

Reusing this material





This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

https://creativecommons.org/licenses/by-nc-sa/4.0/

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.

epcc

• ARCHER:

- PBS:
 - qsub: submit a job
 - qsub -I: submit an interactive job
 - qstat: query the status of a job
 - qdel: delete a job
 - qstat -q: query the status of the system
- Job launcher:
 - aprun

• ARCHER2:

- Slurm:
 - sbatch: submit a job
 - salloc: submit an interactive job
 - squeue: query the status of a job
 - scancel: delete a job
 - sinfo: query the status of the system
- Job launcher:
 - srun

adrianj@uan01~> sinfo

PARTITION AVAIL TIMELIMIT NODES STATE NODELIST

standard up 1-00:00:00 45 down* nid[001045,001047,001061,001068...]

standard up 1-00:00:00 10 drain nid[001016,001069,001468,...]

standard up 1-00:00:00 5 resv nid[001000-001003,001021]

standard up 1-00:00:00 513 alloc nid[001004-001015,001017,001022-001044,...]

standard up 1-00:00:00 447 idle nid[001018-001020,001046,001062-001067,...]

standard up 1-00:00:00 1 down nid001138



adrianj@eslogin004:~> qstat -q

server: sdb

Queue	Memory	CPU Time	Walltime	Node	Run	Que	Lm	State
parallel			24:00:00		0	0		D S
phase2			24:00:00		0	0		D S
ppn			24:00:00		0	0		ΕR
high			24:00:00		0	0		ΕR
weekend			24:00:00		0	48		E S
standard			24:00:00		281	125		ΕR
long			48:00:00		75	4		ΕR
short					0	0		ΕR
serial			24:00:00		24	12		ΕR
largemem			48:00:00		4	7		E S
low			03:00:00		0	31		E S
R7327082			00:20:00		3	0		ΕR
R7327794					1	0		ΕR

388 227

adrianj@uan01:~> sacctmgr show assoc where user=adrianj
format=account,user,maxtresmins

Account	User	MaxTRESMins	
cse-admin	adrianj	cpu=0	
y07	adrianj	cpu=0	
z19	adrianj		



adrianj	@eslogin004:	:~> budgets

Remaining kAUs	Budget
89.953	z01
9.960	z01-cse
No resources left	z01-csetds
No resources left	z01-test
23005.127	z19-cse
1999.965	z19-csetds

adrianj@uan01~> sinfo

PARTITION AVAIL TIMELIMIT NODES STATE NODELIST

standard up 1-00:00:00 45 down* nid[001045,001047,001061,001068...]

standard up 1-00:00:00 10 drain nid[001016,001069,001468,...]

standard up 1-00:00:00 5 resv nid[001000-001003,001021]

standard up 1-00:00:00 513 alloc nid[001004-001015,001017,001022-001044,...]

standard up 1-00:00:00 447 idle nid[001018-001020,001046,001062-001067,...]

standard up 1-00:00:00 1 down nid001138



adrianj@eslogin004:~> qstat -q

server: sdb

Queue	Memory	CPU Time	Walltime	Node	Run	Que	Lm	State
parallel			24:00:00		0	0		D S
phase2			24:00:00		0	0		D S
ppn			24:00:00		0	0		ΕR
high			24:00:00		0	0		ΕR
weekend			24:00:00		0	48		E S
standard			24:00:00		281	125		ΕR
long			48:00:00		75	4		ΕR
short					0	0		ΕR
serial			24:00:00		24	12		ΕR
largemem			48:00:00		4	7		E S
low			03:00:00		0	31		E S
R7327082			00:20:00		3	0		ΕR
R7327794					1	0		ΕR

388 227

epcc

adrianj@uan01:~> s

		PARTITION	NAME	USER	ST	TIME	NODES	
NODELIST (REA	SON)							
	30752	standard	bash	grte2001	R	14:31	1	nid001017
001015,]	30749	standard	hpcc	adrianj	R	15:40	512	nid[001004-

adrianj@eslogin004:~> qstat | more

5148849.sdb 12S-2P taibui 0 H standard 5914122.sdb pollutionprac s1879801 0 H standard 6438161.sdb PuWide_1 mzv2c 0 H weekend 6439801.sdb LES_narrow mzv2c 0 H weekend 6452569.sdb DNS_Splitter mzv2c 0 H weekend 6463985.sdb DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vacl.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_atmos_ dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325565.sdb	Job id	Name	User	Time Use S Queue
5914122.sdb pollutionprac s1879801 0 H standard 6438161.sdb PuWide_1 mzv2c 0 H weekend 6439801.sdb LES_narrow mzv2c 0 H weekend 6452569.sdb DNS_Splitter mzv2c 0 H weekend 6463985.sdb DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vac1.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_atmos_ dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_atmos_ dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7024877.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsoh				
6438161.sdb PuWide_1 mzv2c 0 H weekend 6439801.sdb LES_narrow mzv2c 0 H weekend 6452569.sdb DNS_Splitter mzv2c 0 H weekend 6463985.sdb DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vac1.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_cice_e dflocco 0 H serial 7019131.sdb postproc_atmos_ dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	5148849.sdb	12S-2P	taibui	0 H standard
6439801.sdb LES_narrow mzv2c 0 H weekend 6452569.sdb DNS_Splitter mzv2c 0 H weekend 6463985.sdb DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vac1.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	5914122.sdb	pollutionprac	s1879801	0 H standard
OH weekend 6452569.sdb DNS_Splitter mzv2c 0 H weekend 6463985.sdb DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vac1.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	6438161.sdb	PuWide_1	mzv2c	0 H weekend
DNS_Splitter mzv2c 0 H weekend 6952967.sdb tite2M-vac1.5 uccawra 0 H serial 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_atmos_ dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_cice_e dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	6439801.sdb	LES_narrow	mzv2c	0 H weekend
tite2M-vac1.5 uccawra 0 H weekend 7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	6452569.sdb	DNS_Splitter	mzv2c	0 H weekend
7019105.sdb postproc_atmos_ dflocco 0 H serial 7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	6463985.sdb	DNS_Splitter	mzv2c	0 H weekend
7019107.sdb postproc_nemo_e dflocco 0 H serial 7019108.sdb postproc_atmos_ dflocco 0 H serial 7019127.sdb postproc_cice_e dflocco 0 H serial 7019130.sdb postproc_atmos_ dflocco 0 H serial 7019131.sdb postproc_cice_e dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7019136.sdb postproc_atmos_ dflocco 0 H serial 7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	6952967.sdb	tite2M-vac1.5	uccawra	0 H weekend
7019108.sdb postproc_atmos_ dflocco	7019105.sdb	postproc_atmos_	dflocco	0 H serial
7019127.sdb postproc_cice_e dflocco	7019107.sdb	postproc_nemo_e	dflocco	0 H serial
7019130.sdb postproc_atmos_ dflocco	7019108.sdb	postproc_atmos_	dflocco	0 H serial
7019131.sdb postproc_cice_e dflocco	7019127.sdb	postproc_cice_e	dflocco	0 H serial
7019136.sdb postproc_atmos_ dflocco	7019130.sdb	postproc_atmos_	dflocco	0 H serial
7024877.sdb vac-2 uccawra 0 H weekend 7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	7019131.sdb	postproc_cice_e	dflocco	0 H serial
7097417.sdb ave4 gcastigl 0 H long 7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	7019136.sdb	postproc_atmos_	dflocco	0 H serial
7287426.sdb ag100 bsohail 0 H standard 7325564.sdb nogly_new mohdfbs 00:00:02 R standard	7024877.sdb	vac-2	uccawra	0 H weekend
7325564.sdb nogly_new mohdfbs 00:00:02 R standard	7097417.sdb	ave4	gcastigl	0 H long
	7287426.sdb	ag100	bsohail	0 H standard
7325565.sdb nogly_new mohdfbs 0 H standard	7325564.sdb	nogly_new	mohdfbs	00:00:02 R standard
	7325565.sdb	nogly_new	mohdfbs	0 H standard



```
#!/bin/bash
                                                   #!/bin/bash --login
#SBATCH --job-name=Example MPI Job
                                                   #PBS -N hello world
#SBATCH --time=0:20:0
                                                   #PBS -l walltime=0:5:0
#SBATCH --nodes=4
                                                   #PBS -1 select=43
#SBATCH --tasks-per-node=128
                                                  #PBS -A [budget code]
#SBATCH --cpus-per-task=1
#SBATCH --account=[budget code]
#SBATCH --partition=standard
#SBATCH --qos=standard
                                                   cd $PBS O WORKDIR
srun --cpu-bind=cores ./my_mpi_executable.x
                                                  aprun -n 1024 $HOME/ my_mpi_executable.x
```



Interactive run on ARCHER:

```
qsub -IVl select=8, walltime=1:0:0 -A [project code] qsub: waiting for job 492383.sdb to start adrianj@mom3:~> aprun -n 192 ./my exe
```

Interactive run on ARCHER2:

```
salloc --nodes=8 --tasks-per-node=128 --cpus-per-task=1 --time=1:0:0 --partition=standard --
qos=standard --account=[budget code]
salloc: Granted job allocation 30751
salloc: Waiting for resource configuration
salloc: Nodes nid[001019-001020,001062-001067] are ready for job
adrianj@uan01:/work/z19/z19/adrianj/>srun -cpu-bind=cores ./my_exe
```

ARCHER2 configuration



- Partitions:
 - Standard
 - Highmem (for the full system, not currently available)
 - GPU (for the full system, not currently available)*
- QoS:
 - Standard: up to 24 hour jobs, up to the full system
 - 16 running jobs + 16 queued jobs per user
 - Long: from 24-48 hour jobs, up to 64 nodes *
 - 64 nodes in total per user
 - 512 nodes in long queue use for the 4 cabinet system in total across all users
 - Short: up to 20 minutes, up to 4 nodes*
 - 1 running job + 2 queued job per user
 - requires a reservation
 - sbatch -reservation=shortgos ...
 - only active 08.00-20.00 Monday-Friday

*subject to change in the future

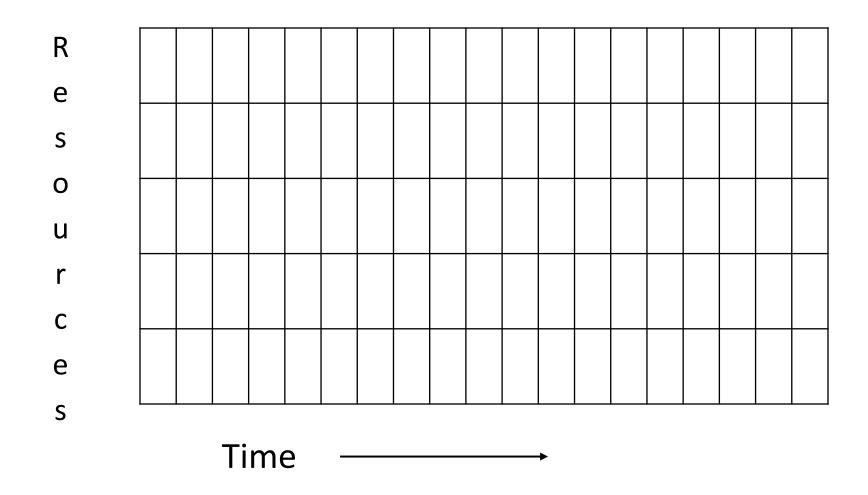
Placement and binding

epcc

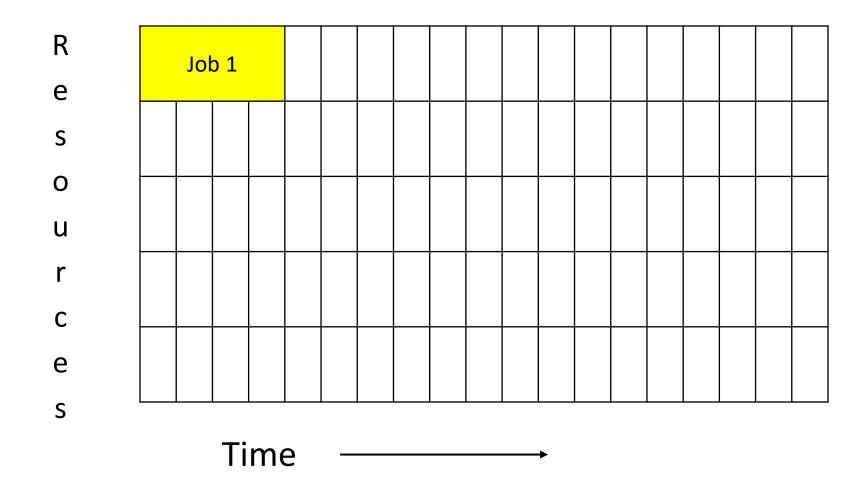
- Slurm (srun) is doing our placement and binding
 - Processes and threads to cores

```
#!/bin/bash
#SBATCH --job-name=Example MPI Job
#SBATCH --time=0:20:0
#SBATCH --nodes=4
#SBATCH --ntasks=32
#SBATCH --tasks-per-node=8
#SBATCH --cpus-per-task=16
#SBATCH --account=[budget code]
#SBATCH --partition=standard
#SBATCH --gos=standard
# Set the number of threads to 16 and specify placement
   There are 16 OpenMP threads per MPI process
   We want one thread per physical core
export OMP NUM THREADS=16
export OMP PLACES=cores
srun --hint=nomultithread --distribution=block:block
./my mixed executable.x arg1 arg2
```

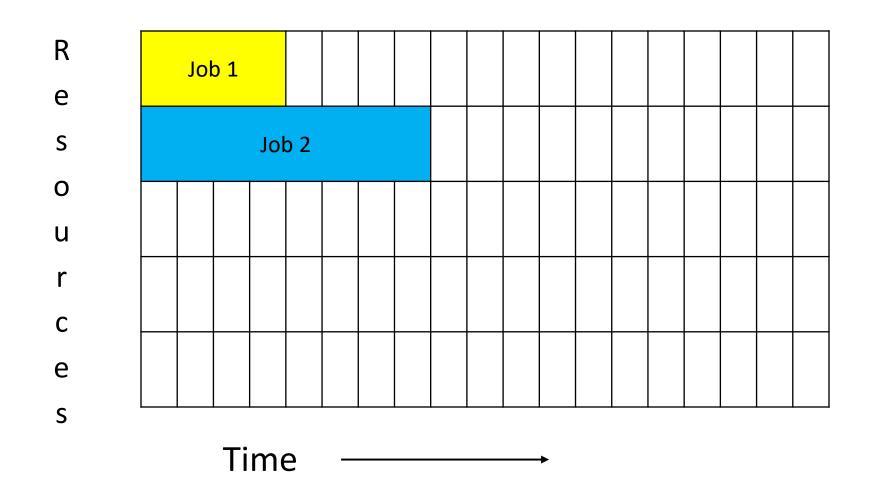




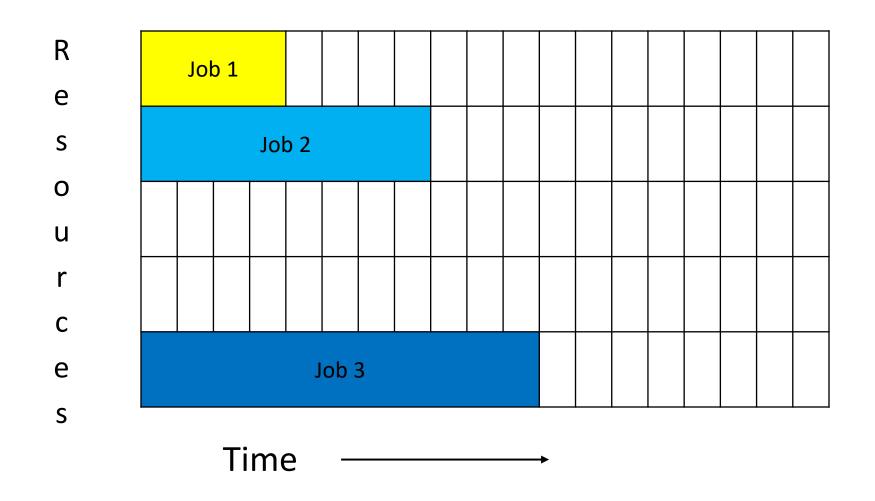




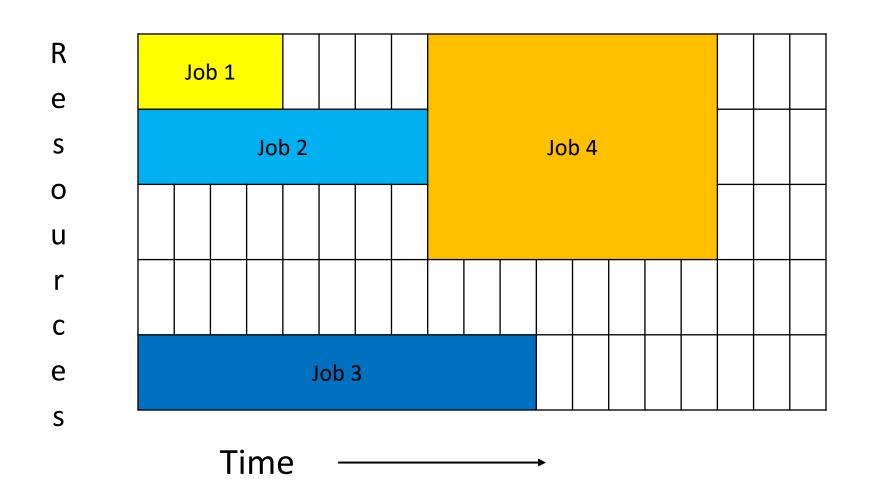




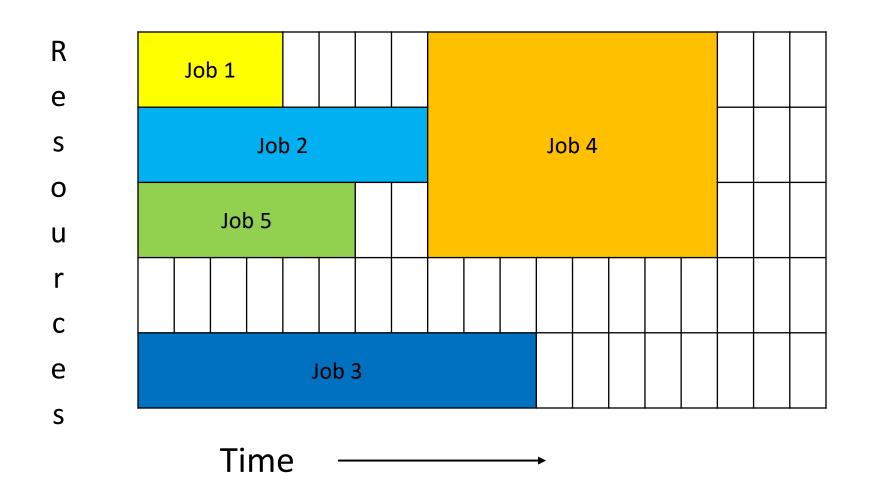




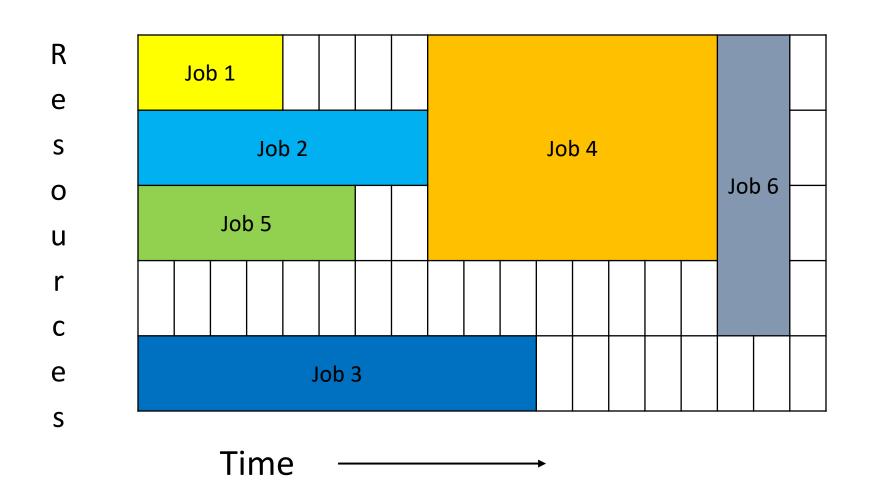




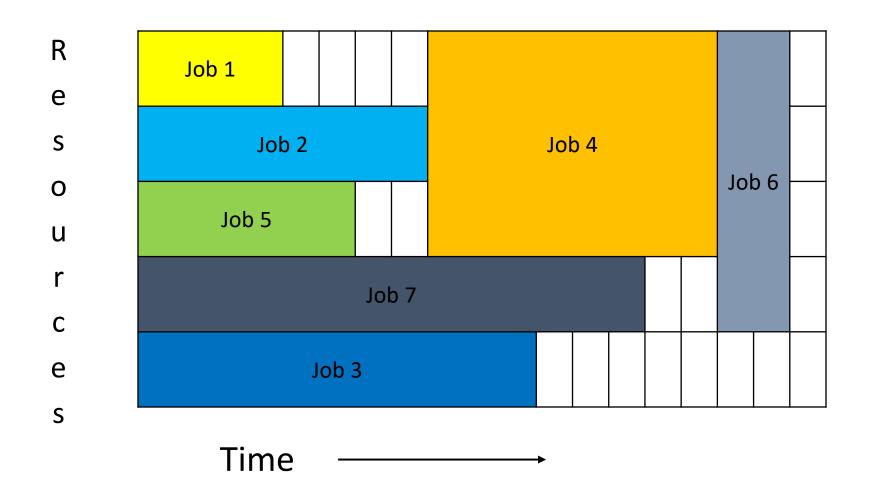




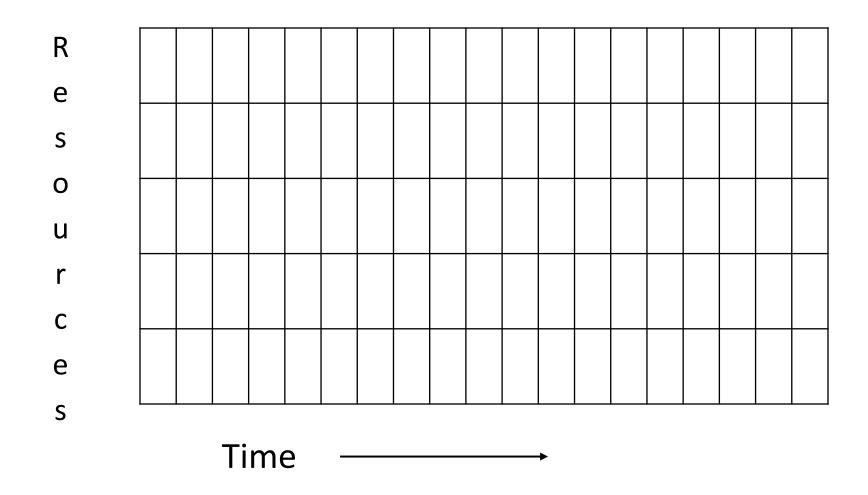




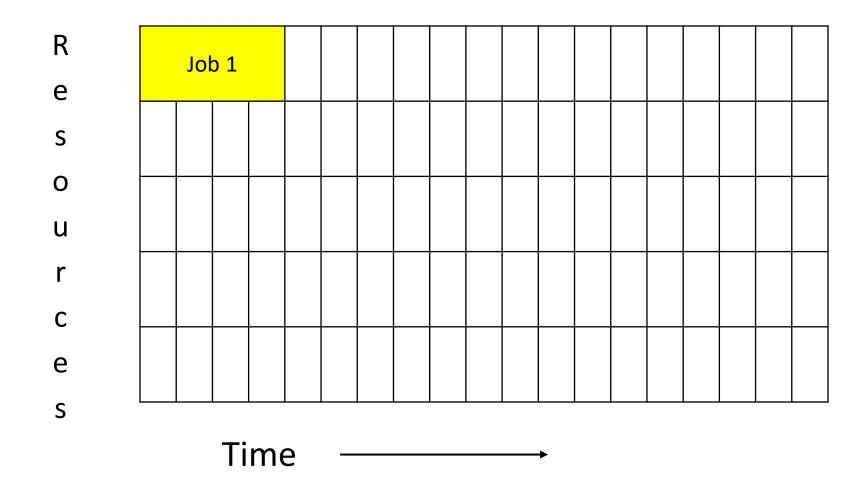




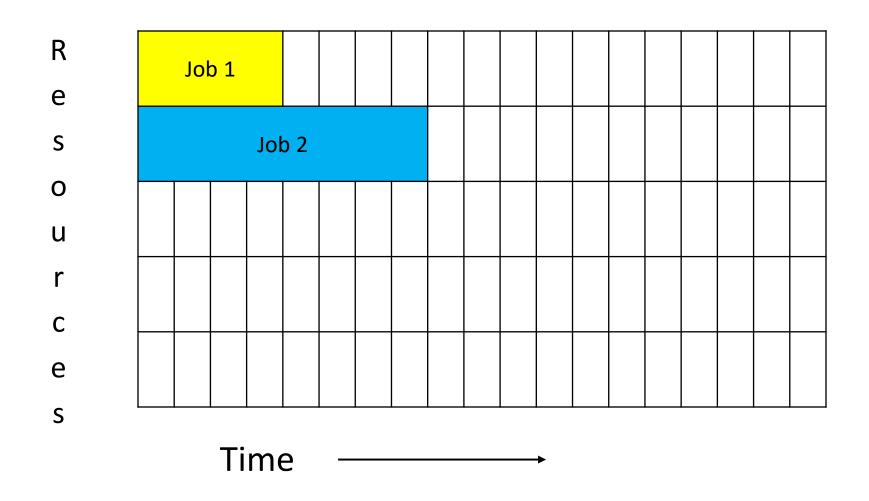




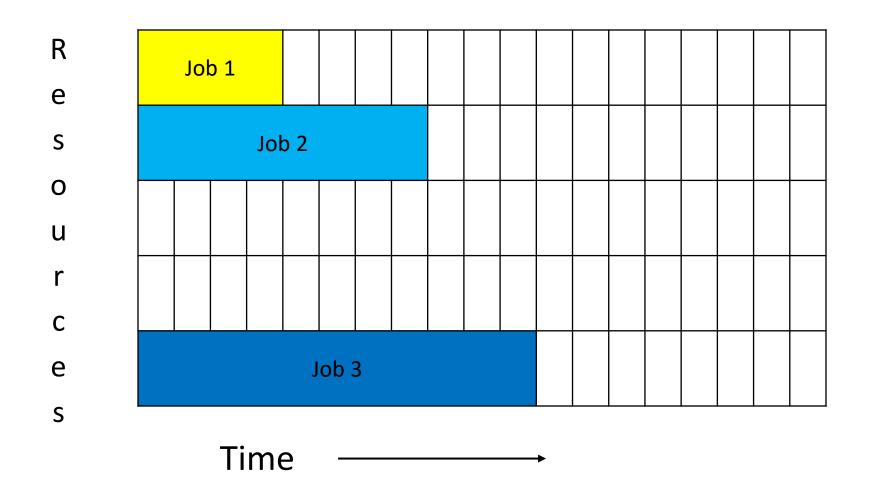




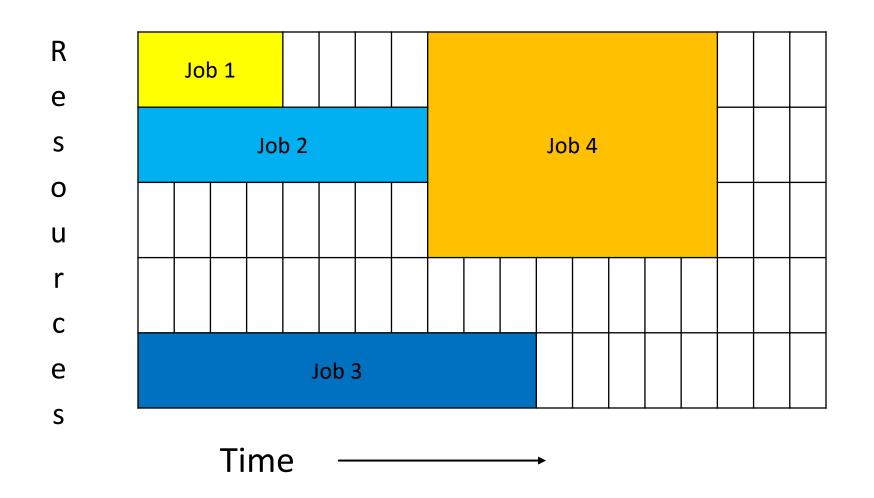




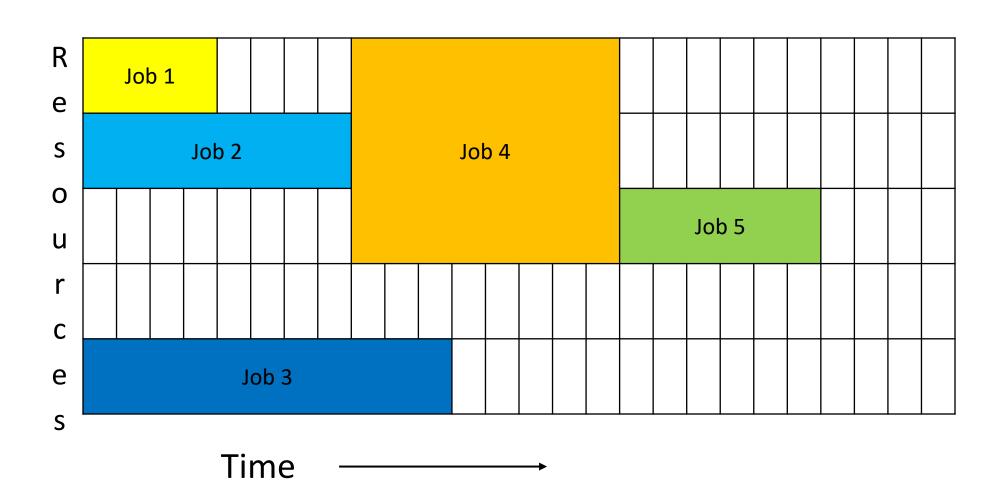




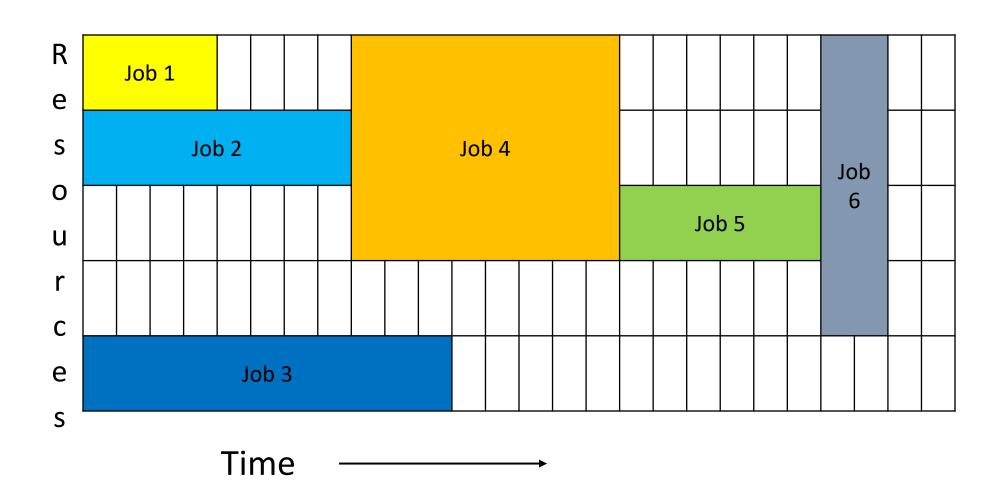




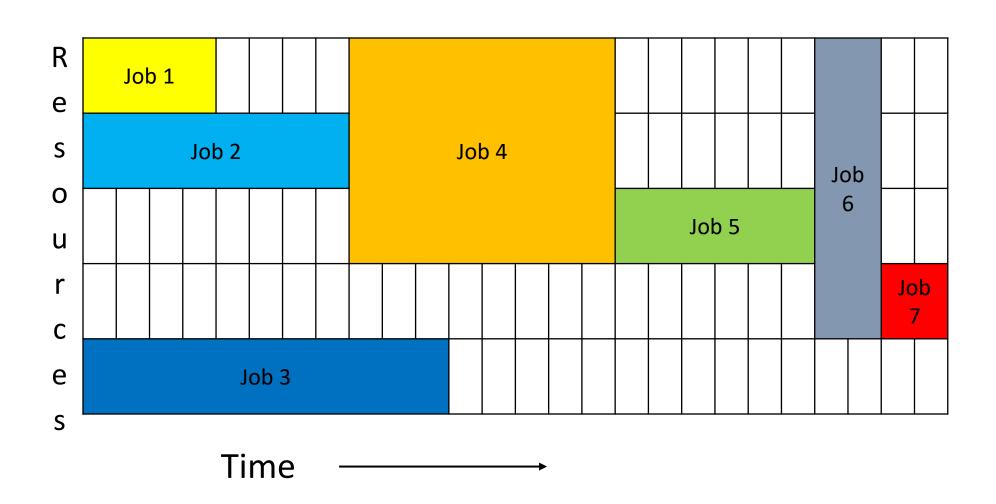




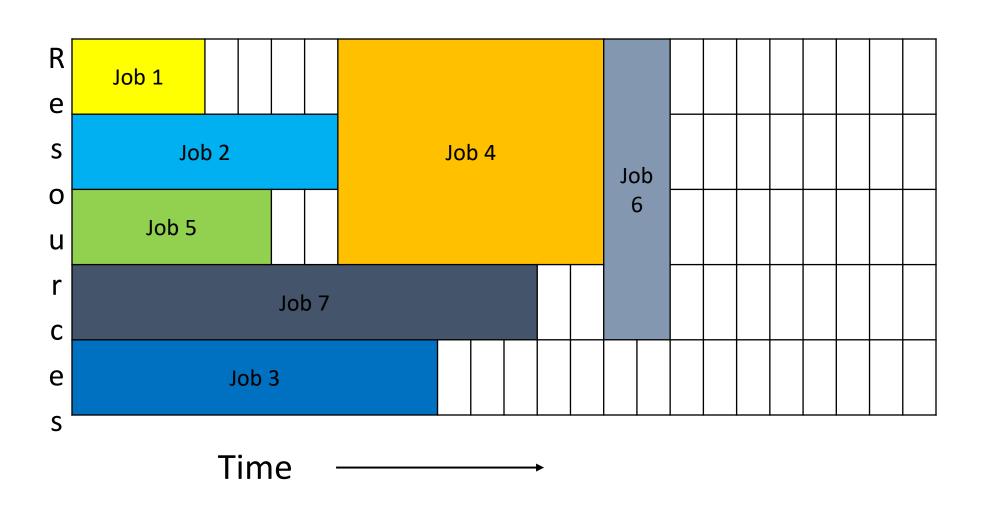












Slurm Scheduling



- Slurm tries to find a better schedule (using quick and simple algorithms)
 when:
 - A job is submitted;
 - A job completes;
 - A configuration change takes place.
- Slurm also performs slower and more expensive scheduling attempts less frequently
- This design allows nearly instant response; even when thousand of job are submitted at the same time.

Slurm – Quick Scheduling



- Slurm only checks the first X (by default 100) entries of the queue for new scheduling opportunities;
- Once a job in a partition is left pending (i.e. no scheduling is possible),
 Slurm ignores the other jobs in that partition;

Slurm – Thorough Scheduling



- Slurm checks all jobs in the queue (or until a configurable time limit is reached);
- Jobs are ordered by priority so this operation has low overhead;
- However, jobs in lower priority partitions (queues) have now more opportunities to start.