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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 --partitions... 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-esb	dp-esb[log:@26-75 "[01-75]"], DEEP-EST ESB nodes connected with IB EDR (Xeon Cascadelake + 1 V100)
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 (.e.g. the maximum walltime) 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

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

[kreutz1@deepv ~]\$ srun -A deep -N 1 -n 8 -p dp-cn -t 00:30:00 --pty --interactive bash [kreutz1@dp-cn22 ~]\$ srun -n 8 hostname dp-cn22

```
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
dp-cn22
```

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 "deepsea" for DEEP-SEA project members. For people not included in the DEEP-SEA project, please use the "Budget" name you received along with your account creation.

Assume you would like to run an MPI task on 4 cluster nodes with 2 tasks per node. It's necessary to use salloc then:

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

Hello World from rank 5 of 8 on dp-cn01
```

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). It's also possible to use less nodes in the srun command. So the following command would work as well:

```
[kreutz1@dp-cn01 Temp]$ srun -N 1 -n 1 ./MPI_HelloWorld
Hello World from rank 0 of 1 on dp-cn01
```

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.

```
[kreutz1@deepv Temp]$ ml GCC/10.3.0 ParaStationMPI/5.4.9-1
[kreutz1@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-cn02
```

```
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
...
[kreutzl@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
```

Information on past jobs and accounting

The ${\tt sacct}$ command can be used to enquire the Slurm database about a past job.

[kreutz1@deepv Temp]\$ sacct -j 69268							
	JobID	JobName	Partition	Account	AllocCPUS	State ExitCode	
69268	3+0	bash	dp-cn	deepest-a+	96	COMPLETED	0:0
69268	3+0.0	MPI_Hello+		deepest-a+	2	COMPLETED	0:0
69268	8+1	bash	dp-dam deepest-a+		384	COMPLETED	0:0

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

This feature will also be for the ESB nodes.

Advanced topics

For further details on the batchsystem and psslurm which is used on DEEP as well as on the JSC production systems, please refer to the in-depth description for using the ?Batchsystem on Jureca. Among extended examples for allocation of nodes you can find information on job steps, dependency chains and multithreading there. If you are interested in pinning of threads and tasks to certain CPUs or cores, please also take a look into the ?Processor Anffinity sections of the Jureca documentation. Most of the information provided there will also refer to the DEEP System.

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 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). A graphical overview can be displayed using slurmtop command.

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:

PARTITION sdv knl knl knl256 knl256	AVAIL up up	bridhello]\$ TIMELIMIT 20:00:00	sinfo NODES	STATE	NODEL TOTAL
sdv kn1 kn1 kn1256 kn1256	up up		NODES	STATE	NODEL TOP
knl knl knl256 knl256	up	20:00:00			NODELISI
knl knl256 knl256	_		11	idle	deeper-sdv[06-16]
kn1256 kn1256		20:00:00	1	drain	kn101
kn1256	up	20:00:00	3	idle	knl[04-06]
	up	20:00:00	1	drain	kn101
	up	20:00:00	1	idle	kn105
kn1272	up	20:00:00	2	idle	knl[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-cluste	er up	20:00:00	1	idle	nfgw01
psgw-booste	er 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:

```
#!sh ... #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.