

Introduction to High-Performance Computing (HPC) at USC

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Advanced Cyberinfrastructure Research and Education Facilitation

USC Center for High-Performance Computing

Welcome!

- Sign in at <https://goo.gl/Qan5Kg>
- Presentation handouts are available on HPC
 - /home/rcf-proj/workshop/handouts
- Log in and cd to your project directory
- Make a workshop directory and copy the course materials
 - \$ mkdir workshop
 - \$ cd workshop
 - \$ cp -r /home/rcf-proj/workshop/intro-hpc/* .
- Ask questions!



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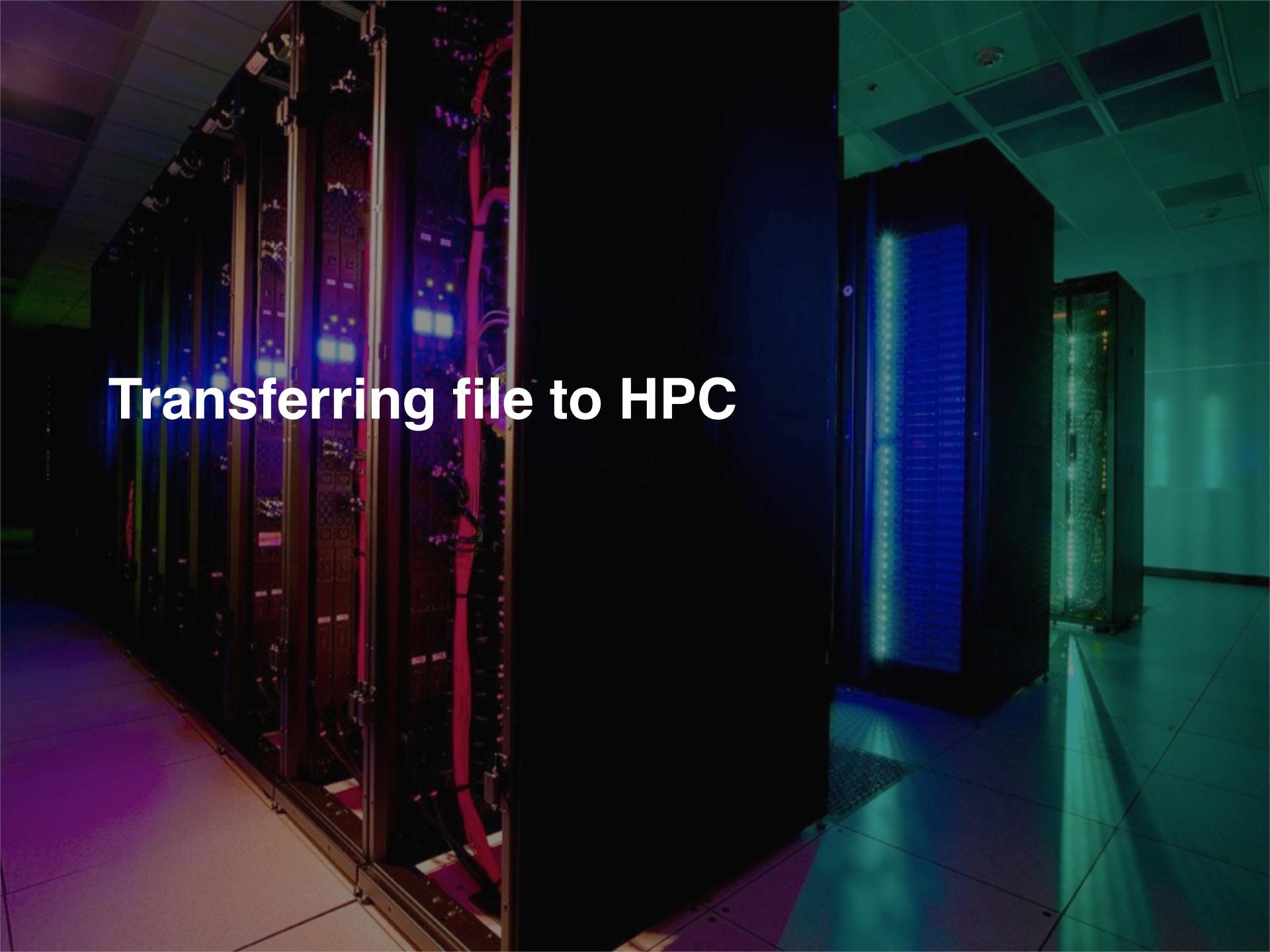
Outline

- Setup
- Running /usr/usc programs
- Running interactive jobs
- Monitoring jobs
- Running batch jobs
- Running MPI jobs
- Other slides...



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A photograph of a server room filled with tall server racks. The racks are illuminated from within, showing glowing blue and green lights along their vertical sides. The floor is a polished grey, and the ceiling is white with recessed lighting. The overall atmosphere is dark and tech-oriented.

Transferring file to HPC

Transferring files

- Between HPC and Linux/macOS computers (small files)
 - scp
 - sftp (command line, FileZilla, Cyberduck,...)
- Between HPC and Linux/macOS computer (large files)
 - rsync
 - High speed transfer utilities: Globus, ascp, bbcp,...
- Between HPC and Google Drive and OneDrive
 - rclone
- From Internet to HPC
 - wget, git clone, curl



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Transferring files

- Documentation for setting up FileZilla
 - [hpcc.usc.edu -> Documentation -> Transferring Data -> Transferring Files between Your Computer and HPC](#)
- Let's practice by downloading workshop slides to your laptop
 - [/home/rcf-proj/workshops/handouts/](#)
 - *HPCIntroHPC-yyymmdd.pdf*



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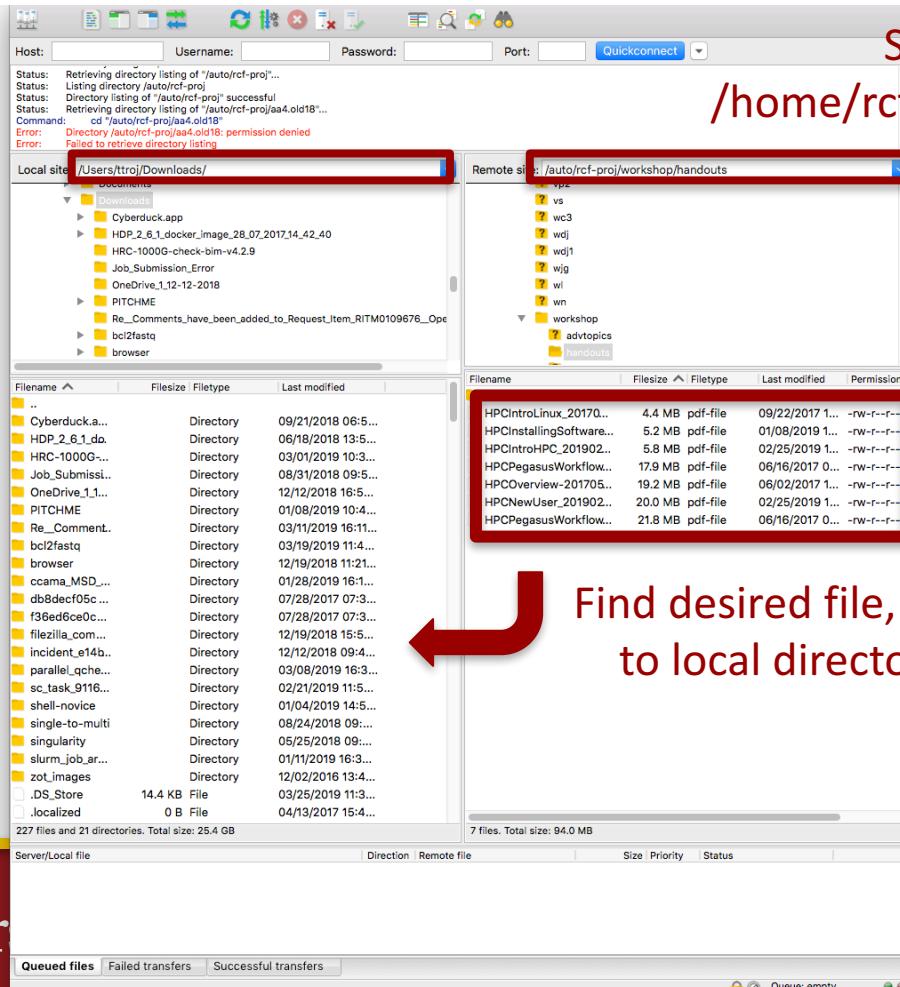
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Transferring files

- Download remote file to your computer

Set local path

Set remote path to
/home/rcf-proj/workshops/handou



Find desired file, drag to local directory



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Running programs on HPC

- software under /usr/usr

Software repository: /usr/usc

- HPC installs and maintains university licensed and other commonly used software in /usr/usc
 - Compilers: *gnu, intel, pgi*
 - Numerical libraries: *mpich, openmpi, cuda, fftw, petsc*
 - Molecular simulation: *NAMD, gromacs, amber*
 - Quantum chemistry: *gaussian, schrodinger*
 - Numerical computation: *MATLAB, Python*
 - Statistical computing: *R, SAS, Stata*
- You can also install software in your project directory
 - HPC can help with this



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Software repository: /usr/usc

- Let's take a field trip to the software repository

```
$ ls -F /usr/usc
```

acml/	cmake/	glog/	jdk/	mpich/	petsc/	schrodinger/
amber/	conf/	gnu/	julia/	mpich2/	pgi/	sgems/
antiword/	cuda/	graph-tool/	lam/	mpich-mx/	protobuf/	singularity/
aspera/	cuDNN/	gromacs/	lammps/	mvapich2/	pstotext/	sox/
bazel/	cula/	gurobi/	leveldb/	NAMD/	python/	stata/
bhcp/	dict@	hadoop/	libroadrunner/	ncview/	qchem/	subversion/
bcl2fastq/	dmtcp/	hdf5/	llvm/	netcdf/	gespresso/	swig/
bin/	etc/	hdfview@	lmod/	netcdf-fortran/	qiime/	taxila/
blast/	fdtd/	hello_usc/	lua/	nwdb/	QT/	tdk/
boost/	fftw/	hpctoolkit/	magma/	opencv/	R/	tensorflow/
caffe/	gaussian/	igraph/	mathematica/	OpenGeos/	root/	trilinos/
cellprofiler/	gcc_wrap/	imp/	matlab/	openmpi/	ruby/	udunits/
cellranger/	gflags/	intel/	modulefiles/	papi/	rust/	valgrind/
CGAL/	git/	iperf/	mongo2k/	patchelf/	samtools/	VisIt/
clang/	globus/	java@	moose/	perl/	sas/	



Software repository: example

- Let's run the program `hello_usc`

```
$ ls /usr/usc/hello_usc  
1.0/ 2.0/ 3.0/ @default  
  
$ ls -l /usr/usc/hello_usc  
<listing>  
  
$ ls /usr/usc/hello_usc/default  
bin/ setup.csh setup.sh  
  
$ ls /usr/usc/hello_usc/default/bin  
hello_usc*
```



Software repository: example

- What happens when I run the program?

```
$ hello_usc
```

```
-bash: hello_usc: command not found
```

- Bash cannot find a program named hello_usc because it is not in your path (\$PATH)

```
$ which hello_usc
```

- “which” searches \$PATH

- echo \$PATH

- Exercise: What happens if you type echo PATH?



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Software repository: example

- Setup scripts add a directory to your path

```
$ source /usr/usc/hello_usc/2.0/setup.sh
```

```
$ which hello_usc
```

```
/usr/usc/hello_usc/2.0/bin/hello_usc
```

```
$ hello_usc
```

```
Hello USC!!!
```

```
I am version 2.0 running on host: hpc-login3
```



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Software repository: setup.sh

What is in the setup script?

```
$ cat /usr/usc/hello_usc/2.0/setup.sh
1. HELLO_PREFIX=/usr/usc/hello_usc/3.0
2. PATH=${HELLO_PREFIX}/bin:$PATH
```

What happens?

1. The variable HELLO_PREFIX is set to the location of your program (/usr/usc/hello_usc/3.0)
2. The location \${HELLO_PREFIX}/bin is then prepended to your current path (\$PATH). Bash will find the program when it searches your path.



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Software: system vs. /usr/usc programs

- Try this

```
$ which python3  
/usr/bin/python3
```

```
$ source /usr/usc/python/3.6.0/setup.sh
```

```
$ which python3  
/usr/usc/python/3.6.0/bin/python
```



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Software: system vs. /usr/usc programs

- Some programs and libraries (python, gcc, fftw) are installed with Linux and are updated when OS updates are installed
 - The **name** is the same as the one under /usr/usc but the programs may differ in version, libraries used, developer, etc.
 - Researchers should not use the OS version if they want reproducible results!
- Check that the software you use is correct
 - HPC creates a “default” symlink when it installs programs under /usr/usc/. The “default” version is the most recently installed and tested version of the software
 - We recommend that you replace “default” symlinks in /usr/usc/, with actual version numbers when you write your job script

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Running jobs on the cluster

- Interactive jobs

6. Running on HPC: Easy as 1-2-3!

1. Plan ahead

- Organize project directory
- Install software, transfer data
- Think about your job requirements
 - amount of memory
 - number of i/o files
 - size of data

2. Test interactively

- Use salloc/srun
 - test run commands
 - check paths, results
- Experiment with resource allocation
 - number cores (cpus)
 - amount of memory
- Start small, then scale
- Prepare Slurm script
 - e.g., myjob.slurm

3. Run remotely

- Submit your job to the queue:
`$sbatch myjob.slurm`
- Monitor your job to make sure it starts
`$myqueue`
`$squeue --user <uname>`
- Check results
`$less slurm-<jobid>.out`



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Running a job interactively

- Let's request resources

- cd to your workshop directory and type the following

```
$ salloc --ntasks=8 --time=00:20:00
salloc: Granted job allocation 991
salloc: Waiting for resource configuration
```

- While we're waiting for our resources...

- open a second terminal window and log in to a head node



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Running a job interactively (2 windows)



```
erinshaw@hpc2283 workshop]$ source /usr/usc/hello_usc/  
1.0/ 2.0/ 3.0/ default/  
[erinshaw@hpc2283 workshop]$ source /usr/usc/hello_usc/2.0/  
bin/ setup.csh setup.sh  
shrinshaw@hpc2283 workshop]$ source /usr/usc/hello_usc/2.0/setup.  
[erinshaw@hpc2283 workshop]$ which hello_usc  
/usr/usc/hello_usc/3.0/bin/hello_usc  
[erinshaw@hpc2283 workshop]$ hello_usc  
  
Hello USC!!!.  
I am version 3.0 running on host: hpc2283  
  
[erinshaw@hpc2283 workshop]$
```

This is your original hpc-login shell

When ‘salloc’ succeeds, a shell on
your compute node will open here

Run your program here



```
top - 23:29:58 up 31 days, 10:32, 1 user, load average  
Tasks: 227 total, 1 running, 226 sleeping, 0 stopped  
Cpu(s): 0.0%us, 0.0%sy, 0.0%ni,100.0%id, 0.0%wa, 0.  
Mem: 12190944k total, 956000k used, 11234944k free,  
Swap: 8388604k total, 61900k used, 8326704k free,  
  
 PID USER      PR  NI    VIRT    RES    SHR S %CPU %MEM  
1676 erinshaw  20   0 13132 1324  920 R  0.3  0.0  
2073 root     20   0 100m 52m 10m S  0.3  0.4  
  1 root     20   0 19232 1016  824 S  0.0  0.0  
  2 root     20   0      0    0    0 S  0.0  0.0  
  3 root     RT   0      0    0    0 S  0.0  0.0  
  4 root     20   0      0    0    0 S  0.0  0.0
```

Now open a new window and log in
to head node (...ssh hpc-slurm)

Monitor your program here
(\$squeue or \$scontrol)

You can ‘ssh hpcxxx’ to your
compute node from here



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Got compute nodes?

```
[ttrojan@hpc-login3 ~]$ salloc --ntasks=8 --time=00:20:00
```

```
salloc: Granted job allocation 991
```

```
salloc: Waiting for resource configuration
```

```
salloc: Nodes hpc0981 are ready for job
```

```
-----  
Begin SLURM Prolog Tue 27 Feb 2018 09:49
```

```
Job ID: 991
```

```
Username: ttrojan
```

```
Accountname: lc_tt1
```

```
Name: sh
```

```
Partition: quick
```

```
Nodes: hpc[0981,1407]
```

```
TasksPerNode: 8
```

```
CPUSPerTask: Default[1]
```

```
TMPDIR: /tmp/991.quick
```

```
Cluster: uschpc
```

```
HSDA Account: false
```

```
End SLURM Prolog
```

Slurm Prolog: Things to notice

Job ID:

An useful number (give to us when ticketing)

Name: sh

Indicates an interactive job (typically job name)

Nodes: hpc0981 hpc1407

Shell opens on first node, run your commands here

TMPDIR:

This is an environment variable you can use for moving data on and off the compute node

SCRATCHDIR: (When there are multiple nodes)

This is an environment variable you can use for sharing files across programs on multiple nodes



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Got compute nodes!

- We can now test our program on the cluster

```
hpc1736 $ source /usr/usc/hello_usc/3.0/setup.sh
```

```
hpc1736 $ which hello_usc  
/usr/usc/hello_usc/3.0/bin/hello_usc
```

```
hpc1736 $ hello_usc  
Hello USC!!!  
I am version 3.0 running on host: hpc1736
```



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Monitoring jobs on the cluster

Job monitoring

\$ **myqueue** Display jobs status and allocated node list for your jobs

On login nodes only: Use **squeue -u <me>** on compute nodes

\$ **squeue -u ttrojan**

JOBID	PARTITION	NAME	USER	ST	START_TIME	NODES	SCHEDNODES	NODELIST
937	quick	sh	ttrojan	R	2018-02-26T14:27:03	1	(null)	hpc0981

Column **ST** displays the job status

PD (pending) job is queued and waiting to be executed

R (running) job is currently running

CD (completed) job has completed

Job monitoring

```
$ squeue -j <job_id> --start
```

Displays approximate start time for <job_id>

```
$ scontrol show job <job_id>
```

Display status properties of <job_id>

#Look for problems with your job

```
$ scontrol show job {jobid}
```

```
$ squeue --start --job {jobid}
```

JOBID	PARTITION	NAME	USER	ST	START_TIME	NODES	SCHEDNODES	NODELIST
937	quick	star-lac	ttrojan	PD	2018-02-26T14:27:03	2	(null)	hpc0981



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Processes

- When you run a program on HPC, one or more processes are created
- You can view the processes running on a node

```
$ ps -aux
```

```
$ top
```

```
$ htop
```

(Can you find the sysadmin? ;)

- You can view node information, too.

```
$ head -5 /proc/cpuinfo
```

```
$ head -2 /proc/meminfo
```



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Linux processes

\$top

```
top - 11:39:54 up 5:35, 30 users, load average: 1.11, 0.86, 1.67
Tasks: 568 total, 1 running, 567 sleeping, 0 stopped, 0 zombie
%Cpu(s): 2.3 us, 0.8 sy, 0.0 ni, 96.8 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
KiB Mem : 65765680 total, 2707772 free, 6511936 used 56545972 buff/cache
KiB Swap: 8380412 total, 8297468 free, 82944 used. 58724840 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
25769	geoffret	20	0	300400	27840	4040	S	72.5	0.0	1:45.34	python
30194	geoffret	20	0	697836	33776	4352	S	8.6	0.1	14:22.32	python2.7
45495	skchoudh	20	0	1061960	368020	11924	S	5.0	0.6	16:56.82	snakemake
28078	alanjuar	20	0	151692	2660	1096	S	3.6	0.0	2:01.84	sshd
28210	alanjuar	20	0	182956	6244	4004	S	3.0	0.0	1:56.38	ssh
26361	shaoyent	20	0	119512	2932	1464	S	1.7	0.0	0:00.57	htop
35095	ztchu	20	0	151584	2488	1052	S	1.0	0.0	0:15.40	sshd
5118	root	20	0	160880	2632	1632	S	0.7	0.0	2:16.67	top
5702	root	20	0	0	0	0	S	0.7	0.0	2:05.83	kworker/1:2
26447	erinshaw	20	0	160752	2740	1580	R	0.7	0.0	0:00.10	top
28811	dcampo	20	0	160892	2872	1624	S	0.7	0.0	1:16.21	top
10	root	20	0	0	0	0	S	0.3	0.0	1:04.32	rcu_sched
3342	mdougher	20	0	160860	2872	1620	S	0.3	0.0	0:24.85	top



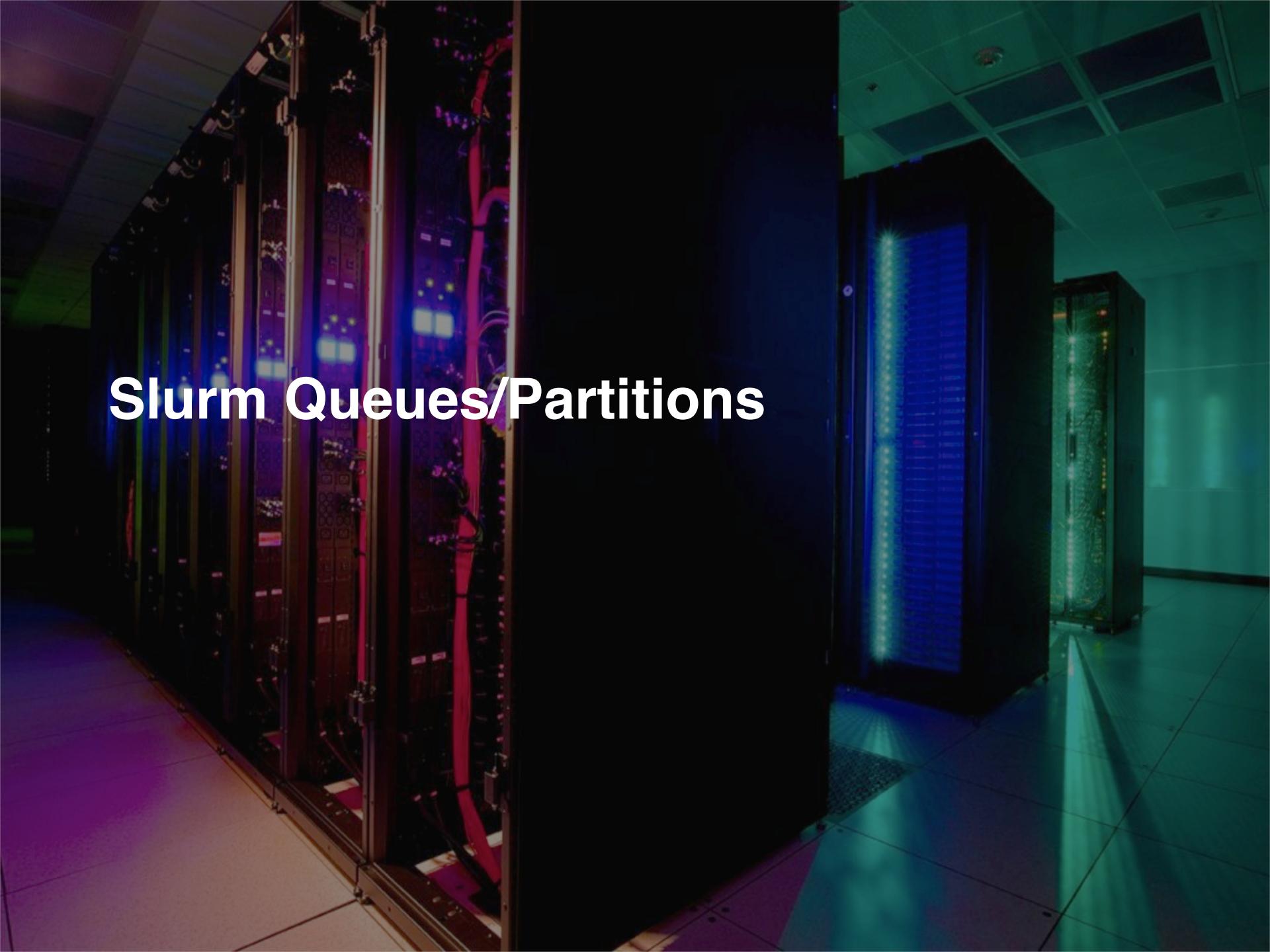
Linux processes

\$ htop

```
1 [|||     8.0%] 3 [|||     6.0%] 5 [|||     20.9%] 7 [|||     19.9%
2 [|||     7.4%] 4 [|||     9.3%] 6 [|||     21.6%] 8 [|||     18.8%
Mem[|||||||||||||||||711M/15.5G]
Swp[|          2.58M/8.00G] Tasks: 152, 74 thr; 1 running
                                Load average: 1.53 1.38 1.27
                                Uptime: 05:07:43
```

PID	USER	PRI	NI	VIRT	RES	SHR	S	CPU%	MEM%	TIME+	Command
3490	bk_143	20	0	149M	3668	984	S	10.7	0.0	1:03.03	sshd: bk_143@notty
3908	scottcal	20	0	263M	12388	4244	D	5.3	0.1	2:33.76	python /home/scec-00/
9997	georgiou	20	0	9568	1408	1168	S	4.7	0.0	0:00.41	bash /home/rcf-42/geo
9757	joshuakl	20	0	143M	2504	1932	S	2.7	0.0	0:00.34	wget ftp://ftp.sra.eb
3491	bk_143	20	0	71048	3196	2028	S	2.0	0.0	0:11.06	scp -r -t /staging/gr
15681	rahromos	20	0	148M	3208	1016	S	2.0	0.0	2:11.16	sshd: rahromos@notty
10229	georgiou	20	0	141M	27048	1164	S	1.3	0.2	0:06.55	/home/rcf-42/georgiou
9646	erinshaw	20	0	118M	2516	1796	R	1.3	0.0	0:00.41	htop
17801	mdougher	20	0	156M	2736	1840	S	1.3	0.0	0:14.36	top
15682	rahromos	20	0	70680	2664	1936	S	0.7	0.0	0:58.22	/usr/libexec.openssh/
20297	root	20	0	156M	2692	1748	S	0.7	0.0	0:47.19	top
1769	root	20	0	679M	38920	5684	S	0.7	0.2	0:10.27	/usr/bin/python /usr/
10791	root	20	0	147M	5680	4396	S	0.0	0.0	0:00.03	sshd: zlan [priv]
10019	georgiou	20	0	148M	2336	992	S	0.0	0.0	0:00.89	sshd: georgiou@pts/8
763	root	20	0	463M	11492	6812	S	0.0	0.1	0:01.91	/usr/sbin/NetworkMana
1784	munge	20	0	221M	2732	1560	S	0.0	0.0	0:00.64	/usr/sbin/munged --ke
27894	bk_143	20	0	147M	2172	884	S	0.0	0.0	0:00.13	sshd: bk_143@pts/0

Slurm Queues/Partitions



HPC queues/partitions

- There are 4 default queues in the general (public) partition
 - A partition is automatically selected for you based on wall time and node count
 - Each partition has different constraints

Queue Name	Maximum Wall Time	Max Node Count	Max Jobs/User
main	24 hours	99	10
quick	2 hours	4	10
large	24 hours	256	1
long	336 hours	1	1
largemem (must request)	336 hours (14 days)	1	1
scavenge (must request)	168 hours (7 days)	500 cores	200



HPC queues/partitions

- General queue: 'largemem'
 - --partition=largemem
 - Requests from pool of 4 40-core 1TB nodes
- Private queues
 - --partition=<name>
 - Research labs with condo nodes have private partitions with their own constraints

Queue Name	Maximum Wall Time	Max Node Count	Max Jobs/User
main	24 hours	99	10
quick	2 hours	4	10
large	24 hours	256	1
long	336 hours	1	1
largemem (must request)	336 hours (14 days)	1	1
scavenge (must request)	168 hours (7 days)	500 cores	200

HPC queues/partitions

- General queue: 'scavenge'
 - --partition=scavenge
 - Requests idle private partition nodes
 - Short wait time, jobs may be preempted
- See compute node allocation table on website
 - <https://hpcc.usc.edu/support/infrastructure/node-allocation/>

Queue Name	Maximum Wall Time	Max Node Count	Max Jobs/User
main	24 hours	99	10
quick	2 hours	4	10
large	24 hours	256	1
long	336 hours	1	1
largemem <small>(must request)</small>	336 hours <small>(14 days)</small>	1	1
scavenge <small>(must request)</small>	168 hours <small>(7 days)</small>	500 cores	200

Queue monitoring

■ Inspect jobs in queue

```
squeue
```

```
squeue --user ttrojan (myqueue, on head nodes)
```

```
sacct -a --allocations --partition=main,large,quick,long |  
grep FAILED
```

■ Inspect job status

```
sacct -a --allocations --partition=main,large,quick,long | grep FAILED
```

```
sacct --format=jobname%20,elapsed,maxrss%8,ntasks%4,allocgres%50,allocgres
```



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Queue monitoring

■ Inspect node status

`sinfo`

`sinfo --help` (or “`man sinfo`” for full manual page)

`sinfo --partition=main`

PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
main	up	1-00:00:00	3	drain*	hpc[3210,3780,4659]
main	up	1-00:00:00	1	down*	hpc3211
main	up	1-00:00:00	1	drng	hpc4433
main	up	1-00:00:00	2	drain	hpc[4434,4665]
main	up	1-00:00:00	677	alloc	hpc[0965-0969,0981-1012,1015-1020,1040,11
main	up	1-00:00:00	36	idle	hpc[1013-1014,1021,1041-1050,1123-1126,11

`sinfo --partition=main --states=idle`

`sinfo --partition=main --states=idle -o "%6t %N %10G" | grep -e gpu`



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Running jobs on the cluster

- Batch jobs

Slurm batch jobs

- **Batch jobs**
 - Batch jobs are not interactive, they are submitted to Slurm and run automatically on compute nodes according to the instructions you provide in a shell script
 - *A bash script is a text file containing commands that are interpreted by bash and then run*
 - Your nodes are released when your job finishes
- **Example**
 - Copy the directory and files in helloUSC/ to your workshop directory

```
$ cp -r /home/rcf-proj/workshop/intro-hpc/* .  
$ cd helloUSC/  
$ ls
```

Example batch job: HelloUSC

- Try this:

```
$ nano helloUSC.slurm
```

- Edit the script

- What is "#SBATCH --export=none"?
 - Change the path

- Submit the job and check results

```
$ sbatch helloUSC.slurm  
$ squeue -user {userid}  
$ ls  
$ cat slurm_{jobid}.out
```

- Exercise: Edit job script so that it runs on multiple cores

Slurm sbatch options

Syntax	Meaning
--account=<account>	Which account to charge cpu time
--partition=<partition_name>	Which partition to submit to, for condo owners
--ntasks=<amount>	Number of CPUs to use
--mem_per_cpu=<amount>	RAM per CPU
--gres=gpu:<GPU_TYPE>:<amount>	Type and number of GPU to request
--time=<amount>	How long job will run
--constraint=<attribute>	Node property to request (avx, IB, xeon)
--mail-user=<email>	Where to send email alerts
--mail-type=<BEGIN END FAIL REQUEUE ALL>	When to send email alerts
--output=<out_file>	Name of output file
--error=<error_file>	Name of error file
--job-name=<job_name>	Job name

For more details see <https://slurm.schedmd.com/sbatch.html>

Slurm environment variables

- Slurm sets a number of environment variables

Slurm	Meaning
SLURM_JOB_ID	Job ID
SLURM_SUBMIT_DIR	Directory job was submitted from
SLURM_JOB_NODELIST	File containing allocated hostnames
SLURM_NTASKS	Total number of cores for job
SLURM_SUBMIT_HOST	Hostname job was submitted from

- See more environment variables

```
$ env | grep SLURM
```

- <https://slurm.schedmd.com/sbatch.html>

Example batch job: HelloMe.sh

- From your workshop directory

```
$ cd helloMe
```

- Run the script

```
$ ./helloMe.sh
```

- Edit the script, follow the exercise and re-run

```
$ nano helloMe.sh
```

```
$ ./helloMe.sh #argument?
```



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Examples batch job: HelloMe.slurm

- Edit the slurm script

```
$ nano helloMe.slurm
```

- Submit the job and check results

```
$ sbatch helloMe.slurm
```

```
$ squeue --user {user}
```

```
$ ls
```

```
$ cat helloMe_{jobid}.out
```



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Requesting GPUs

- Create hellogpu.slurm and submit
- View output

```
#!/bin/bash
#SBATCH --export=none
#SBATCH --ntasks=8
#SBATCH --mem-per-cpu=1G
#SBATCH --time=00:02:00
#SBATCH --gres=gpu:2

# change to your project directory
cd /home/rcf-proj/{myproj}/{mydir}

# source setup file (setup.csh for tcsh)
source /usr/usc/intel/default/setup.sh
source /usr/usc/openmpi/1.8.8/setup.sh.intel
source /usr/usc/cuda/default/setup.sh

# run command
srun nvidia-smi
srun helloWorldMPI
```



The background image shows a server room with multiple rows of server racks. The racks are dark, but the interior components are illuminated with a bright blue light, creating a glowing effect. The floor is made of polished tiles, and the ceiling has a grid of recessed lighting.

Running jobs on the cluster

- Parallel jobs

Got CPU cores?

- How many CPU cores did we run on? Assume one, unless:
 - You are running a multi-core/node application
 - (e.g., *MATLAB*)
 - Your code has multi-core/node support because you are using a library that supports parallel processing
 - (e.g., '*parallel*' for *R*)
- I requested 4 cores, how do I use them?
 - “Pleasingly parallel” (formerly, “embarrassingly parallel”)
 - *Little or no effort is needed to separate the problem into a number of parallel tasks. This is often the case where there is little or no dependency or need for communication between those parallel tasks, or for results between them*

```
hpc1736 $ srun hello_usc
```



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What is MPI*?

- MPI = Message Passing Interface
 - MPI is a *specification* for the developers and users of message passing libraries (for parallel programming).
 - MPI library *implementations* differ in which version and features of the MPI standard they support.
- USC HPC supports OpenMPI
 - And mpitch and mvapitch for compatibility
 - MPI will be covered in the next level HPC course

*<https://computing.llnl.gov>

Using MPI interactively

Let's compile and run an OpenMPI program

```
hpc2062: cp /home/rcf-proj/workshop/introSlurm/helloMPI/* .
```

```
hpc2062: ls
```

```
compile.sh* helloMPI.c helloMPI.slurm README
```

```
hpc2062: cat compile.sh
```

```
#!/bin/sh
```

```
CC=mpicc make helloMPI
```

```
hpc2062: source /usr/usc/openmpi/1.8.8/setup.sh
```

```
hpc2062: ./compile.sh
```

```
mpicc helloWorldMPI.c -o helloWorldMPI
```

```
hpc2062: ls
```

```
compile.sh* helloWorldMPI* helloWorldMPI.c helloMPI.slurm README
```

Using MPI interactively

Results of OpenMPI program

```
hpc2062: which mpirun
```

```
/usr/usc/openmpi/1.8.8/bin/mpirun
```

```
hpc2062: srun ./helloMPI      #use srun instead of mpirun
```

```
Hello World from rank 1 running on hpc2062!
```

```
Hello World from rank 2 running on hpc2062!
```

```
Hello World from rank 3 running on hpc2062!
```

```
Hello World from rank 0 running on hpc2062!
```

```
MPI World size = 8 processes
```

```
Hello World from rank 4 running on hpc2081!
```

```
Hello World from rank 5 running on hpc2081!
```

```
Hello World from rank 6 running on hpc2081!
```

```
Hello World from rank 7 running on hpc2081!
```



Using MPI in batch mode

- Create helloMPI.slurm and submit
- View output

```
#!/bin/bash
#SBATCH --export=none
#SBATCH --ntasks=8
#SBATCH --mem-per-cpu=1G
#SBATCH --time=00:10:00

# change to your project directory
cd /home/rcf-proj/{myproj}/{mydir}

# source setup file (setup.csh for tcsh)
source /usr/usc/openmpi/1.8.8/setup.sh

# run command
#mpirun -np 2 helloWorldMPI
srun -n2 helloWorldMPI
srun -n3 helloWorldMPI
```



Note about node attributes myri and IB

- HPC has two clusters (interconnects)
 - Myrinet (myri) and Infiniband (IB)
 - The networks are not connected to each other
- If the interconnect attribute is not specified, HPC will use any set of nodes that allow your job to start, starting with myri nodes

```
#SBATCH --constraint=myri
```

```
#SBATCH --constraint=IB
```
- Warning!
 - Codes compiled to use MPICH will only run on the Myrinet nodes
 - OpenMPI codes will run on either



A dark server room filled with tall server racks. The racks are illuminated from within, showing glowing blue and green lights along their vertical sides. The floor is a polished grey, and the ceiling is a standard drop ceiling with recessed lighting. The overall atmosphere is mysterious and high-tech.

HPC Downtime.... coming soon!

HPC Downtime Policy

- Twice a year HPC brings the cluster down
 - Add new machines
 - Remove old machines
 - Install patches
 - Upgrade software
 - General maintenance.
- This will never come at a good time!
 - Plan your job submission in advance -- queue will get busy!
 - Clear your data from staging when asked to do so.
 - No exceptions!



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Upgrades for downtime April 2019

- **Update the operating system on all compute nodes and head nodes.** We will apply security and operating system patches on head nodes, compute nodes, the file servers, run file system checks on the majority of the HPC file systems, and install firmware patches on various storage devices.
- **Make default symbolic link (symlink) changes for software installed under /usr/usc to newer versions.**
- **Update head node IP addresses.**
- **Add 68 HPE XL170 or x86 (non-GPU) compute condo nodes to the Infiniband cluster.** The x86 nodes will have dual processor/twelve-core Intel Xeon 4116 2.1GHz CPUs, 2 terabyte (TB) internal drives, and 192 gigabytes (GB) of memory. These new nodes utilize the Intel Skylake chipsets and a 56 gigabit per second (Gbps) Infiniband connection.



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The background image shows a server room with multiple rows of server racks. The racks are dark-colored with glowing blue and green lights from within, indicating active hardware. The floor is a light-colored tile, and the ceiling has a grid of recessed lighting.

Learning more



lynda.com

Want to learn more?

Watching: **The working directory**
From: Unix for Mac OS X Users with Kevin Skoglund

In playlist Exercise files Share Take a tour Use classic layout

Terminal -- bash -- 80x28
ksmac:~ kevin\$

Finder File Edit View Go Window Help

DEVICES PLACES

Name Desktop Documents Downloads Library Music Pictures Public Sites

9 items, 20.49 GB available

Search this course Search Course details Transcript FAQs

My notes Beta

The working directory

In this chapter we're going to take a look at the Unix file system and how we can work with files and directories. I want to start that off by talking about the concept of the working directory. This is an important concept. It's the directory where we are right now. So when we issue commands, it's important to know which working directory we are in, because that's where those

Expand all Collapse all

- Introduction 3m 57s
- Introduction 1m 14s
- Using the exercise files 2m 43s
- 1. Introduction to Unix 32m 2s
- What is Unix? 7m 27s
- The terminal application 4m 23s

- Up and Running with Bash Scripting
 - Unix for Mac OS X Users
 - Using Regular Expressions
 - Perl 5 Essential Training
 - R Statistics Essential Training
 - C/C++ Essential Training
 - Up and Running with Python
 - Python 3 Essential Training
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- and More!

Want to learn more?

<https://carpentries.org>



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We teach foundational coding and data science skills to researchers worldwide.



What we do

The Carpentries teach foundational coding, and data science skills to researchers worldwide. Software Carpentry, Data Carpentry, and Library Carpentry workshops are based on our lessons. Workshop hosts, Instructors, and learners must be prepared to follow our [Code of Conduct](#).

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Who we are

We are a diverse, global community of [volunteers](#). Our community includes [helpers](#), [Trainers](#), [Mentors](#), [community champions](#), [organisations](#), supporters, workers, staff and a whole lot more.

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HPC Carpentry: Teaching basic skills for high-performance computing.

HPC Carpentry is a set of teaching materials designed to help new users take advantage of high-performance computing systems. No prior computational experience is required - these lessons are ideal for either an in-person workshop or independent study.

NOTE: This is the draft HPC Carpentry release. Comments and feedback are welcome.

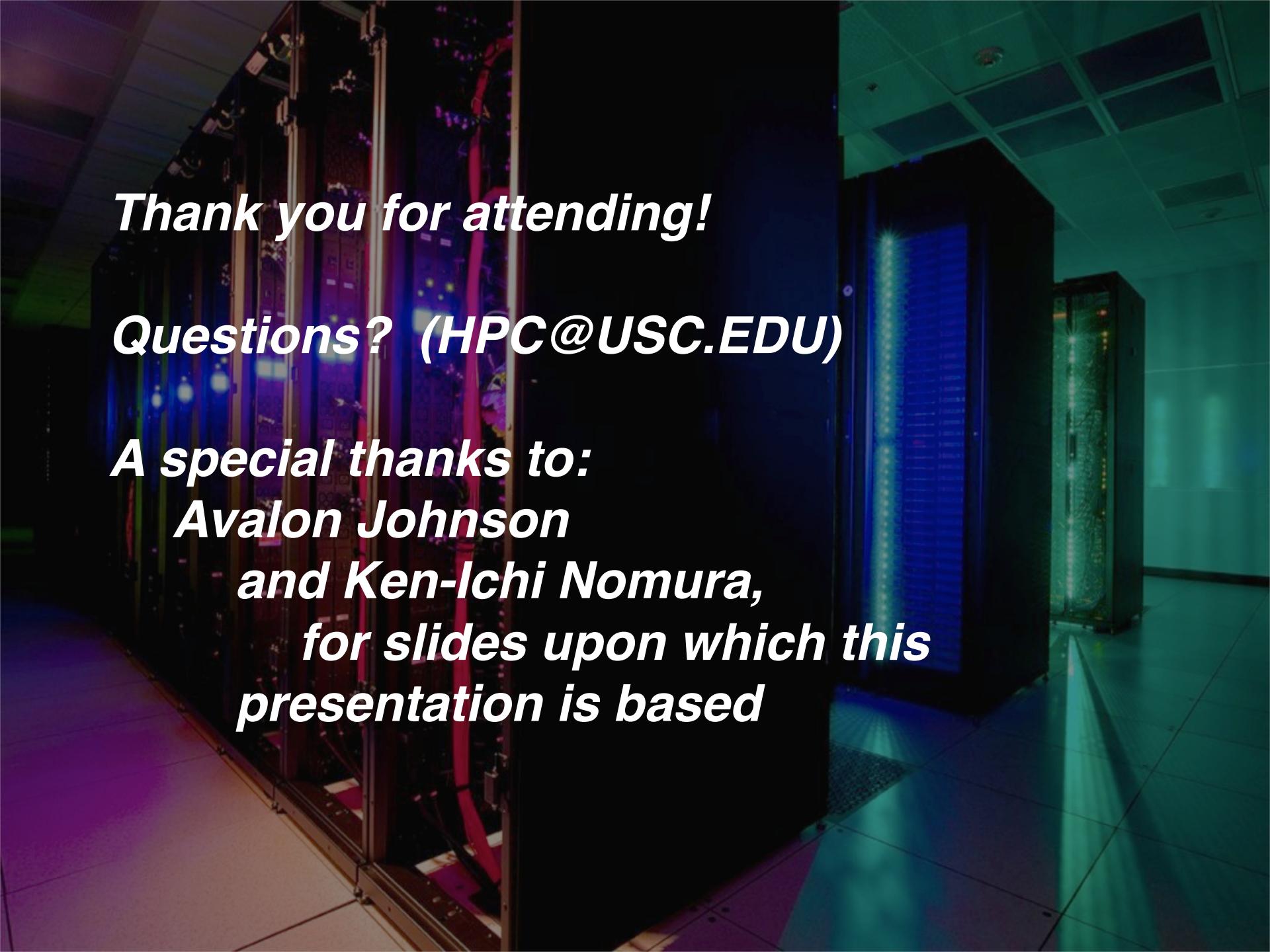
INTRO TO HIGH-
PERFORMANCE
COMPUTING

THE SHELL AND
HIGH-
PERFORMANCE
COMPUTING

ANALYSIS
PIPELINES WITH
PYTHON

Our Core Lessons in English

Lesson	Site	Repository	Reference	Instructor Guide
The Unix Shell				
Version Control with Git				
Programming with Python				
Plotting and Programming in Python				
Programming with R				
R for Reproducible Scientific Analysis				

The background of the slide is a photograph of a server room. On the left, there are several tall server racks with glass doors, through which internal components and cables are visible. The lighting is low, with bright blue and white lights from the server units creating a glowing effect. On the right, there are more server racks and a dark floor. The ceiling has a grid of recessed lights.

Thank you for attending!

Questions? (HPC@USC.EDU)

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