Supercomputing Resources at UCSB

Burak Himmetoglu Enterprise Technology Services & Center for Scientific Computing

e-mail: <u>bhimmetoglu@ucsb.edu</u>

Paul Weakliem

California Nanosystems Institute & Center for Scientific Computing

e-mail: weakliem@cnsi.ucsb.edu

http://www.ets.ucsb.edu/services/supercomputing http://csc.cnsi.ucsb.edu



University of California

Santa Barbara



LINIVERSITY OF CALIFORNIA SANTA BARBARA CENTER FOR SCIENTIFIC COMPUTING

Overview

- Triton Shared Computing Cluster (TSCC) at San Diego Supercomputing Center (SDSC)
- Extreme Science and Engineering Discovery Environment (XSEDE)
- UCSB Center for Scientific Computing (CSC) clusters
- Training resources and workshops

TSCC

- Encourages campus participation, allowing researchers to use time and storage space on SDSC computing and data resources.
- UCSB purchases blocks of computer hours which researchers may request from the supercomputing consultant.
- Primarily used for educational purposes, but some groups also use it for research.

TSCC

System Features

General Computing Nodes

Dual-socket, 12-core, 2.5GHz Intel Xeon E5-2680 (coming) and Dual-socket, 8core, 2.6GHz Intel Xeon E5-2670

GPU Nodes

Host Processors: Dual-socket, 6-core, 2.6GHz Intel Xeon E5-2630v2 GPUs: 4 NVIDIA GeForce GTX 980

Interconnect

10GbE (QDR InfiniBand optional)

Lustre-based Parallel File System Access to Data Oasis

http://www.sdsc.edu/support/user_guides/tscc.html

http://www.sdsc.edu/services/hpc/hpc_systems.html#tscc

TSCC

http://www.ets.ucsb.edu/services/supercomputing/triton-shared-computing-cluster-tscc

- Individuals:
 - <1000 hours/yr, used for training and startup
 - Fill the application form at website
 - XSEDE trial and startup allocations recommended!
- Research Groups:
 - Max 40,000 hrs/yr
 - Fill the application form at website
 - XSEDE research allocations and CSC recommended!
- Class accounts:
 - Generally 300-500 hours per student (supplements available)
 - Syllabus, Number of Students and CV of instructor
 - For advanced topics (GPUs, Mapreduce, Hadoop etc.) XSEDE educational allocations can be more appropriate.



Extreme Science and Engineering Discovery Environment

XSEDE is an NSF sponsored service organization that provides access to computing resources.

https://portal.xsede.org

www.xsede.org

Currently XSEDE supports more than a dozen supercomputers and high-end visualization and data analysis resources.



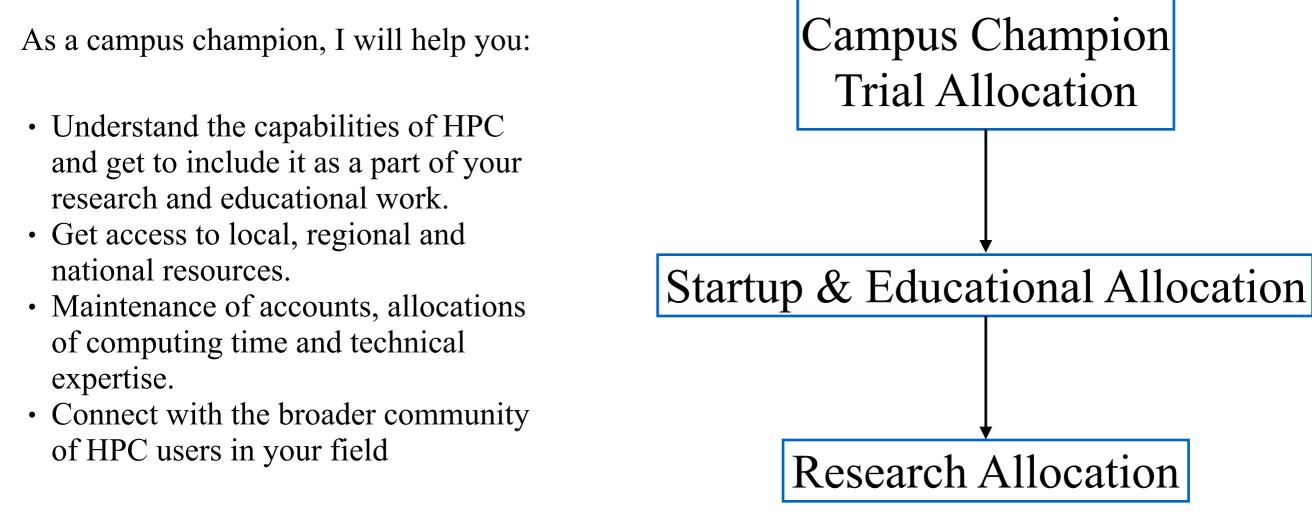
Available XSEDE Resources

	My XSEDE Resources			Jul System Monitor		
	Resource	Status	Load	Username	My Jobs	
Workhorse	Stampede TACC 🛢	✓ Healthy	96%	burak	R: 0 Q: 0 O: 0	
General purpose, more Big Data	Comet SDSC 릗	✓ Healthy	62%	burak	R: 0 Q: 0 O: 0	
Big Data	Gordon Compute Cluster SDSC 릗	✓ Healthy	88%	burak	R: 0 Q: 0 O: 0	
Visualization, data analysis	Maverick TACC 🛢	✓ Healthy		burak		
High throughput	Open Science Grid USC 🛢	✓ Healthy		burak	R: 0 Q: 0 O: 0	
Long term storage	Ranch TACC 🛢	✓ Healthy		burak		
Large memory, big data	Greenfield PSC 🛢	✓ Healthy		himmetog	R: 0 Q: 0 O: 0	

https://www.xsede.org/resources/overview

Campus Champions Program

Represents XSEDE on the campus



https://portal.xsede.org/allocations-overview

Trial Allocation

- Limited number of hours in XSEDE resources available to UCSB through the Campus Champion
- Getting familiar with XSEDE
- Running small tests

To get access

https://portal.xsede.org

- Sign up and get a username
- E-mail your username to the Campus Champion with a short description of your computational needs.

https://portal.xsede.org/allocations-overview

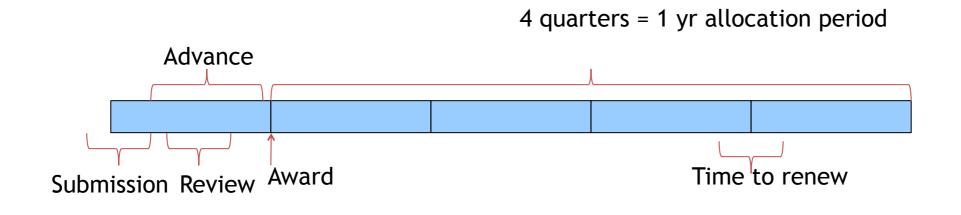
Startup & Educational Allocation

- Requires a one-two page allocation request
- Available all year around
- Available for use ~ two weeks after submission of request
- Max Limit: 200,000 hours per request
- Code development
- <u>Scaling tests</u>
- Training
- <u>Users are expected to apply for Research Allocation after</u> <u>Startup</u>

https://portal.xsede.org/allocations-overview

Research Allocations

- You can get millions of computer hours.
- One PI + researchers (added to the allocation from the portal)
- ~ 10 page research allocation request needs to be submitted
- Awarded 4 times a year
- Renewed each year by a progress report+renewal request

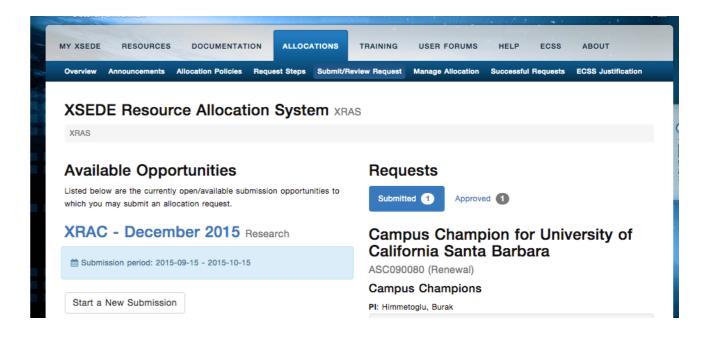


https://portal.xsede.org/allocations-overview

Allocation Periods

SUBMISSION PERIOD	ALLOCATION BEGIN DATE			
Dec 15 thru Jan 15	April 1			
Mar 15 thru Apr 15	Jul 1			
Jun 15 thru Jul 15	Oct 1			
Sep 15 thru Oct 15	Jan 1			

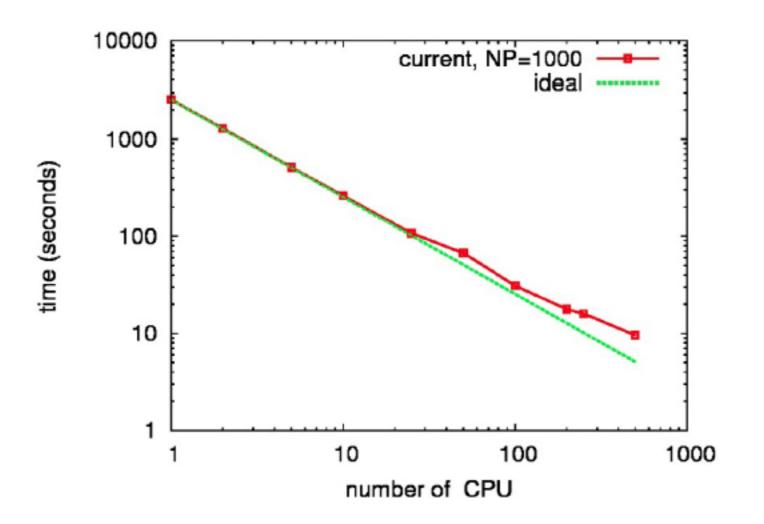
Requests are submitted from the Portal



- Short description of research
- Justification of requested hours
- <u>Scaling tests</u>

Successful allocation requests:

https://portal.xsede.org/successful-requests



Other useful aspects of XSEDE

A nice portal



- Get a username from the portal
- Go to allocations tab, and below you can ask for 1000 hrs from Comet

RESOURCE	TRIAL ALLOCATION LIMIT	REQUEST A TRIAL ACCOUNT
Comet	1000 SUs, 6 months	Please submit an XSEDE help-desk ticket

- Send me your username
- A short description of your computing needs
- You will get limited trial time from any resource!

Other useful aspects of XSEDE

Numerous Training sessions, most of them broadcasted from the web

Training classes

			SEARCH:
START DATE 🔻	END DATE	CLASS NAME	REGISTERED
11/24/2015	11/24/2015	nvidia OpenACC Course (October 1 - November 24, 2015) 😐	Download 🗮
11/13/2015	11/13/2015	R HPC Training 11.13.2015 (Texas Advanced Computing Center)	REGISTER
11/13/2015	11/13/2015	R HPC Training 11.13.2015 😐	REGISTER
11/12/2015	11/12/2015	nvidia OpenACC Course (October 1 - November 24, 2015) 💻	Download 🔛
11/05/2015	11/05/2015	Data sharing from Comet and Gordon clusters using SeedMe.org \square	REGISTER
11/04/2015	11/04/2015	Data sharing from Comet and Gordon clusters using SeedMe.org \square	REGISTER
11/03/2015	11/03/2015	nvidia OpenACC Course (October 1 - November 24, 2015) 💻	Download 🔛
11/03/2015	11/03/2015	XSEDE HPC Monthly Workshop - November 3, 2015 - Big Data (Pittsburgh Supercomputing Center)	SIGN UP FOR WAITLIST
11/03/2015	11/03/2015	XSEDE HPC Monthly Workshop - November 3, 2015 - Big Data (Lehigh University)	REGISTER
11/03/2015	11/03/2015	XSEDE HPC Monthly Workshop - November 3, 2015 - Big Data (University of Houston - Clear Lake)	REGISTER
11/03/2015	11/03/2015	XSEDE HPC Monthly Workshop - November 3, 2015 - Big Data (Harvey Mudd College)	REGISTER
11/03/2015	11/03/2015	XSEDE HPC Monthly Workshop - November 3, 2015 - Big Data (University of Iowa)	REGISTER



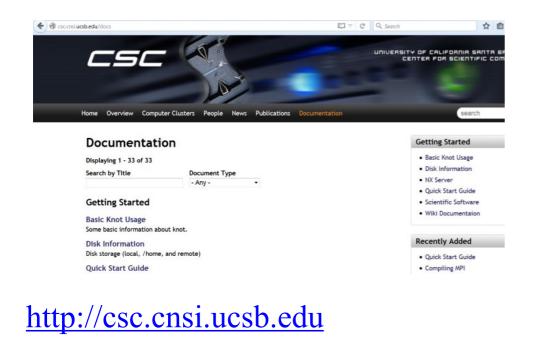
CSC Clusters Campus available clusters: *QSR* (32 node, 4 core Opterons) *Knot* (110 node, ~1400 core) system 4 'fat nodes' (256/512 GB RAM) GPU nodes (12)

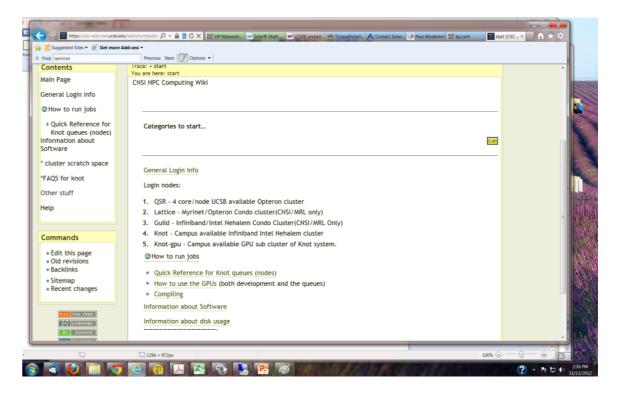




• Free!!

We acknowledge support from the Center for Scientific Computing at the CNSI and MRL: an NSF MRSEC (DMR-1121053) and NSF CNS-0960316.





- Look for wiki
- search









- 'Condo clusters'
 - PI's buy nodes in the clusters
 - □ Lattice (62 node Opteron)
 - Guild (60 node Nehalem)
 - □ Braid (70 node IvyBridge/Haswell and GPUs)
- Groups buy nodes in the cluster, CSC handles infrastructure (disk, network, etc.) and management





- /csc/central for temporary storage
- Globus endpoint (<u>http://globusonline.org</u>)
 - Look for ucsb#knot-storage (can then navigate to / home, /csc directories)

• Move large quantities of connections

ansfer Files				Get Globus Connect Perso Turn your computer into an endpo			
Endpoint pweaklem#ucsb-paul-desktop	Go			Endpoint	ucsb#knot-storage		Go
Path /~/	Go	_		Path	/~/		Go
select all none 🖕 up one folder 🖒 refresh	list	≡	select all	none Ł up	one folder 🖒 refresh list		=
60PXN		Folder *	Abaqusé	9EF1installation		Fo	ider *
Acquisition_Board		Folder	Ansoft			Fo	ider 🗏
BldDirectoryFolder		Folder	Ansoft_F	Projects		Fo	ider
CNSI Networking		Folder	Canopy			Fo	ider
CNSI-ComputingAdmin		Folder	Canopy.	bac		Fo	lder
CNSI-Entire		Folder	E Desktop			Fo	lder
CNSI-images		Folder	Enthoug	ht		Fo	lder
CNSI-psych		Folder	GPUStre	essTest		Fo	lder
CNSI-web		Folder	Helix			Fo	ider
CNT-3		Folder	NAMD 2	2.10 Linux-x86 6	4-ibverbs-smp-CUDA	Fo	lder
Canon Fax Data		Folder	NewFok			Fo	ider
Center		Folder	Python-2	2.7.3		Fo	Ider
Chern10-Winter07		Folder	Results	040412 t1		Fo	lder
ChemComputer		Folder	Results	040412 14		Fo	lder
CommStuff		Folder	MACO	OSX		Fo	Ider
		F				-	



- Local clusters good for development work, 'smaller' jobs.
- Once you exceed the resources, work with Burak to use SDSC, XSEDE resources



Training Sessions at UCSB

- Intel Xeon Phi training will take place in January (2 days)
- Using Python and R in parallel (planned)
- Big Data related subjects: SDSC staff can be invited
- Other requests (e.g. cuda, hadoop etc.)?
- Questions ?