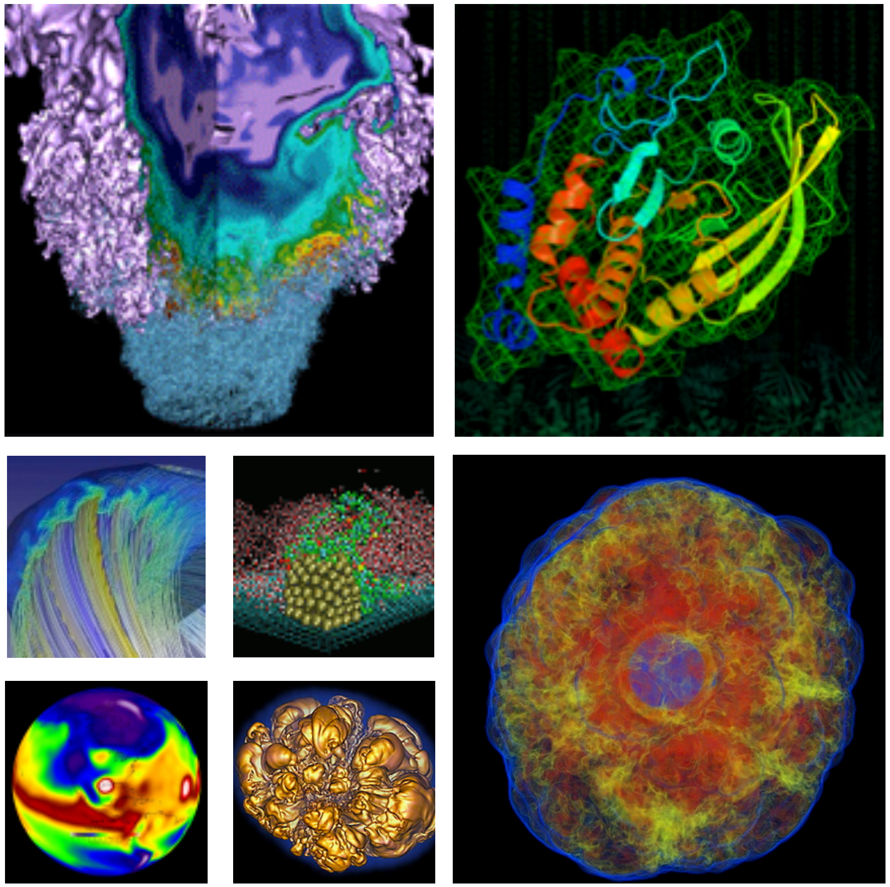
Submitting and Running Jobs



NERSC 40 YEARS at the FOREFRONT 1974-2014

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NERSC User Engagement Group

New User Training

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U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB Lawrence Berkeley National Laboratory

Jobs at NERSC

- **Most are parallel jobs (10s to 100,000+ cores)**
- **Also a number of "serial" jobs**
  - Typically "pleasantly parallel" simulation or data analysis
- **Production runs execute in batch mode**
- **Our batch scheduler is SLURM (native)**
- **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 6,000 users' jobs

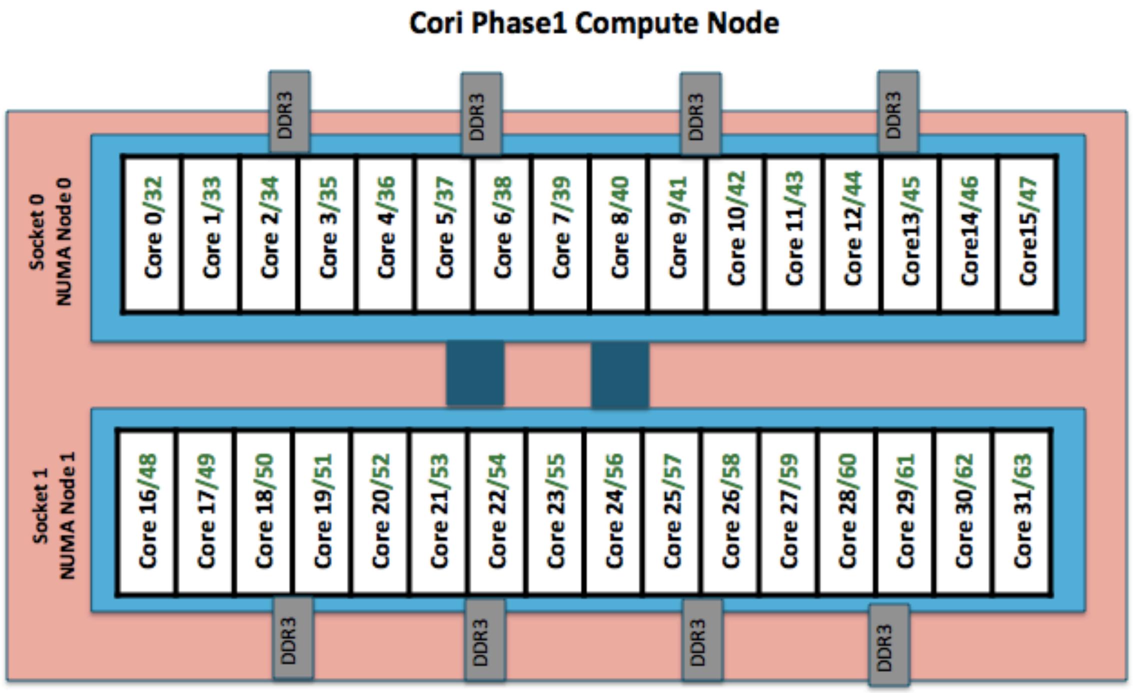
Edison - Cray XC30

- 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

Cori Phase 1 - Cray XC40

- 52,160 cores, 1,630 nodes
- “Aries” interconnect
- 2 x 16-core Intel ’Haswell' 2.3 GHz processors per node
- 32 processor cores per node, 64 with hyperthreading
- 128 GB of memory per node
- 203 TB of aggregate memory
- 4 GB memory / core for applications
- /scratch disk quota of 20 TB
- 30 PB of /scratch disk
- Choice of full Linux operating system or optimized Linux OS (Cray Linux)
- Intel, Cray, and GNU compilers

Cori Phase 1 Compute Nodes



To obtain processor info:

Get on a compute node:
% salloc –N 1

Then:
% cat /proc/cpuinfo
or
% hwloc-ls

- **Cori Phase 1: NERSC Cray XC40, 1,630 nodes, 52,160 cores.**
  - **Each node has 2 Intel Xeon 16-core Haswell processors.**
  - **2 NUMA domains per node, 16 cores per NUMA domain. 2 hardware threads per core.**
- **Memory bandwidth is non-homogeneous among NUMA domains.**

Login Nodes and Compute Nodes

Each machine has 2 types of nodes visible to users

- **Login nodes (external)**
  - Edit files, compile codes, submit batch jobs, etc.
  - Run short, serial utilities and applications
- **Compute nodes**
  - Execute your application
  - Dedicated resources for your job

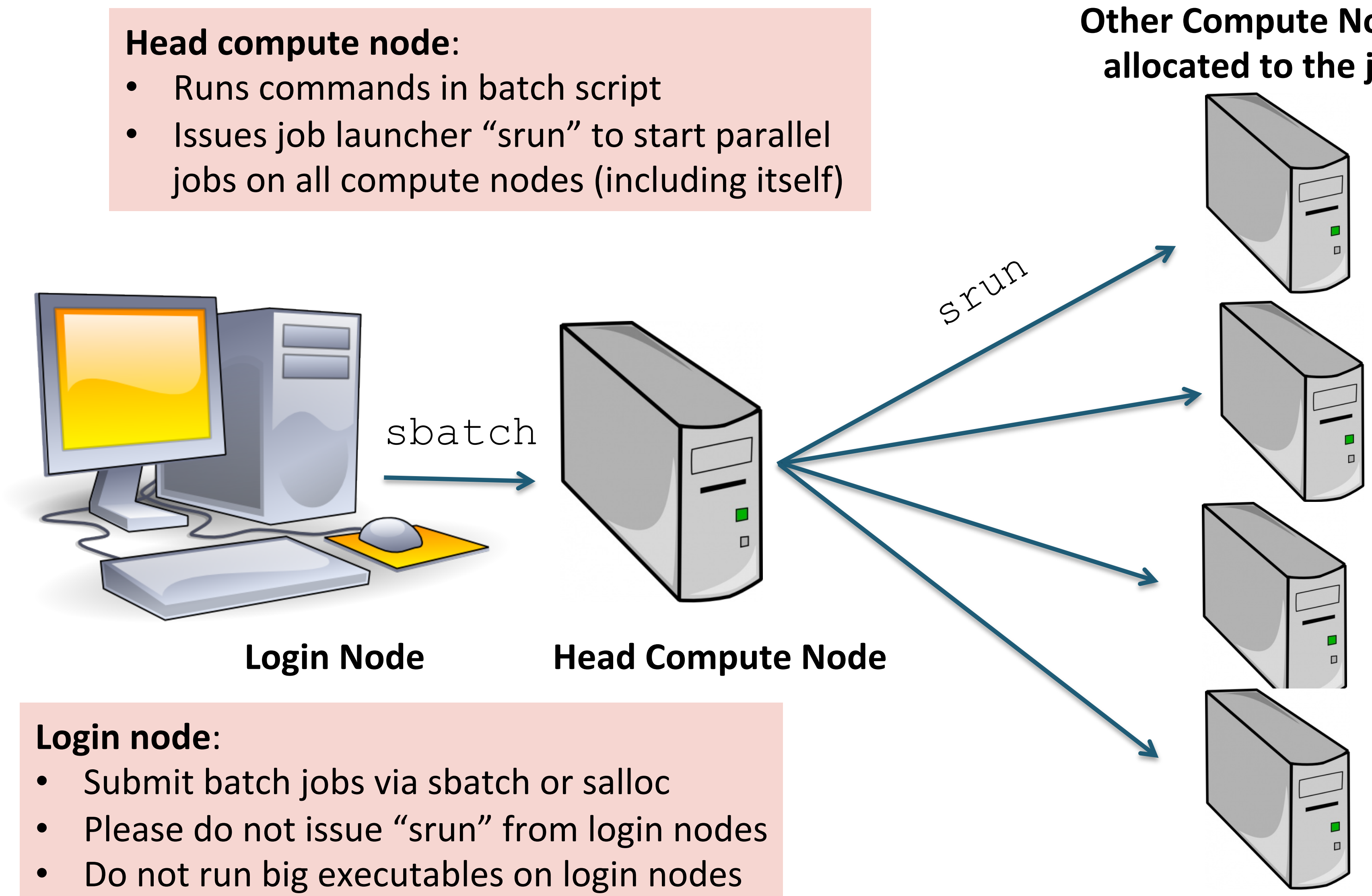
Submitting Batch Jobs

- **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 `srun` command that launches your parallel executable
- **Submit the job to the queuing system with the sbatch command**
  - `% sbatch my_batch_script`

Launching Parallel Jobs with SLURM

Head compute node:

- Runs commands in batch script
- Issues job launcher "srun" to start parallel jobs on all compute nodes (including itself)



Login node:

- Submit batch jobs via sbatch or salloc
- Please do not issue "srun" from login nodes
- Do not run big executables on login nodes

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP_NUM_THREADS=1
srun -n 1280 ./mycode.exe
```

Sample Cori Batch Script - MPI

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srun -n 1280 ./mycode.exe
```

- Need to specify which shell to use for batch script
- Use "-l" as login shell is optional.
- Environment is automatically imported

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP_NUM_THREADS=1
srun -n 1280 ./mycode.exe
```

Job directives: instructions for the batch system

- Submission partition (default is "debug")
- How many compute nodes to reserve for your job
- How long to reserve those nodes
- More optional SBATCH keywords

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP_NUM_THREADS=1
srun -n 1280 ./mycode.exe
```

SBATCH optional keywords:

- how many instances of applications to launch (# of MPI tasks)
- which QOS to use via "#SBATCH --qos=…" (default is normal)
- what to name STDOUT files
- what account to charge
- whether to notify you by email when your job finishes
- …

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP_NUM_THREADS=1
srun -n 1280 ./mycode.exe
```

- By default, hyperthreading is on. SLURM sees 2 threads are available for each of the 32 physical CPUs on the node.
- No need to set this if your application programming model is pure MPI.
- If your code is hybrid MPI/OpenMP, set this value to 1 to run in pure MPI mode.

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP NUM THREADS=1
srun -n 1280 ./mycode.exe
```

"srun" command launches parallel executables on the compute nodes

- srun flags overwrite SBATCH keywords
- No need to repeat flags in srun command if already defined in SBATCH keywords. (e.g. "srun ./my_executable" will also do in above example)

Sample Cori Batch Script - MPI

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00
#SBATCH -n 1280
#SBATCH -J myjob

export OMP_NUM_THREADS=1
srun -n 1280 ./mycode.exe
```

- There are 64 logical CPUs on each node
- With 40 nodes, using hyperthreading, up to 40*64=2,560 MPI tasks can be launched: “srun -n 2560 ./my_executable” is OK

Hybrid MPI/OpenMP

```
#!/bin/bash -l
#SBATCH -p regular
#SBATCH -N 40
#SBATCH -t 1:00:00

export OMP_NUM_THREADS=8
srun -n 160 -c 8 ./mycode.exe
```

- srun does most of optimal process and thread binding automatically. Only flags such as “-n” “-c”, along with OMP_NUM_THREADS are needed for most applications
- Hyperthreading is enabled by default. Jobs requesting more than 32 cores (MPI tasks * OpenMP threads) per node will use hyperthreads automatically.

Interactive Parallel Jobs

- **You can run small parallel jobs interactively for up to 30 minutes**

```
login% salloc -N 2 -p debug -t 15:00
[wait for job to start]
compute% srun -n 64 ./mycode.exe
```

Serial Jobs on Cori

- The "shared" partition on Cori allows multiple executables from different users to share a node
- Each serial job run on a single core of a "shared" node
- Up to 32 jobs from different users depending on their memory requirements

```
#SBATCH -p shared
#SBATCH -t 1:00:00
#SBATCH --mem=4GB
#SBATCH -J my_job
./mycode.x
```

- Do not specify #SBATCH -N"
- Default "#SBATCH -n" is 1
- Default memory is 1,952 MB
- Use -n or --mem to request more slots for larger memory
- Do not use "srun" for serial executable (reduces overhead)

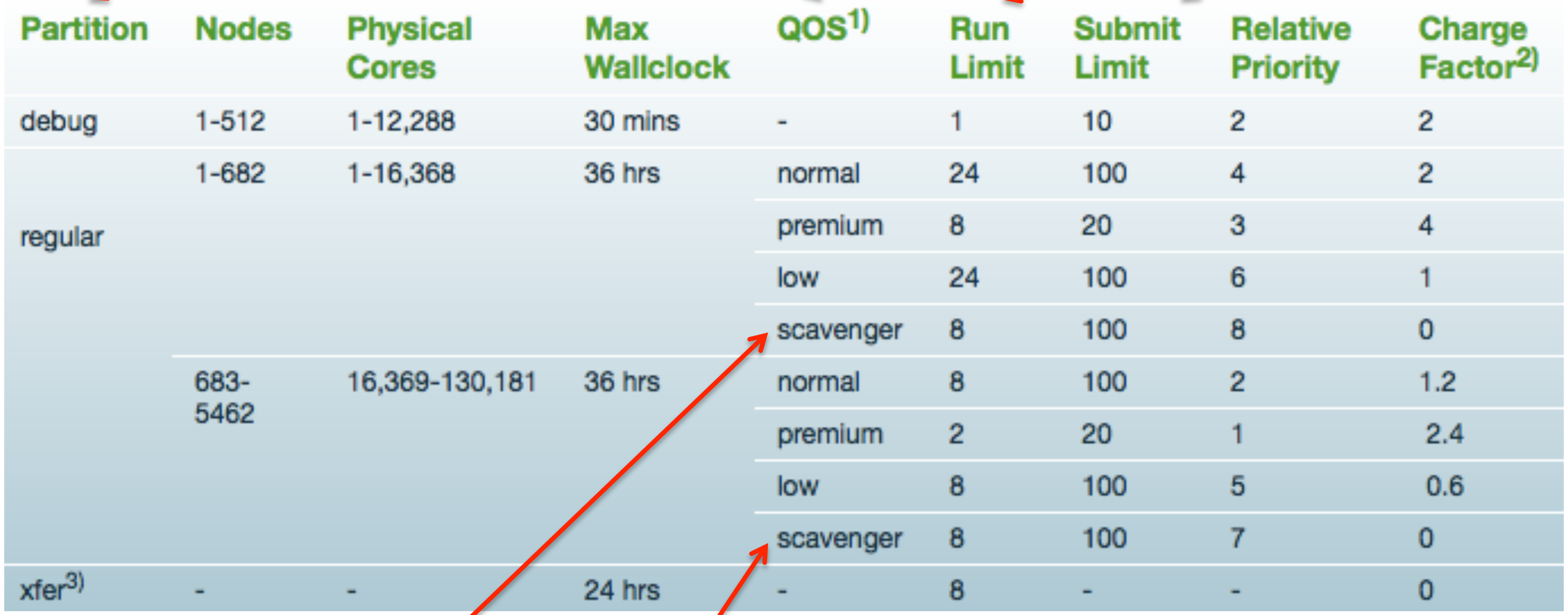
- Small parallel job that use less than a full node can also run in the "shared" partition

Edison Queue Policy (as of March 2016)

Specify these partitions with
`#SBATCH -q partition_name`

Specify these QOS with
`#SBATCH --qos=premium`

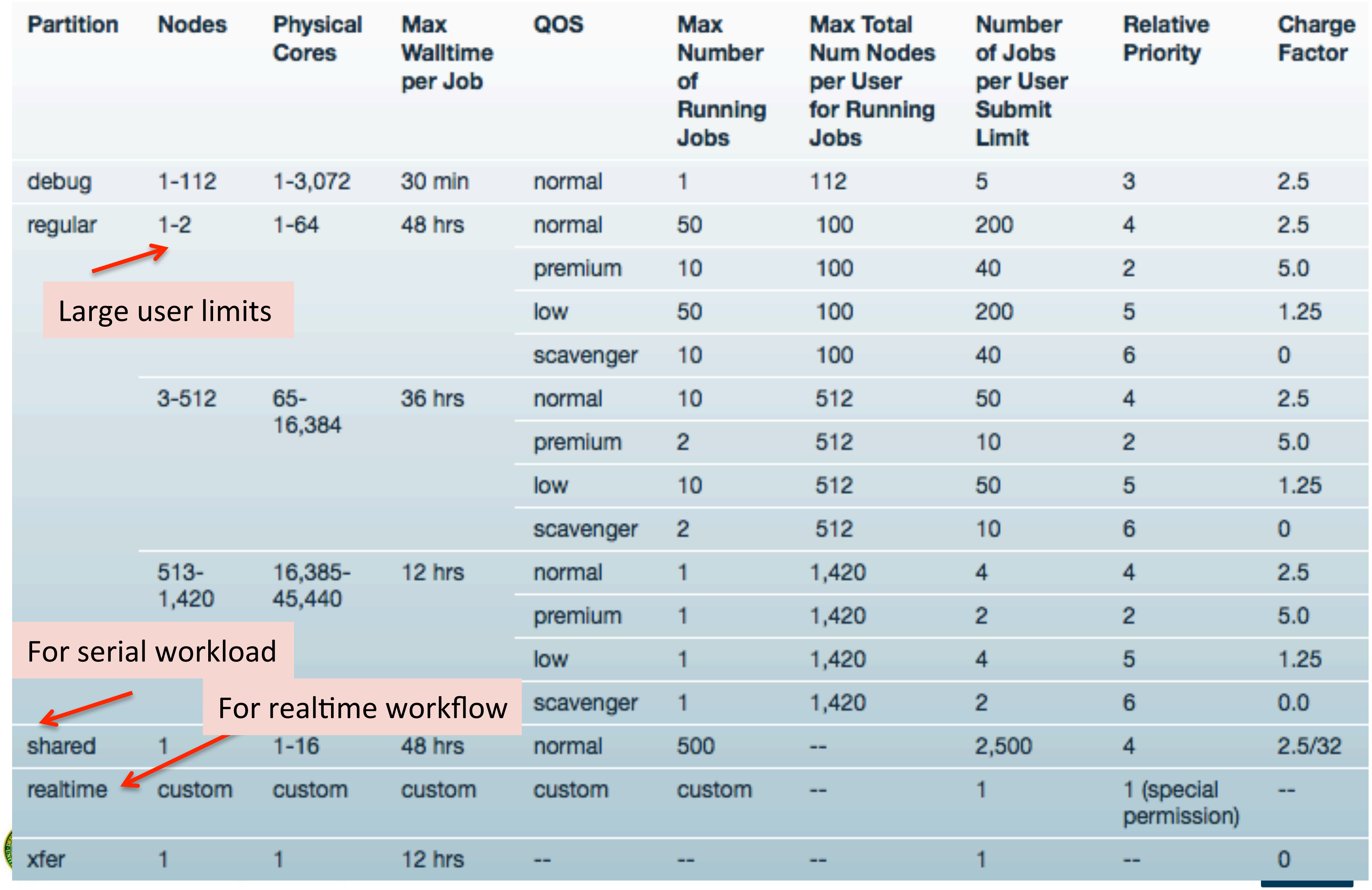
These limits are per user per partition/QOS limits



Partition	Nodes	Physical Cores	Max Wallclock	QOS[1]	Run Limit	Submit Limit	Relative Priority	Charge Factor[2]
debug	1-512	1-12,288	30 mins	-	1	10	2	2
regular	1-682	1-16,368	36 hrs	normal	24	100	4	2
				premium	8	20	3	4
				low	24	100	6	1
				scavenger	8	100	8	0
	683-5462	16,369-130,181	36 hrs	normal	8	100	2	1.2
				premium	2	20	1	2.4
				low	8	100	5	0.6
				scavenger	8	100	7	0
xfer[3]	-	-	24 hrs	-	8	-	-	0

Jobs with insufficient allocations to run are directed to "scanvenger"

Cori Queue Policy (as of March 2016)



Partition	Nodes	Physical Cores	Max Walltime per Job	QOS	Max Number of Running Jobs	Max Total Num Nodes per User for Running Jobs	Number of Jobs per User Submit Limit	Relative Priority	Charge Factor
debug	1-112	1-3,072	30 min	normal	1	112	5	3	2.5
regular	1-2	1-64	48 hrs	normal	50	100	200	4	2.5
				premium	10	100	40	2	5.0
				low	50	100	200	5	1.25
				scavenger	10	100	40	6	0
	3-512	65-16,384	36 hrs	normal	10	512	50	4	2.5
				premium	2	512	10	2	5.0
				low	10	512	50	5	1.25
				scavenger	2	512	10	6	0
	513-1,420	16,385-45,440	12 hrs	normal	1	1,420	4	4	2.5
				premium	1	1,420	2	2	5.0
				low	1	1,420	4	5	1.25
				scavenger	1	1,420	2	6	0.0
shared	1	1-16	48 hrs	normal	500	--	2,500	4	2.5/32
realtime	custom	custom	custom	custom	custom	--	1	1 (special permission)	--
xfer	1	1	12 hrs	--	--	--	1	--	0

Large user limits

For serial workload

For realtime workflow

Which System to Run My Jobs

- **Queue configuration and policies are still under tuning for max throughput and system utilization.**
- **The Cori Phase 1 (also known as the "Cori Data Partition") system is designed to accelerate data-intensive applications.**
  - 1-2 node jobs in “regular” partition for high throughput jobs: larger user limits, longer wall time limits
  - “shared” partition for serial workload: very large user limits
  - “realtime” partition for realtime workflow (special arrangement)
- **Users are encouraged to run large size massive parallel jobs on Edison. Jobs use 683+ nodes on Edison get 40% charging discount.**

Monitoring Your Job

- **Once your job is submitted, it enters the queue and will start when resources are available**
- **Overall job priorities are a combination of partition, QOS, queue wait time, job size, wall time request, and fair share.**
- **You can monitor it with:**
  - `sqs`
  - `squeue`

  On the web:

  https://my.nersc.gov

  https://www.nersc.gov/users/live-status/ : “Queue Look”

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

SLURM User Commands

- **sbatch:** submit a batch script
- **salloc:** request nodes for an interactive batch session
- **srun:** launch parallel jobs
- **scancel:** delete a batch job
- **sqs**: NERSC custom queue display with job priority ranking info
- **squeue:** display info about jobs in the queue
- **sinfo:** view SLURM configuration about nodes and partitions
- **scontrol**: view and modify SLURM configuration and job state
- **sacct:** display accounting data for jobs and job steps
- https://www.nersc.gov/users/computational-systems/cori/running-jobs/monitoring-jobs/

Tips for Getting Better Throughput

- **Line jumping is allowed, but it may cost more**
- **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
- **Queue wait time statistics**
  - https://www.nersc.gov/users/queues/queue-wait-times/

Advanced Workflow Management

- **Bundle jobs (multiple “srun”s in one script, sequential or simultaneously)**
- **Use Job Arrays for submitting and managing collections of similar jobs**
  – Better managing jobs, not necessary faster turnaround
  – Each array task is considered a single job for scheduling
- **Use job dependency features to chain jobs that have dependency**

Charge Factors & Discounts

- **Each machine has a "machine charge factor" (MCF) that multiplies the "raw hours" used**
  - Edison MCF = 2.0
  - Cori MCF = 2.5
- **Each QOS has a "QOS charge factor" (QCF)**
  - premium QCF = 2.0
  - normal QCF = 1.0 (default)
  - low QCF = 0.5
  - scavenger QCF = 0
- **On Edison:**
  - Jobs requesting 683 or more nodes get a 40% discount

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 "shared" partition on Cori*). Edison have 24 cores/node and Cori has 32 cores/node.

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

  - Example: 4 Cori nodes for 1 hour with "premium" QOS
    MPP hours = (4) * (32) * (1 hour) * (2) * (2.5) = 640 MPP hours
  - "shared" jobs are charged with physical CPUs used instead of entire node.
- **If you have access to multiple repos, pick which one to charge in your batch script**

```
#SBATCH -A repo_name
```

More Information

NERSC Web pages:

- **Edison**
  http://www.nersc.gov/users/computational-systems/edison/running-jobs/
- **Cori**
  http://www.nersc.gov/users/computational-systems/cori/running-jobs/

Contact NERSC Consulting:

- Toll-free 800-666-3772
- 510-486-8611, option #3
- Email *consult@nersc.gov*

Thank You