

# **USC Center for High- Performance Computing**

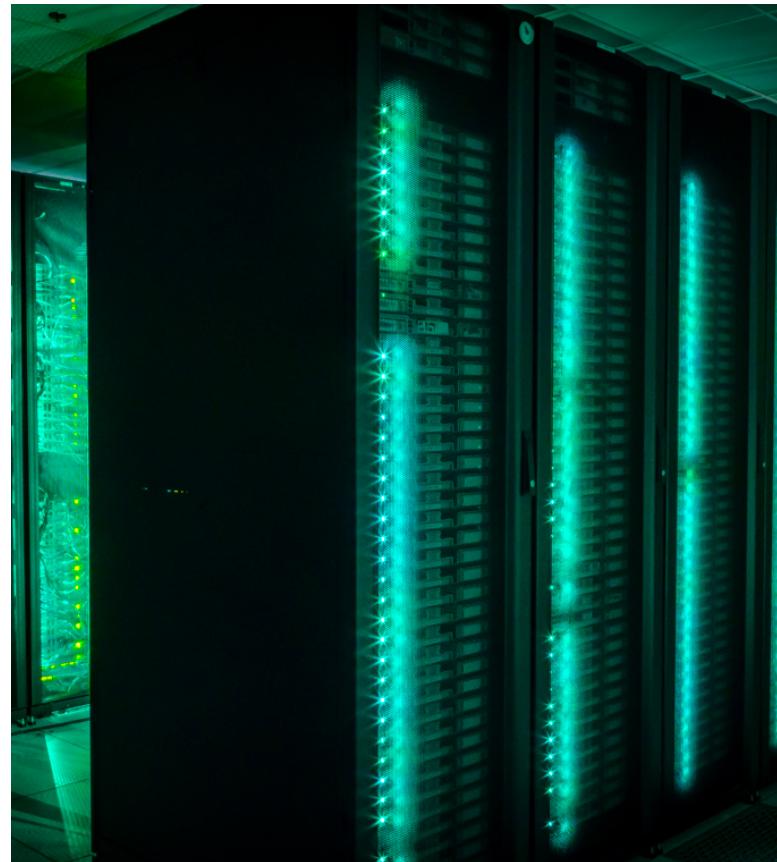
**Erin Shaw, Cesar Sul, and HPC Team**

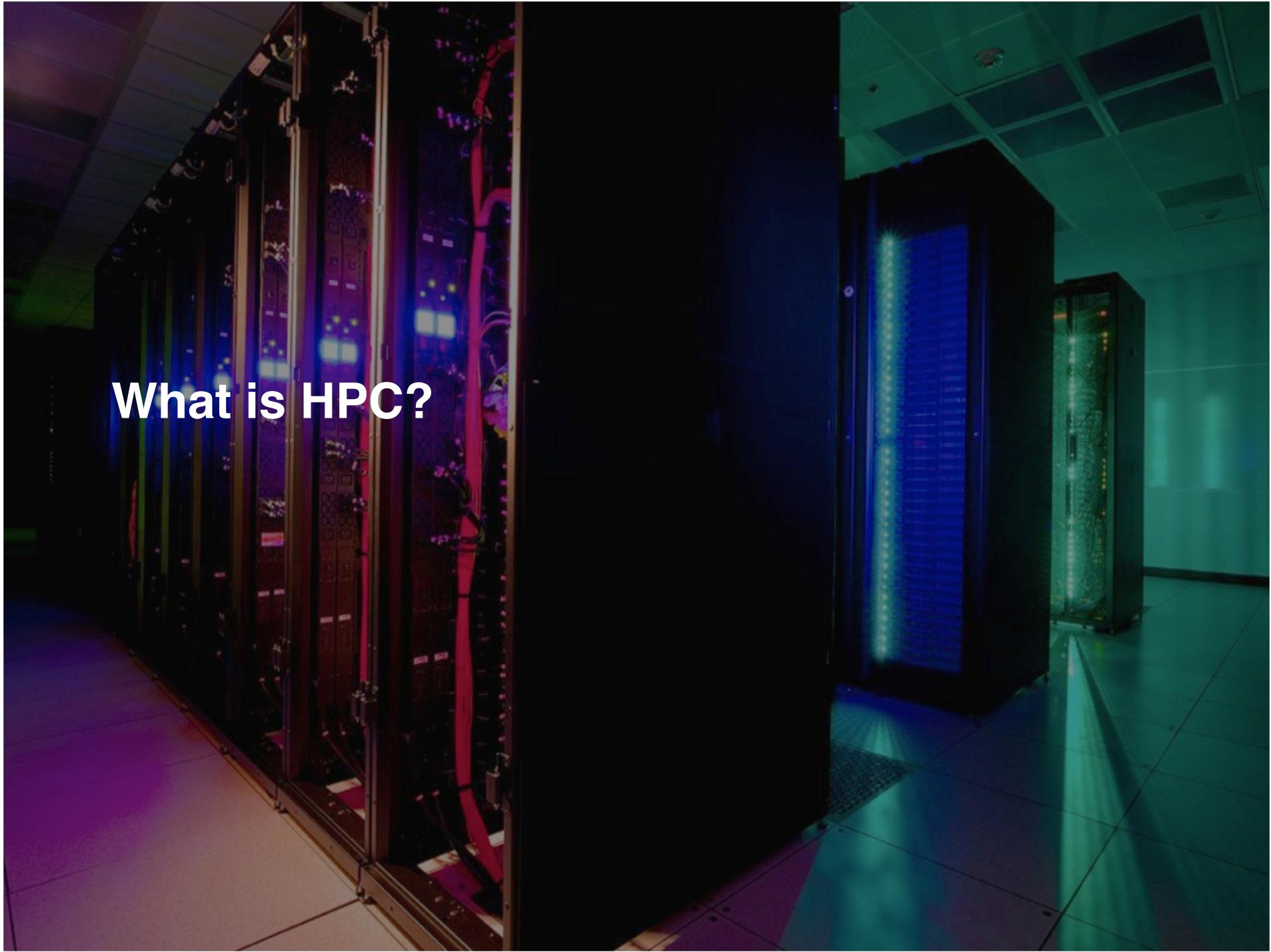
**ACI Research & Education Facilitator**

**USC Center for High Performance Computing**

# Talk Outline

- HPC Introduction
- Computing Cluster
- Accounts/Secure Data
- Cluster Access/Use
- Condo Options
- HPC Policies
- Facilitation
- Inquiries





# What is HPC?

# HPC Introduction

- HPC is USC's Center for High-Performance Computing.
  - HPC advances USC's mission by providing the infrastructure and support necessary for **research computing**.
  - It exists to help advance scientific discovery at USC.
- HPC is a world-class super-computing center!
  - As part of “standing up” an upgraded system, HPC runs and publishes standard performance benchmarks.
  - It is currently ranked the 12<sup>th</sup> fastest academic supercomputer in U.S. by TOP500.org, the international supercomputer ranking site.



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# HPC ITS (Information Technology Services)



Douglas Shook  
USC CIO



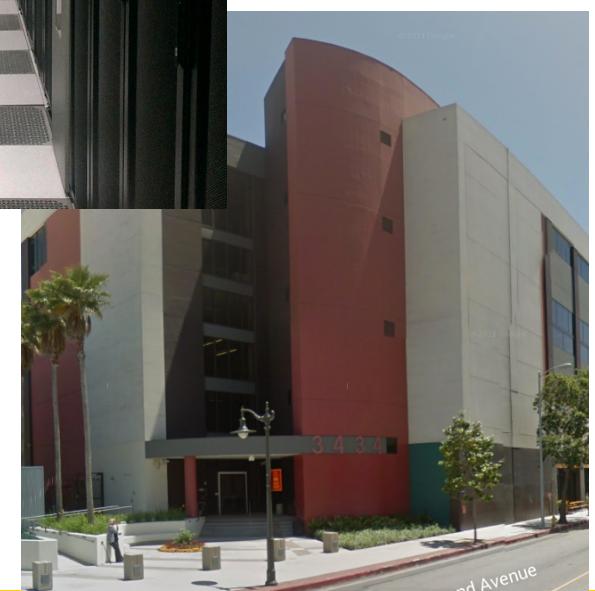
Randolph Hall  
*USC VP of Research &  
Faculty Executive  
Director, HPC\**



Maureen Dougherty  
USC HPC Director

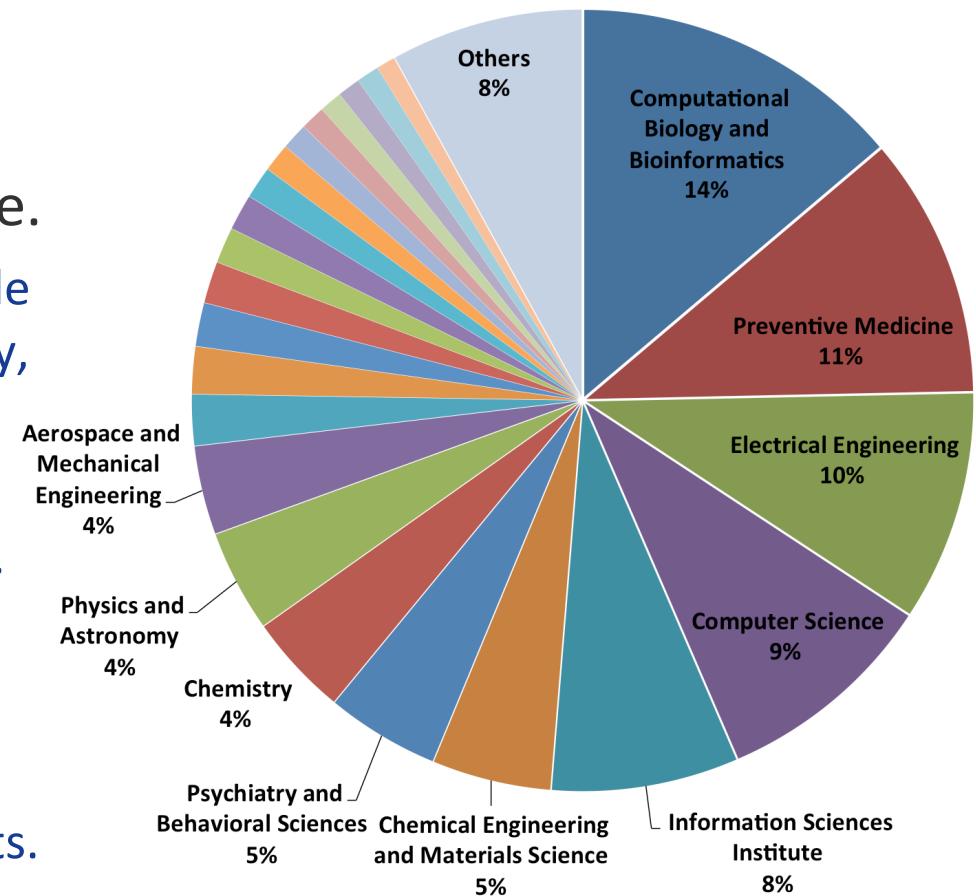


HPC  
ITS Data Center



# HPC User Base

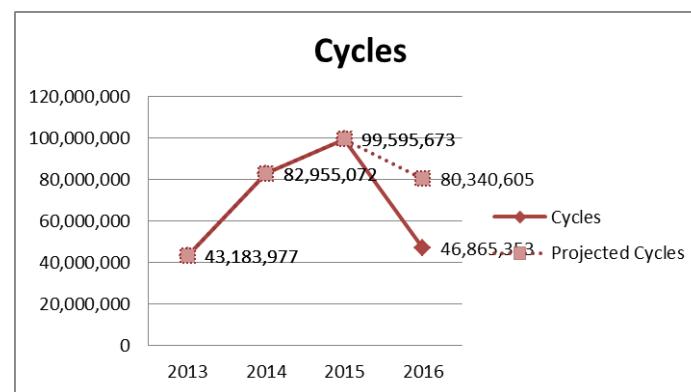
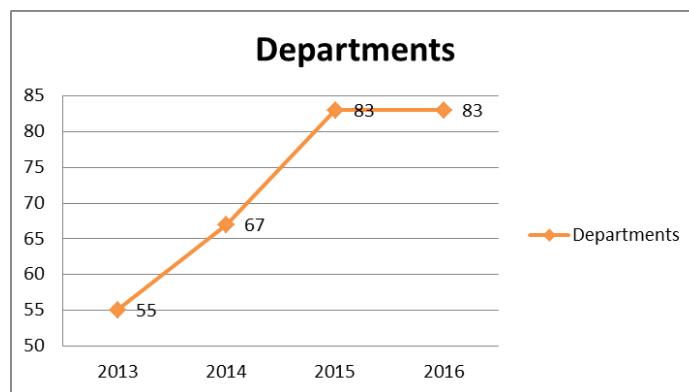
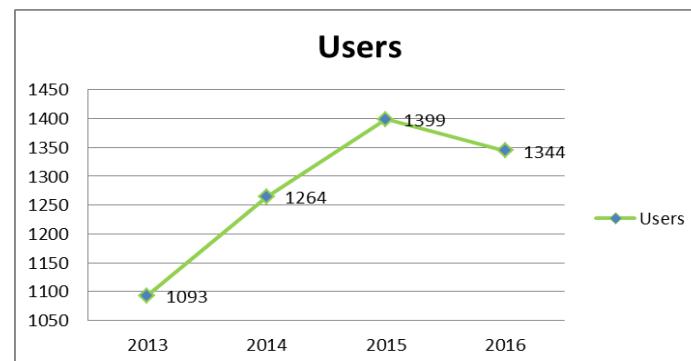
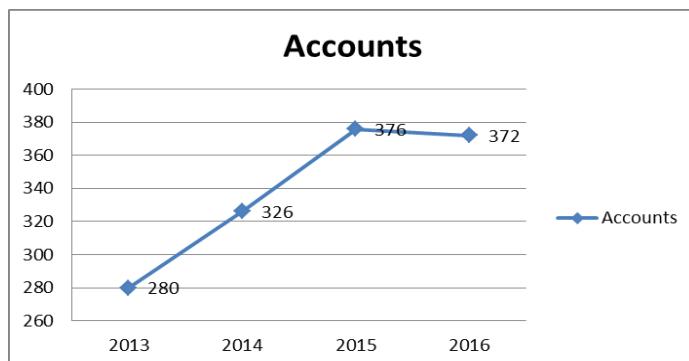
- HPC is a USC-wide resource.
  - HPC resources are available at no charge to USC faculty, researchers and students.
  - Most users are from Dornsife, Viterbi and Keck.
  - Others are from business, psychology, cinema, pharmacy and elsewhere.
  - There are 11 class accounts.
- HPC is housed within the ITS data center and is monitored around-the-clock by ITS staff.



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# HPC User Base (as of January 2017)



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# HPC Website: <http://hpcc.usc.edu>

The screenshot shows the homepage of the USC HPC website. At the top, there's a navigation bar with links for About, Research, User Support, New User Guide, HPC Computing Workshops, Frequently Asked Questions, Contact Us, and a Search bar. The main content area features a news item about a National Science Foundation award, a photo of several people in a server room, and a sidebar with a "Popular Topics" list. Below this are four profiles of faculty members: Maryam Shanechi, Daniel Lidar, Naomi Levine, and Arieh Warshel.

**HPC**  
*Center for High-Performance Computing*

**National Science Foundation Award To Benefit USC Researchers**

The National Science Foundation has awarded a \$5.3 million grant to a consortium of six universities, including USC, to fund the collaborative project "Advanced CyberInfrastructure—Research and Educational Facilitation: Campus-

**Popular Topics**

- ▶ Applying for an HPC Account
- ▶ Managing and Renewing Your Account
- ▶ Office Hours and Consultations
- ▶ New User Guide
- ▶ Documentation
- ▶ Education and Training
- ▶ Outreach

**Maryam Shanechi**  
Maryam M. Shanechi is an assistant professor and the Viterbi early career chair in electrical engineering at USC.

**Daniel Lidar**  
Daniel Lidar is a professor of electrical engineering, chemistry, and physics at the Viterbi School of Engineering.

**Naomi Levine**  
Naomi Levine is Gabilan assistant professor of biological sciences and earth sciences in the marine and environmental biology program at the USC Dana and David Dornsife College of Letters, Arts and Sciences.

**Arieh Warshel**  
Arieh Warshel is a nobel laureate, distinguished professor of chemistry at the Dornsife College of Arts, Letters and Sciences, and a founder of the field of computational enzymology.

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# HPC Computing Cluster

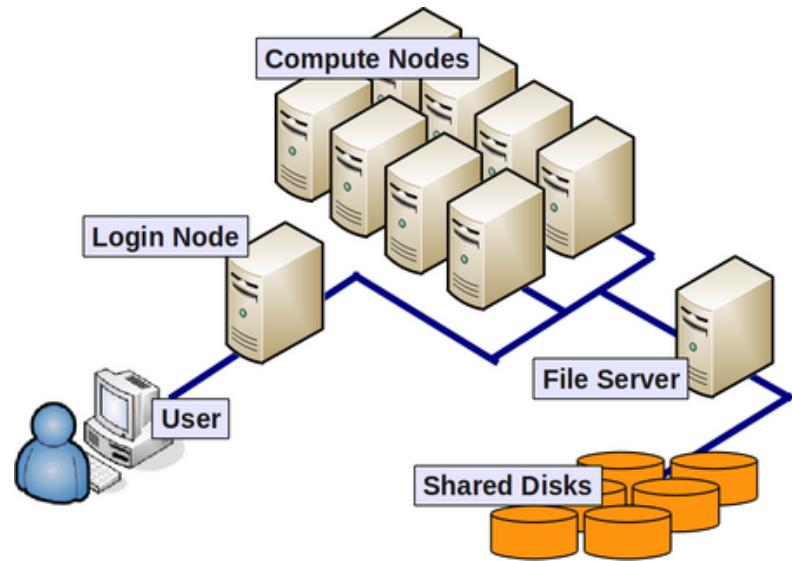


# What is a Computing Cluster?



## A computer cluster

- ... consists of connected computers (nodes) that work together
- ... nodes are connected to each other through fast local area networks
- ... with each node running its own instance of an operating system
- ... usually includes software for high-performance distributed computing



# HPC Computing Cluster

Simple, home-built cluster One rack in HPC cluster



Rows of racks in HPC cluster!



Networked nodes



Multiple racks in HPC cluster

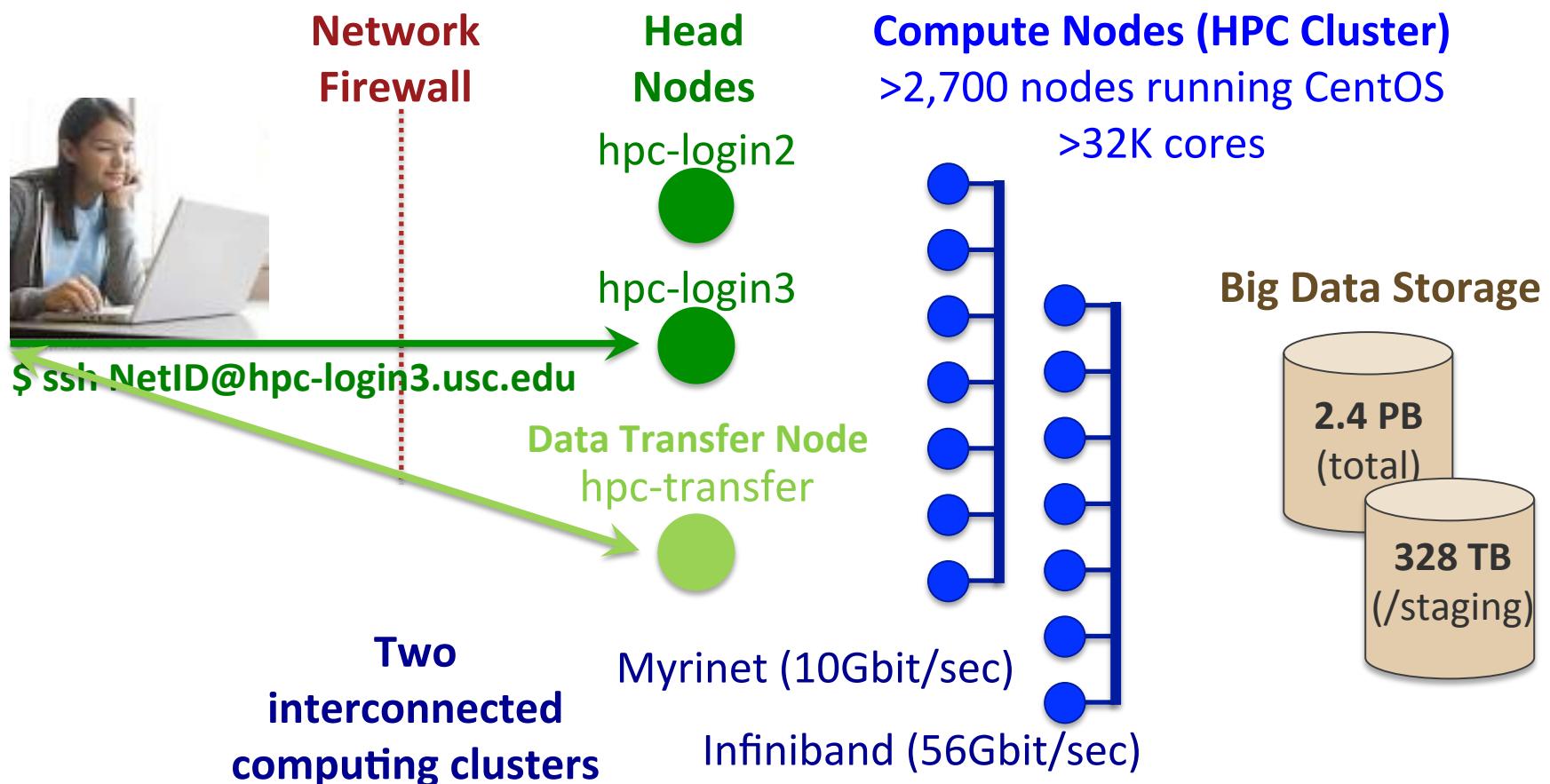


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# HPC Computing Cluster



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# HPC Computing Cluster

- As an example, the newer IB cluster has the following nodes:
  - **264** Hewlett-Packard SL250, dual Xeon 8-core 2.6GHz, dual NVIDIA K20 GPUs containing 2,496 cores, each with 64GB memory
  - **448** Hewlett-Packard SL230, dual Xeon 8-core 2.6GHz CPUs, 64GB mem.
  - **288** Lenovo nx360m5 dual Xeon 8-core 2.6GHz CPUs with 64GB mem.
  - **19** Lenovo nx360m5 2.6GHz dual NVIDIA K40 GPUs containing 2,880 cores, each with 64GB memory
  - **5** Lenovo nx360m5 2.6GHz dual NVIDIA K80 GPUs containing 2 x 2,496 cores, each with 64GB memory (These are condo nodes.)



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# HPC Computing Cluster (June 2016)

Index	Vendor Model	CPU Number Type Core Speed	Memory	GPU Number & Type
1	Dell R910	Quad Intel Xeon Decacore 2.0GHz	1TB	
2	HP SL160	Dual Intel Xeon Hexcore 3.0GHz	24GB	
3	HP DL165	Dual Intel Xeon, Dodecacore 2.3GHz	48GB	
4	Oracle X2200	Dual AMD Opteron Dualcore 2.3GHz	16GB	
5	Dell PE1950	Dual Intel Xeon Quadcore 2.5GHz	12GB	
6	Oracle X2200	Dual AMD Opteron Quadcore 2.3GHz	16GB	
7	IBM DX360	Dual Intel Xeon Hexcore 2.6GHz	24GB	
8	HP SL250S	Dual Intel SB Xeon Octocore 2.6GHz	64GB	Dual NVIDIA K20
9	HP SL230S	Dual Intel SB Xeon Octocore 2.6GHz	64GB	
10	Lenovo NX360 M5	Dual Intel Xeon Octocore GHz	64GB	
11	Lenovo NX360 M5	Dual Intel Xeon Octocore 2.6 GHz	64GB	Dual NVIDIA K40

queue	nodes	ppn	gpus	avx	/tmp	core	cpu	model	net-work	node names	node type
large-mem	4	40	-	-	1.8T	decacore	xeon	r910	myri	hpc-1t-1 hpc-1t-2 hpc-1t-3 hpc-1t-4	1
large main quick	8	12	-	-	140 GB	hexcore	xeon	sl160	myri	hpc0965-0972	2
large main quick	67	24	-	-	895 GB	dodeca-core	xeon	dl165	myri	hpc0981-1021 hpc1044-1050 hpc1123-1128 hpc1196-1200 hpc1223-1230	3
large main quick	26	8	-	-	60 GB	dualcore	opteron	x2200	myri	hpc1723-1728 hpc1734-1739 hpc1741-1742 hpc1744-1754 hpc1756	4
large main quick	54	8	-	-	60 GB	quadcore	xeon	pe1950	myri	hpc2283-2318 hpc2320-2337	5
large main quick	138	8	-	-	60 GB	quadcore	opteron	x2200	myri	hpc2349-2370 hpc2470 hpc2472-2481 hpc2483 hpc2486-2505 hpc2510-2544 hpc2546-2559 hpc2561-2580 hpc2582-2597 hpc2600	6
large main quick	4	12	-	-	200 GB	hexcore	xeon	dx360	myri	hpc2758-2761	7
large main quick	237	16	2	avx	850 GB	octocore	xeon	sl250s	IB	hpc3025-3027 hpc3031-3264	8
large main quick	45	16	-	avx	5500 GB	octocore	xeon	sl230s	IB	hpc3648-3688 hpc3695 hpc3766-3768	9

# HPC Software

- HPC provides various scientific software packages, as well as standard compilers and libraries, for use on the cluster.
  - e.g., Amber, Gaussian, MATLAB, R, MPICH, CUDA, and SAS.
  - We also collaborate with the developers of Globus and Pegasus for job workflow.
- Researchers can install software packages or develop their own code within their project's allotted storage.
  - Condo owners can purchase network licenses and we will manage them from our license server.
  - Different vendors address licensing in different ways so it is something to inquire about when purchasing.



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# Benefits of Using HPC

- There are many reasons to use HPC
  - HPC's professional staff manages and maintains compute nodes, the job scheduler/resource manager software and storage.
    - *PIs do not have to depend on graduate students for computer maintenance*
  - Researchers may have large computational or storage needs.
    - *e.g., for running engineering simulations, analyzing space data, processing MRI scans or sequencing DNA files*
    - *e.g., they may need to use graphics processing units (gpus) or lots of memory*
  - Researchers may need to use software on HPC.
    - *e.g., licensed software like MATLAB, SAS, Stata, Compilers*
    - *e.g., bioinformatics applications that run on HPC*



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# Benefits of Using HPC

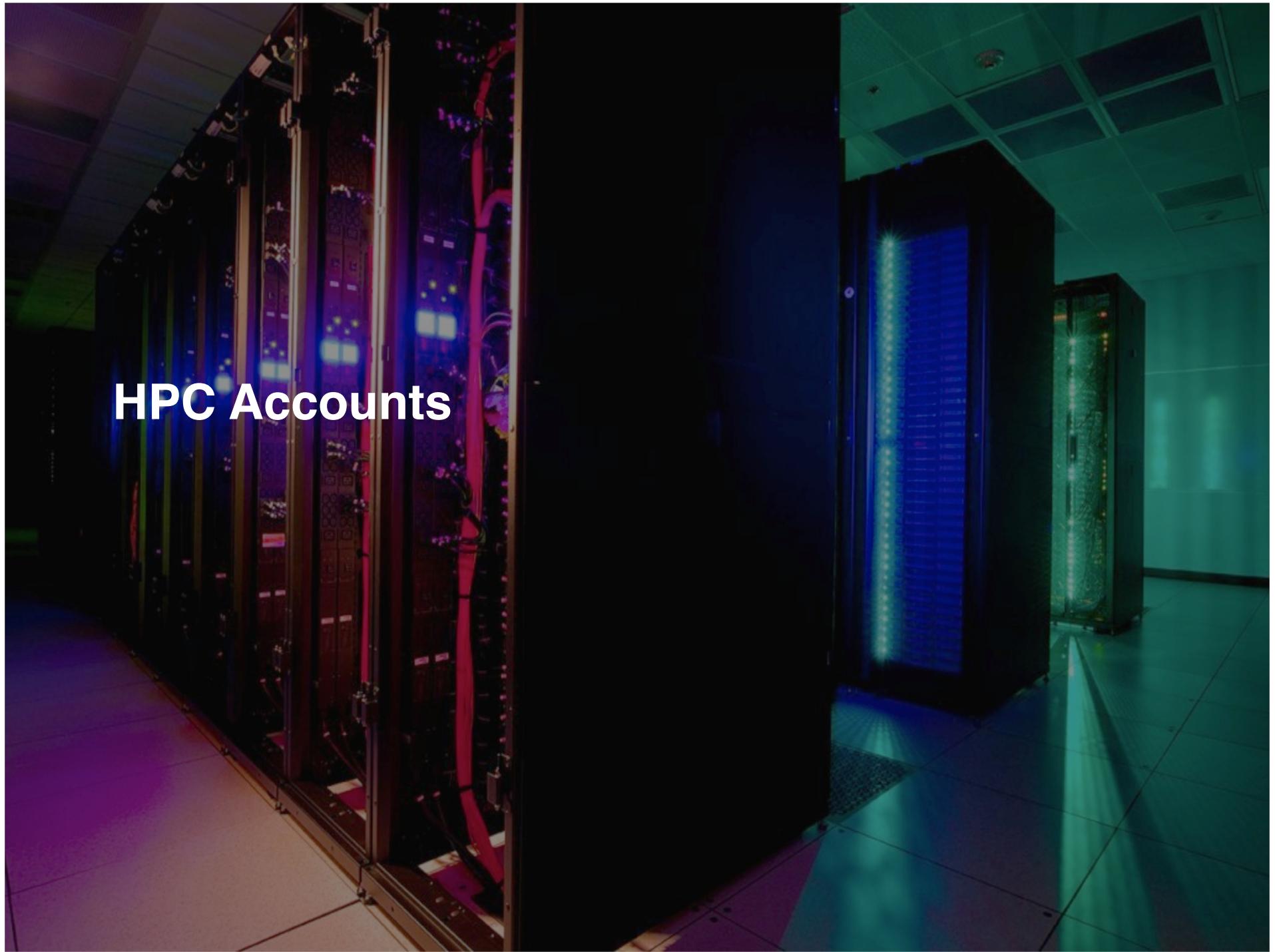
- Access to computational resources may not be available locally to all researchers and students.
  - *e.g., for remote students*
- Outreach, training and consultation services are available to aid in the optimal use of cluster resources.
- Educators can leverage HPC for teaching.
  - *Introduce students to 21<sup>st</sup> century research techniques*
  - *Train researchers for their eventual use of commercial web services such as Amazon, Microsoft and Google*
- HPC is free-of-charge, unlike commercial services.



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# HPC Accounts



# Applying for an Account

- All USC faculty, staff, researchers and graduate students can apply for HPC project accounts.
  - HPC accounts are project-based.
  - HPC refers to the project applicant as the **PI (Primary Investigator)** of the project/account, regardless of their funding status.
  - PIs must have a USC Network ID (NetID).
  - Researchers may apply for iVIP accounts through ITS for collaborators outside the university.
  - HPC requires PIs to re-apply annually for a project account.



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# Applying for an Account

- Project members:
  - A PI can add **members** to their project group (or be the sole member).
    - *e.g., a professor can add students to a class project*
    - *e.g., an investigator can add graduate students to a research project*
  - Anyone, including undergraduate students, can be members of projects.
  - Members can belong to multiple projects, including their own.
- Projects are allocated compute hours and disk space quotas.
  - PIs can request an increase to these quotas through the website.
  - Members use \$mybalance/\$myquota to monitor compute/disk quotas.



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# Applying for an Account

- Compute time is “charged” by accounting convention, but there is no fee for compute cycles.
- Storage
  - Storage is shared among all members of the project.
  - If you require more storage, or dedicated computing resources, we have purchase options.
  - Additional storage that can be made available to the cluster can also be purchased through USC Digital Repository (ITS) for approximately \$70/TB/month. See <http://repository.usc.edu> for more information.
- The account application site can be found at:  
<http://hpcc.usc.edu/support/accounts/applying-for-a-hpcc-account>



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# Return on Investment

- We ask that any form of publication, including webpages, resulting from work done on HPC machines include a citation similar to the following:

*Computation for the work described in this paper was supported by the University of Southern California's Center for High-Performance Computing (<http://hpcc.usc.edu>).*

- For ROI purposes, we ask that you tell us about these publications through the publications page on our account website.



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# Special Accounts

- Class accounts
  - Instructors can create class accounts for their students, for teaching and class assignments.
    - *We had eleven courses across the academic year*
- Secure data accounts 
  - As of January, 2017, HPC can now be used with sensitive and restricted-access data.
  - Previously, you could not store or process data or documents on HPC if they belonged to a category of legally protected or high-risk information.



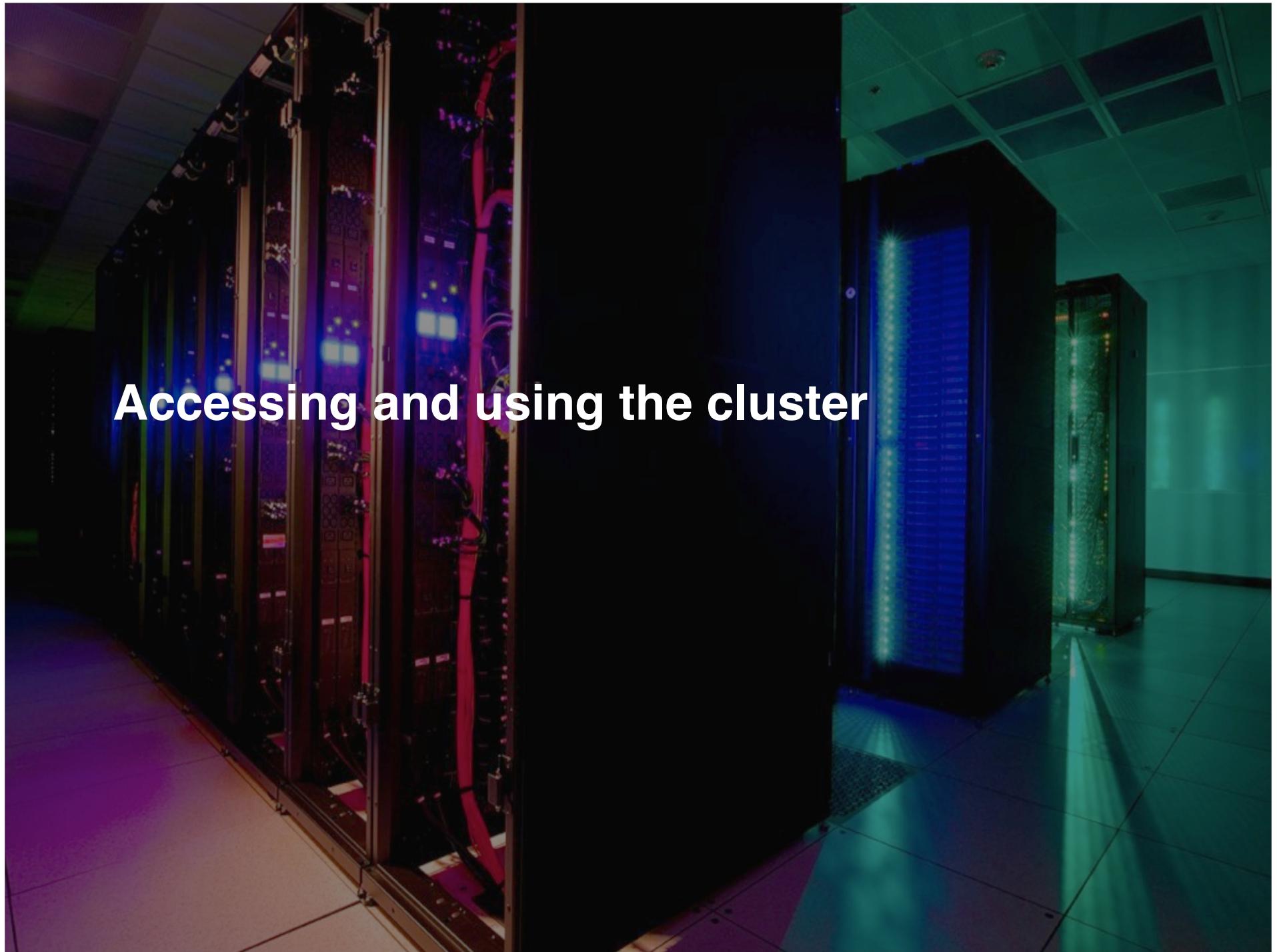
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# HPC Secure Data Account (HDSA)

- HPC researchers who require secure data computation for their projects may additionally apply for an HPC secure data account (HDSA).
  - Data stored in these accounts will be encrypted automatically upon upload and at rest. These accounts allow researchers to work in a secure environment that meets the requirements of HIPAA regulations.
- Researchers requesting a secure data account:
  - Must submit an HDSA agreement.
    - <https://hpcc.usc.edu/files/2012/11/HPC-Secure-Data-Agreement-1.pdf>
  - Must have IRB authorization/approval if they are doing a human subjects study.
  - Must be registered for Duo (two-factor authentication is required).

# Accessing and using the cluster



# Accessing the Cluster

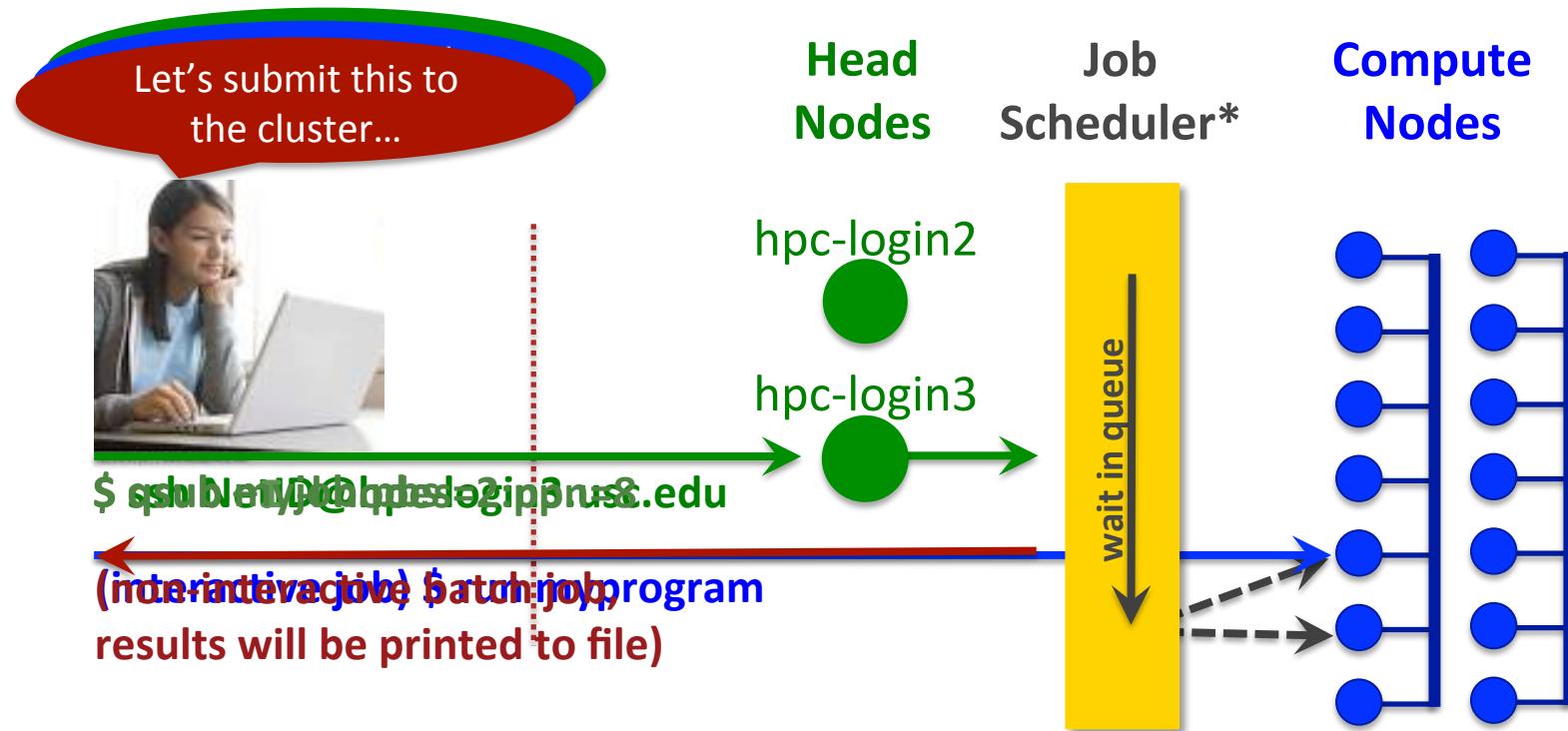
- A secure network is required.
  - Use USC Secure Wireless or USC Ethernet to connect from USC.
  - Use a Virtual Private Network (VPN) client to connect from outside USC.
- A secure shell (ssh) is required for connecting to HPC.
  - The Terminal application is built-in on Macs.
  - There are numerous clients available for Windows.
- A secure file transfer protocol (sftp) is required for transferring data files to/from HPC.
  - There are many applications available for transferring files.
  - HPC has a fast, dedicated Data Transfer Node for this purpose.
- Duo registration is required for secure data accounts.



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# Running jobs on the Cluster



\*HPC uses the TORQUE/PBS resource manager and the Moab cluster scheduler

# Running Jobs on the Cluster

1. Prepare your job on a head node.
  - Download software and data, edit, compile and organize directories.  
(Note that only head nodes can connect to public Internet.)
2. Test your job interactively on a compute node.
  - Set up and test run job, and plan resource allocation request.  
(How much memory? How many nodes/cores?)
3. Run your job on the cluster.
  - Submit your job to the queue via a PBS script.
  - Use monitoring tools and email options to see progress.
  - Results are provided within 24 hours.



## Condo compute node and storage options

# Condo Compute Nodes

- HPC provides the opportunity for USC researchers, who are active HPC account PIs, to condo (purchase) compute nodes.
  - Condo nodes can be purchased through HPC, at any time, if we have new nodes in our existing pool of compute nodes, for the cost we purchased them.
    - *HPC is able to leverage vendors to provide resources at costs typically unavailable to individual research groups.*
  - Condo prices include taxes and three years of vendor support.
  - This is a one time fee. HPC covers infrastructure costs to incorporate these resources into the cluster.



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# Condo Compute Nodes

- Memorandum of Understanding
  - A three year MOU is signed between the researcher and HPC, stating that HPC will manage and maintain these nodes, presenting them as a dedicated queue with dedicated rulesets on the HPC cluster for the duration of the MOU.
  - After the MOU expires, we will continue to manage and maintain the nodes until either we run out of spare parts, or the nodes are decommissioned for our next upgrade. An average condo node is available for approximately five years.



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# Condo Compute Nodes

- Configuration
  - HPC condo nodes are configured for the exclusive use of the condo owner while at the same time remaining part of the HPC cluster.
  - They are configured with a dedicated queue that is only accessible to authorized users, typically all members of the PI's account.
  - The internal storage is for operating system and computational use only and is not presented as standard use storage.



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# Condo Storage

- Similarly, researchers can purchase condo storage through HPC.
  - All storage requires mandatory vendor support on the hardware.
  - A three-year MOU between the researchers and HPC will indicate that HPC will manage, maintain the hardware, and present the file system to the researcher at no additional cost.
  - If you are interested in this option, inform us of the amount of storage required and we will provide a quote from vendors that we have utilized, whose products we know will work with our infrastructure.



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# Condo Storage

- Configuration
  - We provide limited backup of data (up to 100TB) at no cost to the condo owner for nodes using HPC's standard file system type.
    - *Option is not available for file systems like GPFS, Lustre or panfs*
  - The condo storage is only available on the cluster, we do not share the file system outside of HPC.
- Alternatively, researchers can lease storage from USC Digital Repository (DR).
  - USC DR resources are available to both HPC and user space.
  - USC DR is a separate group under ITS. See <http://repository.usc.edu>.

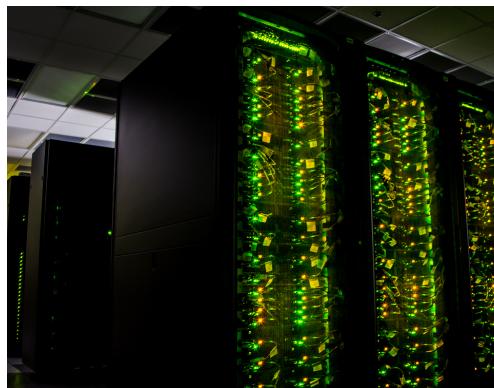


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# Current Pricing

- Please inquire with HPC
  - Pricing and configuration change often so we do not advertise prices on condo nodes or condo storage.
  - We recommend that the users try our general resources first, unless they have large storage needs, then contact us.



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# Grant Proposals

- Start-up budgets
  - General HPC cluster resources are free.
  - Request condo pricing if needed.
- Grant submissions
  - HPC will provide a description of cluster resources and letter of support.
  - A flyer is available from our website.
    - <http://hpcc.usc.edu/research/grant-app/>
  - If condo resources are required, a letter of support detailing your condo requirements and costs will be provided by HPC.



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# HPC Policies



# HPC Policies

- Resource use policies reflect the fact that HPC is a shared resource.
  - There are limits on compute node use:
    - *run time for each job limited to 24 hours*
    - *allocation limited to 99 simultaneous nodes*
    - *number of jobs limited to 1 or 10, depending on node*
    - *the four nodes that allow 300 hour jobs are large memory systems, each with 1TB and 40 cores, and have additional restrictions*
  - There are also limits on cluster access at certain times of the year.
- HPC strictly enforces secure data account regulations and all ITS users must comply with all appropriate laws and regulations.
  - e.g., information security, network use, privacy, copyright compliance

# Downtime Policy

- HPC cluster use is available all year, 24/7, with two exceptions.
  - Approximately every six months, all nodes including condo nodes are brought down for one week, for upgrades and maintenance.
    - *Data on the shared disks are deleted and jobs that have not ended are terminated.*
  - Per the MOU, we provide at least 30 days notice of scheduled downtimes.
    - *Dear HPC Researchers:*  
*From 8:00 a.m. on Monday, May 2, until 9:00 a.m. on Monday, May 9, the entire HPC cluster—including all head nodes, file systems, almaak machines, and compute nodes—will be unavailable for use during our annual spring upgrade.*



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# Downtime Policy

- For example, during the 10/16 downtime we...
  - Performed the following hardware upgrades:
    - *Upgraded the operating system to CentOS on all nodes*
    - *Applied security and firmware patches and ran checks*
    - *Upgraded HPC resource and job schedulers, Torque and Moab*
    - *Upgraded memory on /staging file servers to 64GB*
  - Installed new hardware and software, including:
    - *New versions of software under /usr/usc*
    - *92 Lenovo nx360m5 non-GPU compute condo nodes*
    - *48 Lenovo nx360m5 dual K40 GPU compute nodes*



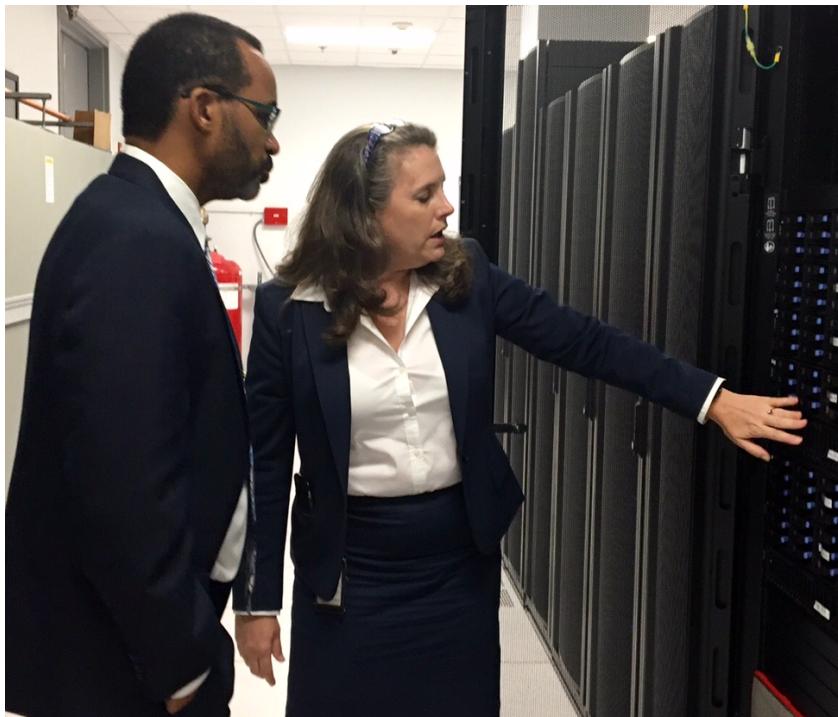
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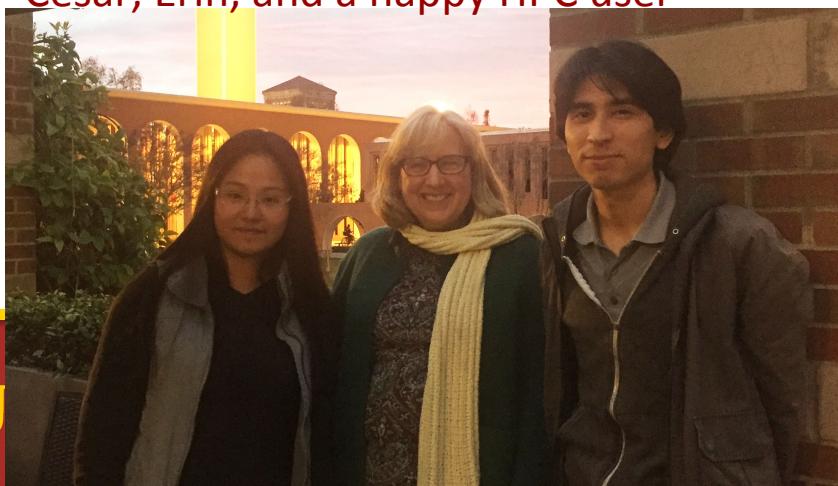


# Facilitation and outreach

## HPC tour with VP Research after orientation



Cesar, Erin, and a happy HPC user



U

Avalon teaching an HPC workshop.



Cesar teaching an optimization workshop



ia

# HPC Facilitation



In 2014, USC and five partnering universities were the recipients of a two-year \$5.3M NSF award to support HPC leadership and two facilitators at each site.

## The ACI-REF Project

Advancing scientific discovery  
through a national network of  
Advanced Cyberinfrastructure  
Research and Education Facilitators



HPC Director Dougherty is a Co-PI.



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# HPC Facilitation

- The addition of two dedicated Facilitators at USC has broadened the services and support levels offered to researchers.
  - Allows us to address high-priority researcher needs, and provide in-depth and/or long-term assistance.
  - Provides the flexibility to address both non-traditional researcher issues and offer broad spectrum knowledge of cyberinfrastructure.
- Facilitators participate in a national network.
  - Share ideas, collaborate on projects, write papers, etc.
  - Clemson U, Harvard, U Hawaii, USC, U Utah, U Wisconsin-Madison, U Oklahoma, U Miami, UCSD, UCB, U Virginia



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# HPC Facilitation

- Examples of solutions that USC Facilitators have provided and the feedback they have received:
  - Assisted a long-time faculty member with 6 terabytes of code and data spanning 20 years in adjusting to changing technology.
    - *... Cesar has been very successful in developing this crucial work-around for RLINE. Thanks are definitely in order.*
  - Assisted a new medical biology student in moving from a tedious laptop workflow to an efficient HPC workflow.
    - *Thank you tremendously for all the help these past few weeks! I was able to analyze a month's worth of data in just a few days!*



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# HPC Facilitation – Assistance with Jobs



Suhn Rhee, Senior Research Associate, Cancer Center

- Was affiliated with multiple research groups and had trouble keeping python environments separate. Provided debugging for ‘virtual environment’ tool.



Jungyeon Kim, Ph.D. Student, Computer Science

- Doing deep learning on millions of tiny images, which was affecting performance for everyone. Showed her how to use an LMDB database to quickly store and access images.



Hoda El Safty, Ph.D. Student, Civil Engineering

- Had irreproducible problem while running code. Showed her how to run debugger and put in checkpoints. Discovered a memory error in the code she was using.



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## Use Case Study: Jasmin Alves

Ph.D. Student, Medical Biology, KSOM  
Researcher in Dr. Katie Page's Lab for Brain  
Regulation of Appetite Control and Eating Behavior



Before: Was analyzing fMRI data on laptop and could not let laptop turn off for weeks.

What we did: Provided HPC and Unix training, helped her install software and run analysis on many patients in parallel.

“Thank you tremendously for all the help these past few weeks! I was able to analyze a month's worth of data in just a few days!”

## Use Case Study: Stephen Pinkerton

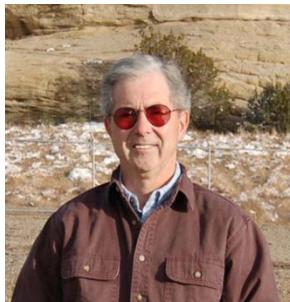
Ph.D. Student, Physics & Astronomy, LASN  
Researcher in Dr. Ed Rhodes' Lab for  
Helioseismology



Before: Significant research computing was done on an old 16 core machine that was being decommissioned.

What we did: Develop workflows to take advantage of increased resources. Found software packages for ones that no longer worked on alternate system.

## HPC Facilitation - Assistance for Labs



Dr. Robert Farley, Professor Biophysics

Students were running 300 hour jobs to create one graph (and needed six). Sent us code for single core job and we analyzed and suggested saving state and also ways to parallelize parameter sweep.



Dr. Erin Baggot Carter, Asst. Prof. International Relations.

Student was web scraping with a single core process. We reprogrammed to run on multiple cores, improving time and efficiency.

## HPC Facilitation - Assistance for Labs



Dr. Stephen Gruber, Prof. Medicine, Director Norris Cancer Center

Helped lab members (8) get started with / transfer data to HPC where new storage array was located.



Dr. Kathleen Page, Asst. Prof. Internal Medicine, Endocrinologist

Helped lab members (4) install FSL and Freesurfer software and configure for HPC.



Dr. Rehan Kapadia, Asst. Prof. Electrical Engineering  
Help lab members (5) with software licensing and running jobs on six new HPC compute nodes.

# HPC Facilitation - Classes, lectures, assignments

## ■ Lectures



- BISC 478 Undergraduate Biological Sciences class, Dr. Andrew Smith, Assoc. Professor
- EE 5xx Graduate Electrical Engineering class, Dr. Rehan Kapadia, Asst. Prof.

## ■ New opportunities



- Spatial Sciences Institute (Online Master's Program).
- Dr. Karen Kemp (Professor (Teaching)), Dr. Jennifer Swift (Assoc. Prof. (Teaching)), Dr. Yao-Yi Chiang (Asst Prof. Research)
- Discussed integrating HPC assignments into curriculum to enable students to do more authentic problems.

# HPC Facilitation

- We recommend speaking with a Facilitator.
  - We find that there is often a need for additional directed discussion and education to ensure that HPC users can be as productive as possible.
  - PIs who feel that this would benefit their team can contact HPC and ask that a Facilitator contact them or their designee to coordinate.
- There are many ways to request assistance.
  - Email [hpc@usc.edu](mailto:hpc@usc.edu) or drop-in to office hours.
    - *UPC office hours are every Tuesday, 2:30pm (LVL 3M)*
    - *HSC office hours are after Wednesday workshops (NML 203)*
  - Request a consultation or getting-started class.
    - *Individual or research lab, remote, at CAL or on-site*



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# HPC Facilitation

- You can also learn more by attending scheduled events.
  - New user meetings
  - Hands-on workshops
    - *We teach 3-5 workshops a month on Linux, HPC, MATLAB, etc.*
    - *Fridays, 2:30-4:30p (UPC) and Wednesdays, 1:30-3:30p (HSC)*
  - Invited speaker talks (Mathworks, Nvidia);
- Activities listed on website.
  - <https://hpcc.usc.edu/education>



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# HPC Outreach

- HPC reaches out to faculty and graduate students through the following venues:
  - We speak at new faculty and department meetings, and at talks like these.
  - We invite researchers to give talks at our Supercomputing exhibition booth each year.
  - We give data center tours.
- Email [hpc@usc.edu](mailto:hpc@usc.edu) to request.



# The End

- Thank you for attending.
- To inquire about something you heard today, please email [hpc@usc.edu](mailto:hpc@usc.edu) or use the ITS service portal ([itsservices.usc.edu](https://itsusc.service-now.com/ess_services))

The screenshot shows the USC ITS Service Portal interface. On the left, there's a sidebar with a red header "Research Computing" featuring a molecular structure icon. Below it, there are sections for "Condo Resources", "General Inquiry", and "Software Management". The main content area has a title "High Performance Computing" and a brief description of the HPC center. To the right, a larger window displays a service request form for "Nodes". The form includes fields for "Required Service" (set to "Nodes"), "Which HPC account will utilize this?", "If nodes are to be added to an existing queue, which queue?", "Do you need accelerators (GPUs/PHI)? Yes or No" (set to "None"), "Quantity of Nodes required" (with a "More information" link), and "Projected Due Date".