Example serial job scripts on the Linux-Cluster

- Introductory remarks
- Time and Memory Requirements
- Serial jobs
- Shared Memory jobs
- TSM Archivation

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 multiple cores of a node are shared with other users.

<table>
<thead>
<tr>
<th>Serial job</th>
<th>Serial job (long running)</th>
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</table>
| #!/bin/bash  
#SBATCH --job-name 
#SBATCH --o ./%x.%j.%N.out 
#SBATCH --D ./ 
#SBATCH --get-user-env 
#SBATCH --clusters=serial 
#SBATCH --partition=serial_mpp2 
#SBATCH --mail-type=end 
#SBATCH --mem=800mb 
#SBATCH --cpus-per-task=1 
#SBATCH --mail-user=insert_your_email_here 
#SBATCH --export=NONE 
#SBATCH --time=24:00:00 
./myprog.exe | #!/bin/bash  
#SBATCH --job-name 
#SBATCH --o ./%x.%j.%N.out 
#SBATCH --D ./ 
#SBATCH --get-user-env 
#SBATCH --clusters=serial 
#SBATCH --partition=serial_long 
#SBATCH --mail-type=end 
#SBATCH --mem=800mb 
#SBATCH --cpus-per-task=1 
#SBATCH --mail-user=insert_your_email_here 
#SBATCH --export=NONE 
#SBATCH --time=8-00:00:00 
./myprog.exe |

The above example requests 1 core of a node and assumes the binary is located in the submission directory (-D)

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>Shared memory job on HP DL580 &quot;teramem1&quot;</th>
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</thead>
<tbody>
<tr>
<td>up to 28 cores with up to 50 GByte memory</td>
<td>with shared memory multithreading with up to 96 cores and 6 TByte of memory</td>
</tr>
</tbody>
</table>
```bash
#!/bin/bash
#SBATCH -J job_name
#SBATCH -o ./%x.%j.%N.out
#SBATCH -D ./
#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=insert_your_email_here
#SBATCH --export=NONE
#SBATCH --time=8:00:00

export OMP_NUM_THREADS=7
./myprog.exe
```

```bash
#!/bin/bash
#SBATCH -J job_name
#SBATCH -o ./%x.%j.%N.out
#SBATCH -D ./
#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=insert_your_email_here
#SBATCH --export=NONE
#SBATCH --time=8:00:00

export OMP_NUM_THREADS=32
./myprog.exe
```

The above example requests 7 cores of a node and assumes the binary is located in the submission directory (-D) and can make use of OpenMP for multi-threading across the 7 cores. If you do not specify --mem then 1.7GB*cpus_per_task will be used, which is also a good balance.

To avoid wasting resources, the number of cores requested should be commensurate with the memory requirement, i.e. at around 60 GB per core. This may imply that you need to parallelize your code if not done yet.

### 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.