May 3, 2017

XSEDE New User Tutorial



Extreme Science and Engineering Discovery Environment Jay Alameda National Center for Supercomputing Applications

XSEDE Training Survey

- Please complete a short on-line survey about this module at <u>http://bit.ly/xsedejackson</u>. We value your feedback, and will use your feedback to help improve our training offerings.
- Slides from this workshop are available at http://hpcuniversity.org/trainingMaterials/238/



Learning Outcomes

After completing this tutorial, you will be able to:

SEI

- Use the XSEDE User Portal
- Access your XSEDE resources
- Manage files
- Run jobs
- Get help

XSEDE User Portal (XUP)

- URL: portal.xsede.org
- Single point-of-entry to information about XSEDE services and utilities for using them
- Anyone can create an XUP user account and access non-project features
- Only XSEDE allocation project members can access project features

Using the XUP

- Create and login to your XUP Account
- Use XSEDE resources responsibly
- Get added to your XSEDE project
- Navigate your personal My XSEDE webpage

• Navigate the information in the XUP

Create and login to your XUP account

portal.xsede.org

Enter the Portal	
USER NAME	
PASSWORD	
Sign In REMEMBER ME	
Other Sign In Options	ME
$\overline{\boldsymbol{\boldsymbol{\lambda}}}$	

- 1. From the XUP homepage, click CREATE ACCOUNT
- 2. Complete the User Account Form
- 3. Verify your account request
- 4. Select your username and password

5. Login to the XUP

Click the CREATE ACCOUNT link to access the XUP User Account Form

Other Sign In Options

Extreme Science and Engineering Discovery Environment	CiLogon 🥿
XSEDE User Portal" requests that y	rou select an Identity Provider and click "Log On". If you do not approve this request, do not proceed.
By proceeding you agree to share yo	our name and email address with "XSEDE User Portal".
Site Name: Site URL:	XSEDE User Portal https://portal.xsede.org
Service ORL.	https://poltai.ksede.org/delegate/services/ready
	Select An Identity Provider:
	University of Illinois at Urbana-Champaign University of Iowa University of Kansas University of Kansas Medical Center
	Search:
	Remember this selection:
	By selecting "Log On", you agree to Cilcopon's privacy policy.
Fo	r questions about this site, please see the FAQs or send email to help @ cilogon.org

Example: Logging in with Illinois credentials

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Enter y	our NetID: alameda	
Enter your Active Directory (AD)	bassword:	
	Login	
	Forgot your Active Directory password?	
	To change or reset your Active Directory password, go to the <u>CITES</u>	
Nore Information		
Where to Cat Usin	Technical Information	



Link your campus identity and portal identity

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MY XSEDE Summary Allocations/Usage	Connect RESOURCES Systems Monitor Remote	DOCUMENTATION > Get Started > Access	ALLOCATIONS	Create TRAINING > Overview > Course Calendar	USER FORUMS	HELP > Overview > Help Desk	ABOUT > Welcome > Portal Password	

Login to the portal to link identities

https://portal.xs/	ede.org/cilogc 🔎 👻	🔒 🖻 🖒 🔀 XSEDE U:	ser Port 🔀 XSED	E User Port 🔀 XSED	E User Port 🔀 XS	EDE User Port 🔀 XS	EDE User P ×	□ × ∰
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Summary Allocati	ons/Usage Accounts	s Jobs Profile Put	blications Tickets	Change Password A	dd User Communit	y Accounts SSH Terr	minal	
Please log in to	o your XSEDE accou	unt to proceed. This	will connect your F	Federated Identity Pro	vider			
account with yo	our XSEDE account.							
You will only h	ave to do this one ti	me After connecting	your accounts w	hon you log in Eedera	tod			FE
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Summary	- Designation					- Halo Daak	- HOTTOL LOCOMORD	
Summary Allocations/Usage Accounts	> Remote Visualization	Access	> Allocation Policies	> Course Calendar		Security Incident	Reset	

And inspect your new linked identity, via user profile

MY XSEDE RESOURCES	DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS	HELP ABOUT
Summary Allocations/Usage	Accounts Jobs Profile Publications Tickets Change Password Add User Co Jay Alameda University of Illinois at Urbana-Champaign N.C.S.A. Center Researcher Staff MC 257 - 1008 NCSA 1205 W. Clark St. Urbana Illinois 61801 United States Jalameda@ncsa.illinois.edu	OMMUNITY Accounts SSH Terminal Publications Add a new publication • No publications to display
	work: 217-244-4696 Demographic information XSEDE collects this information for reporting purposes to the NSF and other governing bodies. Your personal information will not be reported with this demographic information. Gender: Not Specified Race: Not Specified	
	Other XSEDE Login Identities To add a new identity please login to portal.xsede.org and select 'Other Login Options'. IDENTITIY STATUS CN=Jay Alameda A7281, O=University of Illinois at Urbana-Champaign, C=US, DC=cilogon, DC=org Display Inactive Logins	

XSEDE Acceptable Use Policy

- Must accept the <u>User Responsibilities Form</u> after creating your XUP account and again at the beginning of each allocation you receive.
 - Available on the portal Documentation, Usage Policy https://portal.xsede.org/web/xup/usage-policy
- Choose a strong password and protect it.
- Close SSH terminals and log out of the User Portal when you are finished with your session.
- Report Suspicious Activity : email <u>help@xsede.org</u> or call 1-866-907-2383 immediately, regardless of the time of day.

XSEDE Cybersecurity Tutorial

https://portal.xsede.org/web/xup/online-training

Get Added to Your XSEDE project

- PIs automatically have full access to their project's account.
- The PI is responsible for managing users on their account.
- Ask the PI, or their allocation manager, to add your XUP username to the project.

Your My XSEDE webpage

MY XSEDE RESOURCES DOCUMENTATION ALLOCATIONS TRAINING USER FORUMS HELP ECSS ABOUT Publications Tickets SSH Terminal Summary Allocations/Usage Accounts Jobs Profile Change Password Add User Community Accounts Share your feedback on XSEDE Training Services with a quick 5 question survey! Share the impact of XSEDE!

- For all publications, please acknowledge your use of XSEDE and allocated resources and add publications your User Profile
- Tell us about your achievements with XSEDE
- Help us improve our reporting by keeping your XSEDE User Profile up to date and completing the demographic information



(1)

Welcome to the XUP

 Quick access to commonly used features.

(2) Latest updates

Latest information specific to your user account.

(3)

•

My Resources and Allocations

Summary of the active projects for which you are either a PI or member.



Update your XUP User Profile

MY XSEDE→Profile

- View and or change your user information (organization, address).
- Make sure your email address is correct. XSEDE staff will use it to communicate with you regarding your allocation.

Summary Alloca	tions/Usage	Accounts	Jobs P	Profile	Publications	Tickets	Change	Password	Add User	Communi	ty Accounts	SSH Terminal
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Navigating the XUP



- My XSEDE
- Resources
- Documentation
- Allocations

- Training
- Help
- About

SEDE

View the XSEDE Systems Monitor

Resources -> Systems Monitor

- Provides technical and status information for all of XSEDE's resources.
- The STATUS column indicates whether the system is up or down. If down, can click on status to find when the machine is expected to come back up.

ystems Monitor Re	emote Visualization	File Manager	Software Queue Pre	ediction Science Ga	teways Scheduled Do	wntimes	
	Second Second						
🗱 Compute	Resources					1	
Name	Status	CPUs	Peak TFlops	Utilization	Running Jobs	Queued Jobs	Other Jobs
Stampede ₽ ∳ User Guide	✓ Healthy	102400	9600.0	67%	334	2202	129
comet ⊒ ⁰ User Guide	✔ Healthy	47616	2000.0	86%	1560	6481	109
(Stream	✓ Healthy	1300	1001.7	78%	262	174.	225

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Accessing XSEDE Resources



Authentication Methods

- 1. Password
 - XUP credentials
 - Site-password
 - One-time password
- 2. Key-based

Single Sign-On

Enables logging in once to access all of your allocated resources

SEI

Connection Methods

- 1. GSI-OpenSSH
- 2. OpenSSH

XSEDE SSO Login Hub



SSH to login.xsede.org using your XUP credentials with 2 Factor Authentication

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Set up 2 Factor Authentication



• After logging into the XSEDE User Portal, select your profile

XSEDE

Adding 2 Factor Authentication





What is Duo?

🔀 XSEDE User Portal | My x 🔀 XSEDE User Portal | My x 🔀 XSEDE User Portal | Prot x

← C a Secure https://portal.xsede.org/group/xup/profile#

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What is Duo?

Duo Enrollment Details

You can choose to protect SSH login attempts to your accounts at certain XSEDE Service Providers that have implemented XSEDE Multi-Factor Authentication (XSEDE MFA) using your XSEDE portal account username/password as the primary authentication factor and Duo Security Authentication as the secondary authentication factor. What is 19µ/2

It is strongly encouraged that you register at least 2 authentication devices so that in case you lose one, you have another way to authenticate with Duo and replace the lost token, Example: Your mobile device/phone + desk phone.

Currently, SSH access for the following XSEDE systems can be protected in this fashion.

- XSEDE SSO (Single SignOn) Hub at login.xsede.org
- NICS Darter SP duo.darter.nics.xsede.org

You would be able to login to the above systems using your XSEDE portal usemane and password in conjunction with Duo Authentication. Other types of authentication that you might currently use such as GSI authentication (X 609 certificates), Public Key, etc., will NOT be affected by enrollment in XSEDE MFA. Raher, enrolling in XSEDE MFA enables an additional authentication method, a multi-factor authentication method as described above, for login to the above mentioned Service Provider systems

Please note that the protection offered by XSEDE MFA is currently limited to certain SSH login attempts to the above systems and as such is NOT a comprehensive solution that protects your access to all XSEDE resources from a compromise of your XSEDE password (or Duo authentication factor if you erroll in XSEDE MFA). One significant omission is the XSEDE MyProxy service which will continue to issue certificates with just XSEDE portal username/password authentication. XSEDE may enlarge the scope of protection offered by XSEDE MFA to other types of access to XSEDE resources in the future. If you erroll in XSEDE MFA and find that it negatively impacts your workflow, you can come back to the profile page and cities on Unenroll from Duo

To opt in to protect above SSH access using Duo Security, please click on the Enroll button below. To later opt out of Duo Security protection, return to the profile page and click on Unerroll from Duo. You will be able to manage your Multi-Factor Authentication methods/devices after initial enrollment by returning to the profile page and clicking on Manage Duo. To report a lost authentication token/device or to request assignment of a hardware token or for any other issues related to your enrollment in XSEDE MFA, please submit a help desk ticket or send an email to help@xsede.org.

ENROLL

Note that DUO 2 Factor Authentication is required for access to the XSEDE Single Signon Hub

- Select enroll



Duo Enrollment:

DEU	SEF	} P	OR	TAL	94 1					Search
RESOURCES	DOCUN	IENTAT	ION	ALLOCATIONS	TR	AINING	USER	FORUMS	HELP	ECSS
Allocations/Usage	Accounts	Jobs	Profile	Publications	Tickets	Change	Password	Add User	Community	Account
				Duo	« Back Enrol	Iment				
			To proce	ed, please verify	your XS	EDE Use	r Portal pas	ssword		
				Password		S	ивміт			

 To verify your identity in your current session, you will need to enter your XSEDE User Portal password

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 Start the process of setting up 2 factor authentication

XSEDE

Choose the device for 2 Factor Auth



- Mobile Phone is recommended
 - Tablet, Landline also OK (though not preferred)

SEDE

Connect Duo to your phone

age Accounts Jobs	Profile Publicati	ons Tickets	Change Password	Add User	Community Accounts	55
			Iment			
Please setup v	our device(s) then	slick 'Login'	at the final step to	complete er	rollment	
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XSEDE	Entery	our pho	ne number			
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1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	+1					
	ex	(201) 234-567	8			
	Back					
	Data					

• Add phone number

SEDE

- Continue

Verifying phone number ownership



Duo calls your phone
Enter code from Duo call to your phone

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Download Duo app (if desired)



- Set authentication method (push, text, call)
 - And continue to login

SEDE

Choose authentication method

		. Back		
	Duc	Enrollment		
 Please setup your	device(s), then clic	k 'Login' at the final step to	complete enrollment.	
XSEDE	Choose an a	uthentication method		
What is this? Ef	Duo Pust	n RECOMMENDED	Send Me a Push	
Add a new device My Settings & Devices Need help?	🛞 Call Me		Call Me	
Powered by Duo Security	Passcode		Enter a Passcode	

• Duo push (to app)

SEDE

- Call phone
- Text passcode

Success!



Indication of successful setup

XSEDE

Following along with today's tutorial:

- Verify that everyone has an ssh client on their laptop!
- For ssh to XSEDE SSO login hub (today!) ssh –l username login.xsede.org username on handout
- And from there go to your XSEDE resource, for example:

SEI

gsissh comet.sdsc.edu

2 factor authentication



Managing your XSEDE files

1. Where to store files

- Home directory
- Scratch directory
- Archival storage

2. How to move files

- Command line using globus-url-copy, uberftp, scp, or sftp
- Globus Online







XSEDE File Systems

Home directory

- Location specified in the environment variable \$HOME.
- Use to store project files you want to keep long term such as source code, scripts, and input data sets.
- Not backed up regularly and not purged.
- Quotas typically set to limit amount of disk space available.

Scratch directory

- Location specified in environment variable varies among resources but will include the term SCRATCH, e.g. \$SCRATCH_DIR.
- Use to temporarily store files produced during application runs.
- Not backed up and routinely purged.
- No quotas. Available space depends on cumulative use by all users.
- Archival storage
 - Must request through allocation process

Your XSEDE Compute Environment

- Your default XSEDE compute environment provides access to the compilers, directories, and software you will need to efficiently use your XSEDE resources.
 - Environment: An area of a computer's memory used by the operating system and some programs to store certain variables to which they need frequent access
- Customize environment using Modules
 XSEDE Customizing Environment Tutorial https://portal.xsede.org/web/xup/online-training
Modules Package

- A command line interface used to configure the shell for an application. Two components:
 - 1. Modulefiles contain configuration information
 - 2. Module command interprets modulefiles
- Pre-written modulefiles available for compilers, mpi implementations
- Pre-written modulefiles available for common software, e.g. NAMD, GAMESS

Module Commands

Module command	Description
module avail [path]	List all modulefiles available on the system.
module list	List the modulefiles currently loaded in the shell environment.
module help modulefile	Print help information for the modulefile specified in the argument.
module display modulefile	Display the changes made to the environment when the specified modulefile is loaded.
module load modulefile	Interpret the commands contained within the specified modulefile.
module switch modulefile1 modulefile2	Remove the environment changes made by modulefile1 and make the changes specified in modulefile2 .
module unload modulefile	Remove the environment changes made by modulefile .



Module Commands Example





Moving Files - Globus

- A fast, reliable, and secure file transfer service geared to the big data needs of the research community.
- Moves terabytes of data in thousands of files
- Automatic fault recovery
- Easy to use
- No client software installation
- Consolidated support and troubleshooting
- Supports file transfer to any machine
- Accounts are free <u>https://www.globus.org/</u>

Globus Dashboard



Focus on your research, not IT problems. We make it easy to move, manage, and share big data.

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GET GLOBUS PLUS



Globus gives you more control over your data infrastructure, while providing excellent ease-of-use for your

researchers LEARN MORE

GLOBUS PROVIDER PLANS

Globus' tools and services help connect people and HPC resources, so that no researcher is an island.

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LEARN MORE

Login to use Globus Web App

🞐 glo	bus	Globus Account Log	j In	
	Log in to use Globus Web App			
	Use your existing organizational login			
	e.g. university, national lab, facility, project, Google or Globus ID (Your Globus username and password used prior to February 13, 2016 is now Glob	us ID)		
	Look up your organization	*		
	Continue			
	Why has this page changed?			
	Didn't find your organization? Then use Globus ID to sign up.			

Use XSEDE Identity Provider



XSEDE

Sign in with XSEDE credentials

XSEDE User Portal Delega ×	Jay — — ×
← → C _ https://oa4mp.xsede.org/oauth/authorize?oaut	th_token=myproxy%3Aoa4mp%2C2012%3Aoauth1%3A%2FtempCred%2F1 🖉 📣 🚍
Extreme Science and Engineering Discovery Environment	
Welcome to the XSEDE's Client Authorization Page	
Science Gateway Access The XSEDE Science Gateway or Service below is requesting access to you Note: Only members of active XSEDE project allocations will be able to sig	ur XSEDE account. If you approve, please sign in with your XSEDE username and password. In in on this page.
SCIENCE GATEWAY INFORMATION	SIGN IN
The XSEDE Science Gateway listed below is requesting access to your XSEDE account. If you approve, please sign in.	Username Password
Name: Globus URL: http://www.globus.org/	SIGN IN CANCEL
Please send any questions or comments about this site to help exsect one	



Globus Online File Transfer

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Choosing a file to move...

globus		Manage Data Groups Sup	port jalameda
		Transfer Files Activity Manage Endp	ooints Dashboard
ransfer Files		Get Turn you	Globus Connect Personal r computer into an endpoint.
Endpoint xsede#comet Go		Endpoint xsede#blacklight	× Go
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select all none 🖕 up one folder 💪 refresh list	=	select all none L up one folder C refresh lis	st 📃
intel	Folder	PweTest	Folder
newfolder	Folder	shallow-sr1-kepler-jan2014	Folder
shallow	Folder	shallow-trestles-icc	Folder
shallow-12jun2014	Folder	shallow_43_SR2_SEA	Folder
shallow-43-SR2-nightly	Folder	trainingSC12_C	Folder
shallow-SR1_kepler_try2	Folder	ptp_job.e1286924	96 b
shallow-SR2-RC1-23jan2014	Folder		
n shallow-gordon-icc	Folder		
shallow-luna-SR1-RC4-candidate	Folder		
shallow-luna-sr1-rc1-candidate	Folder		
shallow-sr1-kepler-jan2014	Folder		
shallow-trestles-icc	Folder		
shallow-trestles-icc-43SR2	Folder		
shallow_43_SR2_SEA	Folder		
test-synch	Folder		
trainingSC12_C	Folder		
a.out	7.84 kB		
hellompi-slurm.sb	341 b		
ptp_job.e1286924	96 b 🗸		
ptp_job.e1286961	837 b		

Running Jobs Overview



Compute Nodes

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Login Nodes

- When you login to an XSEDE resource, you connect to a login node.
- Use login nodes for basic tasks such as file editing, code compilation, data backup, and job submission.
- Do not run compute jobs on the login nodes.



Running Compute Jobs

- Jobs are run on the compute nodes by submitting a batch script on a login node
- All jobs are placed in a batch queue after they are submitted.
- All XSEDE compute resources use a batch scheduler for running jobs.
- Resource User Guides on the XUP have details on your system's scheduler.

Batch Scripts

- Batch scripts include scheduler specific directives, comments, and executable commands, e.g.:
 - Number and type of nodes needed
 - Time needed to run the job
 - Where to write output files
- Script commands are system specific see the resource's User Guide on the XUP for details

Batch Script for PSC's Blacklight

- 1. #!/bin/csh
- **2.** #PBS -1 ncpus=16
- 3. #ncpus must be a multiple of 16
- **4. #PBS** -1 walltime=5:00
- 5. #PBS -j oe
- 6. #PBS -q batch
- 7. set echo
- **8.** ja
- 9. #move to my \$SCRATCH directory
- **10.** cd \$SCRATCH
- 11. #copy executable to \$SCRATCH
- 12. cp \$HOME/mympi
- 13. #run my executable
- 14. mpirun -np \$PBS_NCPUS ./mympi
- 15. ja -chlst

Blacklight uses the Portable Batch System (PBS) scheduler. Lines 2,4,5, and 6 are PBS directives.

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Submitting Batch Scripts

- Commands are machine specific, but follow general principles
- With PBS batch scripts, use the qsub command qsub myscript.job
- Can also specify PBS directives as commandline options:

qsub -1 ncpus=16 -1 walltime=5:00 -j oe -q batch myscript.job

SEI

• Command-line directives override directives in your scripts.

More PBS commands

• qstat - displays the status of batch jobs.

-a	gives the status of all jobs on the system.
qstat -n	lists nodes allocated to a running job in addition to basic information.
qstat -f PBS_JOBID	gives detailed information on a particular job.
-q	provides summary information on all the queues.

 qdel – deletes a queued job or kills a running job.

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• See the qsub manpage for more

Example Batch Command

qsub amb	per.job									
qstat -a										
Job ID	Username	Queue	Jobname	SessID N	NDS	Tasks	Memory	Time	S Tim	е
29668	user1	batch	job2	21909	1	256		08:00	R	02:28
29894	user2	batch	run128		1	128		02:30	Q	
29895	user3	batch	STDIN	15921	1	1		01:00	R 00	:10
29896	user2	batch	jobL	21988	1	2048		01:00	R 00:	09
29897	user4	batch	STDIN	22367	1	2		00:30	r 0	0:06
29898	user1	batch	amber	25188	1	1		01:10) R	
00:00	C									

qdel 29668

• After job 29898 runs: user1 should get file amber.job.o29898 with output/errors (log file)

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Job Scheduling

- All XSEDE compute resources use a batch scheduler for running jobs.
- All jobs are placed in a batch queue after they are submitted.
- Resource User Guides on the XUP have details on your system's scheduler.

Batch Schedulers

• Attempt to balance queue wait times of competing jobs with efficient system utilization.



- Job prioritization influenced by number of cores and wall clock time requested
- FIFO queues with fair use mechanisms to keep a single user from dominating the queue
- Backfilling unused nodes with smaller jobs
- Will not start jobs if they will not finish before scheduled system maintenance.

Common problems encountered when running jobs:

- Invalid number of cores were requested
- Job runs out of CPU time
- Files can't be found
- Inadequate software permissions

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Improving job turnaround

- Request accurate walltime
- Use flexible walltime
- Pack your job
 - Running many small jobs places a great burden on the scheduler and is also inconvenient for you.
 - Pack many executions into a single job, which you then submit to PBS with a single qsub command.

Requesting flexible walltime

- -1 walltime_min=HH:MM:SS
- -1 walltime max=HH:MM:SS

Example: Your job requests 64 cores and a walltime between 2 and 4 hours. If there is a 64 core slot available for 3 hours, your job could run in this slot. However, if your job had requested a fixed walltime of 4 hours it would not run until the larger time slot becomes available.

Packing Serial Jobs

Run each program execution in the background and place a wait command after each execution.

```
#!/bin/csh
#PBS -1 ncpus=96
#PBS -1 walltime=5:00
#PBS -q batch
dplace -c 0 ./myserial1 < serial1.dat &
dplace -c 32 ./myserial2 < serial2.dat &
dplace -c 64 ./myserial3 < serial3.dat &
wait
```

Packing OpenMP Jobs

To pack OpenMP executables, replace the dplace command with the omplace command. Sample job to pack OpenMP executables:

```
omplace -nt 32 -c 0 ./myopenmp1 < myopenmp1.dat &
omplace -nt 32 -c 32 ./myopenmp2 < myopenmp2.dat &
omplace -nt 32 -c 64 ./myopenmp3 < myopenmp3.dat &
omplace -nt 32 -c 96 ./myopenmp4 < myopenmp4.dat &
wait</pre>
```

Managing Your Environment: Modules

- Allows you to manipulate your environment.
- 'module list' shows currently loaded modules.
- 'module avail' shows available modules.
- 'module show' <name> describes module. http://modules.sourceforge.net/

```
% module load gcc/3.1.1
% which gcc
/usr/local/gcc/3.1.1/linux/bin/gcc
```

```
% module switch gcc/3.1.1 gcc/3.2.0
% which gcc
/usr/local/gcc/3.2.0/linux/bin/gcc
```

```
% module unload gcc
% which gcc
gcc not found
```



For the following exercise (same steps as before):

- Check to see if connection is still live, if not:
- For ssh to XSEDE SSO login hub (today!) ssh –l username login.xsede.org username on handout
- And from there go to your XSEDE resource, for example:

SEI

gsissh comet.sdsc.edu

SDSC comet Cluster & Modules

- Default environment intel compilers, mvapich2 MPI implementation
- We will swap intel compilers with gnu compilers
 - module swap intel gnu
 - which gcc
- And then we'll load the openMPI library module load openmpi_ib which mpicc



Module demo on comet

```
-bash-4.1$ module swap intel gnu
Unloading compiler-dependent module tau/2.23
Need to load an mpi module before loading fftw/2.23
Unloading compiler-dependent module pdt/3.20
Unloading compiler-dependent module papi/5.4.1
Unloading compiler-dependent module tau/2.23
Need to load an mpi module before loading fftw/2.23
-bash-4.1$ module list
Currently Loaded Modulefiles:
 1) gnutools/2.69 2) globus/5.2.5
                                         3) gnu/4.9.2
                                                                4) .intel/tau/2.23
-bash-4.1$ module load openmpi ib
-bash-4.1$ which mpicc
/opt/openmpi/gnu/ib/bin/mpicc
-bash-4.1$
```

XSEDE

Using modules in your job script

• First,

source /usr/share/Modules/init/shell-name module load module-name

SFI

Check on-line documentation

Exercise

- Make sure you are on comet.sdsc.edu
- Run the shallow water model code provided
- No input file needed
- Copy batch script from my home directory:
 cp ~ux400689/shallow-slurm.sb .

Job script

```
#!/bin/bash
#SBATCH --job-name="shallow"
#SBATCH --output="shallow.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=5
#SBATCH --export=ALL
#SBATCH -t 00:30:00
```

#This job runs with 1 nodes, 5 cores per node for a total of 5 cores. #ibrun in verbose mode will give binding detail

ibrun -v ~ux400689/shallow/shallow



Exercise:

- Submit the job (sbatch --res=JSUResDay1 shallow-slurm.sb)
- Monitor the job (squeue –u *username*)
- Make sure you have the output files at job completion

-bash-4.1\$ lscalc.c decs.h eclipse.inc Makefile shallow-batch.sh tstep.f90calc.o diag.c init.c shallow shallow-slurm.sb tstep.ocopy.c diag.o init.o shallow.582135.comet-03-56.out time.c worker.ccopy.o dump.c main.c shallow.591445.comet-04-66.out time.o worker.oCVS dump.o main.o shallow.591474.comet-04-66.out tstep.c -bash-4.1\$

more shallow*out (for this case, yours will be different!)

Output files: need to show successful completion

📲 Remote System Details 🛛 Tasks 🧬	Terminals 🛛 🔥 Re	mote Environments			
🕼 login.xsede.org 🖾					
jstart=0, jend=7, next jstart=8, jend=15, nex jstart=16, jend=23, nex jstart=24, jend=31, nex	=2, prev=4 t=3, prev=1 xt=4, prev=2 xt=1, prev=3				
Shallow water weather i	model - Distr	ributed Memory	Version 0.6		
Number of points in the	e X direction	n 32			
Number of points in the	e Y direction	n 32			
Grid spacing in the X	direction	100000.00			
Grid spacing in the Y	direction	100000.00			
Time step		90.000			
Time filter parameter		0.001			
Cycle number 1 1	Model time in	n days 0.00			
Potential energy	0.000 k	Kinetic Energy	48036.828		
Total Energy	48036.828 F	Pot. Enstrophy	0.000000e+00		
Cycle number 50 H	Model time ir	n days 0.05			
Potential energy	1256.284 k	Kinetic Energy	46526.969		
Total Energy	47783.254 F	Pot. Enstrophy	-nan		
Cycle number 100 N	Model time ir	n days 0.10			
				1,1	Тор

Need help? Reporting and Tracking Issues

- portal.xsede.org → Help
 Submit ticket
- portal.xsede.org \rightarrow My XSEDE \rightarrow Tickets
 - Submit ticket
 - View past tickets (both open and closed)
- Can also email help@xsede.org or call 1-866-907-2383, at any hour (24/7)

More "helpful" resources

xsede.org \rightarrow User Services

- Resources available at each Service Provider
 - User Guides describing memory, number of CPUs, file systems, etc.
 - Storage facilities
 - Software (Comprehensive Search)
- Training: portal.xsede.org → Training
 - Course Calendar
 - On-line training
- Get face-to-face help from XSEDE experts at your institution; contact your local Campus Champions.

 Extended Collaborative Support (formerly known as Advanced User Support (AUSS))
XSEDE Training Survey

- Please complete a short on-line survey about this module at <u>http://bit.ly/xsedejackson</u>. We value your feedback, and will use your feedback to help improve our training offerings.
- Slides from this workshop are available at http://hpcuniversity.org/trainingMaterials/238/

May 3, 2017

Thanks for listening and welcome to XSEDE!



Extreme Science and Engineering Discovery Environment