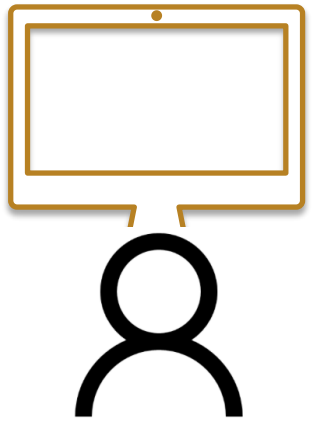
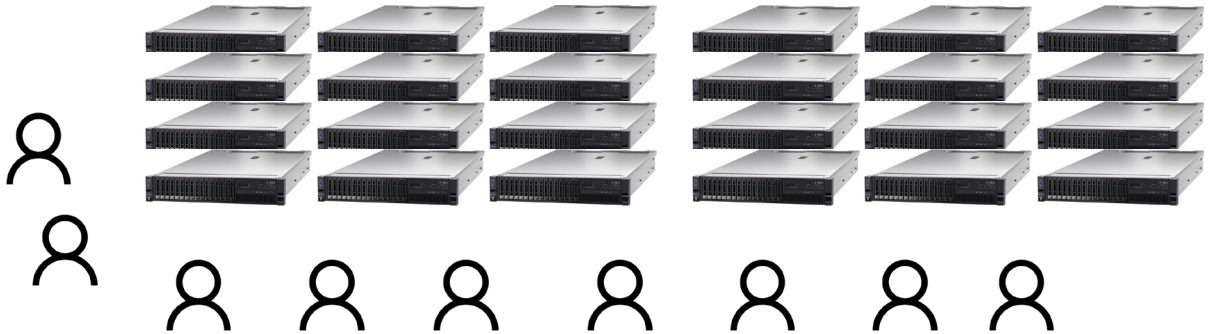
# HMS Research Computing

# Optimizing O2 Jobs

# Optimize how YOU run on a shared environment



VS



Desktop Scenario

Limited amount of computational resources available only to a single user.

Use all you can, even if not at peak efficiency.

HPC Cluster scenario

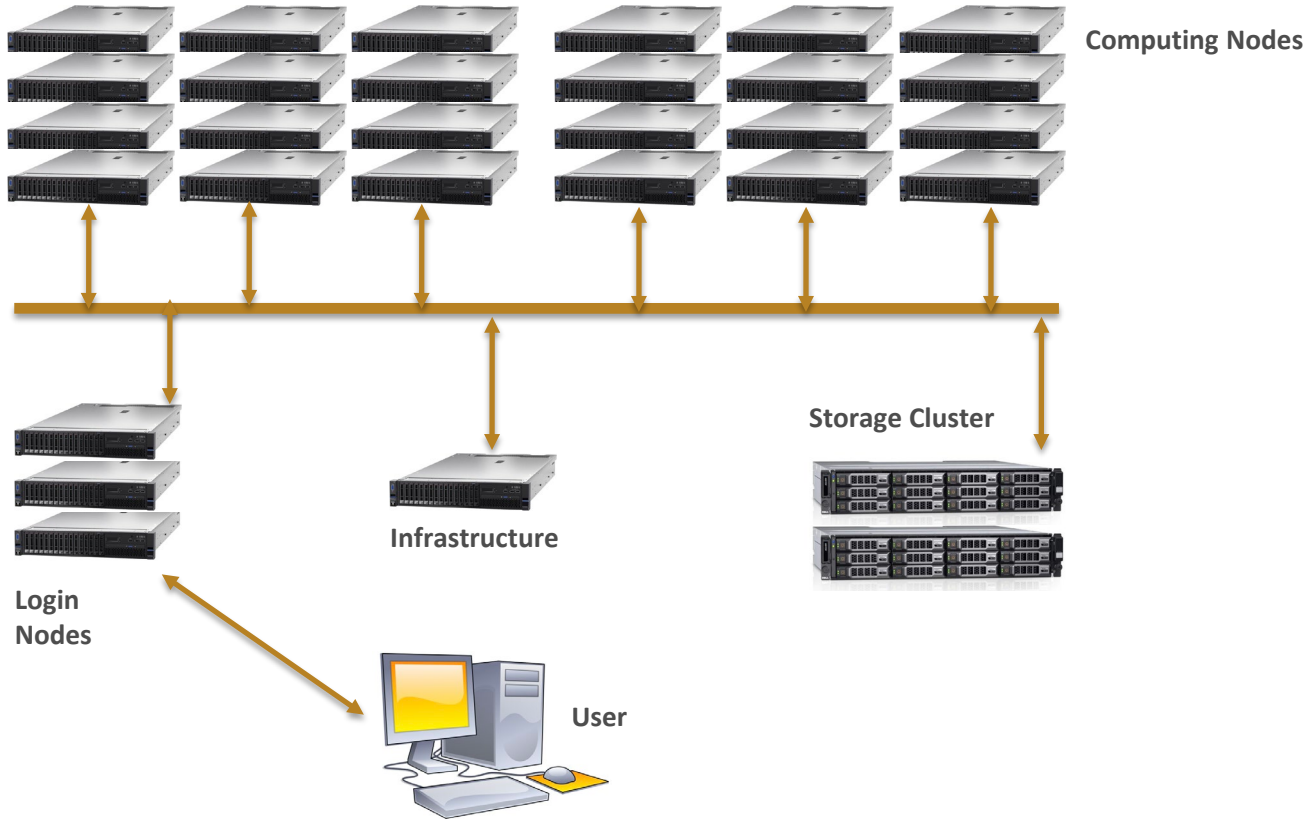
Large amount of computational resources shared between many users.

Using resources efficiently will benefit you and everyone in the system.

# 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.

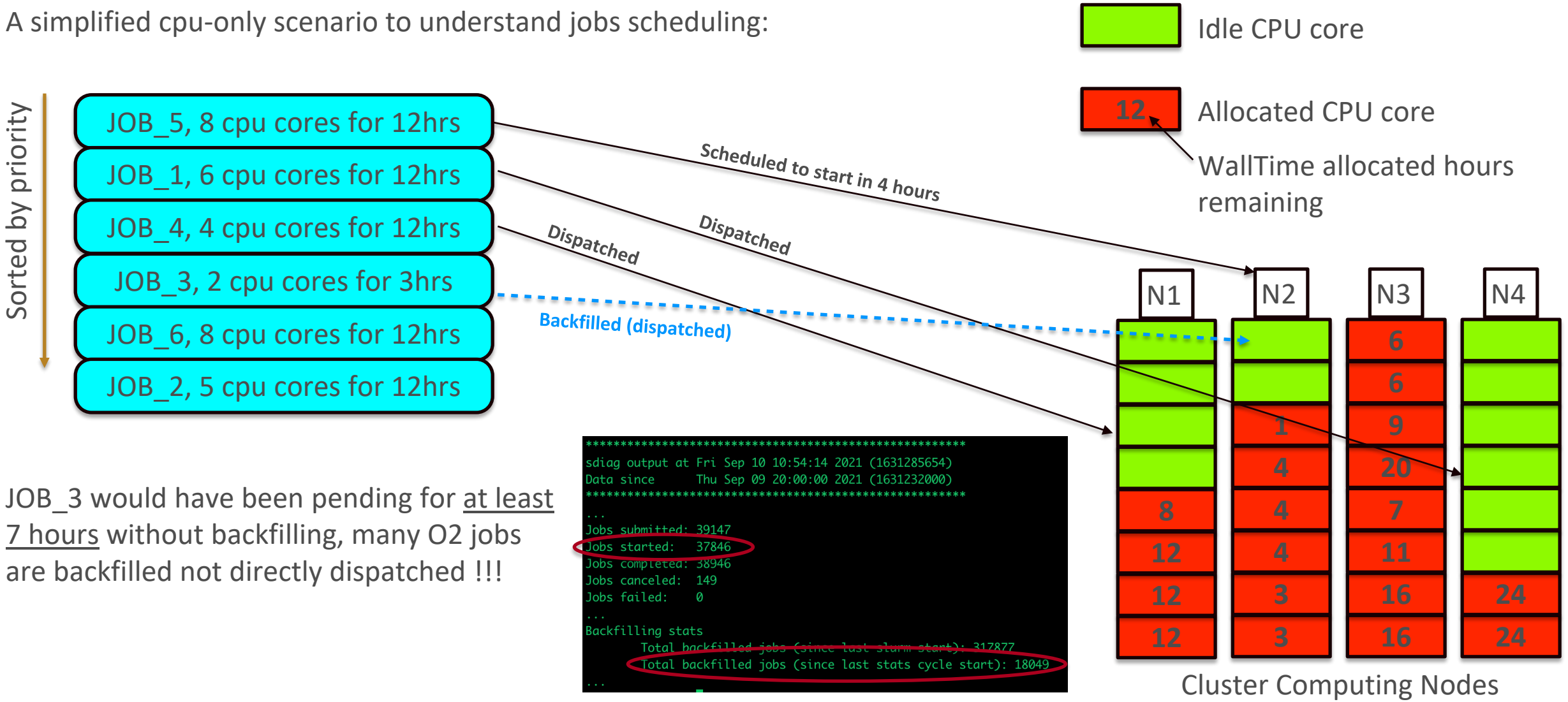
- ***Backfill Scheduling***

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 <u>at least 7 hours</u> without backfilling, many O2 jobs are backfilled not directly dispatched !!!

```
**************************************************
sdiag output at Fri Sep 10 10:54:14 2021 (1631285654)
Data since      Thu Sep 09 20:00:00 2021 (1631232000)
**************************************************
...
Jobs submitted: 39147
Jobs started:   37846
Jobs completed: 38946
Jobs canceled:  149
Jobs failed:    0
...
Backfilling stats
        Total backfilled jobs (since last slurm start): 317877
        Total backfilled jobs (since last stats cycle start): 18049
...
```

# 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 to optimize your jobs

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

- Wasted resources on FAILED jobs

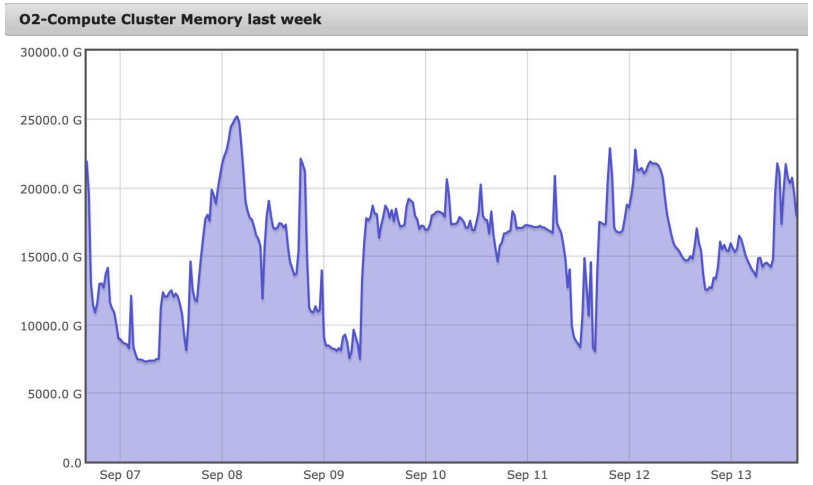
- Allocated but unused RAM

- Allocated but unused CPU cores

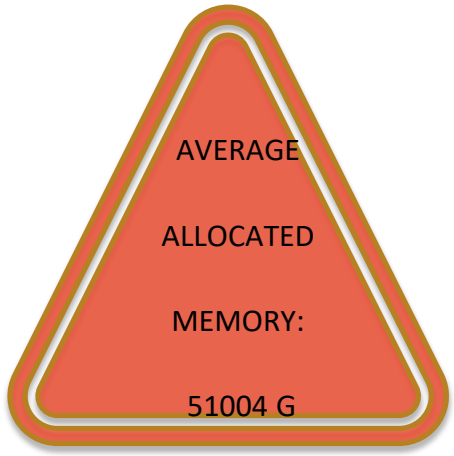

- Overestimated or arbitrary wall-time

# 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 |

B

| 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)

# 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
```

# Questions ?