Example serial job scripts on the Linux-Cluster

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Introductory remarks

The job scripts for SLURM partitions are provided as templates which you can adapt for your own settings. In particular, you should account for the following points:

- Some entries are placeholders, which you must replace with correct, user-specific settings. In particular, path specifications and e-Mail addresses must be adapted. Always specify the appropriate directories instead of the names with the three periods in the following examples!
- In case you have to work with the environment modules package in your batch script, you also have to source the file /etc/profile.d/modules.sh.

Time and Memory Requirements

Try to estimate the time and mem require as close as possible to your needs. This help to prevent idling nodes or CPUs.

Serial jobs

This job type normally uses a single core on a shared memory node of the designated SLURM partition. The CPUs of the node are shared with other users.

<table>
<thead>
<tr>
<th>Serial job</th>
<th>Serial job (long running)</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>#!/bin/bash</code></td>
<td><code>#!/bin/bash</code></td>
</tr>
<tr>
<td><code>## a job which uses 1 core of a node</code></td>
<td><code>## a job which uses 1 core of a node</code></td>
</tr>
<tr>
<td><code>#SBATCH -o /home/hpc/.../.../myjob.%j.%N.out</code></td>
<td><code>#SBATCH -o /home/hpc/.../.../myjob.%j.%N.out</code></td>
</tr>
<tr>
<td><code>#SBATCH -D /home/hpc/.../.../mydir</code></td>
<td><code>#SBATCH -D /home/hpc/.../.../mydir</code></td>
</tr>
<tr>
<td><code>#SBATCH -J Jobname</code></td>
<td><code>#SBATCH -J Jobname</code></td>
</tr>
<tr>
<td><code>#SBATCH --get-user-env</code></td>
<td><code>#SBATCH --get-user-env</code></td>
</tr>
<tr>
<td><code>#SBATCH --clusters=serial</code></td>
<td><code>#SBATCH --clusters=serial</code></td>
</tr>
<tr>
<td><code>#SBATCH --partition=serial_mpp2</code></td>
<td><code>#SBATCH --partition=serial_long</code></td>
</tr>
<tr>
<td><code>#SBATCH --partition=shared_mem</code></td>
<td><code>#SBATCH --partition=shared_mem</code></td>
</tr>
<tr>
<td><code>#SBATCH --mail-type=end</code></td>
<td><code>#SBATCH --mail-type=end</code></td>
</tr>
<tr>
<td><code>#SBATCH --mem=800mb</code></td>
<td><code>#SBATCH --mem=800mb</code></td>
</tr>
<tr>
<td><code>#SBATCH --cpus_per_task=1</code></td>
<td><code>#SBATCH --cpus_per_task=1</code></td>
</tr>
<tr>
<td><code>#SBATCH --mail-user=xyz@xyz.de</code></td>
<td><code>#SBATCH --mail-user=xyz@xyz.de</code></td>
</tr>
<tr>
<td><code>#SBATCH --export=NONE</code></td>
<td><code>#SBATCH --export=NONE</code></td>
</tr>
<tr>
<td><code>#SBATCH --time=24:00:00</code></td>
<td><code>#SBATCH --time=24:00:00</code></td>
</tr>
<tr>
<td><code>source /etc/profile.d/modules.sh</code></td>
<td><code>source /etc/profile.d/modules.sh</code></td>
</tr>
<tr>
<td><code>cd mydir</code></td>
<td><code>cd mydir</code></td>
</tr>
<tr>
<td><code>. /myprog.exe</code></td>
<td><code>. /myprog.exe</code></td>
</tr>
</tbody>
</table>

Shared Memory jobs

For very large memory jobs (more than 8 GByte and up to 240 GBytes) or (going beyond 1 TByte) the teramem_inter partition in the interactive segment should be used.

<table>
<thead>
<tr>
<th>Shared memory job</th>
<th>Large memory job</th>
</tr>
</thead>
<tbody>
<tr>
<td>up to 28 cores with up to 50 GByte memory</td>
<td>with a single core and up to 240 GB memory</td>
</tr>
</tbody>
</table>
```bash
#!/bin/bash
#SBATCH -o /home/hpc/.../.../myjob.%j.%N.out
#SBATCH -D /home/hpc/.../.../mydir
#SBATCH -J Jobname
#SBATCH --get-user-env
#SBATCH --clusters=serial
#SBATCH --partition=serial_mpp2
#SBATCH --mem=10000mb
#SBATCH --cpus_per_task=7
#SBATCH --mail-type=end
#SBATCH --mail-user=xyz@xyz.de
#SBATCH --export=NONE
#SBATCH --time=8:00:00
source /etc/profile.d/modules.sh
cd mydir
export OMP_NUM_THREADS=7
./myprog.exe
```

If you do not specify `mem` then 1.7 GB*cpus_per_task will be used, which is also a good balance.

<table>
<thead>
<tr>
<th>Large memory job with shared memory multithreading with up to 20 cores and up to 240 GB memory</th>
<th>Shared memory job on HP DL580 &quot;teramem1&quot; with shared memory multithreading with up to 96 cores and 6 TByte of memory</th>
</tr>
</thead>
</table>
| ```bash
#!/bin/bash
#SBATCH -o /home/hpc/.../.../myjob.%j.%N.out
#SBATCH -D /home/hpc/.../.../mydir
#SBATCH -J Jobname
#SBATCH --get-user-env
#SBATCH --clusters=
#SBATCH --partition=
#SBATCH --cpus-per-task=10
#SBATCH --mem=200000mb
#SBATCH --mail-type=end
#SBATCH --mail-user=xyz@xyz.de
#SBATCH --export=NONE
#SBATCH --time=8:00:00
source /etc/profile.d/modules.sh
cd mydir
export OMP_NUM_THREADS=10
./myprog.exe
``` | ```bash
#!/bin/bash
#SBATCH -o /home/hpc/.../.../myjob.%j.%N.out
#SBATCH -D /home/hpc/.../.../mydir
#SBATCH -J Jobname
#SBATCH --get-user-env
#SBATCH --clusters=inter
#SBATCH --partition=teramem_inter
#SBATCH --mem=2000gb
#SBATCH --cpus-per-task=32
#SBATCH --mail-type=end
#SBATCH --mail-user=xyz@xyz.de
#SBATCH --export=NONE
#SBATCH --time=8:00:00
source /etc/profile.d/modules.sh
cd mydir
export OMP_NUM_THREADS=32
./myprog.exe
``` |

Use teramem only if you need more than 240 GByte memory! Try to parallelize your application, otherwise some cores will be kept idle. Then, use more cpus_per_task and more OpenMP threads (OMP_NUM_THREADS). A good balance is 600GB per core.

### TSM Archivation

TSM archivation is only supported on the login nodes of the cluster, not on the SLURM-controlled batch nodes. Please consult the document describing tape archivation on our HPC systems for more details on TSM usage.