tools on HPC resources

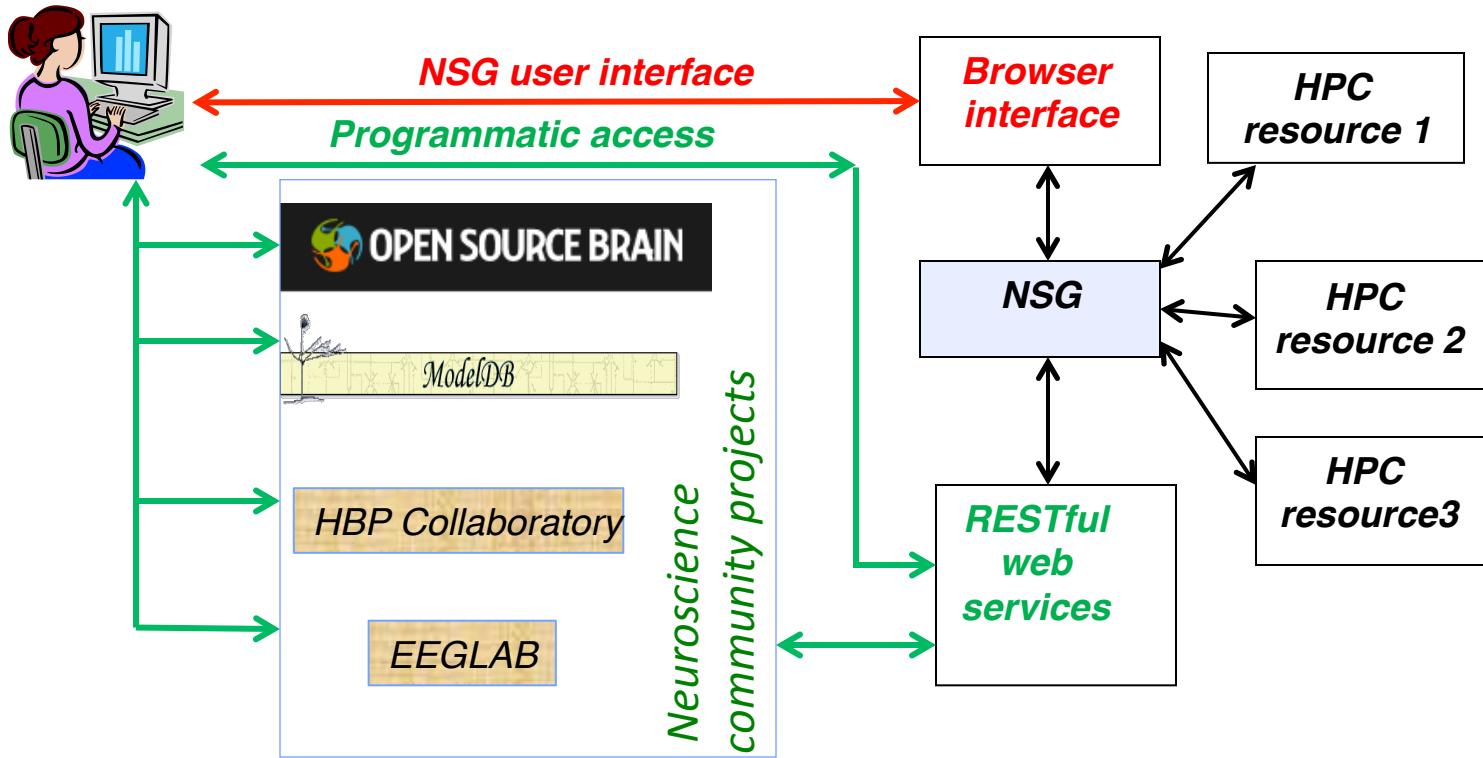
<http://www.nsgportal.org>

1. Developed using CIPRES SDK framework, customized for neuroscience research.
2. Easy user interface – providing easy model/input data upload, running of codes
3. Provide neuronal simulation and data processing tools – widely used by neuroscientists
4. Ability to easily get to the results, download results

NSG backend

- Access to XSEDE HPC resources, NSG/HPC software stack
- Access to various architectures such as GPUs, KNLs.
- Support “bundling” of jobs, i.e multiple single core executions in parallel – parameter sweep studies
- Support custom workflows , e.g. The TVB pipeline

NSG – Portal and Programmatic Access



Trees

CARLsim

TVB -
Empirical
pipeline

NetPyNE

HNN

EEGLAB

DynaSim

LSNM

current

Computational
neuroscience software

NEURON

MATLAB

TensorFlow

Brian

Python

PyNN

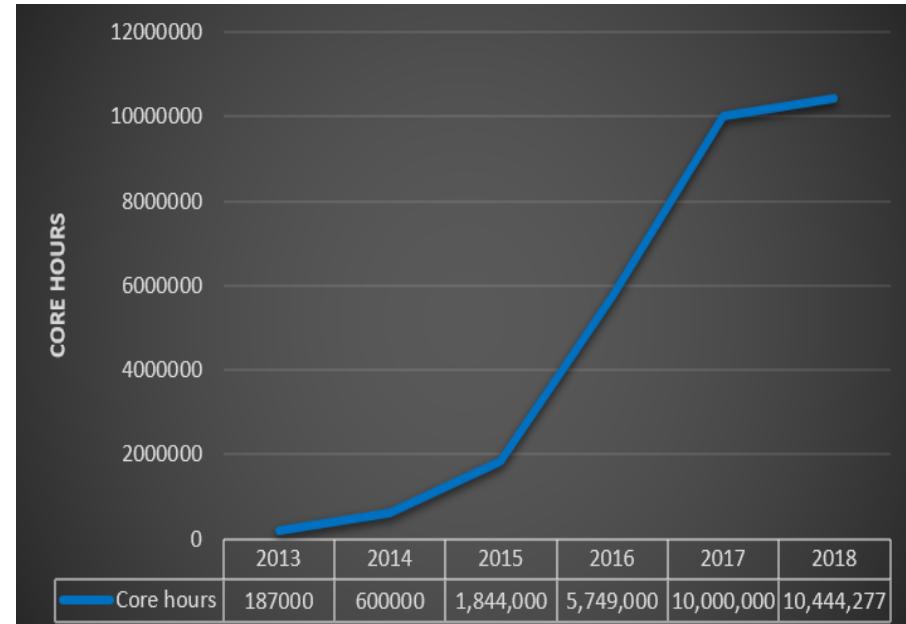
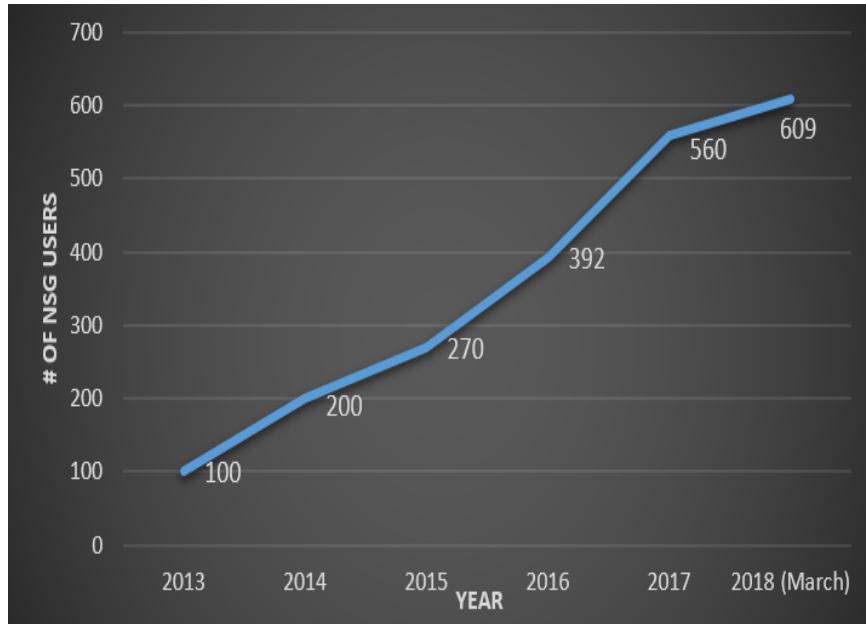
Octave

NEST

R

2012

NSG usage growing – since 2013



Evolving NSG

- **Tool Dissemination**
- **Education and Training**
 - NEURON Summer course
 - NIH funded Computational Neuroscience Training Course (U. Missouri)
 - SFN, CNS workshops
 - NSF funded Cyberinfrastructure Neuroscience training
- **Collaborative Environment**

Thoughts and Tactics for Success

- 1: identify a user population in need**
- 2: commit to responding to users' needs**
- 3: let user behavior/needs drive improvements**
- 4: with limited resources, prioritization is key**
- 5: stay in touch with your community**
- 6: embrace customer service**

Resources available for researchers and developers....

Building a gateway - Challenges

- **Building a gateway requires different types of expertise**
 - Software developer, Graphic designer, Security expert
 - But projects cannot always afford to hire these specialists
 - Short term hires are difficult as well

NSF Awards \$15 Million to Create Science Gateways Community Institute

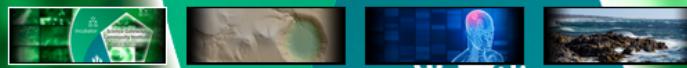
The Institute will accelerate the development and application of highly functional, sustainable science gateways that address the needs of researchers across the full spectrum of NSF directorates

[READ MORE](#)

Incubator

Science Gateways Community Institute

a synergistic focal point



Innovate, Educate, Collaborate:

FOR
UC/UCSD Researchers

FOR
National HPC Users

FOR
Industry & Sponsors

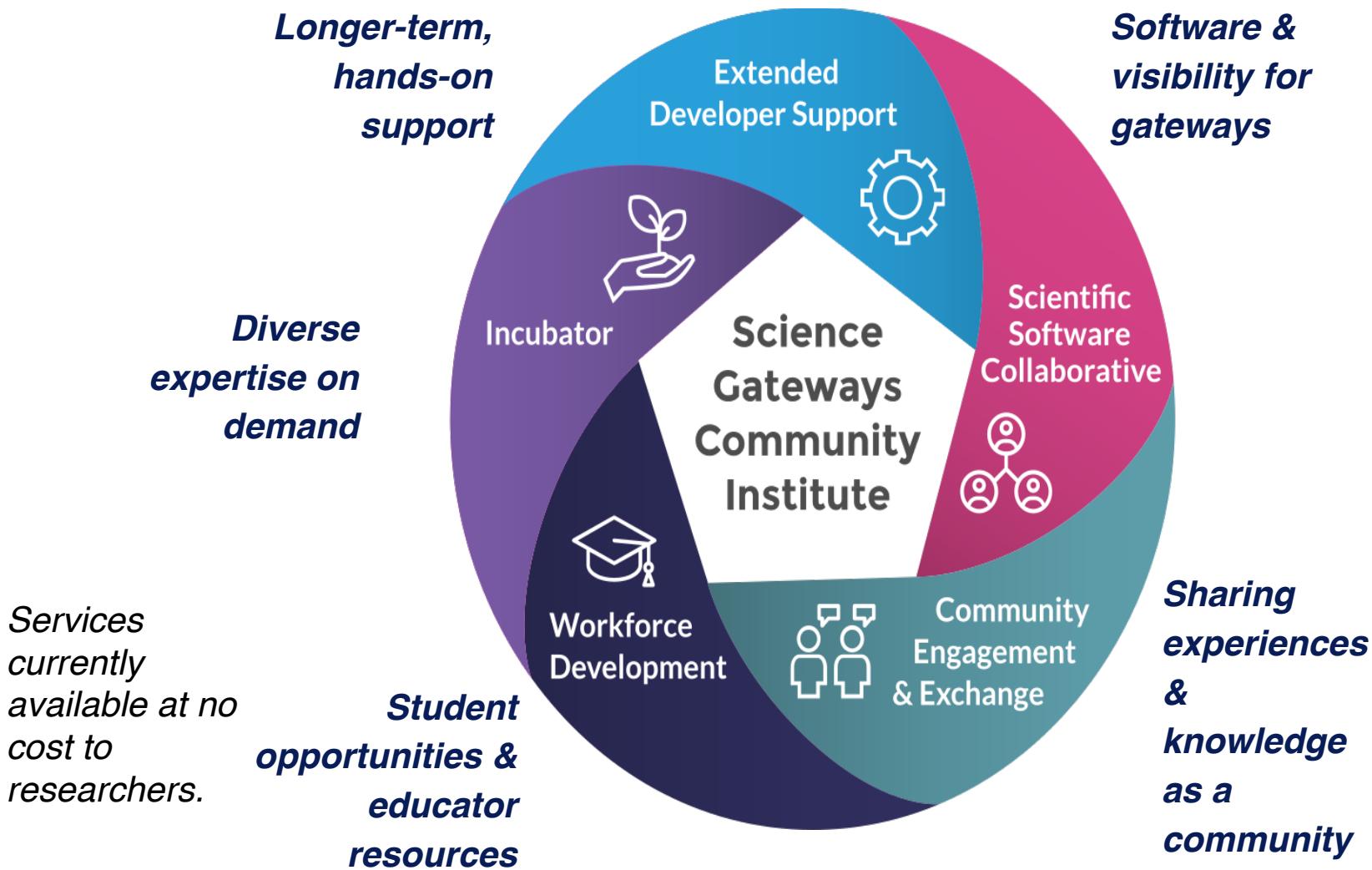
FOR
Students & Educators

Nancy Wilkins-Diehr, SDSC – PI - <http://sciencegateways.org/>

Other institutions: Elizabeth City State in North Carolina, Indiana University, University of Notre Dame, Purdue University, the Texas Advanced Computing Center at the University of Texas, Austin, and the University of Michigan at Ann Arbor

Science Gateways Community Institute

Designed to help researchers build gateways more effectively



Science Gateways for Principal Investigators

This section brings together information required by principal investigators (PIs) of XSEDE allocations to plan, organize, and oversee an XSEDE Science Gateway. Content on this page focuses on decision-making and management. For information on developing and operating a science gateway, see [Science Gateways for Developers and Administrators](#).

Science gateways provide communities of users with simplified mechanisms for accessing scientific applications, tools, and data. By using XSEDE, gateway providers can obtain access to a wide range of computational resources professionally managed by XSEDE service providers. XSEDE resources may allow gateway providers to bring their applications and data to a wider community, to free up their own departmental or campus resources that have become overwhelmed by community usage, or to acquire access to fundamentally different systems than are available at their home institutions or through commercial cloud providers.

Are You Eligible?

XSEDE Science Gateways are community provided resources. PIs must have an active XSEDE allocation in order to provide a functioning science gateway. Eligibility of a PI for sponsoring an XSEDE Science Gateway is the same as for an XSEDE allocation; in brief, you must be a U.S. researcher, or collaborating with a U.S. researcher. For details on eligibility guidelines, see [NSF Resource Allocations Policies: Eligibility](#). For more eligibility details please view the [Allocations section](#). PIs should also take responsibility for managing renewals, supplements, and extensions for their gateways to ensure continuous access to XSEDE resources.

Access Diverse Resources

XSEDE maintains a diverse set of resources through its constituent service providers. These include some of the largest academically operated supercomputers in the country, high throughput resources optimal for running large numbers of serial jobs, high memory and I/O optimized resources, storage-optimized resources, cloud computing resources, and hybrid CPU/co-processor machines. To support science gateways, XSEDE service providers offer both cloud computing resources and novel, hybrid clusters that support the direct hosting of gateways and other persistent services that are co-located with more conventional, batch scheduling clusters. Thus a gateway's web server, database and other services could be located at the PI's home institution and access XSEDE resources remotely, or it could run entirely in an XSEDE allocated academic cloud, or could it run in a virtual machine or virtual cluster that has direct access to a co-located standard cluster with a shared file system for closer integration.

Get Support for Your Gateway

XSEDE supports science gateways directly through its [Extended Collaborative Support Services](#) (ECSS) program. PIs can include ECSS support in their startup and XRAC allocation requests, and they can add ECSS support to existing allocations through a supplemental request. See [XRAS - Submit Allocation Requests](#). XSEDE recommends that all gateway requests include ECSS support. ECSS consultants will help you comply with XSEDE policies and make the best use of XSEDE resources as well as help with technical integration.

Join the Science Gateway Community

The XSEDE gateway program fosters the gateway community. PIs, their developers, and their gateway operators join the [XSEDE gateway community mailing list](#). This list can be used to request community help or input on best practices. It can also be used to ensure that everyone on the PI's team receives important XSEDE announcements.

To subscribe to the mailing list, send an email with "subscribe gateways" in the message body.

If you are a researcher/end user

- Existing gateway listings at XSEDE, SGCI
 - <http://www.xsede.org>
 - <https://sciencegateways.org>
- Follow good practices and provide feedback
- Cite the gateway used in your research in your publication, annual reports

Thanks...

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