Overview of SDSC Resources and Capabilities and XSEDE

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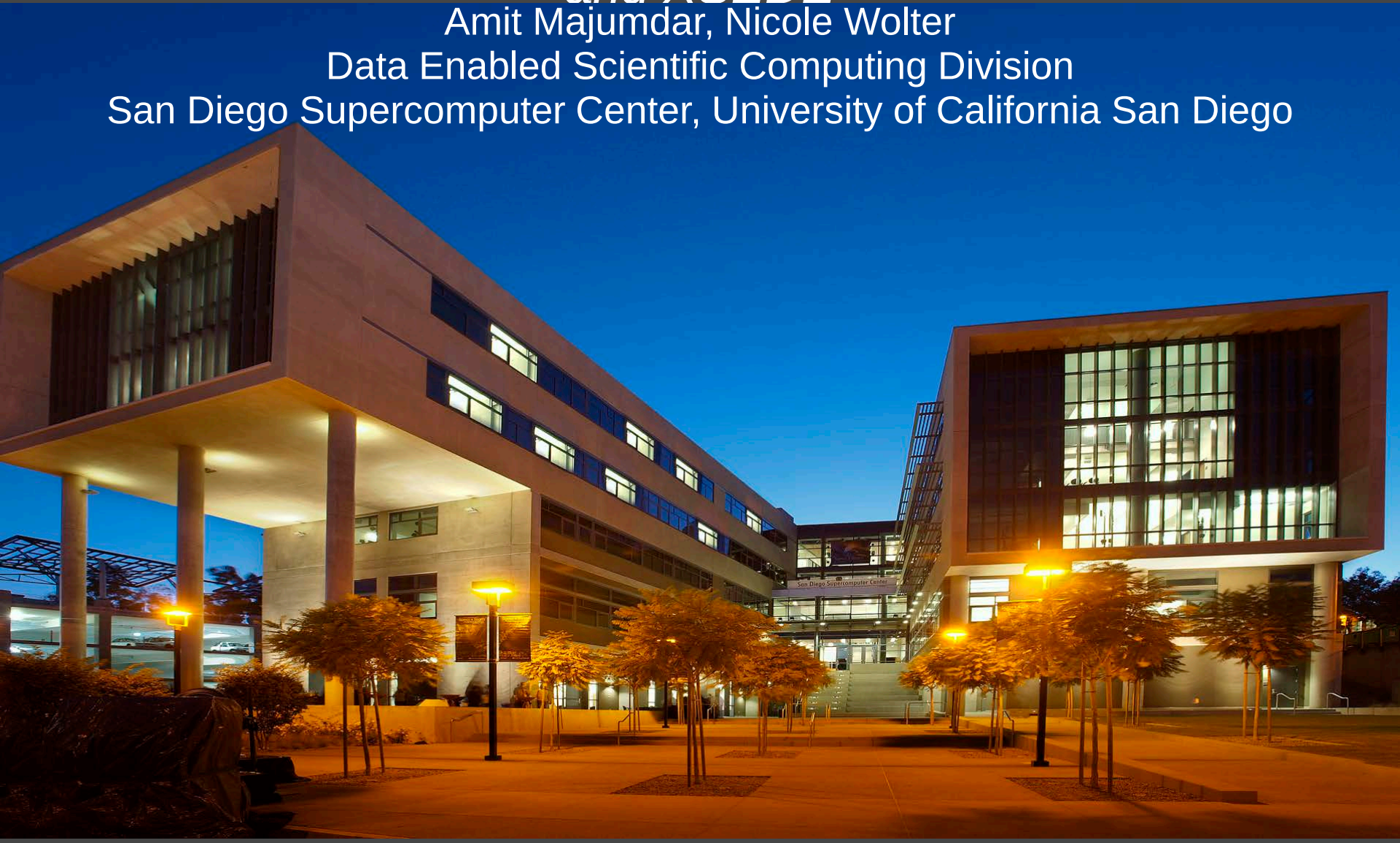


SDSC has Powerful HPC and Data Resources

System	Capabilities	User Community
Comet ~ 2Petaflop	**1,944 nodes, Haswell, 24 cores/node ; 72 GPU nodes; 4 large memory nodes; FDR IB interconnect**	**National, UC, Industry**
Triton Shared computing cluster (TSCC) Condo cluster	~375 dual socket, 8-12-core compute nodes 50 GPU Nodes; 10GbE interconnect, with option for QDR InfiniBand	UC, Industry
SDSC Data Oasis	13 PB of Lustre-based storage; 10/40 GbE fabric	National, UC, Industry
SDSC Universal Scale, Cloud and Project storage	200TB USS; 3PB OpenStack storage; 4 PB NSF/CIFS; VM's based on OpenStack	National, UC, Industry
Data Center	19,000 sq. ft., 13MW, 10/100Gbpfs 24/7 operations, UPS	National, UC, Industry
Sherlock	Compliant data compute solutions	National, UC

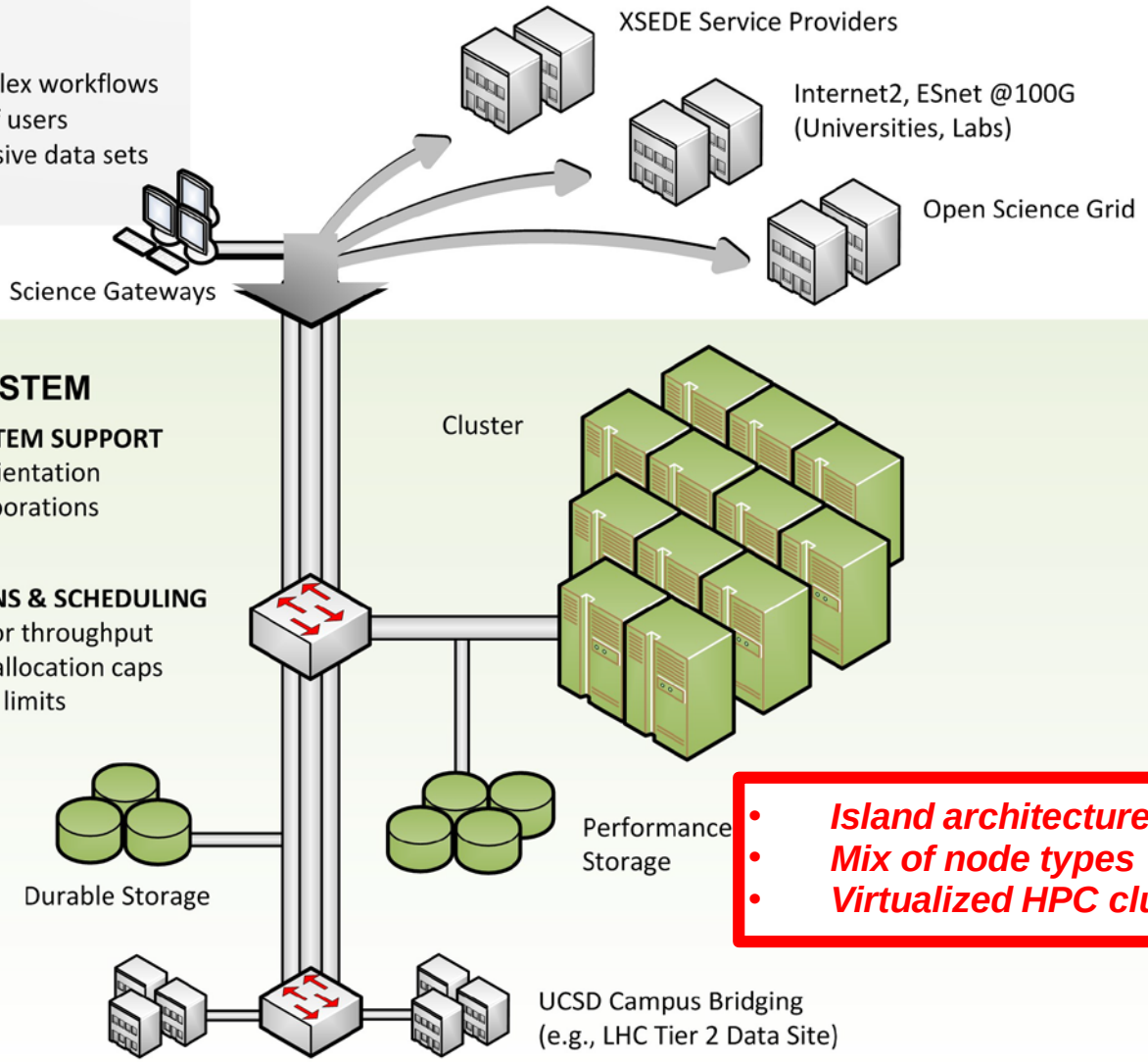
Comet
“HPC for the long tail of science”
Funding - NSF

iPhone panorama photograph of 1 of 2 server rows

Comet Built to Serve the 99%

CHALLENGES OUR PROPOSAL ADDRESSES

- ✓ Attract new users and communities
- ✓ Support diverse applications with complex workflows
- ✓ Ensure responsiveness for thousands of users
- ✓ Transfer, store, analyze, and share massive data sets
- ✓ Integrate with XSEDE



COMET COMPUTE SYSTEM

Cluster architecture
Fast standard nodes
Large-memory nodes
GPU-accelerated nodes
FDR InfiniBand

Storage architecture
Performance Storage
Durable Storage

Software
Science Gateways
Rich base of installed apps
Virtualization

USER & SYSTEM SUPPORT
New user orientation
XSEDE collaborations
FutureGrid

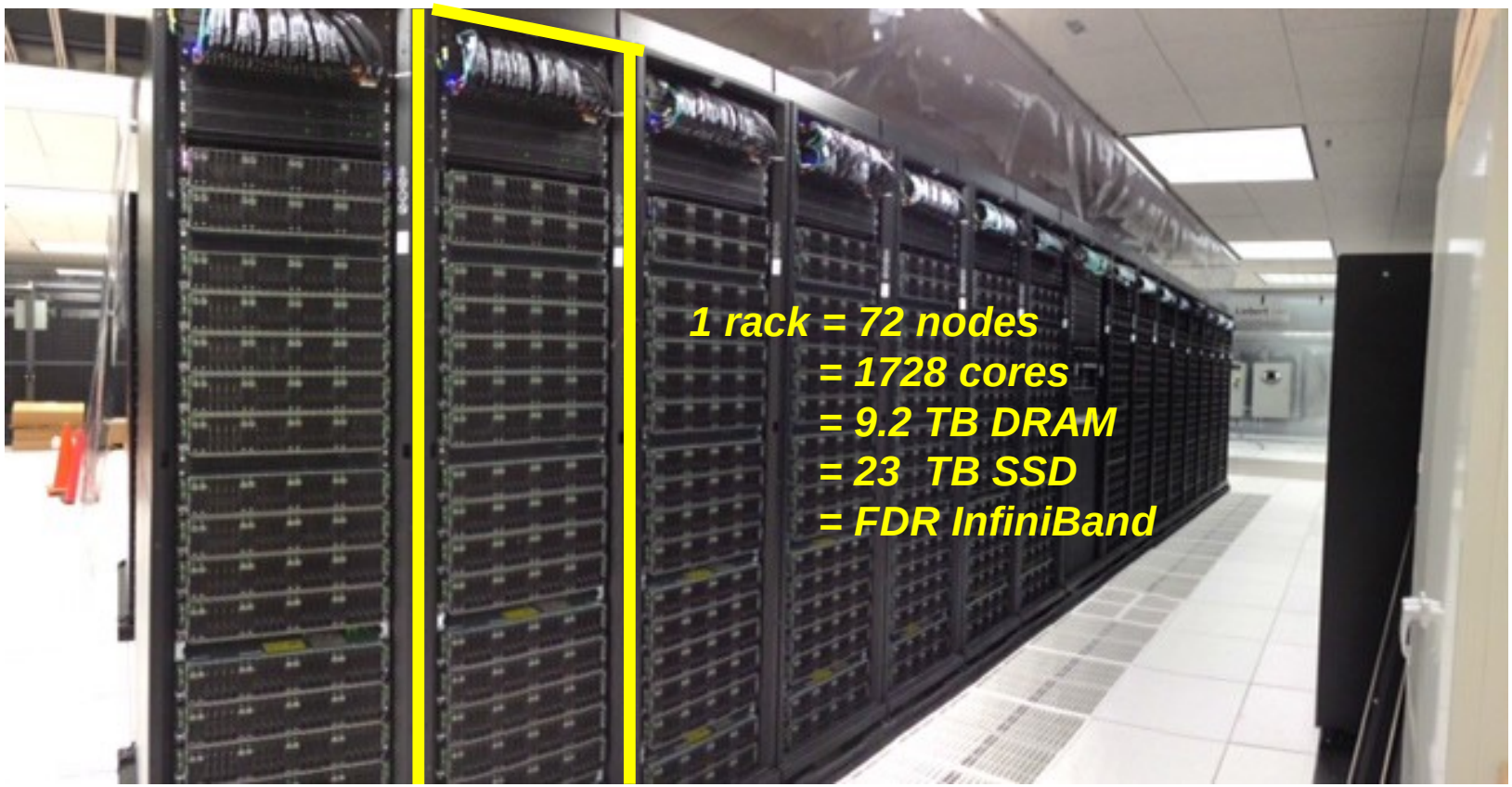
ALLOCATIONS & SCHEDULING
Optimized for throughput
Per-project allocation caps
Per-job core limits

- ***Island architecture***
- ***Mix of node types***
- ***Virtualized HPC clusters***

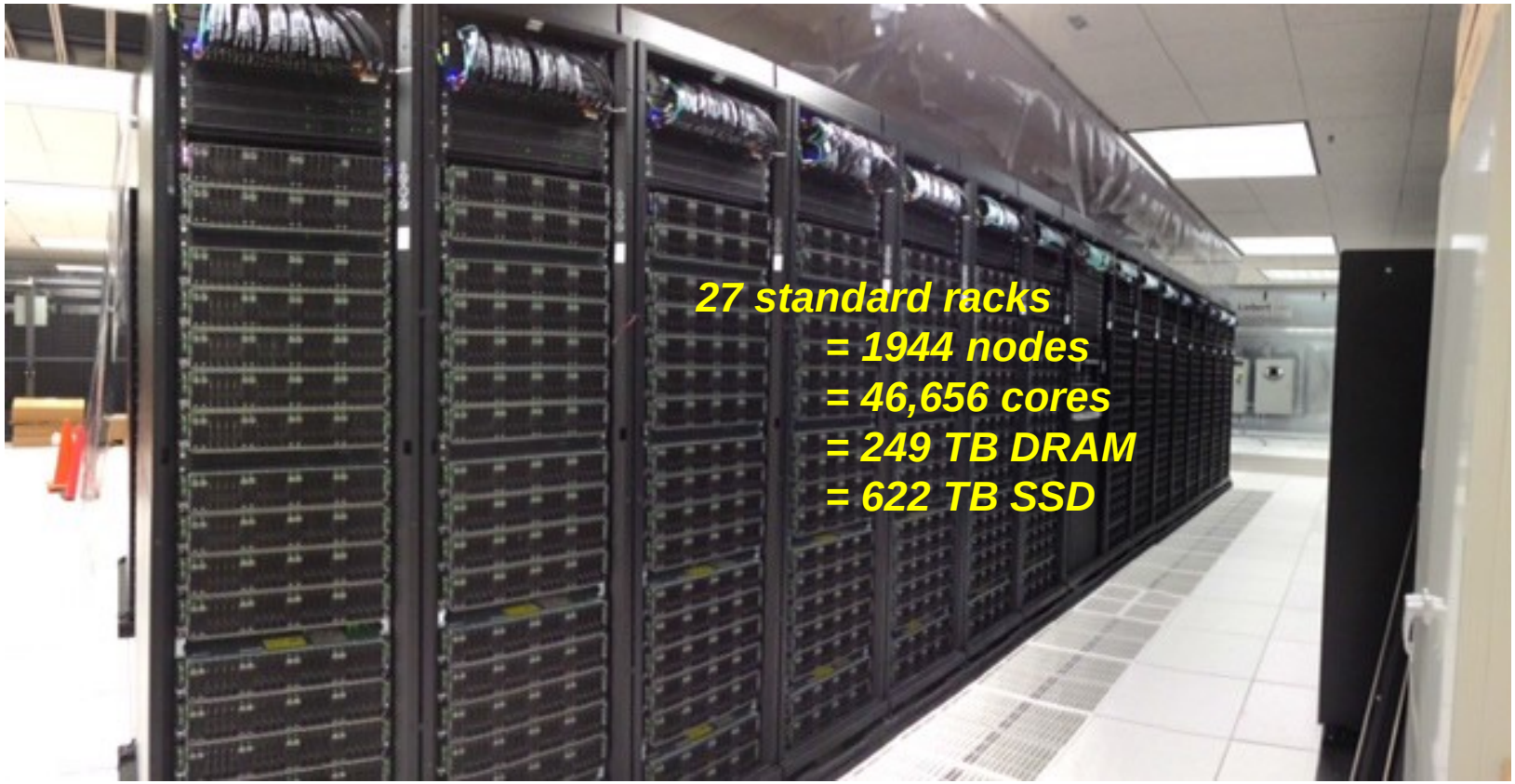
Comet: System Characteristics

- ***Total peak flops ~2.1 PF***
- ***Dell primary integrator***
  - *Intel Haswell processors w/ AVX2*
  - *Mellanox FDR InfiniBand*
- ***1,944 standard compute nodes (46,656 cores)***
  - *Dual CPUs, each 12-core, 2.5 GHz*
  - *128 GB DDR4 2133 MHz DRAM*
  - *2*160GB GB SSDs (local disk)*
- ***72 GPU nodes***
  - *36 nodes same as standard nodes plus Two NVIDIA K80 cards, each with dual Kepler3 GPUs*
  - *36 nodes with 2 14-core Intel Broadwell CPUs plus 4 NVIDIA P100 GPUs*
- ***4 large-memory nodes***
  - *1.5 TB DDR4 1866 MHz DRAM*
  - *Four Haswell processors/node*
  - *64 cores/node*
- ***Hybrid fat-tree topology***
  - *FDR (56 Gbps) InfiniBand*
  - *Rack-level (72 nodes, 1,728 cores) full bisection bandwidth*
  - *4:1 oversubscription cross-rack*
- ***Performance Storage (Aeon)***
  - *7.6 PB, 200 GB/s; Lustre*
  - *Scratch & Persistent Storage segments*
- ***Durable Storage (Aeon)***
  - *6 PB, 100 GB/s; Lustre*
  - *Automatic backups of critical data*
- ***Home directory storage***
- ***Gateway hosting nodes***
- ***Virtual image repository***
- ***100 Gbps external connectivity to Internet2 & ESNet***

~67 TF Supercomputer in a Rack

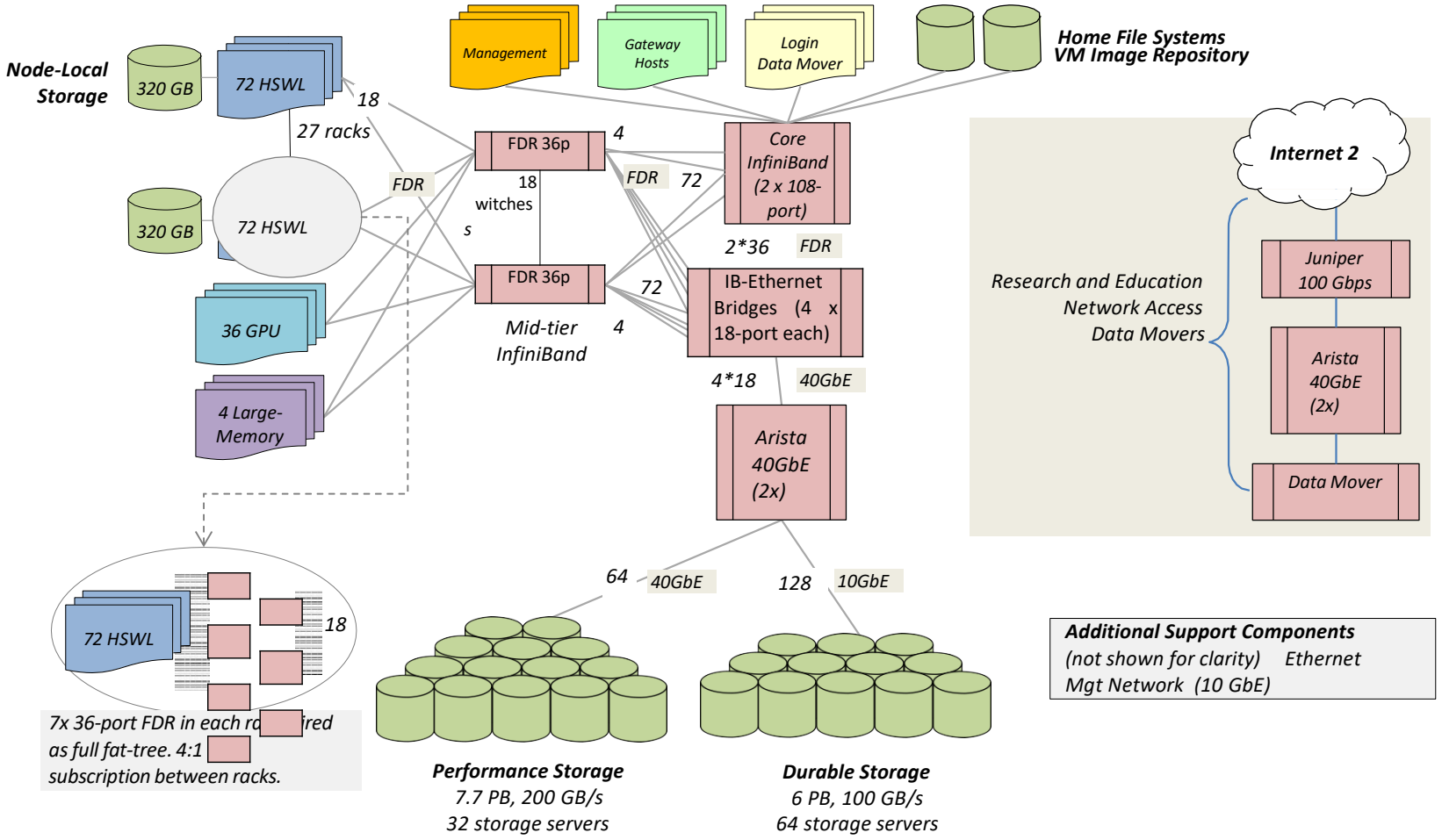


…and 27 Single-Rack Supercomputers



Comet Network Architecture

InfiniBand compute, Ethernet Storage



Comet: MPI options, RDMA Enabled Software

MVAPICH2 v2.1 is the default MPI on Comet. v2.2 and v2.3 also available
Intel MPI and OpenMPI also available.

MVAPICH2-X v2.2a *to provide unified high-performance runtime supporting both MPI and PGAS programming models.*

MVAPICH2-GDR (v2.2) on the GPU nodes featuring NVIDIA K80s and P100s.

Version ***RDMA-Apache-Hadoop-2.x 1.1.0*** *(based on Apache Hadoop 2.6.0) available on Comet*

Version ***RDMA-Spark 0.9.5*** *(based on Apache Spark 2.1.0 available on Comet)*

RDMA-Hadoop (2x-1.1.0), RDMA-Spark (0.9.5) (from Dr. Panda's HiBD lab at Ohio State) also available.

SDSC Comet – HPC for the 99%

- **Comet part of emerging CI for *long tail of science***
  - *Architecture for traditional and non-traditional science*
  - *Science Gateway friendly*
  - *HPC virtualization*
  - *GPU nodes, large memory nodes*
  - *Many PetaBytes of storage*
  - *User friendly allocation policies, trial accounts*

Comet - ~3 years of operation
# of unique standard users 4,700+
# of unique gateway users 33,000+

Triton Shared Computing Cluster(TSCC):

High Performance Computing for UC Researchers

Funding UCSD + Individual PIs

- **Mid-scale campus research cluster**
- **Hybrid business model: "condo" (buy in) and "hotel" (pay-as-you-go) options**
- **Mixed architecture:**
  - ~375nodes (>7,000 cores, not incl. GPU cores) + 50 GPU nodes (~300 GPUs with mix of NVIDIA 980/1080/TitanX GPUs)
  - 850TB parallel file system, home file system, add'l storage services
  - High bandwidth external networks
- **30 participating labs/groups**
- **Prof. Chia-en Chang (UCR) has GPU nodes in cluster**

Program Objectives

- **Provide a robust research computing program for UCSD researchers that:**
  - Enhances research competitiveness
  - Provides a medium- to large-scale computing resource
  - Access to a larger resource than most PI's could afford just for their lab
  - Is readily accessible (without competitive proposals or long wait times)
  - Follows best practices at other universities
  - Is cost-effective and energy-efficient
  - Provides for professional administration/maintenance (freeing up postdocs & grad students to focus on research)

Condo Model Mechanics

Group 1's Purchased Nodes

Group 2's Purchased Nodes

Nodes are purchased directly and are property of the lab/group or funding agency

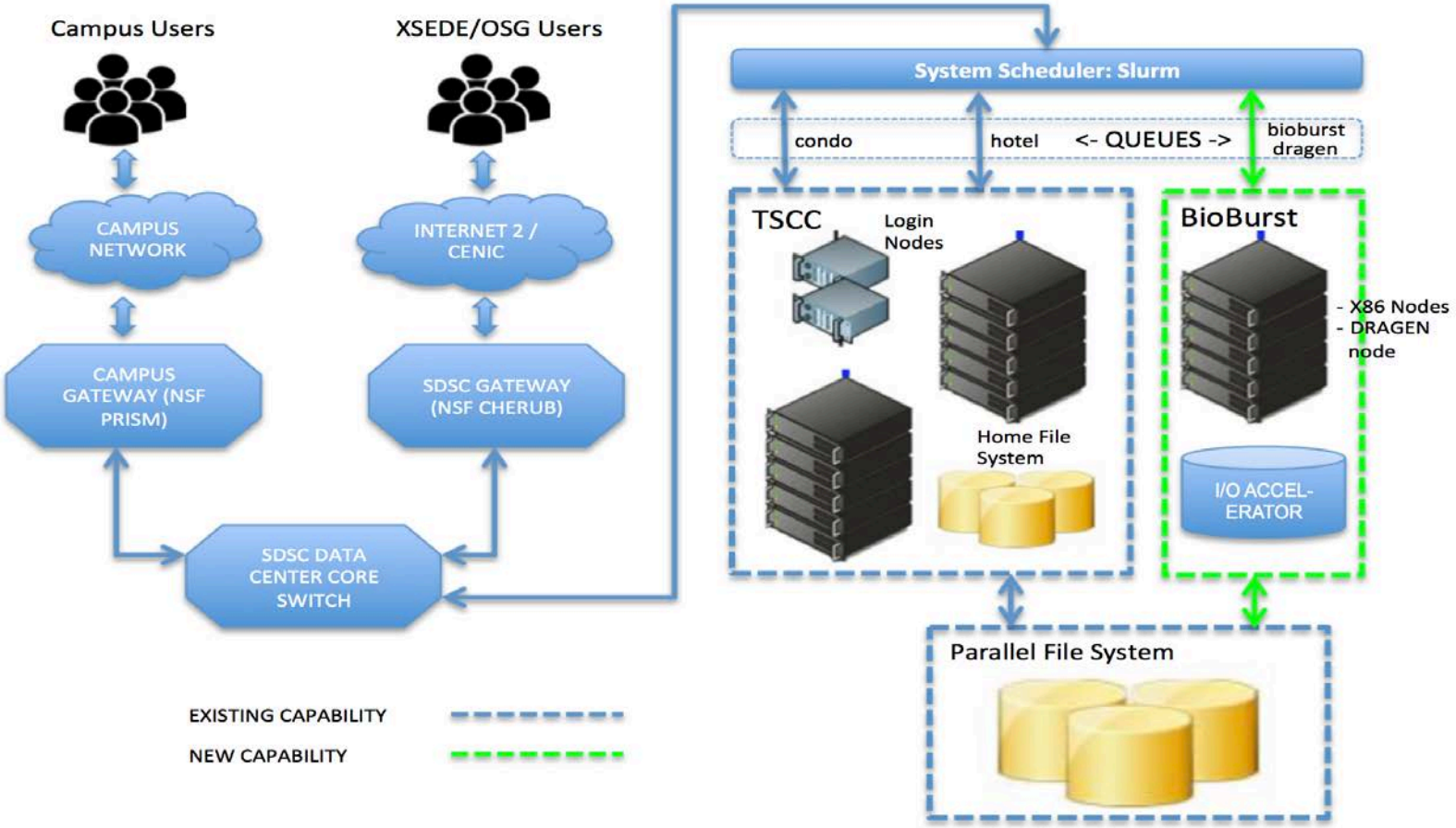
- *Once purchased nodes are in place, group may run on purchased nodes or entire cluster according to usage rules*
- *Labs/groups are assessed an annual per-node operations fee*

Condo Cluster

Common equipment is purchased via assessment of a one-time, per-node "infrastructure fee"

TSCC Group Purchases Common Infrastructure

Overall Architecture



TSCC: Types of Allocations

- **TSCC**
  - Trial Accounts
  - Co-Lo

TSCC Trial Accounts

- **Purpose**
  - Rapid, limited access to the TSCC resource for preliminary system evaluation
- **Startup Request are accepted and reviewed continuously**
  - Expect 1 day response time
- **Awards Available**
  - 250 core hours TSCC for 90 days
  - NO storage award available
- **Eligibility**
  - UC educator or researcher
- **To Apply**
  - email tscc-info@ucsd.edu and provide
  - Full Name, Department, UC affiliation (grad student, post-doc, faculty, etc.),

For More Information Contact:

- **Ron Hawkins**
  - Email rhawkins@sdsc.edu or tscc-info@sdsc.edu
  - Tel (858) 534-5045
  - http://www.sdsc.edu/services/hpc/hpc_systems.html

- **TSCC Purchasing Information**
  - Purchase resources or time on TSCC
  - http://www.sdsc.edu/services/hpc/tscc-purchase.html

Comet/Comet-GPU: Types of Allocations

- **UC (Comet, Comet-GPU, Persistent Storage)**
  - Up to 1Million SUs
- **XSEDE (Comet, Comet-GPU, Persistent Storage)**
  - Trial Accounts
  - Campus Champions
    - Bill Strossman: bill.strossman@ucr.edu
    - Charles Forsyth: forsythc@ucr.edu
  - Startup
    - Up to 50K SUs on Comet
    - 2,500 GPU hours on Comet GPU
    - 500G storage (additional storage provided justification)
  - Research
    - UP to 10 Millions SUs

UC: HPC@UC

- **Purpose**
  - Help UC researchers expand their overall research program.
- **Applications are committee reviewed on an ongoing basis.**
  - Turnaround time less then 10 business days
- **Awards Available**
  - Up to 1 Millions Comet SUs, an storage
- **Eligibility**
  - New XSEDE/HPC PIs
  - Only 1HPC@UC allocation available per PI
  - Then apply for XSEDE allocation
- **Apply**
  - http://www.sdsc.edu/support/hpc_uc_apply.html

For More Information Contact:

- **HPC at UC or SDSC HPC support staff**
  - Email hpc@uc@sdsc.edu or consult@sdsc.edu
  - http://www.sdsc.edu/collaborate/hpc_at_uc.html

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National: XSEDE 2.0

- **$110 million award to 18 institutions**
  - SDSC received $15 M; Bob Sinkovits SDSC XSEDE PI
  - Coordinates NSF funded supercomputing and cyberinfrastructure resources
- **Provides Cyberinfrasture and Support for**
  - 12 Compute Resources
    - Multi-core and many-core high-performance computing (HPC) systems, distributed high-throughput computing (HTC) environments, visualization and data analysis systems, large-memory systems, data storage, and cloud system
  - 5 Storage Resources
    - Data management, Data Collections, Large-Scale persistent storage
  - Provides advanced user services – Extended Collaborative Support Services(ECSS)
  - Online and in person training

Trial Accounts

- **Purpose**
  - Rapid, limited access to the Comet resource for preliminary system evaluation
- **Startup Request are accepted and reviewed continuously**
  - Expect 1 day response time
- **Awards Available**
  - 1000 SUs on Comet
  - 100 GPU hours on Comet GPU
  - NO storage award available
- **Eligibility**
  - PI of Research allocation must be faculty/researcher, including postdoctoral researchers, at a U.S.-based institution. Undergraduate and graduate students can apply with proof of association to eligible PI, or NSF fellowship award
- **To Apply**
  - Create and XSEDE Portal account and send request via ticket to help@xsede.org

Startup Allocations

- **Purpose**
  - Small-scale computational activities
  - Research Proposal development (benchmarking and scaling studies)
- **Startup Request are accepted and reviewed continuously**
  - Expect 1 week turnaround
- **Awards**
  - Up to 50,000 Comet SUs (1 SU = 1 core hour, each comet node has 24 cores)
  - Up to 2,500 GPU hours (Each GPU node consists of 4 GPUs)
  - Default 500G storage, additional storage if justified
  - PIs can request that other users be given accounts to use the allocation.
- **Eligibility**
  - PI of Research allocation must be faculty/researcher, including postdoctoral researchers, at a U.S.-based institution. Undergrad with NSF fellowship award or honorable mention

Startup Proposal: Required Components

- **Project Abstract:**
  - Describe the research objectives of the project
  - Explain need for access to XSEDE resources
  - Justify resource request
    - How amounts were estimated
    - Why the requested resources were selected.
- **CVs (2 pages per CV):**
  - PI and any listed co-PI's
- **NSF Fellowship award letter (if applicable):**
  - Graduate students with NSF Fellowship or Honorable Mention awards are eligible to be PIs on a Startup allocation request.

Research Allocations

- **Purpose**
  - For projects that have progressed beyond the Startup phase, either in purpose or scale of computational activities
- **Research requests are accepted and reviewed quarterly by the XSEDE Resource Allocations Committee (XRAC)**
  - https://portal.xsede.org/allocations/research#schedule
- **Awards**
  - Up to 10 Millions Comet SUs (1 SU = 1 core hour, each comet node has 24 cores)
  - Up to 50TB (default 500G)
  - PIs can request that other users be given accounts to use the allocation.
- **Eligibility**
  - PI of Research allocation must be faculty/researcher, including postdoctoral researchers, at a U.S.-based institution

Research Proposal: Required Components

- **Main Document (10 page limit)**
  - Scientific Background, Research , Resource Usage Plan, Justification of the resource request, Resource Appropriateness
    - Resource usage plan should describing how the requested allocations are necessary and sufficient to accomplish the project's research objectives
    - Disclosure of access to other CI resources and why those resources are not available or sufficient for the work proposed in this request
- **Progress Report (for renewal): 3 page limit**
  - Describe how current/prior allocation was used and summarize the findings or results
- **Code Performance & Resource Costs**
- **Curriculum Vitae (CV): (2 page max)**

To Apply for XSEDE Allocation

- **Apply at: https://portal.xsede.org/submit-request#/**

General Proposal Guidance

- **Use startup for Benchmarking and scaling studies**
  - Research proposal will be rejected if solid justification is not provided

XSEDE ECSS – can request with allocation proposal

- **Extended Collaborative Support Services**
  - Code optimization, profiling/tracing, benchmarking
  - Parallelization, scalability analysis/improvement
  - Incorporation of scientific libraries
  - I/O, storage implementation
  - Visualization
  - Workflows
  - Innovative scheduling

ECSS Justification

1. *What will you accomplish with the help?*
2. *How will success benefit your project?*
3. *Which of your team would collaborate with ECSS staff?*
4. *Have you interacted with XSEDE staff?*
   (If we develop interaction, say via HPC@UC, you can mention SDSC staff)
5. *Have you received XSEDE ECSS before? If yes, details.*

For More Information Contact:

- **XSEDE support staff**
  - E-mail help@xsede.org or create ticket at:

  https://portal.xsede.org/group/xup/help-desk
  - http://www.xsede.org

Science Gateways

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

Barriers of entry to HPC

- Write peer-reviewed proposals for computer time
- Understand HPC machines, architectures, policies, complex OS/software
- Install and benchmark complex tools on HPC resources
- Understand and manage multiple remote authentication systems
- Understand the queuing software, policies at different centers
- Figure out data transfer, management, storage issues

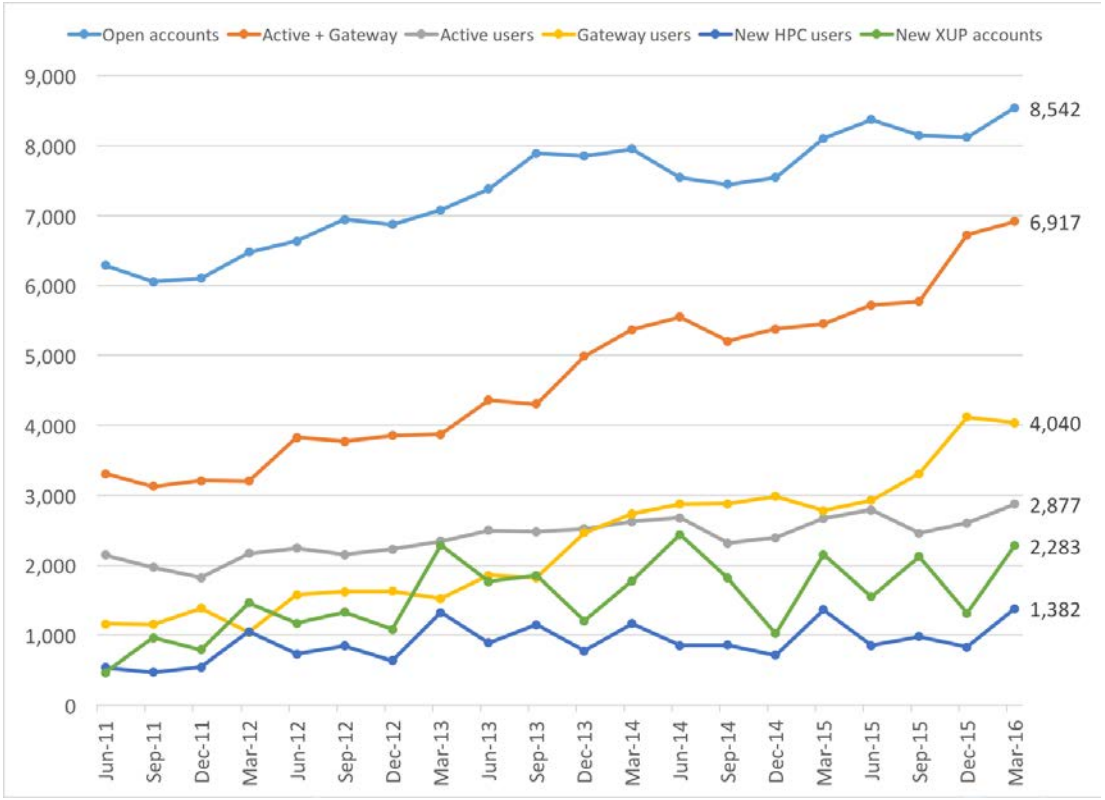
A Science Gateway

1. **Easy user interface to HPC/HTC/Cloud for a domain science**
   1. Primarily secure online web portal
   2. Programmatically also in some cases
2. **Easy web click and submit mode to upload model/input data, run of codes on HPC/HTC/Cloud, notification**
3. **User support from Science Gateway staff**
4. **Provide widely used domain science tools on the backend compute resources**
5. **Ability to easily get to the results, download results**
6. ***No writing of allocation proposals (SGW PI does that for the community)***

A Science Gateway catalyzes and democratizes research for everybody including researchers and students from institutions with less resources

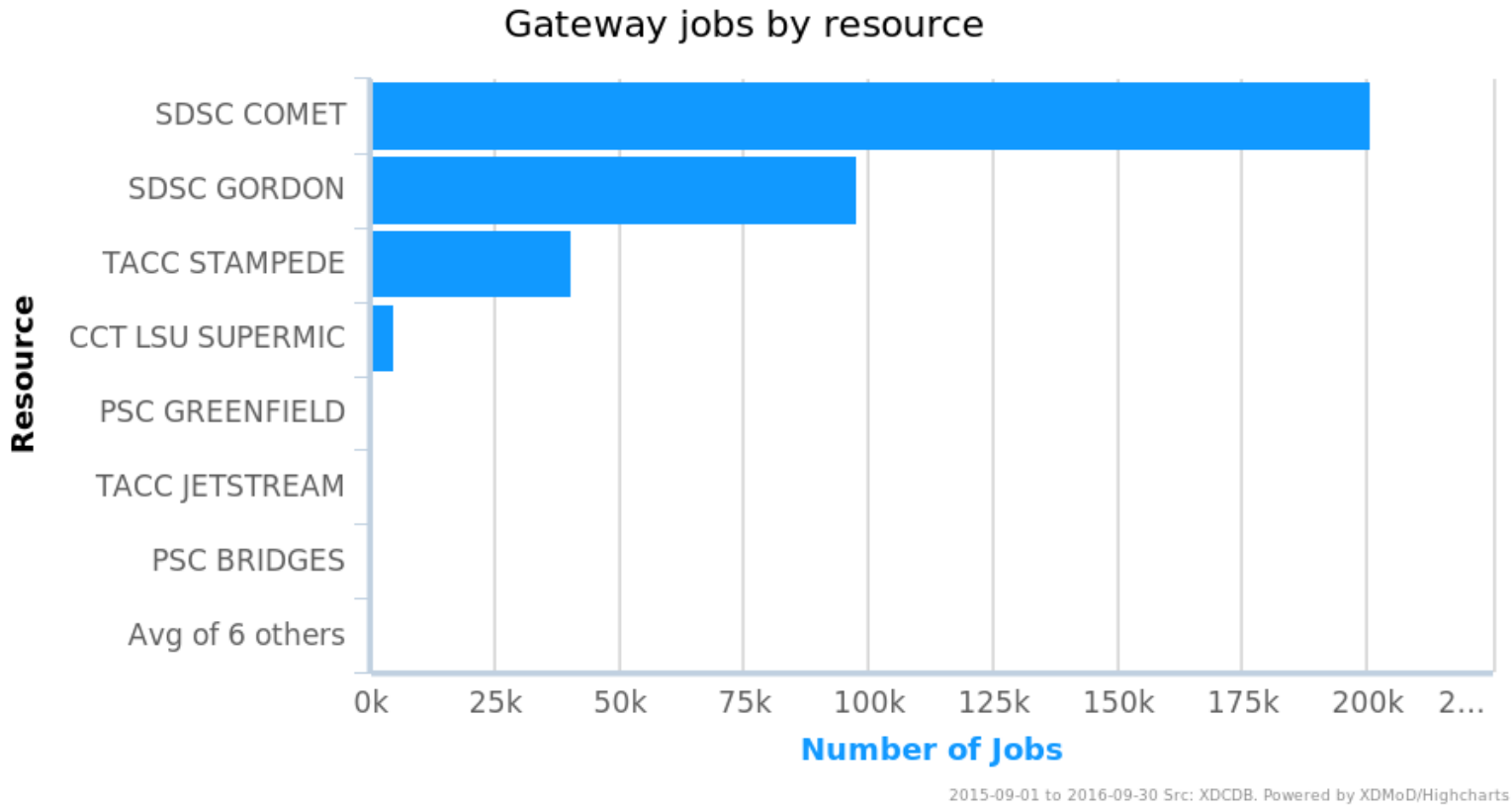
Gateways are revolutionizing and democratizing supercomputer access

- Users can access supercomputers via a browser
- Gateway users exceed login users on XSEDE resources



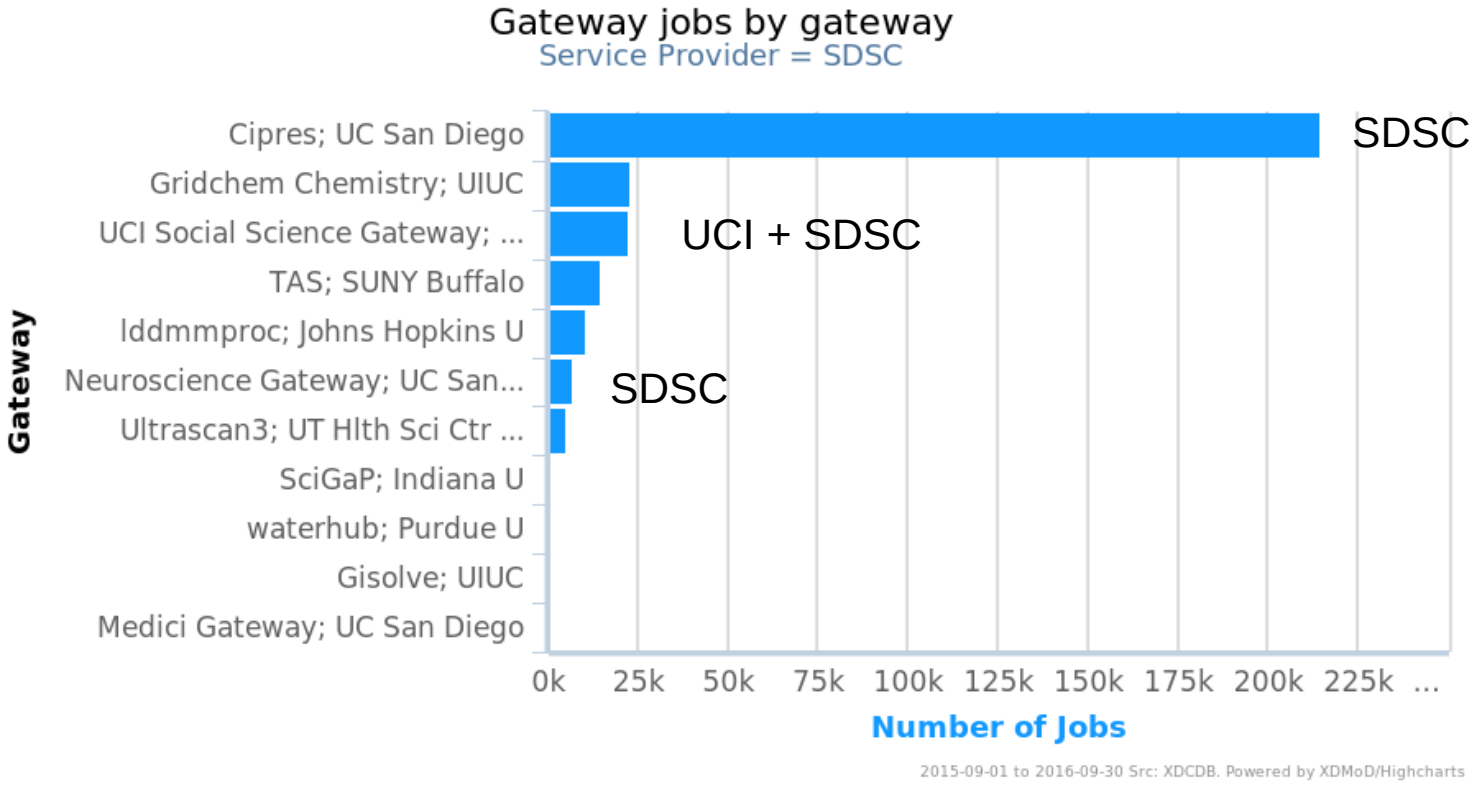
SDSC leads in hosting gateways

- **Comet and Gordon accounted for 86% of gateway jobs on XSEDE resources over the past year (2015-2016)**



SDSC leads in developing and maintaining gateways

- 3 of top 7 gateways that SDSC hosts were developed at or together with SDSC

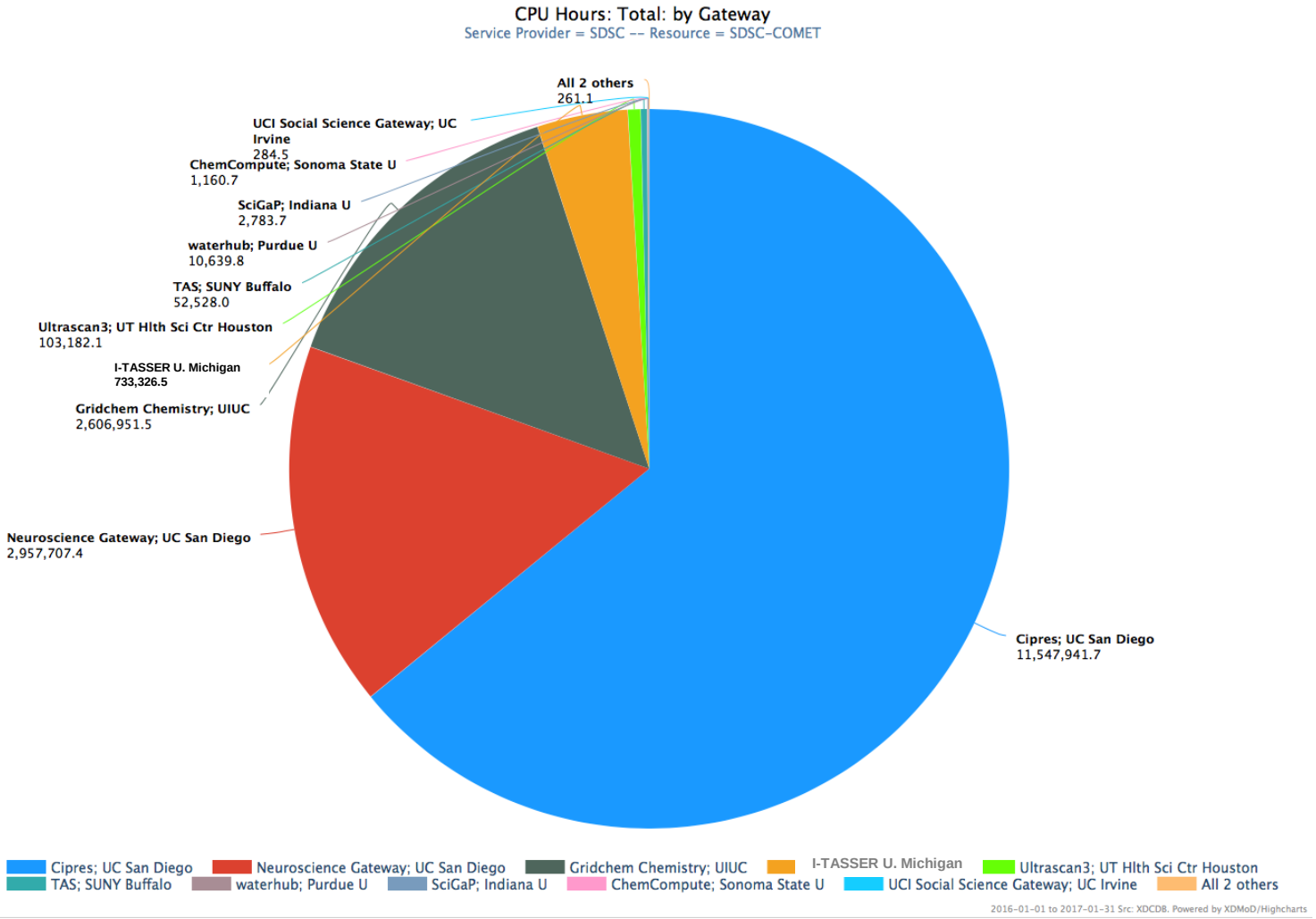


List of SGWs - XSEDE

Title	Field of Science	Portal Homepage
3D-Quantitative Phenotyping Gateway	Biological Sciences	Visit Portal
Asteroseismic Modeling Portal	Stellar Astronomy and Astrophysics	Visit Portal
Chem Compute	Chemistry	Visit Portal
CIPRES Portal for inference of large phylogenetic trees	Systematic and Population Biology	Visit Portal
Computational Anatomy	Neuroscience Biology	Visit Portal
Computational Chemistry Grid (GridChem)	Chemistry	Visit Portal
CyberGIS Gateway	Geography and Regional Science	Visit Portal
DesignSafe: Natural Hazards Engineering Research Infrastructure	Engineering	Visit Portal
Diagrid	Advanced Scientific Computing	Visit Portal
dREG gateway	Genetics and Nucleic Acids	Visit Portal
ENIGMA Bipolar BrainAge Analysis Upload Portal	Neuroscience Biology	Visit Portal
Galaxy	Molecular Biosciences	Visit Portal
GenePattern Server	Biological Sciences	Visit Portal
Globus Online	Engineering Infrastructure Development	Visit Portal
High-Resolution Modeling of Hydrodynamic Experiments with UltraScan	Biophysics	Visit Portal
I-TASSER	Biochemistry and Molecular Structure and Function	Visit Portal
Metaproteomics Gateway	Biochemistry and Molecular Structure and Function	Visit Portal
MP-Complete	Materials Research	Visit Portal
MyGeoHUB	Geosciences	Visit Portal
Nanoparticle Characterization Lab	Materials Research	Visit Portal
Network for Computational Nanotechnology and nanoHUB	Emerging Technologies Initiation	Visit Portal

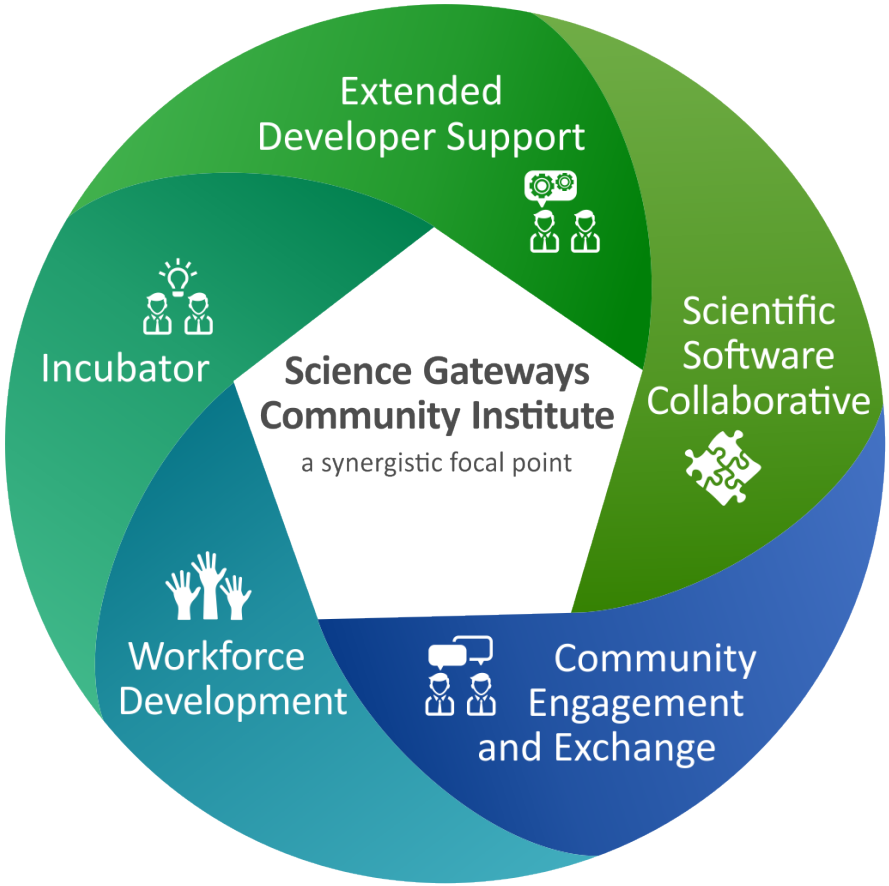
NIST Digital Repository of Mathematical Formulae	Mathematical Sciences	Visit Portal
OpenTopography	Earth Sciences	Visit Portal
ParamChem Gateway	Chemistry	Visit Portal
PGA	Computer and Information Science and Engineering	Visit Portal
PICKSC Science Gateway	Physics	Visit Portal
Proteogenomics Gateway	Biochemistry and Molecular Structure and Function	Visit Portal
Providing a Neuroscience Gateway	Neuroscience Biology	Visit Portal
ROSIE, The Rosetta Online Server that Includes Everyone	Biophysics	Visit Portal
Science Gateways Platform as a Service (SciGaP)	Computer Systems Architecture	Visit Portal
SimCCS Gateway	Geosciences	Visit Portal
SimVascular	Fluid, Particulate, and Hydraulic Systems	Visit Portal
The Earth System Grid	Global Atmospheric Research	Visit Portal
The iPlant Collaborative Agave API	Integrative Biology and Neuroscience	Visit Portal
UCI Complex Social Science Gateway	Anthropology	Visit Portal
Unidata: Data Proximate Services in the Cloud	Atmospheric Sciences	Visit Portal
VLab - Virtual Laboratory for Earth and Planetary Materials	Materials Research	Visit Portal
WaterHUB - Platform for water education, research, data access, partnership and collaboration	Earth Sciences	Visit Portal

There are now 12 gateways on Comet across several domains. More are coming.



SDSC is taking gateway leadership to the next level with the Science Gateways Community Institute

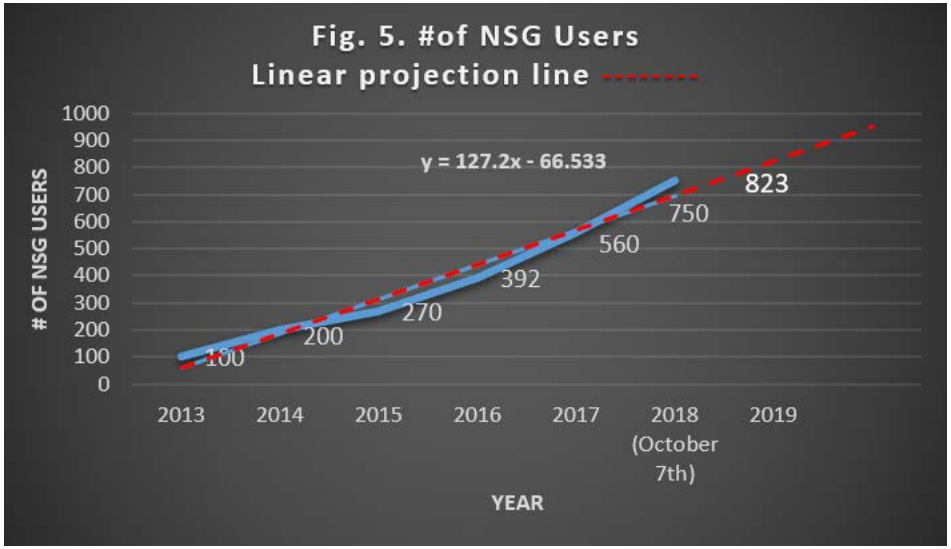
- **$15M NSF award for 5 years with 5-year renewal option**
- **Led by PI Nancy Wilkins-Diehr of SDSC**
- **Co-PIs: Maytal Dahan (TACC), Linda Hayden (ECSU), Katherine Lawrence (Michigan), Marlon Pierce (Indiana), Michael Zentner (Purdue)**
- **Goes beyond ECSS to support**
  - Overall gateway development, both front end and back end
  - Gateways that do not use HPC

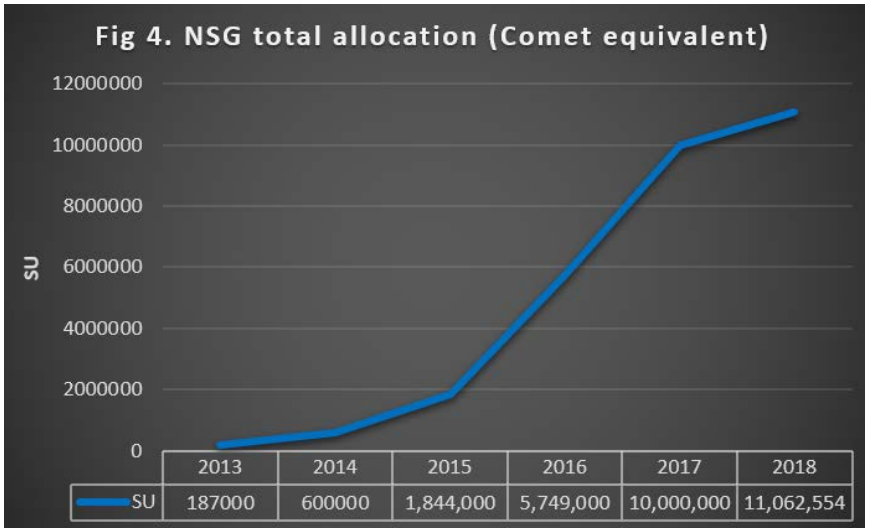


Neuroscience Gateway

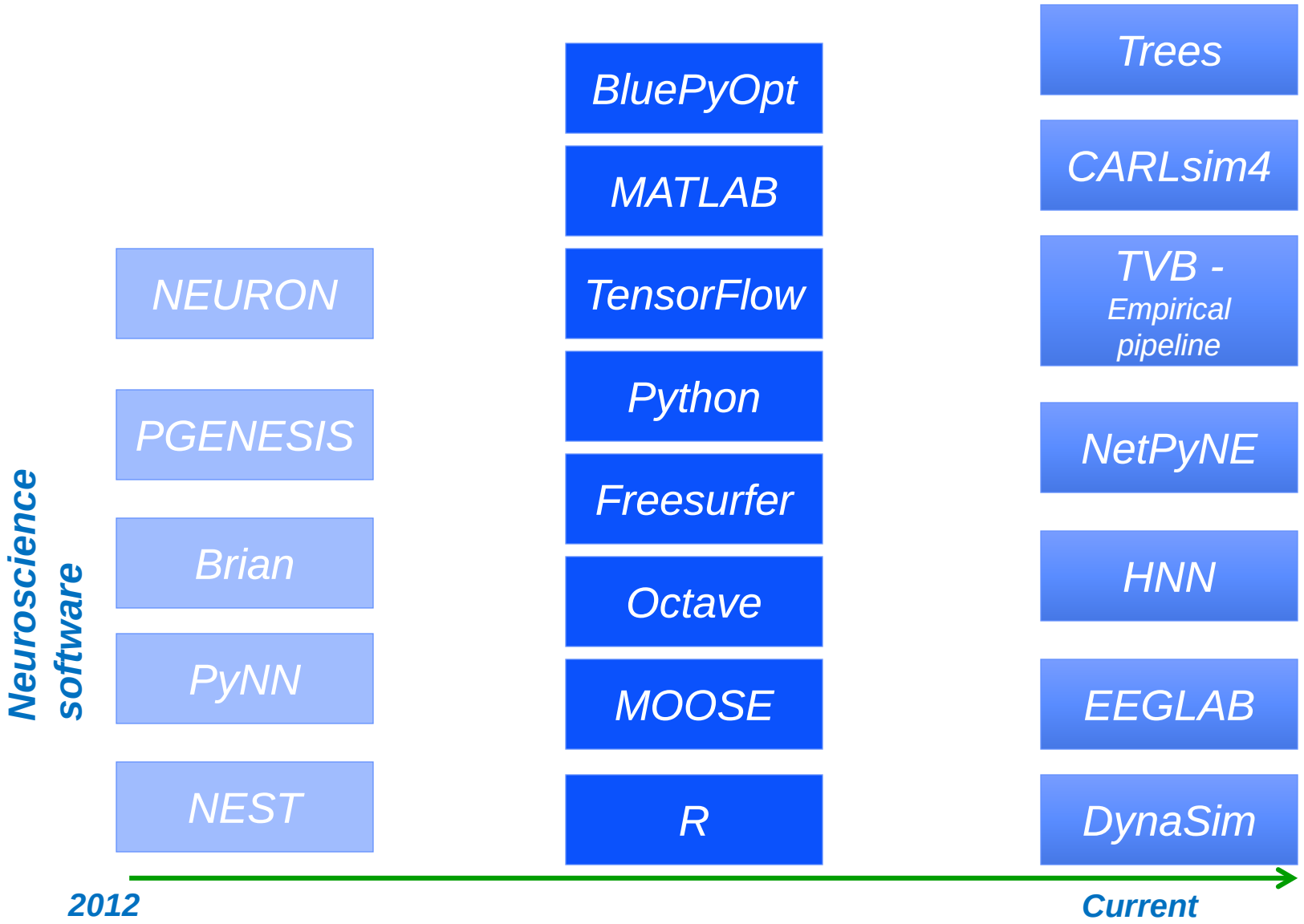
Amit Majumdar, Subhashini Sivagnanam, Kenneth Yoshimoto, SDSC
Ted Carnevale, Yale University

Provide neuroscience tools, libraries, pipelines for computational neuroscience and brain image data processing on HPC, HTC, Cloud
Funded by NSF to build and serve the community; NIH funding for projects



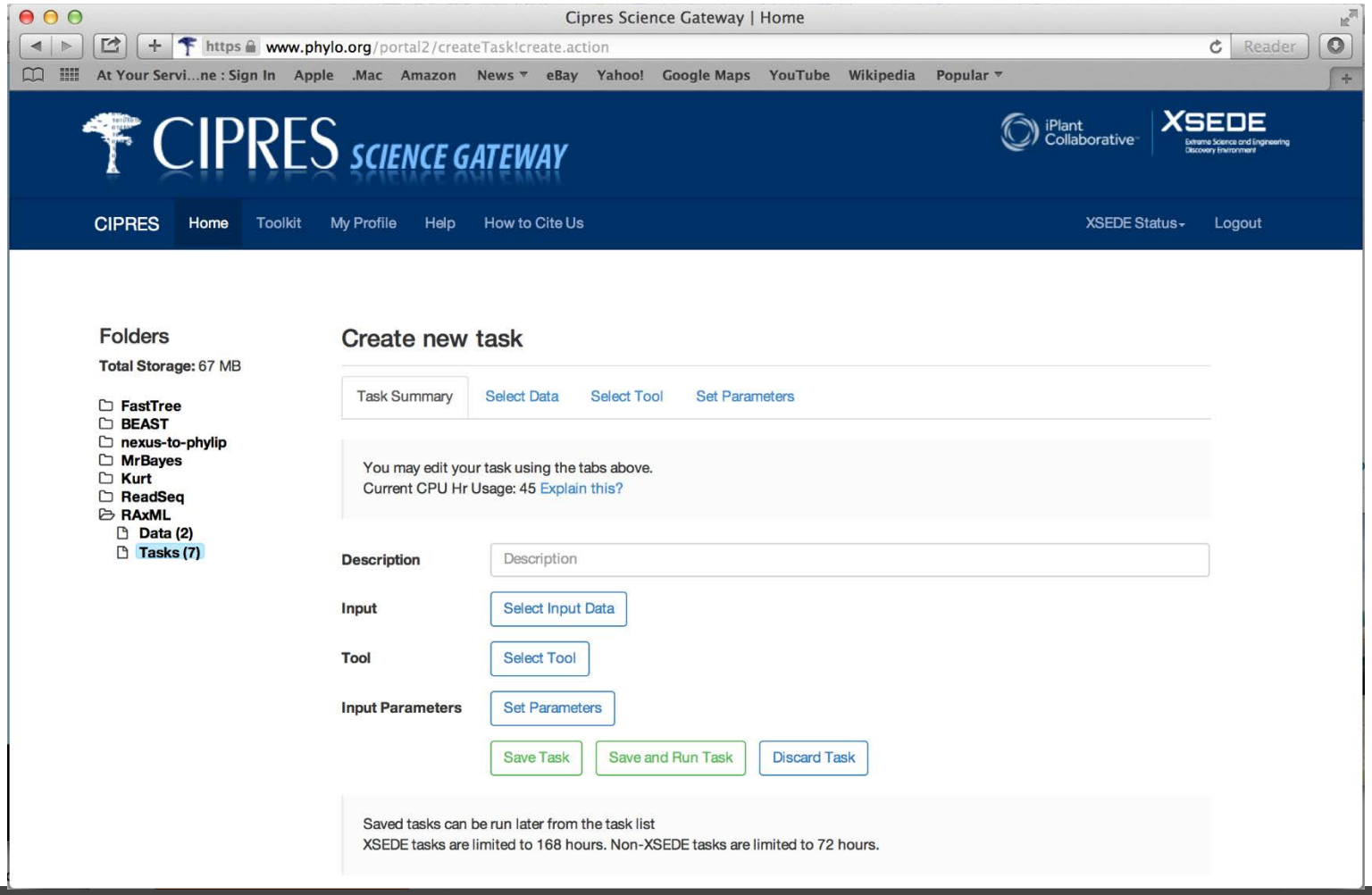


NSG software stack



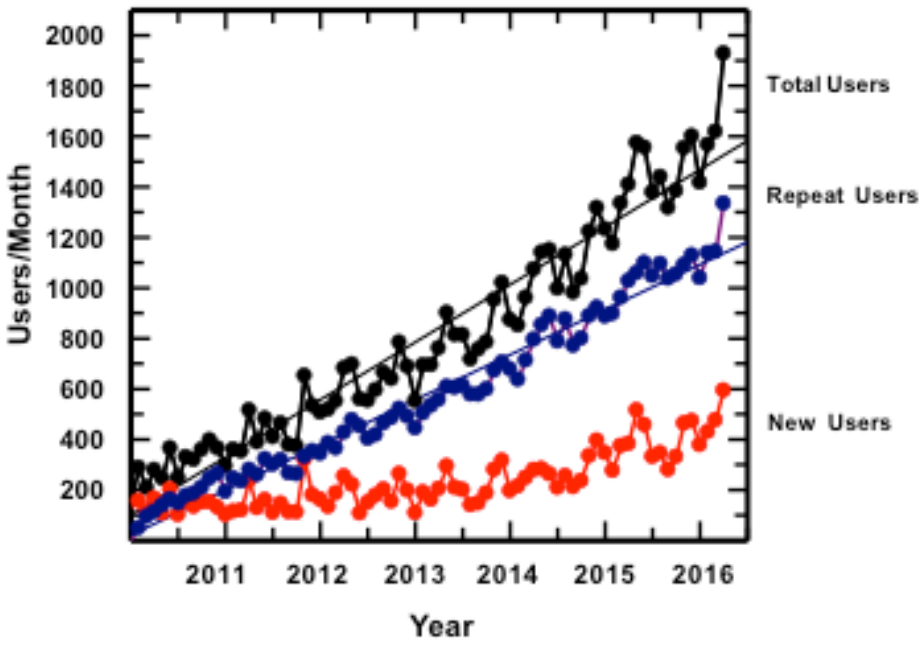
SDSC develops, maintains, & hosts the NSF-funded CIPRES gateway, which runs phylogenetics codes via a browser interface; analyses span the entire tree of life

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

For More Information on XSEDE Gateways in general contact:

- **Marlon Pierce**
  - E-mail marpierc@iu.edu or help@xsede.org

  https://portal.xsede.org/group/xup/help-desk
  - https://www.xsede.org/ecosystem/science-gateways


SHERLOCK
SOLVED @ SDSC
SHERLOCK CLOUD
Sandeep Chandra
Division Director
Health Cyberinfrastructure Divison
A Secure Cloud Solution for UC
San Diego Supercomputer Center @ UC San Diego
SDSC SAN DIEGO SUPERCOMPUTER CENTER
UNIVERSITY OF CALIFORNIA


SHERLOCK
CLOUD
Sherlock Cloud's Managed Infrastructure as a Service (IaaS) Cloud was developed to provide secure end-to-end Cyberinfrastructure for data and computing for academic, state and government partners.
CLOUD COMPUTING
DATA MANAGEMENT
COMPLIANCE & REGULATORY
MODERN COLOCATION
PROFESSIONAL SERVICES
CYBERSECURITY
SDSC SAN DIEGO SUPERCOMPUTER CENTER
UNIVERSITY OF CALIFORNIA

Sherlock Cloud is developed in accordance with NIST controls governing system access, information security, and management processes.

- ✓ Policies, Processes & Procedures
- ✓ Lifecycle Documentation
- ✓ Annual Audits & Assessments
- ✓ Regulatory Know-How
- ✓ Administrative Safeguards
- ✓ Technical & Security Safeguards
- ✓ Physical security

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MANAGING YOUR ENTIRE STACK

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For More Information Contact:

Data Science Hub

İlkay ALTINTAŞ, Ph.D.
Chief Data Science Officer, Founder and Director,
Workflows for Data Science Center of Excellence
https://datascience.sdsc.edu/

Data Science Hub at SDSC

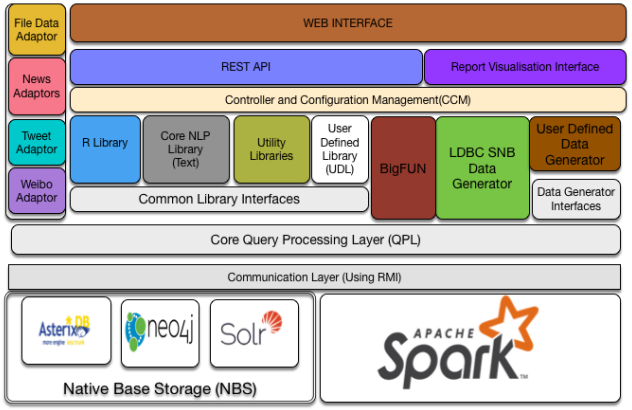
Objectives:

- *Create solutions and applications for data-driven science*
- *Serve as community hub for DS research, collaboration and education*
- *Workforce development*
- *Industry collaboration an entrepreneurial ventures in DS*

Expertise:

- *Data modeling and integration*
- *Data engineering and management*
- *Machine learning and graph analytics*
- *Performance modeling for big data platforms and workloads*
- *Scalable and high performance analytics*
- *Scientific visualization*
- *Advanced computing architectures for DS*

Analytical Workbench for Exploration of SOcial MEdia
Amarnath Gupta, SDSC



Example applications:

- *Machine learning applied to sensor data from weather stations for wildfire monitoring*
- *Deep learning applied to satellite images to detect affluence versus poverty in communities*
- *Graph and network analysis applied to political science and cybersecurity*
- *Management of social data with AWESOME Polystore*
- *Integration and real-time processing of diverse geospatial data*

For More Information Contact:

- **Data Science Hub web page**
  - https://datascience.sdsc.edu/