SLURM – Advanced Usage

October 23, 2024



Bad Job Practices

job submissions within a loop (take a long time)

```
for i in {1..1000}
do
sbatch job.sh $i
done
```

loop inside job script (sequence of mpirun commands): for i in {1..1000} do mpirun -np 16 my_program \$i done





submit/run a series of independent jobs via a single SLURM script



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- example (job_array_vsc5.sh), 10 jobs, SLURM_ARRAY_TASK_ID=1,2,3 ... 10

```
#!/bin/bash
#SBATCH -J array
#SBATCH -N 1
#SBATCH --array 1-10
```

echo "Hi, this is array job number" \$SLURM_ARRAY_TASK_ID sleep \$SLURM_ARRAY_TASK_ID



■ independent jobs: 1, 2, 3 ... 10 VSC-5 > squeue - u \$user 499514 3 zen3_0512 array sh R INVALID 1 n3504-057 sh R 499514 4 zen3 0512 array INVALID 1 n3506-047 499514_5 zen3_0512 array sh R INVALID 1 n3507-013 499514 6 zen3 0512 sh R INVALID n3509-016 arrav 1 499514_7 zen3_0512 arrav sh R INVALID 1 n3511-029 499514_8 zen3_0512 sh R INVALID 1 n3503-010 arrav 499514_9 zen3_0512 sh R INVALID n3503-011 arrav 1 499514_10 zen3_0512 sh R INVALID n3503-028 arrav 1



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corresponding SLURM output files

VSC-5 > ls slurm-*

slurm-499514_10.out	slurm-499514_2.out	slurm-499514_4.out	slurm-499514_6.out	slurm-499514_8.out
slurm-499514_1.out	slurm-499514_3.out	slurm-499514_5.out	slurm-499514_7.out	slurm-499514_9.out



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explicit content of a single SLURM output file

 $VSC-5 > cat slurm-499514_8.out$ Hi, this is array job number 8



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- example of going in chunks of a certain size, e.g. 5, SLURM_ARRAY_TASK_ID=1,6,11,16 #SBATCH --array 1-20:5



- fine-tuning via builtin variables (SLURM_ARRAY_TASK_MIN, SLURM_ARRAY_TASK_MAX etc)
- example of going in chunks of a certain size, e.g. 5, SLURM_ARRAY_TASK_ID=1,6,11,16 #SBATCH --array 1-20:5

example of limiting number of simultaneously running jobs to 2 (perhaps for licences)
 #SBATCH --array 1-20:5%2



■ use an entire compute node for several independent jobs



use an entire compute node for several independent jobs

example single_node_multiple_jobs_vsc5.sh: #!/bin/bash #SBATCH -J snglcre #SBATCH -N 1 #SBATCH -p zen3_0512 #SBATCH --qos zen3_0512

```
for ((i=1; i<=128; i++)) do stress --cpu 1 --timeout $i & done
```

wait



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- "wait" is also important ! waits for all processes in the background to terminate before moving on



Combination of Array and Single Core Job

example combined_array_multiple_jobs_vsc5.sh:

```
. . .
#SBATCH -N 1
#SBATCH --array 1-384:128
i=$SLURM ARRAY TASK ID
((j+=127))
for ((i=$SLURM_ARRAY_TASK_ID; i<=$j; i++))
do
   stress --cpu 1 --timeout $i &
done
wait
```



Exercises

files are located in folder examples/05_submitting_batch_jobs

- look into "job_array_vsc[4, 5].sh" and modify it such that the considered range is from 1 to 20 but in steps of 5
- look into "single_node_multiple_jobs_vsc[4, 5].sh" and also change it to go in steps of 5
- run "combined_array_multiple_jobs_vsc[4, 5].sh" and check whether the output is reasonable



Job Script Enhancements

usage of corresponding environmental variables

#SBATCH	Environmental Variable
-N	SLURM_JOB_NUM_NODES
ntasks-per-core	SLURM_NTASKS_PER_CORE
ntasks-per-node	SLURM_NTASKS_PER_NODE
ntasks [-n]	SLURM_NTASKS



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email notifications

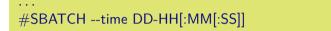
. . .

#SBATCH --mail-user yourmail@example.com #SBATCH --mail-type BEGIN,END



Submission Scripts Tuning

using time constraints less than maximum runtime





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using time constraints less than maximum runtime

```
#SBATCH --time DD-HH[:MM[:SS]]
```

backfilling:

the specified time is an estimate of your required computing time; if this is shorter than the default runtime (mostly 72h) SLURM may squeeze it in on idle nodes waiting for a larger job;



core-h accounting is done for the entire period of reservation



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contact support@vsc.ac.at



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- contact support@vsc.ac.at
- reservations are named after the project id



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check for reservations
 VSC-5> scontrol show reservations



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- contact support@vsc.ac.at
- reservations are named after the project id
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 VSC-5> scontrol show reservations
- using reservations

... #SBATCH --reservation MyRsrv



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- 2. Submit dependent job using the just received parent <job_id>

```
#!/bin/bash
#SBATCH -J myjb
#SBATCH -N 2
#SBATCH -d afterany:<job_id>
mpirun -np 256 my_prog
```

• • •



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mpirun -np 256 my_prog
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```

3. continue with 2. for further dependent jobs



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```
    "srun" example 2 nodes with two MPI processes each
#!/bin/bash
#SBATCH -J myjb
#SBATCH -N 2
#SBATCH --tasks-per-node 2
```

srun --cpu_bind map_cpu:0,64 ./my_mpi_program



"INTEL MPI" example 2 nodes with two MPI processes each

```
#!/bin/bash
#SBATCH -J myjb
#SBATCH -N 2
#SBATCH --tasks-per-node 2
```

```
export I_MPI_PIN_PROCESSOR_LIST=0,64 mpirun -np 4 ./my_mpi_program
```





• check for available reservations. If there is one available, use it

specify an email address that notifies you when your job has finished