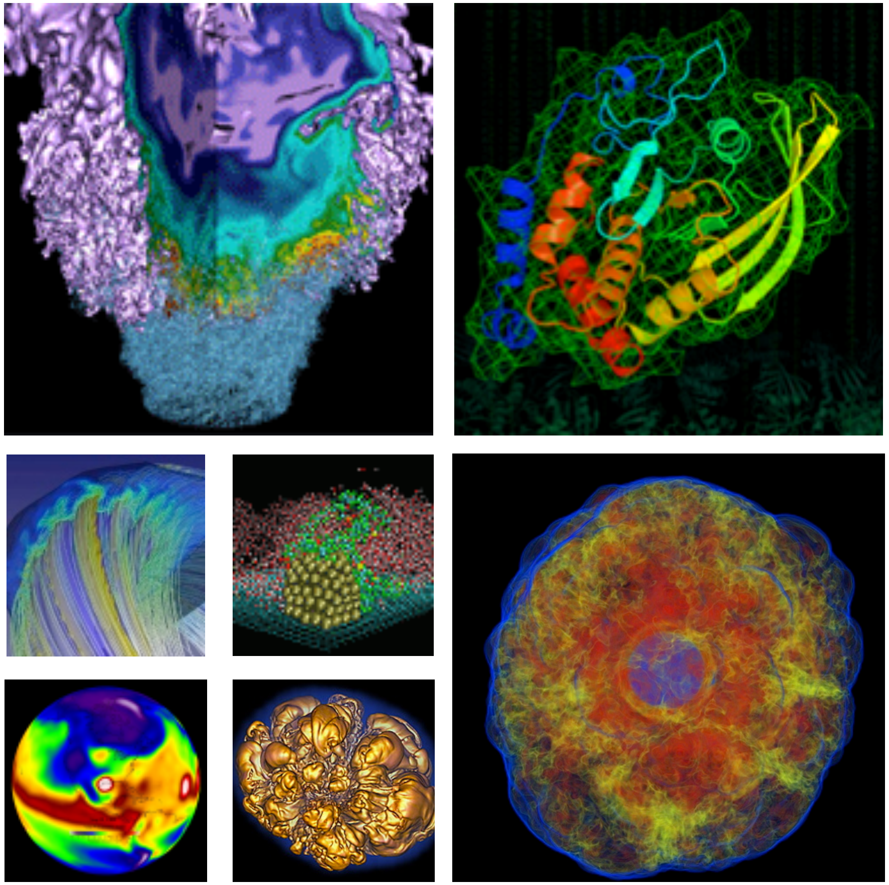
Submitting and Running Jobs



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New User Training
August 13, 2015

NERSC

U.S. DEPARTMENT OF ENERGY | Office of Science

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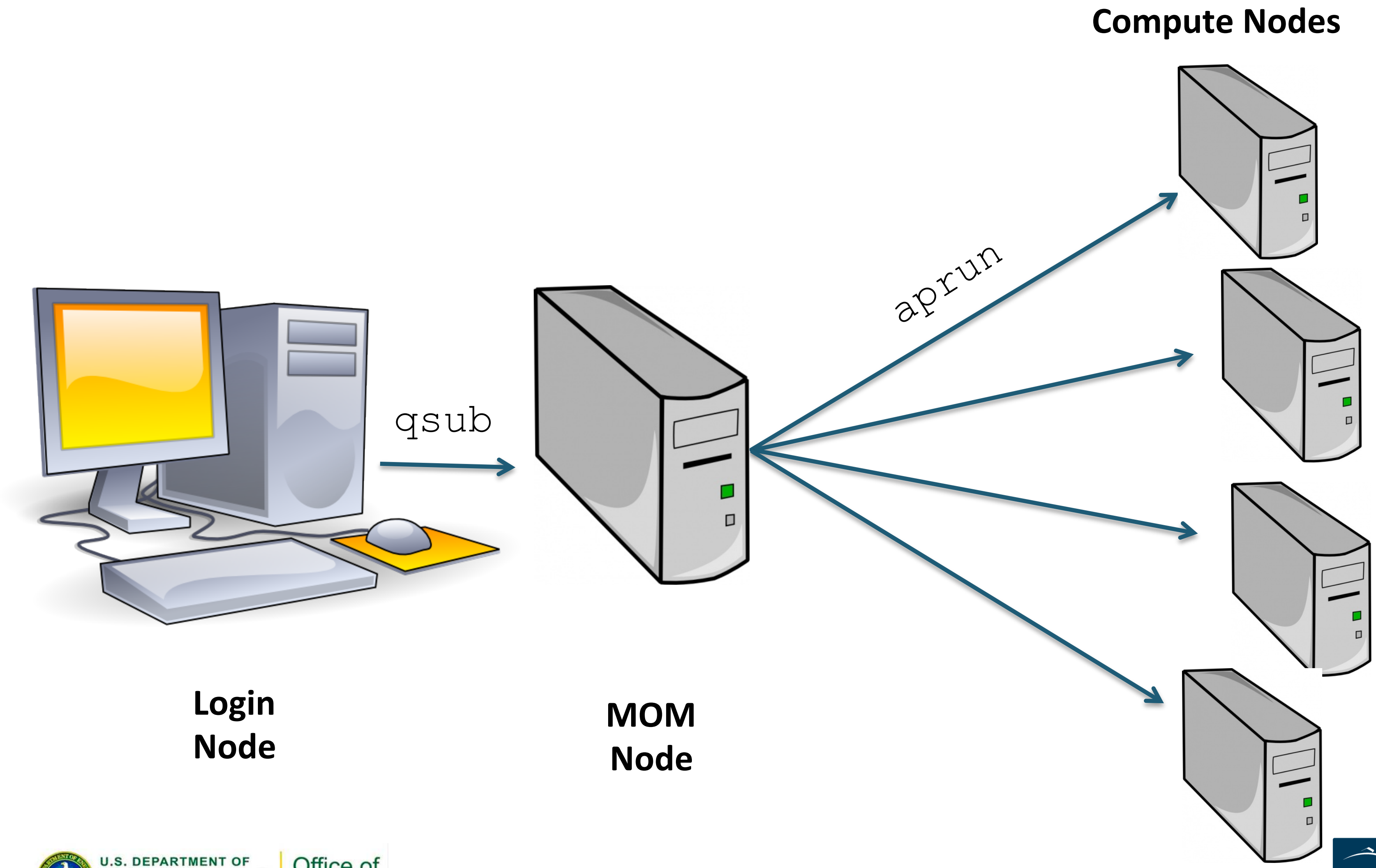
Jobs at NERSC

- **Most are parallel jobs (10s to 100,000+ cores)**
- **Production runs execute in batch mode**
- **Interactive and debug jobs are supported for up to 30 minutes**
- **Typically run times are a few to 10s of hours.**
  - Each machine has different limits.
  - Limits are necessary because of MTBF and the need to accommodate 5,500 users' jobs
- **Also a number of "serial" jobs**
  - Typically "pleasantly parallel" simulation or data analysis

Login Nodes and Compute Nodes

- Each machine has 3 types of nodes visible to users
- **Login nodes**
  - Edit files, compile codes, submit batch jobs, etc.
  - Run short, serial utilities and applications
- **Compute nodes**
  - Execute your application
  - Dedicated resources for your job
- Shared application launcher or “**MOM**” nodes
  - Execute your batch script commands
- **Note**: This will change when we move to SLURM

Launching Parallel Jobs (Cray system)



Launching Parallel Applications

- An “application launcher” executes your code
  - Starts multiple instances of your executable across the compute nodes you were allocated
  - Manages execution of your application
  - On Edison / Hopper: the launcher is called “aprun”
- Only the application launcher can start your application on compute nodes
- You can’t run the launcher from login nodes (only from a batch script or interactive session)

Submitting Batch Jobs

- To run a batch job on the compute nodes you must write a "batch script" that contains
  - Directives to allow the system to schedule your job
  - An `aprun` command that launches your parallel executable (this will change to `srun` under SLURM)
- Submit the job to the queuing system with the `qsub` command
  - `% qsub my_batch_script`

Edison - Cray XC30

- 133,824 cores, 5,576 nodes
- "Aries" interconnect
- 2 x 12-core Intel 'Ivy Bridge' 2.4 GHz processors per node
- 24 processor cores per node, 48 with hyperthreading
- 64 GB of memory per node
- 357 TB of aggregate memory
- 2.7 GB memory / core for applications
- /scratch disk quota of 10 TB
- 7.6 PB of /scratch disk
- Choice of full Linux operating system or optimized Linux OS (Cray Linux)
- Intel, Cray, and GNU compilers

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=96
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#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

Job directives: instructions for the batch system

- Submission queue
- How many compute cores to reserve for your job (/ 24 = # nodes)
- How long to reserve those nodes
- Optional: what to name STDOUT files, what account to charge, whether to notify you by email when your job finishes, etc.

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

Change from home directory to job submission directory

- Script is initially run from your home directory, **which is not advisable** (as we mention in the filesystem intro)
- You will see much better performance if your job reads / writes from one of the high-performance scratch filesystems

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

Launches parallel executable on the compute nodes

- Carries over (partial) login environment
- Controls how your executable:
  - maps to processors on the compute nodes (e.g. how many tasks?)
  - accesses the memory on each processor

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 ./my_executable
```

`mppwidth` is number of compute cores requested for your job

- `mppwidth` = 24 x # of nodes on Edison (and Hopper)
- must be **greater than or equal to** the number of tasks requested (`–n`)

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=192
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 –N 12 ./my_executable
```

–N = number of tasks per node
Might do this to get more memory / task
Note that `mppwidth` has changed accordingly

Sample Edison Batch Script - MPI

```
#PBS -q debug
#PBS -l mppwidth=48
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
aprun -n 96 -j 2 ./my_executable
```

`-j` = Turn on hyperthreading

Hybrid OpenMP/MPI

```
#PBS -q regular
#PBS -l mppwidth=96
#PBS -l walltime=00:10:00
#PBS -N my_job

cd $PBS_O_WORKDIR
export OMP_NUM_THREADS=6
aprun -n 16 -d 6 -N 4 -S 2 ./hybrid.x
```

A more complex example for mixing MPI and OpenMP:

- 16 tasks (**-n**), 4 on each node (**-N**), 6 OpenMP threads per task (**-d**), assign 2 tasks to each NUMA node (**-S**)

Many more examples on www.nersc.gov

Interactive Parallel Jobs

- You can run small parallel jobs interactively for up to 30 minutes (ex. is for Hopper / Edison)

```
login% qsub -I -l mppwidth=48
[wait for job to start]
mom% cd $PBS_O_WORKDIR
mom% aprun -n 48 ./mycode.x
```

Serial Jobs

- Both Hopper and Edison now have a special queue for running serial jobs
  - A single process running on a single core
  - Each serial node can run up to 24 jobs from different users depending on their memory requirements

```
#PBS -q serial
#PBS -l walltime=00:10:00
#PBS -l vmem=4GB
#PBS -N my_job

cd $PBS_O_WORKDIR
./myexecutable
```

Monitoring Your Job

- Once your job is submitted, it enters the queue and will start when resources are available
- Your job's place in the queue is a mix of time and priority, so line jumping is allowed, but it may cost more
- You can monitor it with:
  - `qstat -a`
  - `qstat -u username`
  - `showq`
  - `qs`
  - On the web:

    https://my.nersc.gov

    https://www.nersc.gov/users/live-status/global-queue-look/

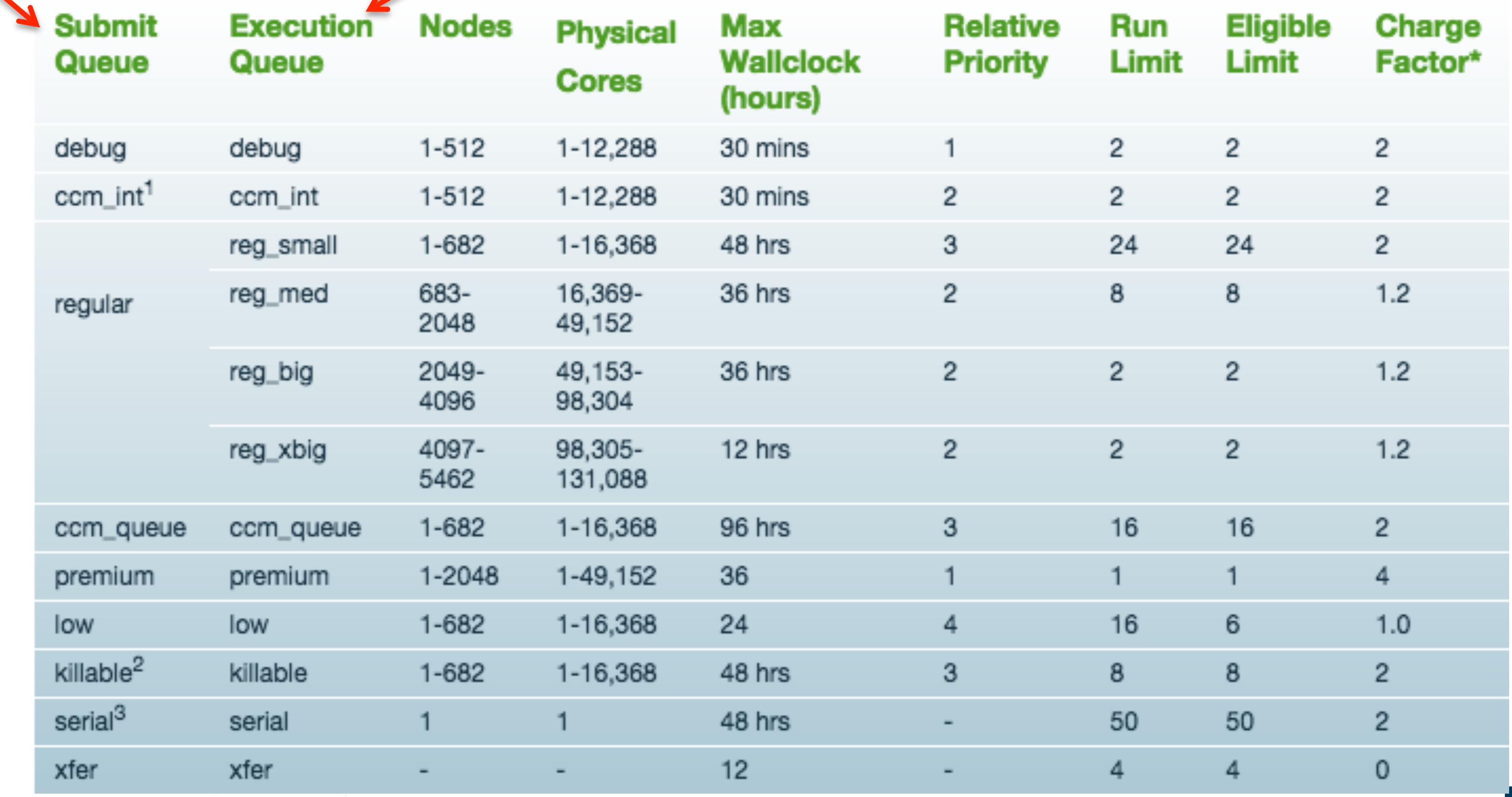
    https://www.nersc.gov/users/job-logs-and-analytics/completed-jobs/

Job Limits

There are per user, per machine job limits. Here are the limits on Edison as of August, 2015.

Specify these queues with
`#PBS -q queue_name`

Not these!



Submit Queue	Execution Queue	Nodes	Physical Cores	Max Wallclock (hours)	Relative Priority	Run Limit	Eligible Limit	Charge Factor*
debug	debug	1-512	1-12,288	30 mins	1	2	2	2
ccm_int[1]	ccm_int	1-512	1-12,288	30 mins	2	2	2	2
regular	reg_small	1-682	1-16,368	48 hrs	3	24	24	2
	reg_med	683-2048	16,369-49,152	36 hrs	2	8	8	1.2
	reg_big	2049-4096	49,153-98,304	36 hrs	2	2	2	1.2
	reg_xbig	4097-5462	98,305-131,088	12 hrs	2	2	2	1.2
ccm_queue	ccm_queue	1-682	1-16,368	96 hrs	3	16	16	2
premium	premium	1-2048	1-49,152	36	1	1	1	4
low	low	1-682	1-16,368	24	4	16	6	1.0
killable[2]	killable	1-682	1-16,368	48 hrs	3	8	8	2
serial[3]	serial	1	1	48 hrs	-	50	50	2
xfer	xfer	-	-	12	-	4	4	0

Tips for jobs

- **Submit shorter jobs, they are easier to schedule**
  - Checkpoint if possible to break up long jobs
  - Short jobs can take advantage of ‘backfill’ opportunities
  - Run short jobs just before maintenance
- **Very important: make sure the wall clock time you request is accurate**
  - As noted above, shorter jobs are easier to schedule
  - Many users unnecessarily enter the largest wall clock time possible as a default

How Your Jobs Are Charged

- **Your repository is charged for each node your job was allocated for the entire duration of your job.**
  - The minimum allocatable unit is a node (*except for the serial queues*). Hopper and Edison have 24 cores / node, so your minimum charge is 24*walltime.

MPP hours = (# nodes) * (# cores / node) * (walltime) * (QCF) * (MCF)

  - Example: 96 Edison cores for 1 hour in regular queue
    MPP hours = (4) * (24) * (1 hour) * (1) * (2) = 192 MPP hours
  - Serial jobs are charged with: (walltime) * (MCF)
- **If you have access to multiple repos, pick which one to charge in your batch script**

```
#PBS –A repo_name
```

Charge Factors & Discounts

- **Each machine has a "machine charge factor" (MCF) that multiplies the "raw hours" used**
  - Edison MCF = 2.0
  - Hopper MCF = 1.0
  - Carver MCF = 1.5
- **Each queue has a "queue charge factor" (QCF) and corresponding relative scheduling priorities**
  - Premium QCF = 2.0
  - Low QCF = 0.5
  - Regular (and everything else) QCF = 1.0 (Hopper: 0.8)
- **On Edison:**
  - Jobs requesting more than 682 nodes (reg_med, reg_big, reg_xbig queues) get a 40% discount (QCF = 0.6)

More Information

NERSC Web pages

Hopper:

http://www.nersc.gov/users/computational-systems/hopper/running-jobs/

Edison:

http://www.nersc.gov/users/computational-systems/edison/running-jobs/

Carver (retiring September, 2015):

http://www.nersc.gov/users/computational-systems/carver/running-jobs/

Contact NERSC Consulting:

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- Email *consult@nersc.gov*.

Thank You