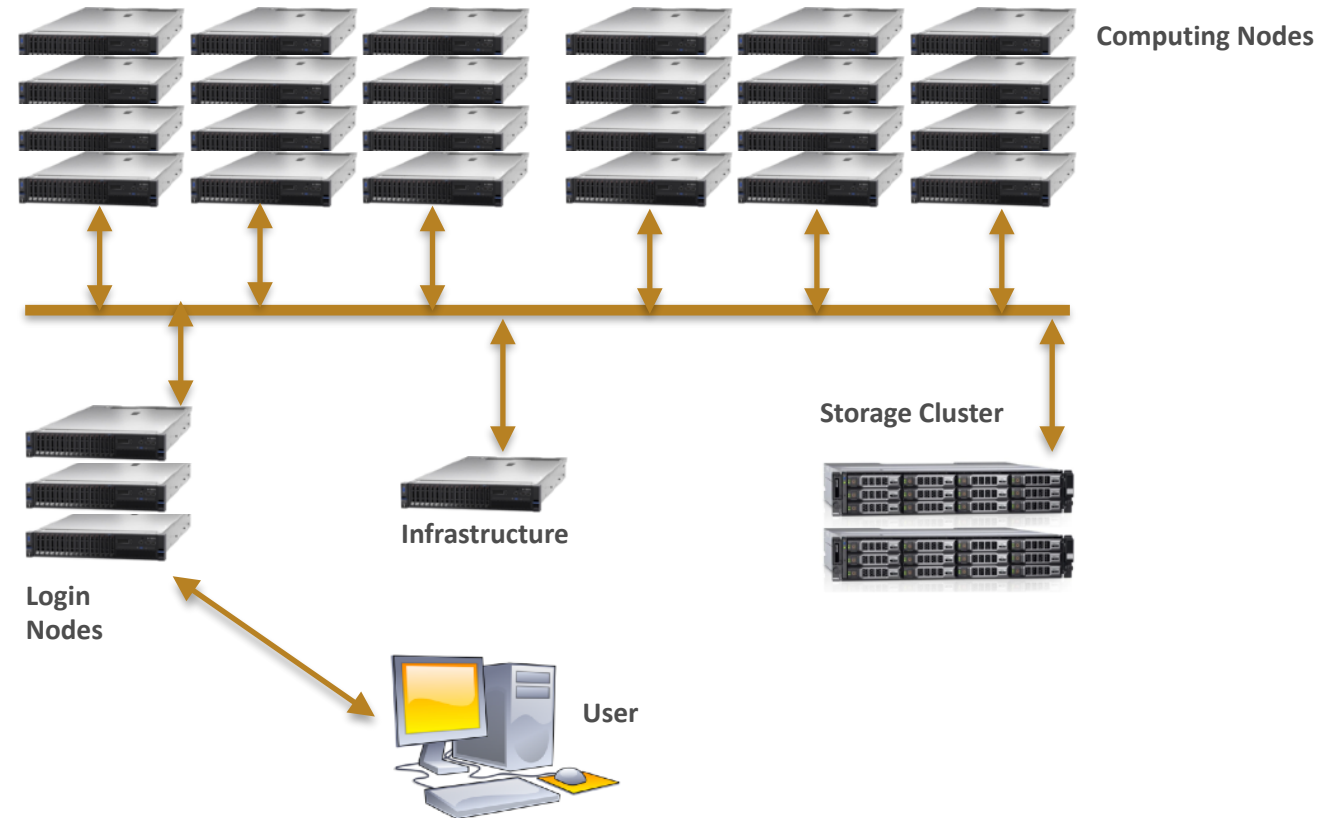


The O2 HPC cluster

The O2 cluster is composed of:

- *Login Nodes*, to connect remotely and submit jobs.
- *Compute nodes*, with high memory and multiple cores, to process many jobs simultaneously
- *Storage nodes*, for hosting the users data in O2
- *Scheduler*, handles O2 resources and dispatches jobs on computing nodes



O2 currently includes:

— **390 Compute Nodes** — **12260 CPU cores** — **106 TiB of RAM** — **136 GPU cards**

The Slurm scheduler



The Slurm scheduler handles resources allocation on the O2 cluster and also provides accounting information about past jobs and cluster utilization. Slurm periodically dispatches O2 jobs in two different ways:

- ***Direct Scheduling***

At every cycle Slurm tries to dispatch pending jobs with the highest priority on available idle resources (memory, cpu cores, gpu). If it cannot find available resources to dispatch a given high priority job, Slurm will determine *when* and *where* the required resources will be available, and will schedule a future start time and node allocation for the high priority job.

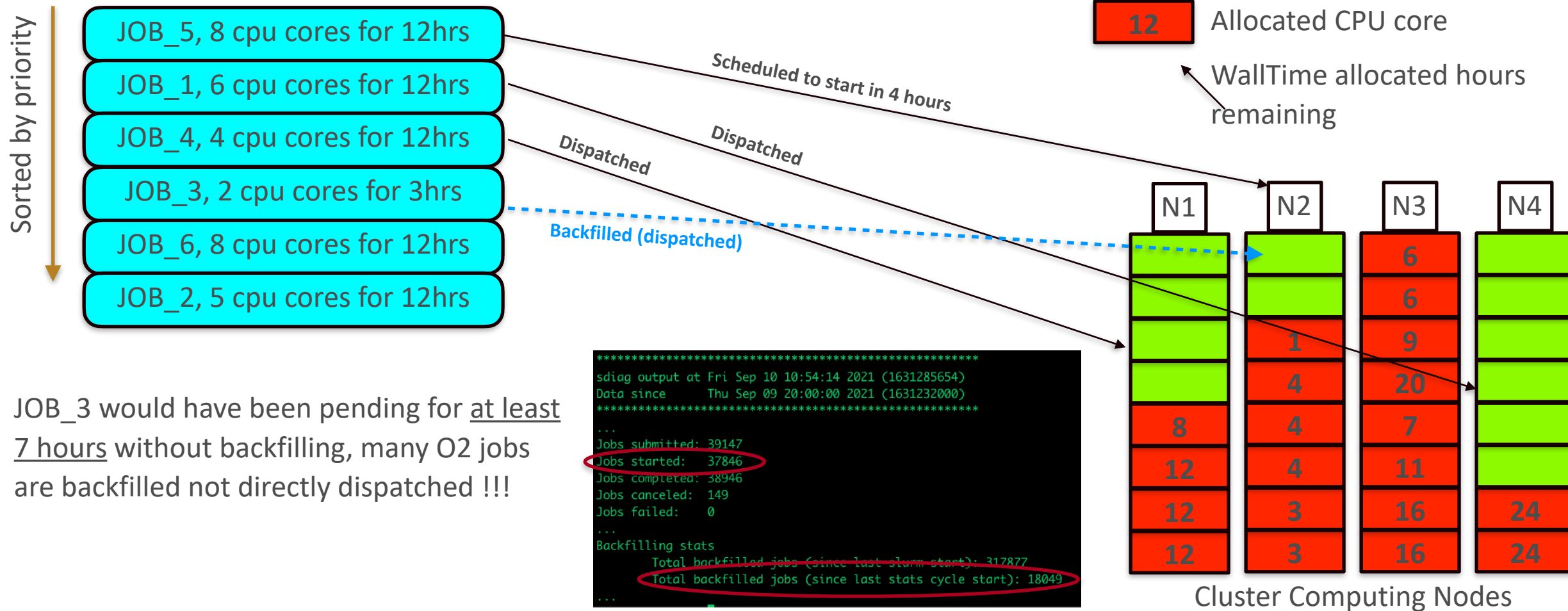
- ***Backfill Scheduling***

At every cycle Slurm tries to dispatch pending jobs with lower priority on available idle resources, as long as dispatching those lower priority jobs will not impact the expected start time of the higher priority jobs

In either cycle Slurm checks only a limited number of jobs per user, and it uses the “priority value” of each job as sorting criteria.

The Slurm scheduler

A simplified cpu-only scenario to understand jobs scheduling:



JOB_3 would have been pending for at least 7 hours without backfilling, many O2 jobs are backfilled not directly dispatched !!!



The Slurm scheduler

The job *priority value* is based on several factors:

- **Age:** proportional to the job's pending time (since eligible), it has a significant impact on overall priority.
- **JobSize:** relates to the resources requested, has negligible contribution.
- **Partition*:** based on the partition used, this factor has a minor impact on jobs overall priority
- **QOS:** “Quality Of Service”, is a custom factor priority, by default set to zero. It can have a significant impact on job's priority.
- **TRES:** not currently active, should always be zero
- **FairShare:** It is the most important factor in determining the overall job priority. It represents the fraction of resources consumed by the user in the last 48 hours respect to all the other users in the cluster.

* The scheduler tries to dispatch first jobs submitted to partitions *interactive* and *priority*, independently by the jobs priority values.

Why should you optimize your jobs ?

There are three good reasons why you should invest some time and optimize how your jobs are being executed on a cluster environment.

1. Reduce pending time, increase your throughput and overall processing speed



2. Reduce the cost, if applicable

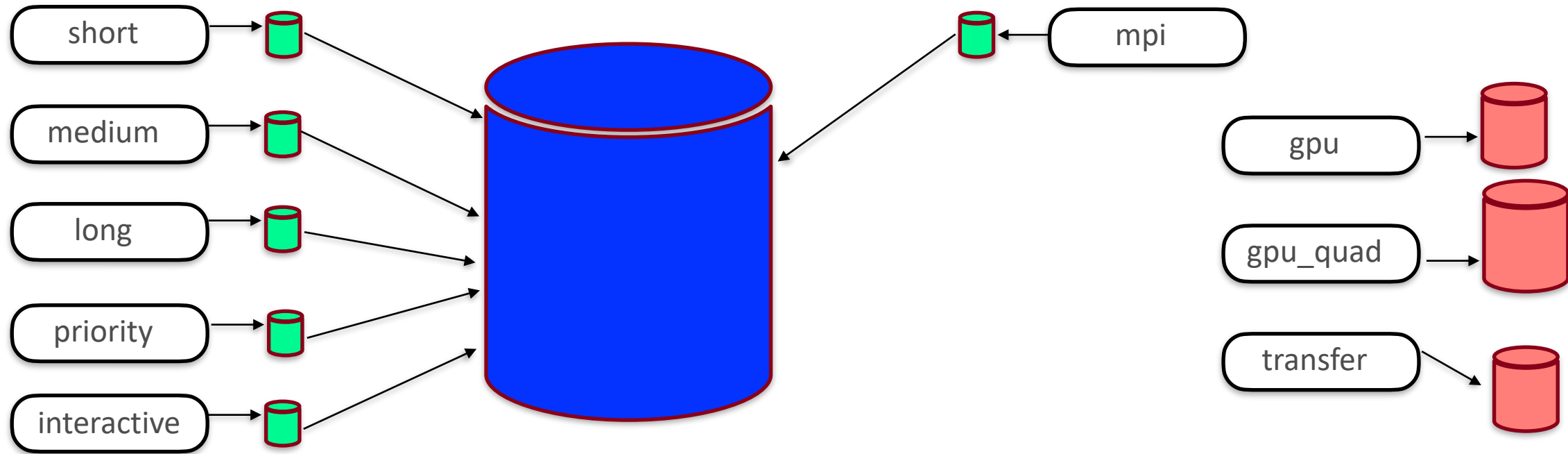


3. Avoid locking idle resources that could be allocated to other users

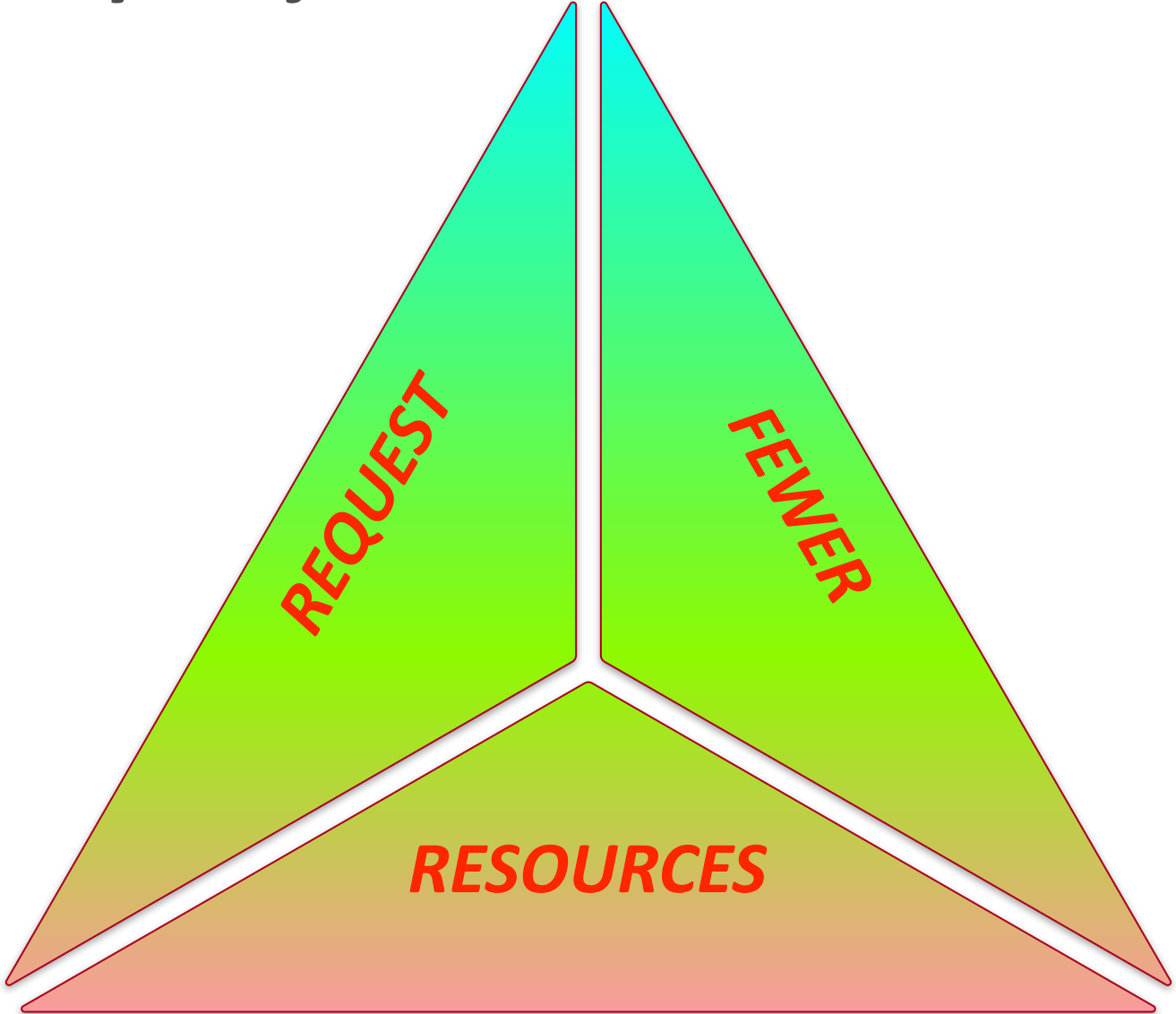


How NOT to optimize your jobs

The O2 cluster currently includes 12 different shared partitions (i.e. queues), one might think to optimize jobs by requesting arbitrary wall time and submitting the jobs across different partitions. This is not a good idea because those partitions share the vast majority of the computing resources.



How to optimize your jobs



How to optimize your jobs

There are four factors that strongly impact jobs' efficiency in O2

- Wasted resources on FAILED jobs



- Allocated but unused RAM



- Allocated but unused CPU cores



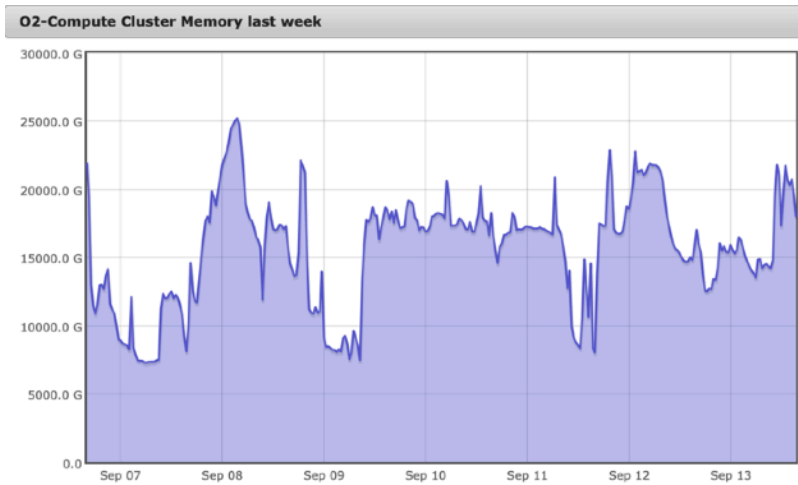
- Overestimated or arbitrary wall-time



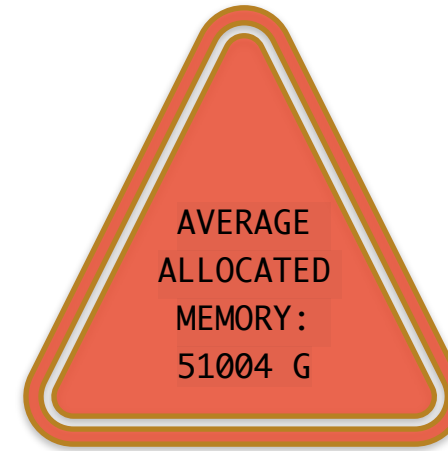
Allocating memory in O2 jobs

The scheduler allocates by default 1000 MiB of RAM for each requested CPU core.

Users can request a custom amount of memory per job using the flag `--mem=` and very often request much more memory than what is really needed.



VS



Allocating more memory than needed will:

- Unnecessarily increase the pending time of each job
- Consume more of your fair share, which will lower your jobs' priority
- Increase the utilization cost (when applicable)
- Stop other people's jobs from starting



Allocating memory in O2 jobs

There are two typical behaviors we see on the cluster:

(A) users over-allocated memory for all jobs

(B) users over-allocated memory for 99% of the jobs. In this case it is always better to plan for the 99% and resubmit the failed 1%

In either case the users below would have increased their throughput and reduced the cost by requesting no more than 1/2 of the memory originally requested.

A

User	Njobs	AvgReqMem(GB)	AvgUsedMem(GB)	AbsMaxUsed(GB)	Njob>1/2Req	AvgCoreEff(%)	AvgWallTimeUsed(%)
	13	199.89	24.96	31.41	0	98.86	27.42
	61	48.24	0.17	1.00	0	98.61	3.92
	14	100.50	4.10	6.28	0	97.74	7.02
	430	50.00	1.39	3.99	0	99.61	3.93
	49	174.99	5.20	5.90	0	57.27	2.26
	7576	50.66	0.86	19.82	0	82.23	11.52

User	Njobs	AvgReqMem(GB)	AvgUsedMem(GB)	AbsMaxUsed(GB)	Njob>1/2Req	AvgCoreEff(%)	AvgWallTimeUsed(%)
	9307	24.68	3.93	81.19	17	95.78	3.09
	252	62.20	11.02	32.53	1	85.54	6.26
	1110	113.92	27.36	181.75	13	27.30	3.67

week_ending_2021-09-13 (END)

B



Allocating CPU cores in O2 jobs

Users can request multiple CPU cores for their jobs. Requesting more cores will not automatically increase the job's performance!

The user requests several CPU assuming the job will run faster but...

- 1. The additional cores remain idle and no speedup is achieved. If your executable supports parallelization, make sure to pass any specific flag required.*
- 2. The parallelization does not scale very well and the overall benefit - cost balance is negative.*

User	TotJobs	AverageCPU	Efficiency
	176	2.98	31.88 %
	126	9.49	14.88 %
	57	3.75	17.55 %
	301	7.86	68.09 %
	146	5.50	31.11 %
	31	6.00	53.57 %
	5	20.00	30.06 %

Allocating more CPU than needed will again:

- Unnecessarily increase the pending time
- Consume fair share, and lower jobs' priority
- Increase the utilization cost (when applicable)



Allocating wall-time in O2 jobs

The majority of users tend to overestimate the wall time required, often setting it to the maximum value allowed.

Requesting too much wall-time does not impact fair-share or cost, however it reduces the possibility of jobs being backfilled.

Combine together very small jobs in larger batches, with each job running at least for 15 minutes, very short jobs can spend more time pending than running.

User	TotJobs	Njobs5X	%_Req_Time_Used	AVGelapsed			%_Partion_used				
	6925	0	0.31 %	0.04		short	100.00 %				
	15965	20	1.61 %	0.10		short	99.97 %	medium	0.03 %		
	2302	172	1.80 %	0.76		short	61.21 %	medium	38.66 %	priority	0.13 %
	11064	2	1.96 %	0.02		short	99.99 %	medium	0.01 %		

Allocating resources efficiently in O2 jobs

How can you check memory, cpu and wall-time utilization to optimize your future jobs?

1. Check the summary reports that RC sends weekly and adjust your required resources accordingly

Hello Raffaele,

Below you can find a short report about the memory, CPU and wall-time efficiencies for the **non-interactive** jobs you *successfully completed* (had state CD) over the last 7 days (since 2021-09-06).

We encourage you to check and, if needed, adjust the amount of memory, CPU and wall-time requested in order to maximize your job throughput and limit the amount of resources allocated but not used. Asking for fewer resources will usually make your jobs start running sooner, and will help other users' jobs run sooner as well.

User	Njobs	AvgReqMem(GB)	AvgUsedMem(GB)	AbsMaxUsed(GB)	Njob>1/2Req	AvgCoreEff(%)	AvgWallTimeUsed(%)
rp189	171	0.98	0.52	0.57	152	68.33	13.10

LEGEND

User = your username (rp189)
Njobs = Number of jobs you ran over the last 7 days marked as completed. Failed, canceled and timed out jobs are not considered.
AvgReqMem = weighted average memory requested (in GB) by your jobs
AvgUsedMem = weighted average memory used (in GB) by your jobs
AbsMaxUsed = Absolute maximum amount of memory (in GB) used by your jobs
Njob>1/2Req = Number of jobs that used at least 1/2 or more memory than what was requested by the job. Ideally this number should match Njobs
AvgCoreEff(%) = Average CPU efficiency. Indicates how much CPU was actually used respect to the reserved CPU. Ideally this number should be at least > 70
AvgWallTimeUsed(%) = Average percent of Wall-Time used. Indicates how much time your jobs actually ran respect to the requested wall-time. Ideally this number should be at least > 50

To get detailed information about resource usage for each job you can run the command O2sacct (O2sacct --help to get more info), and if you have any questions please let us know at rchelp@hms.harvard.edu (or respond to this email).

More information about job accounting and O2sacct can be found here: <https://wiki.rc.hms.harvard.edu/display/O2/Get+information+about+current+and+past+jobs#Getinformationaboutcurrentandpastjobs-O2sacct>

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Allocating resources efficiently in O2 jobs

How can you check memory, cpu and wall-time utilization to optimize your future jobs?

2. Use our **O2sacct** wrapper to see detailed information about a custom subset of jobs, see <https://harvardmed.atlassian.net/l/c/XqnwHpgP> for more details.

```
rp189@login03:~ O2sacct
```

JobID	Partition	State	Nodelist	Start	TimeLimit	Elapsed	CPUefficiency_%	AllocTRES	MaxMemoryUsed
40740675	priority	COMPLETED	compute-e-16-233	2021-09-16T00:15:14	00:05:00	00:00:32	68.75	billing=1,cpu=1,mem=0.98G,node=1	
40740675.batch		COMPLETED	compute-e-16-233	2021-09-16T00:15:14		00:00:32	68.75	cpu=1,mem=0.98G,node=1	0.53G
40740675.extern		COMPLETED	compute-e-16-233	2021-09-16T00:15:14		00:00:32	0.00	billing=1,cpu=1,mem=0.98G,node=1	0
40741499	priority	COMPLETED	compute-a-16-164	2021-09-16T01:15:34	00:05:00	00:00:41	70.73	billing=1,cpu=1,mem=0.98G,node=1	
40741499.batch		COMPLETED	compute-a-16-164	2021-09-16T01:15:34		00:00:41	70.73	cpu=1,mem=0.98G,node=1	0.53G
40741499.extern		COMPLETED	compute-a-16-164	2021-09-16T01:15:34		00:00:42	0.00	billing=1,cpu=1,mem=0.98G,node=1	0
40743060	priority	COMPLETED	compute-a-16-162	2021-09-16T02:15:04	00:05:00	00:00:41	70.73	billing=1,cpu=1,mem=0.98G,node=1	
40743060.batch		COMPLETED	compute-a-16-162	2021-09-16T02:15:04		00:00:41	70.73	cpu=1,mem=0.98G,node=1	0.55G
40743060.extern		COMPLETED	compute-a-16-162	2021-09-16T02:15:04		00:00:41	0.00	billing=1,cpu=1,mem=0.98G,node=1	0
40743774	priority	COMPLETED	compute-a-16-162	2021-09-16T03:15:50	00:05:00	00:00:39	76.92	billing=1,cpu=1,mem=0.98G,node=1	
40743774.batch		COMPLETED	compute-a-16-162	2021-09-16T03:15:50		00:00:39	76.92	cpu=1,mem=0.98G,node=1	0.56G
40743774.extern		COMPLETED	compute-a-16-162	2021-09-16T03:15:50		00:00:39	0.00	billing=1,cpu=1,mem=0.98G,node=1	0

Allocating resources efficiently in O2 jobs

How can you check memory, cpu and wall-time utilization to optimize your future jobs?

3. Build your own custom query using Slurm native *sacct* command.

```
sacct -u $USER --units=G --format=<field1,field2,field3,...>
```

4. Ask for RCC help

rchelp@hms.harvard.edu

<https://it.hms.harvard.edu/our-services/research-computing>

```
Login04:~ sacct -e
Account          AdminComment    AllocCPUS      AllocGRES
AllocNodes       AllocTRES       AssocID        AveCPU
AveCPUFreq       AveDiskRead     AveDiskWrite   AvePages
AveRSS           AveVMSize       BlockID        Cluster
Comment          Constraints     ConsumedEnergy  ConsumedEnergyRaw
CPUTime          CPUTimeRAW     DBIndex        DerivedExitCode
Elapsed          ElapsedRaw     Eligible       End
ExitCode         Flags           GID            Group
JobID            JobIDRaw       JobName        Layout
MaxDiskRead      MaxDiskReadNode  MaxDiskReadTask  MaxDiskWrite
MaxDiskWriteNode  MaxDiskWriteTask  MaxPages        MaxPagesNode
MaxPagesTask     MaxRSS          MaxRSSNode     MaxRSSTask
MaxVMSize        MaxVMSizeNode   MaxVMSizeTask   McsLabel
MinCPU           MinCPUNode     MinCPUTask     NCPUS
NNodes           NodeList       NTasks         Priority
Partition        QOS            QOSRAW         Reason
ReqCPUFreq       ReqCPUFreqMin   ReqCPUFreqMax   ReqCPUFreqGov
ReqCPUS          ReqGRES         ReqMem         ReqNodes
ReqTRES          Reservation     ReservationId   Reserved
ResvCPU          ResvCPURAW     Start          State
Submit          Suspended       SystemCPU       SystemComment
Timelimit        TimelimitRaw    TotalCPU       TRESUsageInAve
TRESUsageInMax   TRESUsageInMaxNode  TRESUsageInMaxTask  TRESUsageInMin
TRESUsageInMinNode  TRESUsageInMinTask  TRESUsageInTot   TRESUsageOutAve
TRESUsageOutMax   TRESUsageOutMaxNode  TRESUsageOutMaxTask  TRESUsageOutMin
TRESUsageOutMinNode  TRESUsageOutMinTask  TRESUsageOutTot   UID
User             UserCPU        WCKey          WCKeyID
WorkDir
```



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Job priority rewards

Users that do not waste too many computational resources are awarded with an extra priority QoS, equivalent to 30% extra fair-share.

Our goal is for O2 users to check resources actually consumed and adjust job submissions accordingly.

It is often not possible to predict exactly memory and/or run time, reasonable memory and wall-time buffers are OK and advised!

More details are available on our wiki page at <https://harvardmed.atlassian.net/l/c/03G8RYP1>

```
Name|Priority|GraceTime|Preempt|PreemptExemptTime|PreemptMode|Flags|UsageThres|UsageFactor|
normalplus|3|00:00:00|||cluster|||1.000000|
```