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Information about the batch system (SLURM)

The DEEP prototype systems are running SLURM for resource management. Documentation of Slurm can be found ?here.

Overview

Slurm offers interactive and batch jobs (scripts submitted into the system). The relevant commands are srun and sbatch. The srun command can be used to spawn processes (**please do not use mpiexec**), both from the frontend and from within a batch script. You can also get a shell on a node to work locally there (e.g. to compile your application natively for a special platform or module).

Available Partitions

Please note that there is no default partition configured. In order to run a job, you have to specify one of the following partitions, using the --partition=... switch:

Name	Description
dp-cn	dp-cn[01-50], DEEP-EST Cluster nodes (Xeon Skylake)
dp-dam	dp-dam[01-16], DEEP-EST Dam nodes (Xeon Cascadelake + 1 V100 + 1 Stratix 10)
dp-dam-ext	dp-dam[09-16], DEEP-EST Dam nodes connected with Extoll Tourmalet
dp-esb-ib	dp-esb[26-75], DEEP-EST ESB nodes connected with IB EDR (Xeon Cascadelake + 1 V100)
dp-esb-ext	dp-esb[01-25], DEEP-EST ESB nodes connected with Extoll Fabri3)
dp-sdv-esb	dp-sdv-esb[01-02], DEEP-EST ESB Test nodes (Xeon Cascadelake + 1 V100)
ml-gpu	ml-gpu[01-03], GPU test nodes for ML applications (4 V100 cards)
knl	knl[01,04-06], KNL nodes
knl256	knl[01,05], KNL nodes with 64 cores
knl272	knl[04,06], KNL nodes with 68 cores
snc4	knl[05], KNL node in snc4 memory mode
debug	all compute nodes (no gateways)

Anytime, you can list the state of the partitions with the sinfo command. The properties of a partition can be seen using

scontrol show partition <partition>

Remark about environment

By default, Slurm passes the environment from your job submission session directly to the execution environment. Please be aware of this when running jobs with srun or when submitting scripts with sbatch. This behavior can be controlled via the --export option. Please refer to the (Slurm documentation to get more information about this.

In particular, when submitting job scripts, it is recommended to load the necessary modules within the script and submit the script from a clean environment.

An introductory example

Suppose you have an mpi executable named ${\tt hello_mpi}$. There are three ways to start the binary.

From a shell on a node

First, start a shell on a node. Assume you would like to run your mpi task on 4 cluster nodes with 2 tasks per node:

```
[kreutz1@deepv /p/project/cdeep/kreutz1/Temp]$ srun -A deep -p dp-cn -N 4 -n 8 -t 00:30:00 --pty --interactive /bin/bash [kreutz1@dp-cn01 /p/project/cdeep/kreutz1/Temp]$
```

The environment is transported to the remote shell, no .profile, .bashrc, ... are sourced (especially not the modules default from /etc/profile.d/modules.sh). As of March 2020, an account has to be specified using the --account (short -A) option, which is "deep" for the project members. For people not included in the DEEP-EST project, please use the "Budget" name you received along with your account creation.

Once you get to the compute node, start your application using srun. Note that the number of tasks used is the same as specified in the initial srun command above (4 nodes with two tasks each):

```
[kreutzl@deepv Temp]$ salloc -A deep -p dp-cn -N 4 -n 8 -t 00:30:00 srun --pty --interactive /bin/bash -i
[kreutzl@dp-cn01 Temp]$ srun -N 2 -n 8 ./MPI_HelloWorld

Hello World from rank 3 of 8 on dp-cn02

Hello World from rank 7 of 8 on dp-cn04

Hello World from rank 2 of 8 on dp-cn02

Hello World from rank 6 of 8 on dp-cn04

Hello World from rank 0 of 8 on dp-cn01

Hello World from rank 4 of 8 on dp-cn03

Hello World from rank 1 of 8 on dp-cn03

Hello World from rank 5 of 8 on dp-cn03
```

You can ignore potential warnings about the cpu binding. ParaStation will pin your processes.

If you just need to one node to run your interactive session on you can simply use the srun command (without salloc), e.g.:

```
[kreutzl@deepv ~]$ srun -A deep -N 1 -n 8 -p dp-cn -t 00:30:00 --pty --interactive bash -i
[kreutzl@dp-cn22 ~]$ srun -n 8 hostname
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
```

Running directly from the front ends

You can run the application directly from the frontend, bypassing the shell. Do not forget to set the correct environment for running your executable on the login node as this will be used for execution with srun.

```
[kreutzl@deepv Temp]$ ml GCC/10.3.0 ParaStationMPI/5.4.9-1
[kreutzl@deepv Temp]$ srun -A deep -p dp-cn -N 4 -n 8 -t 00:30:00 ./MPI_HelloWorld
Hello World from rank 7 of 8 on dp-cn04
Hello World from rank 3 of 8 on dp-cn02
Hello World from rank 6 of 8 on dp-cn04
Hello World from rank 2 of 8 on dp-cn02
Hello World from rank 4 of 8 on dp-cn03
Hello World from rank 0 of 8 on dp-cn01
Hello World from rank 1 of 8 on dp-cn01
Hello World from rank 5 of 8 on dp-cn03
```

It can be useful to create an allocation which can be used for several runs of your job:

```
[kreutzl@deepv Temp]$ salloc -A deep -p dp-cn -N 4 -n 8 -t 00:30:00 salloc: Granted job allocation 69263
[kreutzl@deepv Temp]$ srun ./MPI_HelloWorld
Hello World from rank 7 of 8 on dp-cn04
Hello World from rank 3 of 8 on dp-cn02
Hello World from rank 6 of 8 on dp-cn04
```

```
Hello World from rank 2 of 8 on dp-cn02
Hello World from rank 5 of 8 on dp-cn03
Hello World from rank 1 of 8 on dp-cn01
Hello World from rank 4 of 8 on dp-cn03
Hello World from rank 0 of 8 on dp-cn01
...
# several more runs
...
[kreutz1@deepv Temp]$ exit
exit
salloc: Relinquishing job allocation 69263
```

Note that in this case the -N and -n options for the srun command can be skipped (they default to the corresponding options given to salloc).

Batch script

As stated above, it is recommended to load the necessary modules within the script and submit the script from a clean environment.

The following script hello_cluster.sh will unload all modules and load the modules required for executing the given binary:

```
#!/bin/bash

#SBATCH --partition=dp-esb
#SBATCH -A deep
#SBATCH -N 4
#SBATCH -n 8
#SBATCH -o /p/project/cdeep/kreutz1/hello_cluster-%j.out
#SBATCH -e /p/project/cdeep/kreutz1/hello_cluster-%j.err
#SBATCH --time=00:10:00

ml purge
ml GCC ParaStationMPI
srun ./MPI_HelloWorld
```

This script requests 4 nodes of the ESB module with 8 tasks, specifies the stdout and stderr files, and asks for 10 minutes of walltime. You can submit the job script as follows:

```
[kreutz1@deepv Temp]$ sbatch hello_cluster.sh
Submitted batch job 69264
```

... and check what it's doing:

```
[kreutz1@deepv Temp]$ squeue -u $USER

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

69264 dp-cn hello_cl kreutz1 CG 0:04 4 dp-cn[01-04]
```

Once finished, you can check the result (and the error file if needed)

```
[kreutzl@deepv Temp]$ cat /p/project/cdeep/kreutzl/hello_cluster-69264.out
Hello World from rank 7 of 8 on dp-esb37
Hello World from rank 3 of 8 on dp-esb35
Hello World from rank 5 of 8 on dp-esb36
Hello World from rank 1 of 8 on dp-esb34
Hello World from rank 6 of 8 on dp-esb37
Hello World from rank 2 of 8 on dp-esb35
Hello World from rank 4 of 8 on dp-esb36
Hello World from rank 0 of 8 on dp-esb36
```

Job chains

Please refer to the <u>FAQ</u> for creation of job chains and implementing job dependencies. If you would like to implement workflows, take a look at the <u>Workflows</u> section.

Information on past jobs and accounting

The sacct command can be used to enquire the Slurm database about a past job.

On the Cluster (CM) nodes it's possible to query the consumed energy for a certain job:

```
[kreutz1@deepv kreutz1]$ sacct -o ConsumedEnergy, JobName, JobID, CPUTime, AllocNodes -j 69326

ConsumedEnergy JobName JobID CPUTime AllocNodes

496.70K hpl_MKL_O+ 69326 16:28:48 1

0 batch 69326.batch 16:28:48 1

496.70K xlinpack_+ 69326.0 08:10:24 1
```

This feature will also be for the ESB nodes.

FAQ

Is there a cheat sheet for all main Slurm commands?

Yes, it is available ?here.

Why's my job not running?

You can check the state of your job with

```
scontrol show job <job id>
```

In the output, look for the ${\tt Reason}$ field.

You can check the existing reservations using

```
scontrol show res
```

How can I check which jobs are running in the machine?

Please use the squeue command (the "-u \$USER" option to only list jobs belonging to your user id).

How do I do chain jobs with dependencies?

Please confer the sbatch/srun man page, especially the

```
-d, --dependency=<dependency_list>
```

entry.

Also, jobs can be chained after they have been submitted using the scontrol command by updating their Dependency field.

How can check the status of partitions and nodes?

The main command to use is sinfo. By default, when called alone, sinfo will list the available partitions and the number of nodes in each partition in a given status. For example:

[deamicis1@d	deepv hy	bridhello]\$	sinfo		
PARTITION	AVAIL	TIMELIMIT	NODES	STATE	NODELIST
sdv	up	20:00:00	11	idle	deeper-sdv[06-16]
knl	up	20:00:00	1	drain	kn101
knl	up	20:00:00	3	idle	kn1[04-06]
kn1256	up	20:00:00	1	drain	kn101
kn1256	up	20:00:00	1	idle	kn105
kn1272	up	20:00:00	2	idle	kn1[04,06]
snc4	up	20:00:00	1	idle	kn105
extoll	up	20:00:00	11	idle	deeper-sdv[06-16]
ml-gpu	up	20:00:00	3	idle	ml-gpu[01-03]
dp-cn	up	20:00:00	1	drain	dp-cn33
dp-cn	up	20:00:00	5	resv	dp-cn[09-10,25,49-50]
dp-cn	up	20:00:00	44	idle	dp-cn[01-08,11-24,26-32,34-48]
dp-dam	up	20:00:00	1	drain*	dp-dam08
dp-dam	up	20:00:00	2	drain	dp-dam[03,07]
dp-dam	up	20:00:00	3	resv	dp-dam[05,09-10]
dp-dam	up	20:00:00	2	alloc	dp-dam[01,04]
dp-dam	up	20:00:00	8	idle	dp-dam[02,06,11-16]
dp-dam-ext	up	20:00:00	2	resv	dp-dam[09-10]
dp-dam-ext	up	20:00:00	6	idle	dp-dam[11-16]
dp-esb	up	20:00:00	51	drain*	dp-esb[11,26-75]
dp-esb	up	20:00:00	2	drain	dp-esb[08,23]
dp-esb	up	20:00:00	2	alloc	dp-esb[09-10]
dp-esb	up	20:00:00	20	idle	dp-esb[01-07,12-22,24-25]
dp-sdv-esb	up	20:00:00	2	resv	dp-sdv-esb[01-02]
psgw-cluster	up	20:00:00	1	idle	nfgw01
psgw-booster	up up	20:00:00	1	idle	nfgw02
debug	up	20:00:00	1	drain*	dp-dam08
debug	up	20:00:00	4	drain	dp-cn33,dp-dam[03,07],kn101
debug	up	20:00:00	10	resv	dp-cn[09-10,25,49-50],dp-dam[05,09-10],dp-sdv-esb[01-02]
debug	up	20:00:00	2	alloc	dp-dam[01,04]
debug	up	20:00:00	69	idle	deeper-sdv[06-16],dp-cn[01-08,11-24,26-32,34-48],dp-dam[02,06,11-16],knl[04-06

Please refer to the man page for ${\tt sinfo}$ for more information.

Can I join stderr and stdout like it was done with -joe in Torque?

Not directly. In your batch script, redirect stdout and stderr to the same file:

```
#SBATCH -o /point/to/the/common/logfile-%j.log
#SBATCH -e /point/to/the/common/logfile-%j.log
...
```

(The %j will place the job id in the output file). N.B. It might be more efficient to redirect the output of your script's commands to a dedicated file.