# What are the benefits of using Science Gateways

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# Outline

- **Science Gateways**
  - Examples
- **Hands-on using a Science Gateway**

# Science Gateways

- An online community space for science and engineering research and education
- A web-based resource for accessing data, software, computing services and equipment specific to the needs of a science or engineering discipline

# HPC Resources

- **Available via XSEDE – Extreme Science and Engineering Discovery Environment**
  - NSF funded supercomputers, advanced support, services, allocation, EOT
- **You learned yesterday – how to**
  - Compile codes
  - Launch and manage jobs
  - Manage data on filesystems
  - Use HPC resources effectively
  - etc

# Administrative and Technical tasks (barriers?)

- Write allocation proposals (peer-reviewed) for supercomputer time every year
- Understand HPC machines, policies, complex OS/software
- Install and benchmark complex applications on HPC resources
- Different machines have different schedulers
- Understand and manage remote authentication
- Figure out data transfer, file systems, storage

# Science gateways

- **Easy web based user interface GUI**
  - Upload input files, models
  - Set application and HPC related parameters
  - Run jobs by the click of a button
- **Scientific applications already installed optimally on HPC resources at the backend**
- **Easily access, download output results**
  - Some provide post processing, viz
- **Some provide RESTful services**
- **Gateway team writes annual allocation proposal**

***Catalyzes and democratizes computational science research for researchers and students from all universities, colleges and institutions***

XSEDE
Extreme Science and Engineering Discovery Environment

Search XSEDE...

HOME ABOUT USER SERVICES RESOURCES EDUCATION & OUTREACH GATEWAYS TECHNOLOGY DATABASE

# Science Gateways

A Science Gateway is a community-developed set of tools, applications, and data that are integrated via a portal or a suite of applications, usually in a graphical user interface, that is further customized to meet the needs of a specific community. Gateways enable entire communities of users associated with a common discipline to use national resources through a common interface that is configured for optimal use. Researchers can focus on their scientific goals and less on assembling the cyberinfrastructure they require. Gateways can also foster collaborations and the exchange of ideas among researchers.

## How to Turn Your Project into a Science Gateway

1. Get an XSEDE allocation; Start-up and Educational allocations require only a one paragraph project description. For more information visit the Allocations section of the web site.
2. Register your project as an XSEDE Gateway
3. Build a portal
4. Set up your developer accounts by Adding users to an existing allocation. Also, set up your Gateway community accounts.

## Using Existing Gateways

Gateways are independent projects, each with its own guidelines for access. Most gateways are available for use by anyone, although they usually target a particular research audience. XSEDE Science Gateways are portals to computational and data services and resources across a wide range of science domains for researchers, engineers, educators, and students. Depending on the needs of the communities, a gateway may provide any of the following features:

## Science Gateways

# XSEDE SGW

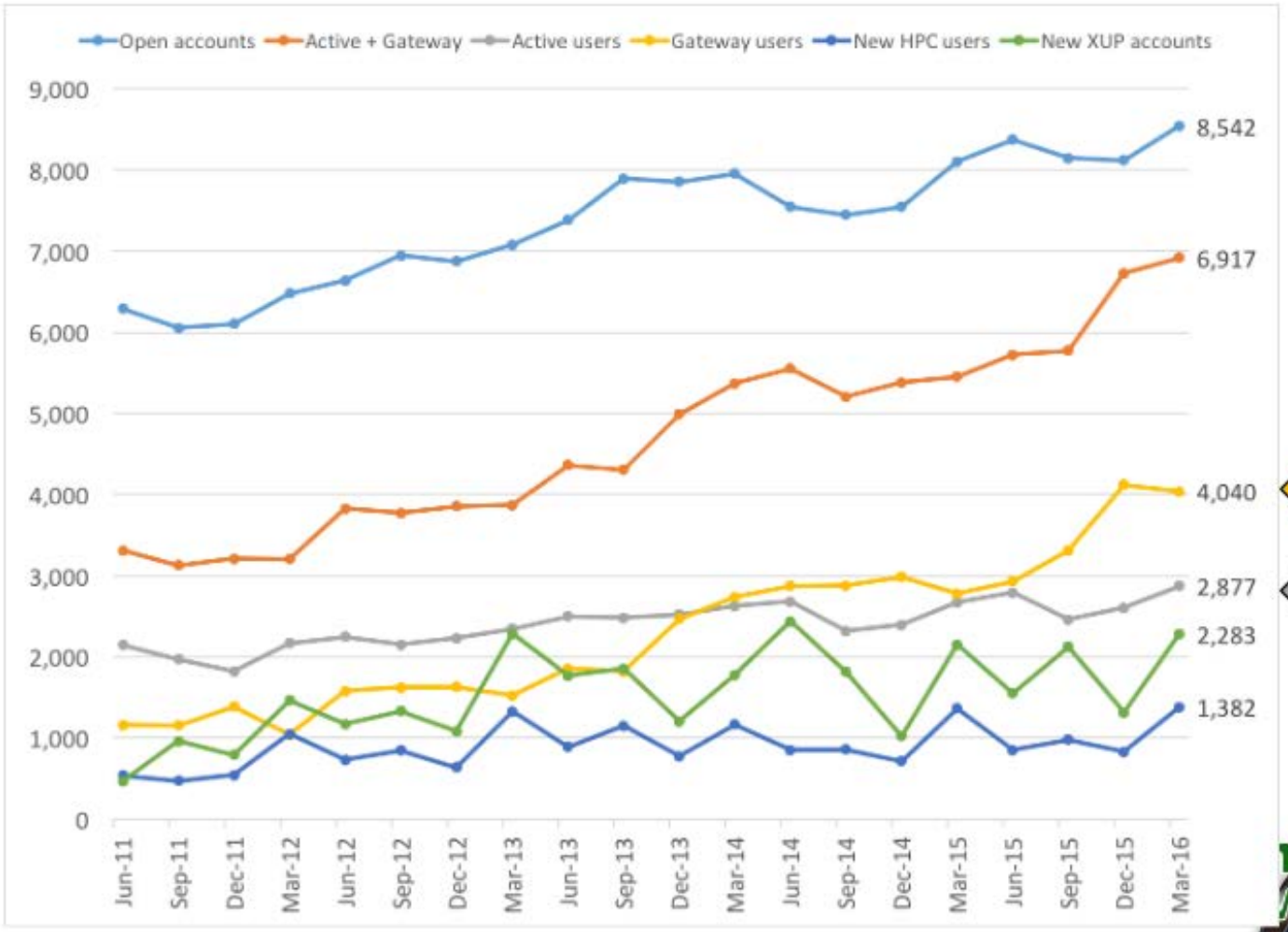
| TITLE | FIELD OF SCIENCE | PORTAL HOMEPAGE |
|---|---|---|
| Diagrid | Advanced Scientific Computing | Visit Portal |
| UCI Complex Social Science Gateway | Anthropology | Visit Portal |
| Massive Pulsar Surveys using the Arecibo L-band Feed Array (ALFA) | Astronomical Sciences | Visit Portal |
| Center for Multiscale Modeling of Atmospheric Processes | Atmospheric Sciences | Visit Portal |
| Biodrugscore: A portal for customized scoring and ranking of molecules docked to the human proteome | Biochemistry and Molecular Structure and Function | Visit Portal |
| High-Resolution Modeling of Hydrodynamic Experiments with UltraScan | Biophysics | Visit Portal |
| ROSIE, The Rosetta Online Server that Includes Everyone | Biophysics | Visit Portal |
| Chem Compute | Chemistry | Visit Portal |
| Computational Chemistry Grid (GridChem) | Chemistry | Visit Portal |
| ParamChem Gateway | Chemistry | Visit Portal |
| User-Friendly Security Solutions for Grid Environments | Communications and Computational Systems | Visit Portal |
| OpenTopography | Earth Sciences | Visit Portal |
| Purdue Environmental Data Portal | Earth Sciences | Visit Portal |
| WaterHUB - Platform for water education, research, data access, partnership and collaboration | Earth Sciences | Visit Portal |
| Network for Earthquake Engineering Simulation | Earthquake Hazard Mitigation | Visit Portal |
| CMS gWMS | Elementary Particle Physics | Visit Portal |
| Network for Computational Nanotechnology and nanoHUB | Emerging Technologies Initiation | Visit Portal |
| Globus Online | Engineering Infrastructure Development | Visit Portal |
| CyberGIS Gateway | Geography and Regional Science | Visit Portal |
| The Earth System Grid | Global Atmospheric Research | Visit Portal |

# XSEDE SGW

| | | |
|---|---|---|
| Network for Computational Nanotechnology and nanoHUB | Emerging Technologies Initiation | Visit Portal |
| Globus Online | Engineering Infrastructure Development | Visit Portal |
| CyberGIS Gateway | Geography and Regional Science | Visit Portal |
| The Earth System Grid | Global Atmospheric Research | Visit Portal |
| The iPlant Collaborative Agave API | Integrative Biology and Neuroscience | Visit Portal |
| MP-Complete | Materials Research | Visit Portal |
| VLab - Virtual Laboratory for Earth and Planetary Materials | Materials Research | Visit Portal |
| NIST Digital Repository of Mathematical Formulae | Mathematical Sciences | Visit Portal |
| Galaxy | Molecular Biosciences | Visit Portal |
| Integrated database and search engine for systems biology (IntegromeDB) | Molecular Biosciences | Visit Portal |
| ROBETTA: Automated Prediction of Protein Structure and Interactions | Molecular Biosciences | Visit Portal |
| Providing a Neuroscience Gateway | Neuroscience Biology | Visit Portal |
| SCEC Earthworks Project | Seismology | Visit Portal |
| Asteroseismic Modeling Portal | Stellar Astronomy and Astrophysics | Visit Portal |
| CIPRES Portal for inference of large phylogenetic trees | Systematic and Population Biology | Visit Portal |
| Computational Anatomy | Visualization, Graphics, and Image Processing | Visit Portal |

# Gateway users surpass login users in 2013

## Automated user-counting in 2015




**Source: David Hart**

# Tactics for Gateway Success:

Step 1: identify a user population in need

Step 2: commit to responding to user's needs

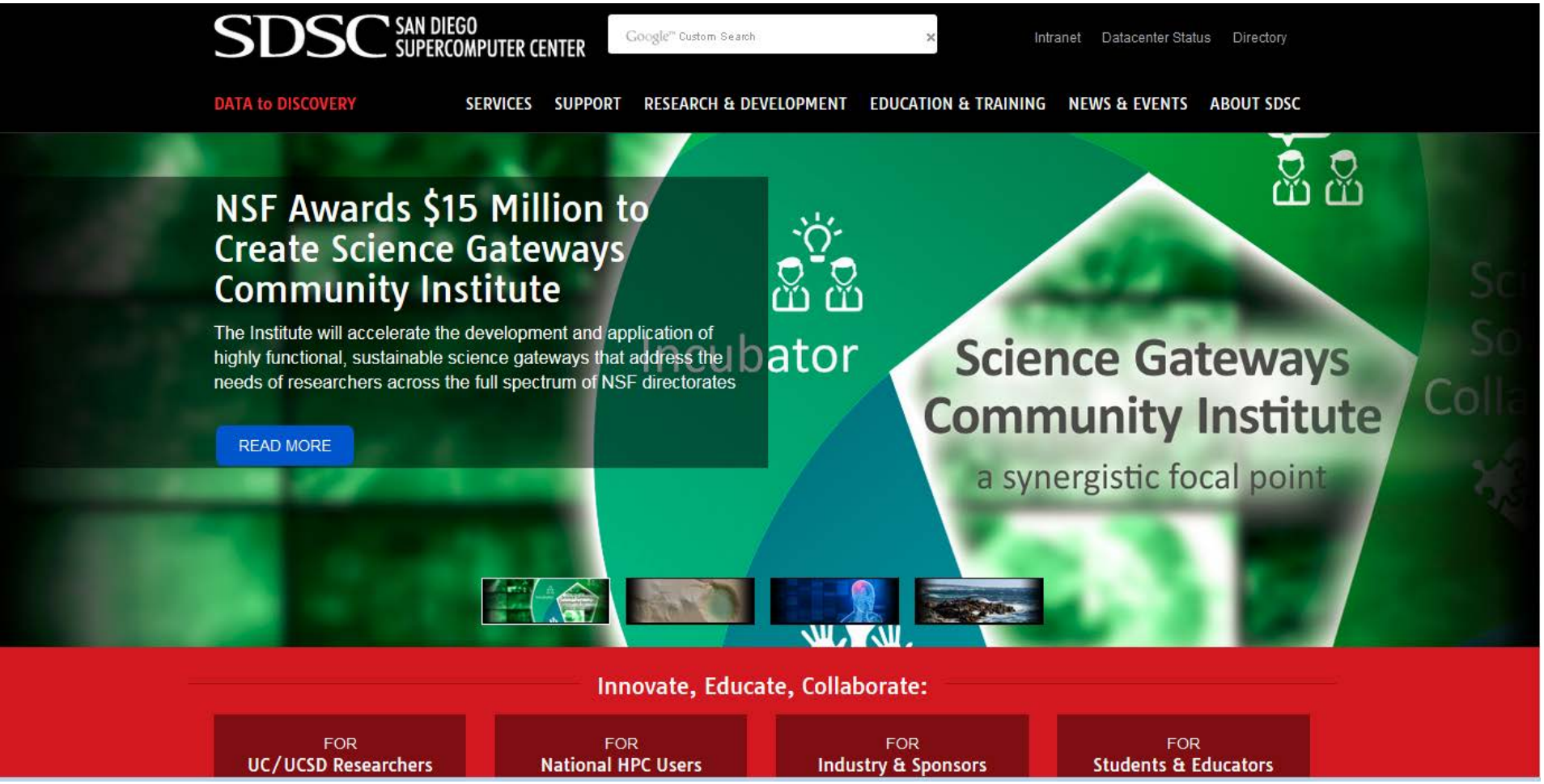
Step 3: let user behavior/needs drive improvements

Step 4: manage challenges that threaten productivity of high end users

Step 5: with limited resources, prioritization is key

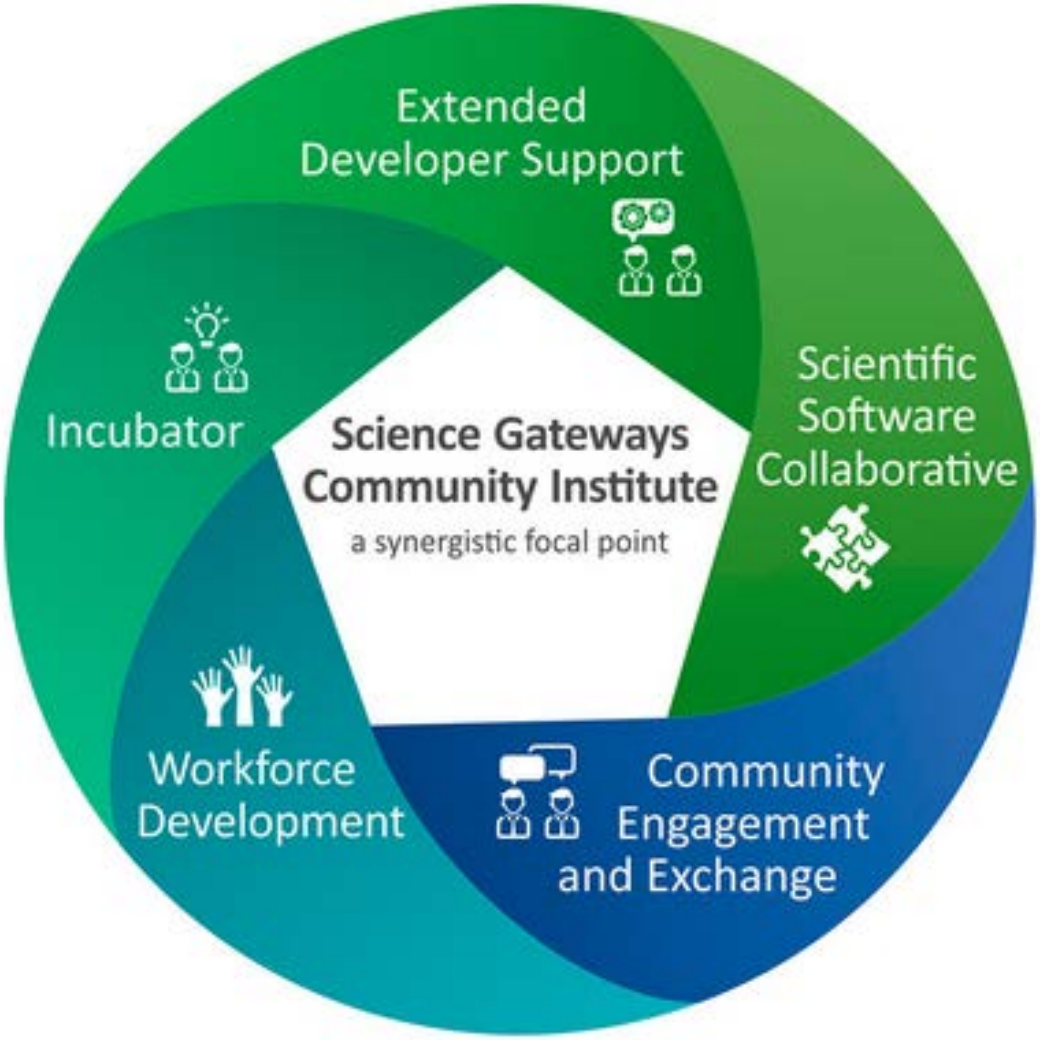
Step 6: stay in touch with your community

Step 7: embrace customer service




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

*Other institutions: Elizabeth City State in North Caronila, 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*

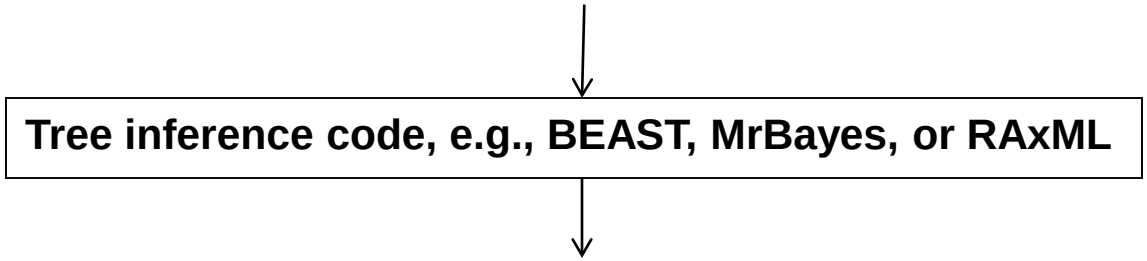



The five key areas for the Science Gateways Community Institute to increase the number, ease of use, and effective application of gateways to serve the greater research and engineering community. *Source: SDSC*

# The advent of DNA sequencing lets scientists infer phylogenetic trees from multiple sequence alignments

**Multiple sequence alignment is a matrix of taxa vs characters**

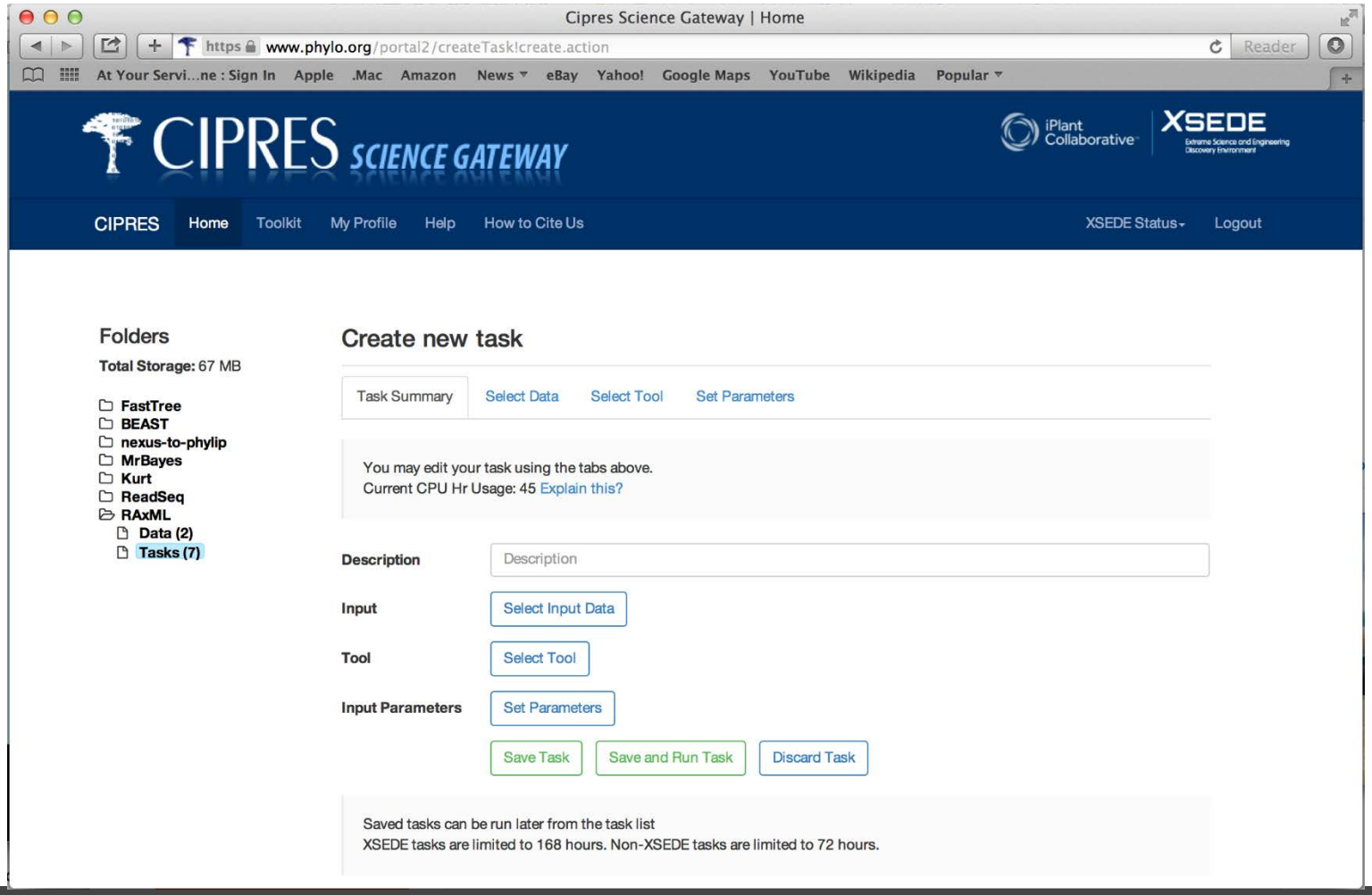
```
                          .   .   .   ......  .   .
Human             AAGCTTCACCGGCGCAGTCATTCTCATAAT...
Chimpanzee        AAGCTTCACCGGCGCAATTATCCTCATAAT...
Gorilla           AAGCTTCACCGGCGCAGTTGTTCTTATAAT...
Orangutan         AAGCTTCACCGGCGCAACCACCCTCATGAT...
Gibbon            AAGCTTTACAGGTGCAACCGTCCTCATAAT...
```




*Phylogeny is represented as tree with taxa at its tips*

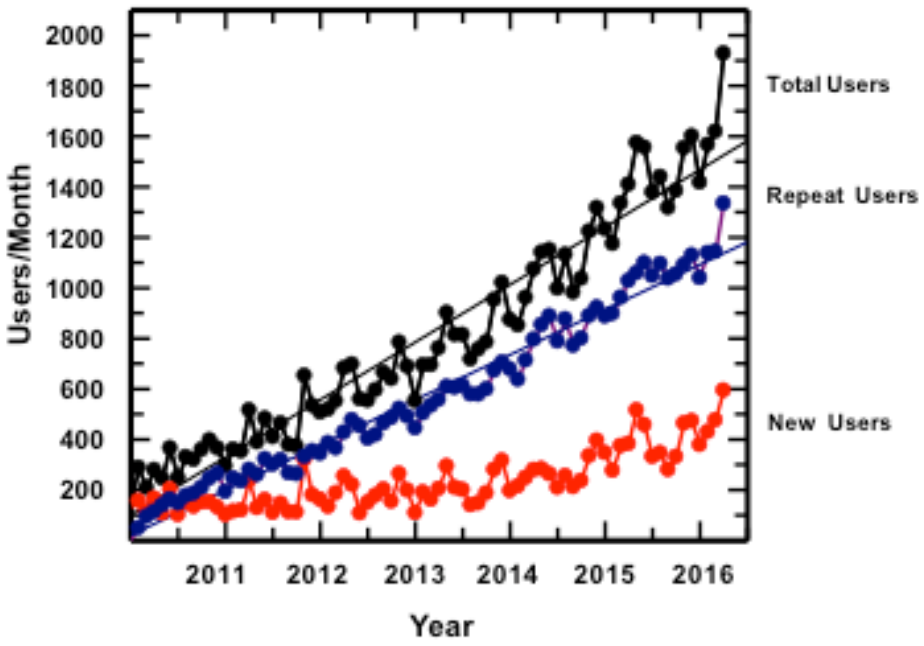
# SDSC develops, maintains, & hosts the NSF-funded CIPRES gateway, which runs phylogenetics codes via a browser interface; analyses span the entire tree of life

Mark Miller, Wayne Pfeiffer, Terri Schwartz, SDSC



# The CIPRES gateway has been extremely popular and supports thousands of researchers around the world

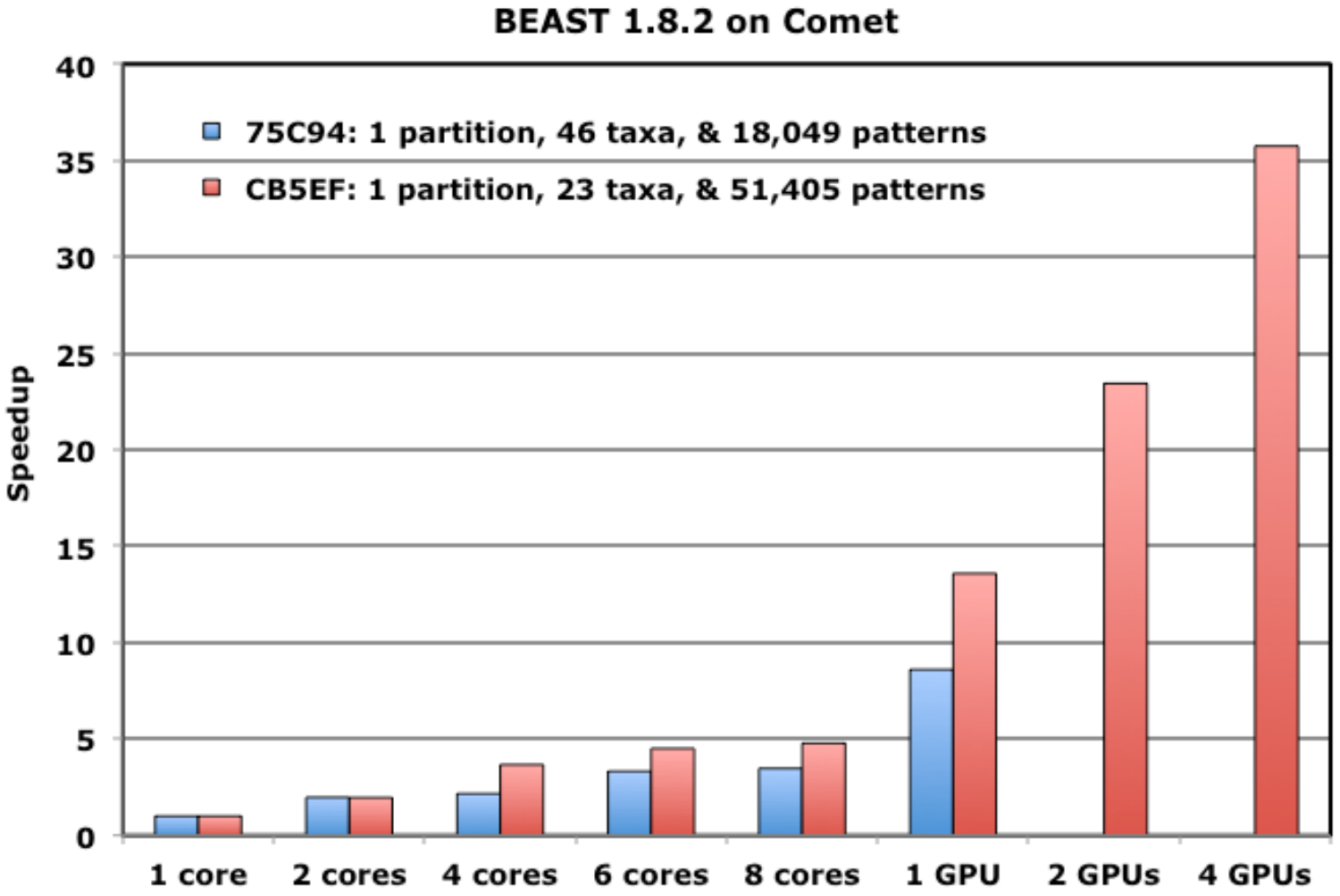
- **>17,000 CIPRES users have run on NSF-funded supercomputers, including 3,152 in 4Q2015 or 47% of all active XSEDE users!**
- **>2,000 publications have been enabled by CIPRES use!**
- **US statistics from 2015**
  - 49 states + 2 territories + DC
  - 252 universities & colleges
  - 18 institutes
  - 22 museums, gardens, & zoos
  - 21 government agencies
  - 4 high schools
- **Non-US statistics from 2015**
  - 85 countries
  - 603 universities & colleges
  - 161 institutes
  - 80 museums, gardens, & zoos
  - 134 government agencies



# 11 codes are supported by CIPRES on Comet & Gordon; most have modest scalability; some run for days

| Code | Version | Language | Computer | Cores charged |
|---|---|---|---|---|
| BEAST | 1.8.3 | Java + C++ | Comet | 2, 4, or GPUs |
| BEAST2 | 2.3.2 | Java + C++ | Comet | 1, 2, or 3 |
| DPPDiv | 1.0 | C++ | Gordon | 16 |
| FastTree | 2.1.8 | C | Comet | 3 |
| GARLI | 2.0.1 | C++ | Comet | 1 to 24 |
| jModelTest2 | 2.1.6 | Java + C | Gordon | 8 |
| MAFFT | 7.187 | C | Gordon | 8 |
| MrBayes | 3.2.6 | C + C++ | Gordon | 8 or 16 |
| Migrate | 3.6.11 | C | Comet | 1 to 72 |
| Phylobayes | 1.5a | C++ | Gordon | 64 |
| RAxML | 8.2.8 | C | Comet | 12, 24, or 48 |

# BEAST phylogenetic tree inference for data sets with many patterns speeds up very well using K80 GPUs instead of Haswell cores on Comet



# NSF funded Neuroscience Gateway at SDSC

Amit Majumdar, Subhashini Sivagnanam, Kenneth Yoshimoto, SDSC

- NSG – in operation since early 2013 – nsgportal.org
- Built using the CIPRES gateway software
- NSG benefits the broader neuroscience research community in several ways, e.g.:
- Researchers can run larger complex neuronal networks, parameter sweep simulations, brain image processing tools
- Fully integrated The Virtual Brain (TVB) connectome pipeline workloads can be processed in parallel
- Easy access to widely used simulation tools such as:
  Brian, NEST, NEURON, pGENESIS, PyNN, MOOSE, and FreeSurfer
- Researchers from EU Human Brain Project providing optimization pipeline
- Access to new HPC resources – GPUs, Intel MICs
- Can be used by researchers with limited local (university-level) resources to address questions that require access to large scale, advanced systems
- Can be used by simulator developers to test, benchmark, and scale codes on large scale resources
- Can be used for classes, workshops, and tutorials

# Neuroscience Tools on NSG

**BluePyOpt on Comet** (1.1.27) - Running BluePyOpt analyses

**Brian on Stampede** (2.0b2) - Brian is a simulator for spiking neural networks

**Brian on Comet** (2.0b2) - Brian is a simulator for spiking neural networks

**The Virtual Brain Personalized Multimodal Connectome Pipeline on Comet** () - Connectome Pipeline on Comet

**FREESURFER on Comet** (5.3.0) - Freesurfer tool on Comet

**PyMOOSE** (3.0.1 Gulab Jamun) - Running Moose models on Comet

**NEST on Stampede** (2.6.0) - Neural Simulation Technology using Python

**NEST using Python on Comet** (2.2.1) - Neural Simulation Technology using Python

**NEST on Stampede** (2.6.0) - Neural Simulation Technology

**NEST on Comet** (2.2.1) - Neural Simulation Technology

**NEURON7.3 Python on Stampede** (7.3) - Using Python to run NEURON 7.3

**NEURON7.3 Python on Comet** (7.3) - Using Python to run NEURON 7.3

**NEURON7.3 on Stampede** (7.3) - Latest NEURON simulation software package on Stampede

**NEURON7.3 on Comet** (7.3) - Latest NEURON simulation software package on Comet

**NEURON7.4 Python on Comet** (7.4) - Using Python to run NEURON 7.4

**NEURON7.4 on Comet** (7.4) - Latest NEURON simulation software package on Comet

**PGENESIS on Stampede** (2.3) - Parallel Genesis software

**PGENESIS on Comet** (2.3) - Parallel Genesis software

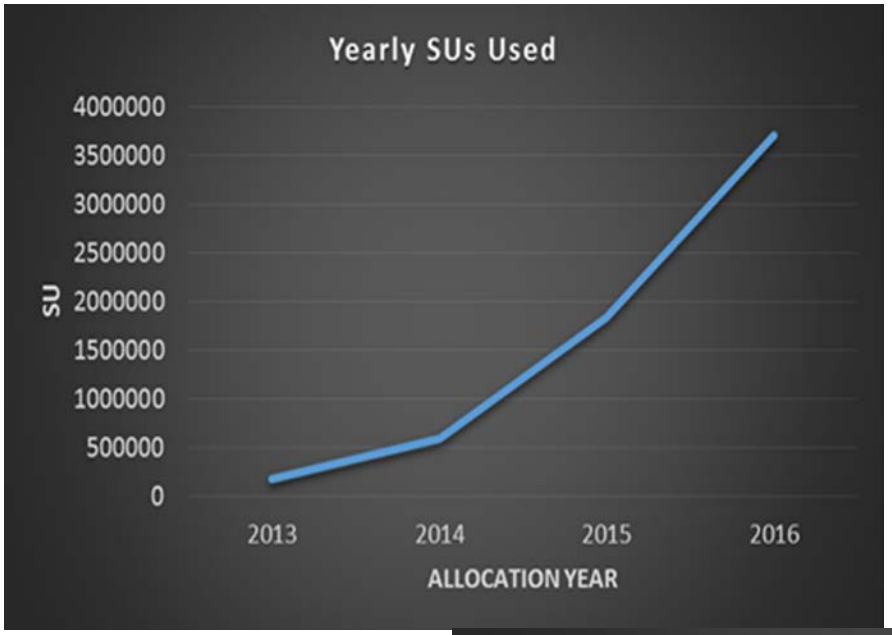
**PyNN on Stampede** (0.7.5) - Python package for simulator-independent specification of neuronal network models

**PyNN on Comet** (0.7.5) - Python package for simulator-independent specification of neuronal network models

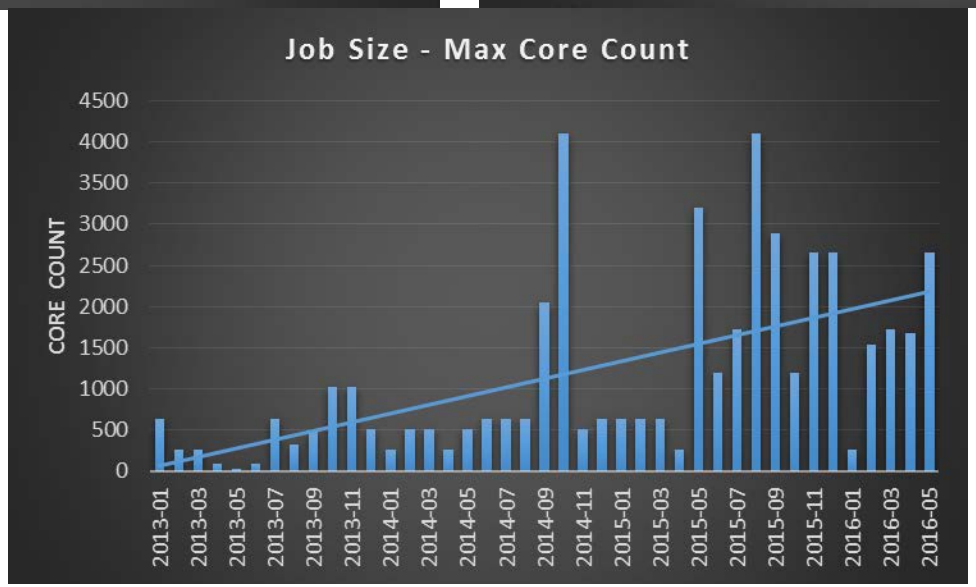
**Python on Stampede** (2.7.9) - Running Python models

**Python on Comet** (2.7.9) - Running Python models

# NSG Usage


Yearly SUs Used
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
SU
2013
2014
2015
2016
ALLOCATION YEAR


Number of NSG Users
400
350
300
250
200
150
100
50
# OF NSG USERS
2013
2014
2015
2016
YEAR


Job Size - Max Core Count
4500
4000
3500
3000
2500
2000
1500
1000
500
0
CORE COUNT
2013-01
2013-03
2013-05
2013-07
2013-09
2013-11
2014-01
2014-03
2014-05
2014-07
2014-09
2014-11
2015-01
2015-03
2015-05
2015-07
2015-09
2015-11
2016-01
2016-03
2016-05

# Hands-on – to show how easy it is!

1. Go to https://www.phylo.org and click on Use the CIPRES Science Gateway.
2. Login as a guest.
3. Upload the attached data set to Data in Guest Folder.
4. Go to Tasks to Create new task.
5. Select Input Data: i.e., the data set just uploaded.
6. Select Tool: BEAST on XSEDE.
7. Select Input Parameters. Use the default parameters with the following exceptions.

. First row folks specify 400 patterns. That will have the job run on 2 cores.
. Second row folks specify 4000 patterns. Then the job will run on 4 cores.
. Other rows specify 4000 patterns and “always” instead of “dynamic” for beagle_scaling. That will run on 4 cores, but be much slower than the default scaling.

8. Save parameters.

9. Save Task and enter an appropriate Description, e.g., benchmark2.dynamic.4000patt

10. Click on Run Task.

11. Click on View Status and then Intermediate Results while job is running or Output when job is done.

12. Then look at stdout.txt. Near the bottom, the time is output in seconds or minutes.

# Science Gateways - Summary

- **Allows anyone from anywhere to *easily* access and use HPC (and data, instrument etc.) for computational science**
  - All users start out with some amount of core hours (depends on the gateway and the science)
  - If you graduate out of a SGW, you can write your own allocation proposal (gateway/XSEDE staff can help)
    - In many cases still use the gateway to charge to your allocation
- **It creates a cyberinfrastructure environment for the science community to enable**
  - Research
  - Education
  - Sharing of information and data