Uni.lu HPC School 2018

PS3: Job scheduling with SLURM and OAR

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http://hpc.uni.lu

Latest versions available on Github:

UL HPC tutorials: https://github.com/ULHPC/tutorials

UL HPC School: http://hpc.uni.lu/hpc-school/

PS3 tutorial sources: ulhpc-tutorials.rtfd.io/en/latest/scheduling/advanced/

Summary

Main Objectives of this Session

- **Design and usage of SLURM**
  - ↪ cluster workload manager of the UL HPC `iris` cluster
  - ↪ . . . and future HPC systems

The tutorial will show you:

- the way SLURM was **configured**, **accounting** and **permissions**
- **common** and **advanced** SLURM tools and commands
  - ↪ `srun`, `sbatch`, `squeue` etc.
  - ↪ job specification
  - ↪ SLURM job types
  - ↪ comparison of SLURM (`iris`) and OAR (`gaia` & `chaos`)
- SLURM generic **launchers** you can use for your own jobs

Documentation & comparison to OAR

`https://hpc.uni.lu/users/docs/scheduler.html`

Summary

SLURM - core concepts

- SLURM manages user jobs with the following **key characteristics**:
  - ↪ set of **requested resources**:
    - ✓ number of computing resources: **nodes** (including all their CPUs and cores) or **CPUs** (including all their cores) or **cores**
    - ✓ number of accelerators (**GPUs**)
    - ✓ amount of **memory**: either per node or per (logical) CPU
    - ✓ the **(wall)time** needed for the user's tasks to complete their work
  - ↪ a set of **constraints** limiting jobs to nodes with specific features
  - ↪ a requested node **partition** (job queue)
  - ↪ a requested **quality of service** (QoS) level which grants users specific accesses
  - ↪ a requested **account** for accounting purposes
- **Example**: run an interactive job Alias: `si [...]`

```
(access)$ srun -p interactive --qos qos-interactive --pty bash -i
(node)$ echo $SLURM_JOBID
2058
```

Simple interactive job running under SLURM

SLURM - job example (I)

```
$ scontrol show job 2058
JobId=2058 JobName=bash
   UserId=vplugaru(5143) GroupId=clusterusers(666) MCS_label=N/A
    Priority =100 Nice=0 Account=ulhpc QOS=qos-interactive
   JobState=RUNNING Reason=None Dependency=(null)
   Requeue=1 Restarts=0 BatchFlag=0 Reboot=0 ExitCode=0:0
   RunTime=00:00:08 TimeLimit=00:05:00 TimeMin=N/A
   SubmitTime=2017-06-09T16:49:42 EligibleTime=2017-06-09T16:49:42
   StartTime=2017-06-09T16:49:42 EndTime=2017-06-09T16:54:42 Deadline=N/A
   PreemptTime=None SuspendTime=None SecsPreSuspend=0
    Partition =interactive  AllocNode:Sid=access2:163067
   ReqNodeList=(null) ExcNodeList=(null)
   NodeList=iris-081
   BatchHost=iris-081
   NumNodes=1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
   TRES=cpu=1,mem=4G,node=1
   Socks/Node=* NtasksPerN:B:S:C=1:0:*:* CoreSpec=*
   MinCPUsNode=1 MinMemoryCPU=4G MinTmpDiskNode=0
   Features=(null) DelayBoot=00:00:00
   Gres=(null) Reservation=(null)
   OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
   Command=bash
   WorkDir=/mnt/irisgpfs/users/vplugaru
   Power=
```

Simple interactive job running under SLURM

SLURM - job example (II)

- Many metrics available during and after job execution
  - ↪ including energy (J) – but with caveats
  - ↪ job **steps** counted individually
  - ↪ enabling advanced application debugging and optimization
- Job information available in easily parseable format (add -p/-P)

```
$ sacct -j 2058 --format=account,user,jobid,jobname,partition,state
   Account       User         JobID    JobName  Partition        State
     ulhpc   vplugaru          2058       bash  interacti +  COMPLETED

$ sacct -j 2058 --format=elapsed,elapsedraw,start,end
   Elapsed ElapsedRaw                Start                  End
  00:02:56         176 2017-06-09T16:49:42 2017-06-09T16:52:38

$ sacct -j 2058 --format=maxrss,maxvmsize,consumedenergy,consumedenergyraw,nnodes,ncpus,nodelist
    MaxRSS MaxVMSize ConsumedEnergy ConsumedEnergyRaw NNodes NCPUS      NodeList
         0    299660K         17.89K       17885.000000      1     1         iris-081
```

Job metrics after execution ended

SLURM - design for iris (I)

Partition	# Nodes	Default time	Max time	Max nodes/user
batch*	148	0-2:0:0	5-0:0:0	unlimited
bigmem	4	0-2:0:0	5-0:0:0	unlimited
gpu	18	0-2:0:0	5-0:0:0	unlimited
interactive	10(~5%)	0-1:0:0	0-4:0:0	2
long	10(~5%)	0-2:0:0	30-0:0:0	2

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long	10(~5%)	0-2:0:0	30-0:0:0	2

QoS	User group	Max cores	Max jobs/user
qos-besteffort	**ALL**	**no limit**	
qos-batch	**ALL**	**2744**	100
qos-bigmem	**ALL**	**448**	100
qos-gpu	**ALL**	**504**	100
qos-interactive	**ALL**	**224**	10
qos-long	**ALL**	**224**	10
qos-batch-001	private	1400	100
qos-interactive-001	private	56	10
qos-long-001	private	56	10

SLURM - design for iris (II)

- **Default partition**: **batch**, meant to receive most user jobs
  - ↪ we hope to see majority of user jobs being able to scale
  - ↪ shorter walltime jobs highly encouraged
- All partitions have a correspondingly named **QOS**
  - ↪ granting resource access (**long** : **qos-long**)
  - ↪ any job is tied to one **QOS** (user specified or inferred)
  - ↪ automation in place to select **QOS** based on partition
  - ↪ jobs may wait in the queue with *QOS*Limit* reason set
    - ✓ e.g. *QOSGrpCpuLimit* if group limit for CPUs was reached

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  - ↪ jobs may wait in the queue with *QOS*Limit* reason set
    - ✓ e.g. *QOSGrpCpuLimit* if group limit for CPUs was reached
- Preemptible **besteffort** QOS available for `batch` and `interactive` partitions (but not *yet* for `bigmem`, `gpu` or `long`)
  - ↪ meant to ensure maximum resource utilization especially on `batch`
  - ↪ should be used together with restartable software
- QOSs specific to particular group accounts exist (discussed later)
  - ↪ granting additional accesses to platform contribuitors

SLURM - design for iris (III)

- **Backfill** scheduling for efficiency
  - ↪ **multifactor job priority** (size, age, fairshare, QOS, . . .)
  - ↪ currently weights set for: job age, partition and fair-share
  - ↪ other factors/decay to be tuned **as needed**
    - ✓ with more user jobs waiting in the queues
- Resource selection: **consumable resources**
  - ↪ **cores and memory** as consumable (per-core scheduling)
  - ↪ **GPUs** as consumable (4 GPUs per node in the gpu partition)
  - ↪ block distribution for cores (best-fit algorithm)
  - ↪ default memory/core: 4GB (4.1GB maximum, rest is for OS)
    - ✓ `gpu` and `bigmem` partitions: 27GB maximum

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  - ↪ default memory/core: 4GB (4.1GB maximum, rest is for OS)
    - ✓ `gpu` and `bigmem` partitions: 27GB maximum
- User process tracking with **cgroups**
  - ↪ cpusets used to constrain cores and RAM (no swap allowed)
  - ↪ task affinity used to bind tasks to cores (hwloc based)
- Hierarchical tree topology defined (for the network)
  - ↪ for optimized job resource allocation

SLURM - design for iris (III)

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Help will be needed on your part to optimize your job parameters!

A note on job priority

```
Job_priority =
    (PriorityWeightAge) * (age_factor) +
    (PriorityWeightFairshare) * (fair-share_factor) +
    (PriorityWeightJobSize) * (job_size_factor) +
    (PriorityWeightPartition) * (partition_factor) +
    (PriorityWeightQOS) * (QOS_factor) +
    SUM(TRES_weight_cpu * TRES_factor_cpu,
        TRES_weight_<type> * TRES_factor_<type>,
        ...)
```

For complete details see: slurm.schedmd.com/priority_multifactor.html

- **TRES** - Trackable RESources
  - ↪ CPU, Energy, Memory and Node tracked by default
- **GRES** - Generic RESources
  - ↪ GPU, available end of 2018/early 2019
- Corresponding weights/reset periods **tuned with your feedback**
  - ↪ we require (your & your group's) usage pattern to optimize them
  - ↪ the target is high interactivity (low time spent by the jobs waiting)

SLURM - design for iris (IV)

Some details on job permissions...

- Partition limits + association-based rule enforcement
  - ↪ association settings in SLURM's accounting database
- **QOS** limits imposed, e.g. you will see (`QOSGrpCpuLimit`)
- Only users with existing **associations** able to run jobs

SLURM - design for iris (IV)

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- **Best-effort** jobs possible through preemptible QOS: **qos-besteffort**
  - ↪ of lower priority and preemptible by all other QOS
  - ↪ preemption mode is **requeue**, requeueing disabled by default

SLURM - design for iris (IV)

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  - ↪ of lower priority and preemptible by all other QOS
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- **On metrics**: Accounting & profiling data for jobs sampled every 30s
  - ↪ tracked: cpu, mem, energy
  - ↪ energy data retrieved through the RAPL mechanism
    - ✓ **caveat**: for energy not all hw. that may consume power is monitored with RAPL (CPUs, GPUs and DRAM are included)

SLURM - design for iris (V)

- **On tightly coupled parallel jobs (MPI)**
  - ↪ Process Management Interface (PMI 2) highly recommended
  - ↪ PMI2 used for better scalability and performance
    - ✓ faster application launches
    - ✓ tight integration w. SLURM's job steps mechanism (& metrics)
    - ✓ we are also testing PMIx (PMI Exascale) support

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  - ↪ PMI2 enabled in default software set for IntelMPI and OpenMPI
    - ✓ requires minimal adaptation in your workflows
    - ✓ (at minimum:) replace **mpirun** with SLURM's **srun**
    - ✓ if you compile/install your own MPI you'll need to configure it
  - ↪ **Many examples at**: `https://hpc.uni.lu/users/docs/slurm_launchers.html`

SLURM - design for iris (V)

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- **SSH-based connections** between computing nodes still **possible**
  - ↪ other MPI implementations can still use `ssh` as launcher
    - ✓ but **really shouldn't need to**, PMI2 support is everywhere
  - ↪ user jobs are tracked, no job == no access to node

SLURM - design for iris (VI)

ULHPC customizations through plugins

- Job submission rule / filter
  - ↪ for now: QOS initialization (if needed)
  - ↪ more rules to come (group credits, node checks, etc.)
- Per-job temporary directories creation & cleanup
  - ↪ better security and privacy, using kernel namespaces and binding
  - ↪ `/tmp` & `/var/tmp` are `/tmp/$jobid.$rstcnt/[tmp,var_tmp]`
  - ↪ transparent for apps. ran through `srun`
  - ↪ apps. ran with ssh cannot be attached, will see base /tmp!
- X11 forwarding (GUI applications)
  - ↪ enabled with `--x11` parameter to `srun/salloc`
  - ↪ being rewritten to play nice with per-job tmpdir
    - ✓ workaround 1: create job and `ssh -X` to head node (need to propagate job environment)
    - ✓ workaround 2: create job using `salloc` and then use `ssh -X`

SLURM - design for iris (VII)

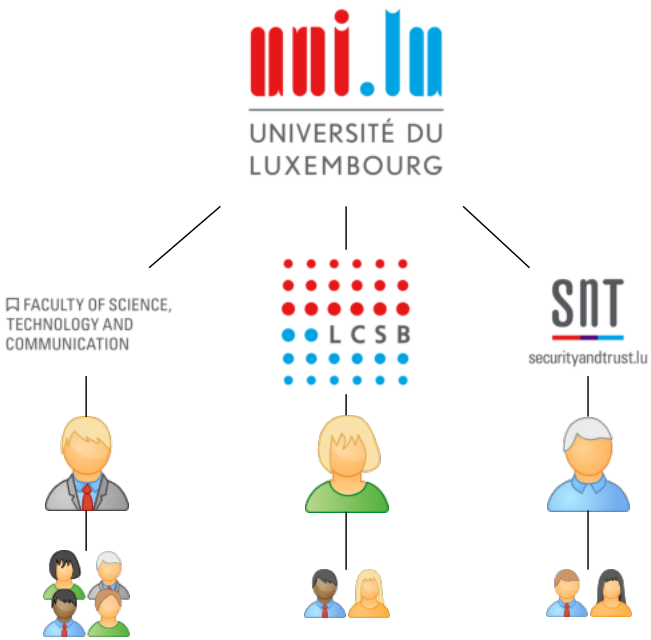
Software licenses in SLURM

- ARM (ex. Allinea) Forge and Performance Reports for now
  - ↪ static allocation in SLURM configuration
  - ↪ dynamic checks for FlexNet / RLM based apps. coming later
- Number and utilization state can be checked with:
  - ↪ `scontrol show licenses`
- Use not enforced, **honor system** applied
  - ↪ `srun [...] -L $licname:$licnumber`

```
$> srun -N 1 -n 28 -p interactive -L forge:28 --pty bash -i
```

SLURM - bank (group) accounts

- Hierarchical **bank (group) accounts**
- UL as root account, then underneath accounts for the 3 Faculties and 3 ICs
- All Prof., Group leaders and above have **bank accounts**, linked to a Faculty or IC
  - ↪ with their own name: **Name.Surname**
- All **user accounts** linked to a bank account
  - ↪ including Profs.'s own user
- Iris accounting DB contains over
  - ↪ 87 group accounts from Faculties & ICs
  - ↪ comprising 578 users



Allows better usage tracking and reporting than was possible before.

SLURM - brief commands overview

- **squeue**: view queued jobs
- **sinfo**: view partition and node info.
- **sbatch**: submit job for batch (scripted) execution
- **srun**: submit interactive job, run (parallel) job step
- **scancel**: cancel queued jobs

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- **scancel**: cancel queued jobs

- **scontrol**: detailed control and info. on jobs, queues, partitions
- **sstat**: view system-level utilization (memory, I/O, energy)
  - ↪ for running jobs / job steps
- **sacct**: view system-level utilization
  - ↪ for completed jobs / job steps (accounting DB)
- **sacctmgr**: view and manage SLURM accounting data

SLURM - brief commands overview

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- **sacct**: view system-level utilization
  - ↪ for completed jobs / job steps (accounting DB)
- **sacctmgr**: view and manage SLURM accounting data

- **sprio**: view job priority factors
- **sshare**: view accounting share info. (usage, fair-share, etc.)

SLURM - basic commands

Action	SLURM command
Submit passive/batch job	`sbatch $script`
Start interactive job	`srun --pty bash -i`
Queue status	`squeue`
User (own) jobs status	`squeue -u $USER`
Specific job status (detailed)	`scontrol show job $jobid`
Job metrics (detailed)	`sstat --job $jobid -l`
Job accounting status (detailed)	`sacct --job $jobid -l`
Job efficiency report	`seff $jobid`
Delete (running/waiting) job	`scancel $jobid`
Hold job	`scontrol hold $jobid`
Resume held job	`scontrol release $jobid`
Node list and their properties	`scontrol show nodes`
Partition list, status and limits	`sinfo`
Attach to running job	`sjoin $jobid [$node]`

QOS deduced if not specified, partition needs to be set if not "batch"

SLURM - basic options for sbatch/srun

Action	sbatch/srun option
Request $n distributed nodes	`-N $n`
Request $m memory per node	`--mem=$mGB`
Request $mc memory per core (logical cpu)	`--mem-per-cpu=$mcGB`
Request job walltime	`--time=d-hh:mm:ss`
Request $tn tasks per node	`--ntasks-per-node=$tn`
Request $ct cores per task (multithreading)	`-c $ct`
Request $nt total # of tasks	`-n $nt`
Request $g # of GPUs per node	`--gres=gpu:$g`
Request to start job at specific $time	`--begin $time`
Specify job name as $name	`-J $name`
Specify required node $feature	`-C $feature`
Specify job partition	`-p $partition`
Specify QOS	`--qos $qos`
Specify account	`-A $account`
Specify email address	`--mail-user=$email`
Request email on event	`--mail-type=all[,begin,end,fail]`
Use the above actions in a batch script	`#SBATCH $option`

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Specify email address	`--mail-user=$email`
Request email on event	`--mail-type=all[,begin,end,fail]`
Use the above actions in a batch script	`#SBATCH $option`

- Diff. between **-N**, **-c**, **-n**, **--ntasks-per-node**, **--ntasks-per-core** ?
- Normally you'd specify **-N** and **--ntasks-per-node**
  - ↪ fix the latter to 1 and add **-c** for MPI+OpenMP jobs
- If your application is scalable, just **-n** might be enough
  - ↪ beware of running across heterogeneous nodes:use '-C'

SLURM - more options for sbatch/srun

Start job when... (dependencies)	sbatch/srun option
these other jobs have started	`-d after:$jobid1:$jobid2`
these other jobs have ended	`-d afterany:$jobid1:$jobid2`
these other jobs have ended with no errors	`-d afterok:$jobid1:$jobid2`
these other jobs have ended with errors	`-d afternok:$jobid1:$jobid2`
all other jobs with the same name have ended	`-d singleton`

Job dependencies and especially "singleton" can be very useful!

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Allocate job at... (specified time)	sbatch/srun option
exact time today	`--begin=16:00`
tomorrow	`--begin=tomorrow`
specific time relative to now	`--begin=now+2hours`
given date and time	`--begin=2017-06-23T07:30:00`

Jobs run like this will wait as PD – Pending with "(BeginTime)" reason

SLURM - more options for sbatch/srun

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Jobs run like this will wait as PD – Pending with "(BeginTime)" reason

Other scheduling requests	sbatch/srun option
Ask for minimum/maximum # of nodes	`-N minnodes-maxnodes`
Ask for minimum run time (start job faster)	`--time-min=d-hh:mm:ss`
Ask to remove job if deadline can't be met	`--deadline=YYYY-MM-DD[THH:MM[:SS]]`
Run job within pre-created (admin) reservation	`--reservation=$reservationname`
Allocate resources as specified job	`--jobid=$jobid`

Can use --jobid to connect to running job (different than sattach!)

SLURM - environment variables

- 53 input env. vars. can be used to define job parameters
  - ↪ almost all have a command line equivallent
- up to 59 output env. vars. available within job environment
  - ↪ some common ones:

Description	Environment variable
Job ID	`$SLURM_JOBID`
Job name	`$SLURM_JOB_NAME`
Name of account under which job runs	`$SLURM_JOB_ACCOUNT`
Name of partition job is running in	`$SLURM_JOB_PARTITION`
Name of QOS the job is running with	`$SLURM_JOB_QOS`
Name of job's advance reservation	`$SLURM_JOB_RESERVATION`
Job submission directory	`$SLURM_SUBMIT_DIR`
Number of nodes assigned to the job	`$SLURM_NNODES`
Name of nodes assigned to the job	`$SLURM_JOB_NODELIST`
Number of tasks for the job	`$SLURM_NTASKS` or `$SLURM_NPROCS`
Number of cores for the job on current node	`$SLURM_JOB_CPUS_PER_NODE`
Memory allocated to the job per node	`$SLURM_MEM_PER_NODE`
Memory allocated per core	`$SLURM_MEM_PER_CPU`
Task count within a job array	`$SLURM_ARRAY_TASK_COUNT`
Task ID assigned within a job array	`$SLURM_ARRAY_TASK_ID`

Outputting these variables to the job log is essential for bookkeeping!

Usage examples (I)

> Interactive jobs

```
srun -p interactive --qos qos-interactive --time=0:30 -N2 --ntasks-per-node=4 --pty bash -i
srun -p interactive --qos qos-interactive --pty --x11 bash -i
srun -p interactive --qos qos-besteffort --cpu-bind=none -N1 -n4 --pty bash -i
srun -C skylake -p batch --time=0:10:0 -N1 -c28  --pty bash -i
```

Usage examples (I)

> Interactive jobs

```
srun -p interactive --qos qos-interactive --time=0:30 -N2 --ntasks-per-node=4 --pty bash -i
srun -p interactive --qos qos-interactive --pty --x11 bash -i
srun -p interactive --qos qos-besteffort --cpu-bind=none -N1 -n4 --pty bash -i
srun -C skylake -p batch --time=0:10:0 -N1 -c28  --pty bash -i
```

> Batch jobs

```
sbatch job.sh
sbatch -N 2 job.sh
sbatch -p batch --qos qos-batch job.sh
sbatch -p long --qos qos-long job.sh
sbatch --begin=2019-06-23T07:30:00 job.sh
sbatch -p batch --qos qos-besteffort job.sh
sbatch -p gpu --qos qos-gpu --gres=gpu:4 job.sh
sbatch -p bigmem --qos qos-bigmem --mem=2T job.sh
```

Usage examples (I)

> Interactive jobs

```
srun -p interactive --qos qos-interactive --time=0:30 -N2 --ntasks-per-node=4 --pty bash -i
srun -p interactive --qos qos-interactive --pty --x11 bash -i
srun -p interactive --qos qos-besteffort --cpu-bind=none -N1 -n4 --pty bash -i
srun -C skylake -p batch --time=0:10:0 -N1 -c28  --pty bash -i
```

> Batch jobs

```
sbatch job.sh
sbatch -N 2 job.sh
sbatch -p batch --qos qos-batch job.sh
sbatch -p long --qos qos-long job.sh
sbatch --begin=2019-06-23T07:30:00 job.sh
sbatch -p batch --qos qos-besteffort job.sh
sbatch -p gpu --qos qos-gpu --gres=gpu:4 job.sh
sbatch -p bigmem --qos qos-bigmem --mem=2T job.sh
```

Status and details for partitions, nodes, reservations

```
squeue / squeue -l / squeue -la / squeue -l -p batch / squeue -t PD
scontrol show nodes / scontrol show nodes $nodename
sinfo / sinfo -s / sinfo -N
sinfo -T
```

Usage examples (II)

Collecting job information, priority, expected start time

```
scontrol show job $jobid          # only available while job is queued + 5 minutes after completion
sprio -l
squeue --start -u $USER
```

Usage examples (II)

Collecting job information, priority, expected start time

```
scontrol show job $jobid          # only available while job is queued + 5 minutes after completion
sprio -l
squeue --start -u $USER
```

Running job metrics – sstat tool

```
sstat -j $jobid / sstat -j $jobid -l
sstat -j $jobid1 --format=AveCPU,AveRSS,AveVMSize,MaxRSS,MaxVMSize
sstat -p -j $jobid1,$jobid2 --format=AveCPU,AveRSS,AveVMSize,MaxRSS,MaxVMSize
```

Usage examples (II)

Collecting job information, priority, expected start time

```
scontrol show job $jobid          # only available while job is queued + 5 minutes after completion
sprio -l
squeue --start -u $USER
```

Running job metrics – sstat tool

```
sstat -j $jobid / sstat -j $jobid -l
sstat -j $jobid1 --format=AveCPU,AveRSS,AveVMSize,MaxRSS,MaxVMSize
sstat -p -j $jobid1,$jobid2 --format=AveCPU,AveRSS,AveVMSize,MaxRSS,MaxVMSize
```

Completed job metrics – sacct & seff tools

```
sacct -j $jobid / sacct -j $jobid -l
sacct -p -j $jobid --format=account,user,jobid,jobname,partition,state,elapsed,elapsedraw,
          start,end,maxrss,maxvmsize,consumedenergy,consumedenergyraw,nnodes,ncpus,nodelist
sacct --starttime 2018-11-23 -u $USER
seff $jobid                  # very useful to see at a glance: CPU/memory efficiency and max. memory
```

Usage examples (III)

Controlling queued and running jobs

```
scontrol hold $jobid
scontrol release $jobid
scontrol suspend $jobid
scontrol resume $jobid
scancel $jobid
scancel -n $jobname
scancel -u $USER
scancel -u $USER -p batch
scontrol requeue $jobid
```

Usage examples (III)

Controlling queued and running jobs

```
scontrol hold $jobid
scontrol release $jobid
scontrol suspend $jobid
scontrol resume $jobid
scancel $jobid
scancel -n $jobname
scancel -u $USER
scancel -u $USER -p batch
scontrol requeue $jobid
```

Checking accounting links and QOS available for you

```
sacctmgr show user $USER format=user%20s,defaultaccount%30s
sacctmgr list association where users=$USER format=account%30s,user%20s,qos%120s
```

Usage examples (III)

Controlling queued and running jobs

```
scontrol hold $jobid
scontrol release $jobid
scontrol suspend $jobid
scontrol resume $jobid
scancel $jobid
scancel -n $jobname
scancel -u $USER
scancel -u $USER -p batch
scontrol requeue $jobid
```

Checking accounting links and QOS available for you

```
sacctmgr show user $USER format=user%20s,defaultaccount%30s
sacctmgr list association where users=$USER format=account%30s,user%20s,qos%120s
```

Checking accounting share info - usage, fair-share, etc.

```
sshare -U
sshare -A $accountname
sshare -A $(sacctmgr -n show user $USER format=defaultaccount%30s)
sshare -a
```

Job launchers - basic (I)

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH --time=0-00:05:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

echo "Hello from the batch queue on node ${SLURM_NODELIST}"
# Your more useful application can be started below!
```

Submit it with: `sbatch launcher.sh`

Job launchers - basic (II)

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH -c 28
#SBATCH --time=0-03:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"

export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
srun ./preprocess_app
srun ./main_app
```

Submit it overriding some settings: `sbatch --time=5:0:0 launcher.sh`

Job launchers - basic (III)

```
#!/bin/bash -l
#SBATCH -J MyTestJob
#SBATCH --mail-type=end,fail
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 2
#SBATCH --ntasks-per-node=2
#SBATCH --time=0-03:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
# Your more useful application can be started below!
```

Job launchers - requesting memory (I)

```
#!/bin/bash -l
#SBATCH -J MyLargeMemorySequentialJob
#SBATCH --mail-type=end,fail
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH --mem=64GB
#SBATCH --time=1-00:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
# Your more useful application can be started below!
```

Use "mem" to request (more) memory per node for low #core jobs

Job launchers - requesting memory (II)

```
#!/bin/bash -l
#SBATCH -J MyVeryLargeMemoryJob
#SBATCH --mail-type=end,fail
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH -c 64
#SBATCH --mem=2TB
#SBATCH --time=1-00:00:00
#SBATCH -p bigmem
#SBATCH --qos=qos-bigmem

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
# Your more useful application can be started below!
```

Iris compute nodes in the bigmem partition (will) have 112C/3TB RAM.

Job launchers - node features selection

```
#!/bin/bash -l
#SBATCH -J MyJobOnSkylakeCPUs
#SBATCH --mail-type=end,fail
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH --mem=64GB
#SBATCH --time=1-00:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch
#SBATCH -C skylake
[...]
```

```
$> sinfo --format="%N %f"
NODELIST AVAIL_FEATURES

iris-[001-108] broadwell

iris-[109-168] skylake
```

Note: above as of Nov.2018; *iris-[169-190]* will have **skylake**, with *iris-[169-186]* additional **volta** feature by 2019

Job launchers - accelerated nodes (I)

```
#!/bin/bash -l
#SBATCH -J MyGPUJob
#SBATCH --mail-type=all
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH -c 14
##SBATCH --gres=gpu:volta:4
#SBATCH --gres=gpu:2
#SBATCH --mem=300G
#SBATCH --time=12:00:00
#SBATCH -p gpu

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
nvidia-smi
```

Iris compute nodes in the gpu partition (will) have 4xVolta V100 GPUs and 768GB RAM.

Job launchers - accelerated nodes (II)

```
#!/bin/bash -l
#SBATCH -J MyGPUJob
#SBATCH -N 1
#SBATCH -c 28
#SBATCH --gres=gpu:4
#SBATCH --time=1-0:0:0
#SBATCH -p gpu

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"

# Load the Singularity HPC containers module
module load tools/Singularity
# Pull the reference TensorFlow (GPU-enabled) image from Docker hub
singularity pull docker://tensorflow/tensorflow:latest-gpu
# Run the TF container w. Singularity's nvidia support on your own model
singularity exec --nv tensorflow-latest-gpu.simg python tf-model.py
```

Job launchers - long jobs

```
#!/bin/bash -l
#SBATCH -J MyLongJob
#SBATCH --mail-type=all
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH --time=3-00:00:00
#SBATCH -p long
#SBATCH --qos=qos-long

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
# Your more useful application can be started below!
```

Long walltime possible but you should not (!) rely on it.
Always prefer parallel, short walltime, requeue-able jobs.

Job launchers - besteffort

```
#!/bin/bash -l
#SBATCH -J MyRerunnableJob
#SBATCH --mail-type=end,fail
#SBATCH --mail-user=Your.Email@Address.lu
#SBATCH -N 1
#SBATCH --ntasks-per-node=28
#SBATCH --time=0-12:00:00
#SBATCH -p batch
#SBATCH --qos=qos-besteffort
#SBATCH --requeue

echo "== Starting run at $(date)"
echo "== Job ID: ${SLURM_JOBID}"
echo "== Node list: ${SLURM_NODELIST}"
echo "== Submit dir. : ${SLURM_SUBMIT_DIR}"
# Your more useful application can be started below!
```

Many scientific applications support internal state saving and restart!
System-level checkpoint-restart possible with DMTCP.

Job launchers - threaded parallel

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=1
#SBATCH -c 28
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
/path/to/your/threaded.app
```

By threaded we mean pthreads/OpenMP shared-memory applications.

Job launchers - MATLAB

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=28
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

module load base/MATLAB
matlab -nodisplay -nosplash < /path/to/infile > /path/to/outfile
```

MATLAB spawns processes, limited for now to single node execution.
We are still waiting for Distributed Computing Server availability.

Job launchers - MATLAB

```
#!/bin/bash -l
#SBATCH -N 1
#SBATCH --ntasks-per-node=28
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

module load base/MATLAB
matlab -nodisplay -nosplash < /path/to/infile > /path/to/outfile
```

MATLAB spawns processes, limited for now to single node execution.
We are still waiting for Distributed Computing Server availability.

A note on parallel jobs

As of 2018 the iris cluster is heterogeneous (Broadwell+Skylake-gen systems)

Its core networking is still non-blocking fat-tree.

- Simply requesting #tasks **may not be optimal**
  - ↪ from hardware POV - slight difference in CPU freq. for now
  - ↪ from software efficiency POV - best to have arch. opt. builds
- Many elements contribute to an optimal (fast!) execution:
  - ↪ correct division of tasks / cores-per-task and application launch
  - ↪ memory allocation
  - ↪ (soon) execution on nodes with GPU accel. and their allocation
- Different MPI implementations will **behave differently**
  - ↪ recent/latest Intel & OpenMPI on **iris**
  - ↪ always prefer launch using **srun**

Job launchers - IntelMPI

```
#!/bin/bash -l
#SBATCH -n 128
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

module load toolchain/intel
srun -n $SLURM_NTASKS /path/to/your/intel-toolchain-compiled-app
```

IntelMPI is configured to use PMI2 for process management (optimal).
Bare mpirun works but not recommended.

Job launchers - OpenMPI

```
#!/bin/bash -l
#SBATCH -n 128
#SBATCH -c 1
#SBATCH --time=0-01:00:00
#SBATCH -p batch
#SBATCH --qos=qos-batch

module load toolchain/foss
srun -n $SLURM_NTASKS /path/to/your/foss-toolchain-compiled-app
```

OpenMPI also uses PMI2 (again, optimal).
Bare mpirun works but not recommended.

You can easily generate a hostfile from within a SLURM job with:
`srun hostname | sort -n > hostfile`

Job launchers - MPI+OpenMP

```
#!/bin/bash -l
#SBATCH -N 10
#SBATCH --ntasks-per-node=1
#SBATCH -c 28
#SBATCH --time=0-01:00:00
#SBATCH -C skylake
#SBATCH -p batch
#SBATCH --qos=qos-batch

module load toolchain/intel
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
srun -n $SLURM_NTASKS /path/to/your/parallel-hybrid-app
```

Compile and use your applications in hybrid MPI+OpenMP mode when you can for better (best?) possible performance.

Notes on optimizing your usage

A note on CPU affinity

- Processes pinned by default to cores (**CPUs** in SLURM docs.)
- `srun` aware of requested tasks/cores configuration and pins processes/threads accordingly
- Many options to control task affinity exist, see:
  - ↪ `https://slurm.schedmd.com/srun.html#OPT_cpu-bind`
  - ↪ `https://slurm.schedmd.com/srun.html#OPT_hint`
- Can be disabled with `srun --cpu-bind=none`

If not disabled for 'interactive' jobs, all your processes will be pinned to 1st core!

Summary

Notes on OAR

- OAR still in use as the workload manager of Gaia and Chaos
  - ↪ celebrating **4.432.531** jobs on Gaia! (2018-11-22)
  - ↪ celebrating **1.657.122** jobs on Chaos! (2018-11-22)

- Many of its features are common to other workload managers, incl. SLURM (**206.045** jobs on Iris as of 2018-11-22)
  - ↪ some things are exactly the same
  - ↪ but some things work in a different way
  - ↪ . . . and some have no equivallent or are widely different
- An adjustment period for you is needed if you've only used OAR
  - ↪ next slides show a brief transition guide

OAR/SLURM - commands guide

Command	OAR (gaia/chaos)	SLURM (iris)
Submit passive/batch job	`oarsub -S $script`	`sbatch $script`
Start interactive job	`oarsub -I`	`srun -p interactive --pty bash -i`
Queue status	`oarstat`	`squeue`
User job status	`oarstat -u $user`	`squeue -u $user`
Specific job status (detailed)	`oarstat -f -j $jobid`	`scontrol show job $jobid`
Delete (running/waiting) job	`oardel $jobid`	`scancel $jobid`
Hold job	`oarhold $jobid`	`scontrol hold $jobid`
Resume held job	`oarresume $jobid`	`scontrol release $jobid`
Node list and properties	`oarnodes`	`scontrol show nodes`
Join a running job	`oarsub -C $jobid`	`sjoin $jobid [$nodeid]`

Similar yet different?
Many specifics will actually come from the way Iris is set up.

OAR/SLURM - job specifications

Specification	OAR	SLURM
Script directive	`#OAR`	`#SBATCH`
Queue request	`-q $queue`	`-p $partition`
Nodes request	`-l nodes=$count`	`-N $min-$max`
Cores request	`-l core=$count`	`-n $count`
Cores-per-node request	`-l nodes=$ncount/core=$ccount`	`-N $ncount --ntasks-per-node=$ccount`
Walltime request	`-l [...],walltime=hh:mm:ss`	`-t $min OR -t $days-hh:mm:ss`
Job array	`--array $count`	`--array $specification`
Job name	`-n $name`	`-J $name`
Job dependency	`-a $jobid`	`-d $specification`
Property request	`-p "$property=$value"`	`-C $specification`
Jobs on GPU nodes	`-t gpu`	`-p gpu`
Jobs on large memory nodes	`-t bigmem`	`-p bigmem`
Besteffort jobs	`-t besteffort`	`--qos qos-besteffort`
Email on job state change	`--notify mail:$email`	`--mail-user=$email`

Job specifications will need most adjustment on your side.
Iris more homogeneous than Gaia/Chaos for now.
Running things in an optimal way is easier.

OAR/SLURM - env. vars.

Environment variable	OAR	SLURM
Job ID	`$OAR_JOB_ID`	`$SLURM_JOB_ID`
Resource list	`$OAR_NODEFILE`	`$SLURM_NODELIST` #List not file! See below.
Job name	`$OAR_JOB_NAME`	`$SLURM_JOB_NAME`
Submitting user name	`$OAR_USER`	`$SLURM_JOB_USER`
Task ID within job array	`$OAR_ARRAY_INDEX`	`$SLURM_ARRAY_TASK_ID`
Working directory at submission	`$OAR_WORKING_DIRECTORY`	`$SLURM_SUBMIT_DIR`

Check available variables: `env | egrep "OAR|SLURM"`
Generate hostfile: `srun hostname | sort -n > hostfile`

Summary

Conclusion and Practical Session start

We've discussed

- ✓ The design of SLURM for the **iris** cluster
- ✓ The permissions system in use through group accounts and QOS
- ✓ Main SLURM tools and how to use them
- ✓ Job types possible with SLURM on **iris**
- ✓ SLURM job launchers for sequential and parallel applications
- ✓ Transitioning from OAR to SLURM

Conclusion and Practical Session start

We've discussed

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- ✓ Transitioning from OAR to SLURM

And now...

Q&A & practical

ulhpc-tutorials.readthedocs.io/en/latest/scheduling/advanced

Questions?

http://hpc.uni.lu

High Performance Computing @ uni.lu

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