Running jobs with dependencies on the Peregrine computer cluster

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https://github.com/richelbilderbeek/Peregrine



What, Why, Mastery

- I will show how to set up jobs with one or more dependencies
- Starting each step manually is tedius and might lead to irreproducible research
- You can create jobs that are dependent on one or more jobs

Not: running a program in parallel on multiple cores

Overview

- bash #1
- Job without dependencies
- bash #2
- Job dependent on one job
- Job dependent on multiple jobs
- bash #3
- Conclusion

bash #1

echo "Hello world"

Display 'Hello World'

ls

List directory content

echo "Hello world" > tmp.txt

Streams the text 'Hello world' to file tmp.txt in overwrite mode

cat tmp.txt

Shows the file tmp.txt

./run.sh

Run the local executable bash script called run.sh

Job without dependencies



Run and check it

```
p230198@pg-login:simple_job ./run.sh
Submitted batch job 7144352
```

```
p230198@pg-login:simple_job cat out.txt
Created by simple_job.sh
```

run.sh

```
#!/bin/bash
sbatch simple_job.sh
```

simple_job.sh

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH --job-name=simple job
#SBATCH --output=simple job.log
echo "Created by simple job.sh" > out.txt
```

bash #2

```
echo "Hello world" | cut -d " " -f 1
```

Pipe the words 'Hello world' to cut. Show, using space as a delimiter, the first field

Pipe the words 'Hello world' to cut.

Stream, using space as a delimiter, the first field to tmp.txt in overwrite mode

Pipe the words 'Hello world' to cut.

Append, using space as a delimiter, the second field to tmp.txt

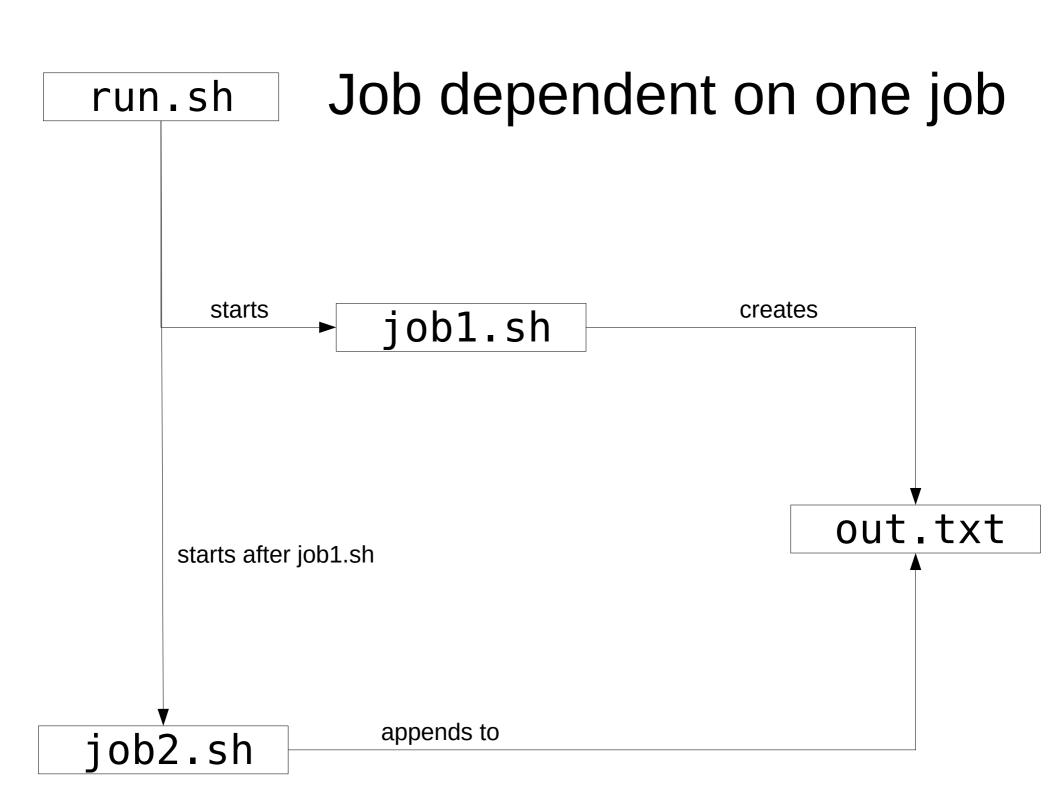
```
hi=$(echo "Hello world" | cut -d " " -f 1)
echo $hi
```

Pipe the words 'Hello world' to cut.

Extract, using space as a delimiter, the first field.

Store this result in the variable called 'hi'

Display the content of the variable 'hi'



Run and check it

```
p230198@pg-login:jobs_in_sequence ./run.sh
Submitted batch job 7144425
```

```
p230198@pg-login:jobs_in_sequence cat out.txt
Created by job1.sh
Appended by job2.sh
```

run.sh

```
#!/bin/bash
# Submit job1, store job ID
jobid=$(sbatch job1.sh | cut -d ' ' -f 4)
# Submit job2 after job1
sbatch --dependency=afterok:$jobid job2.sh
```

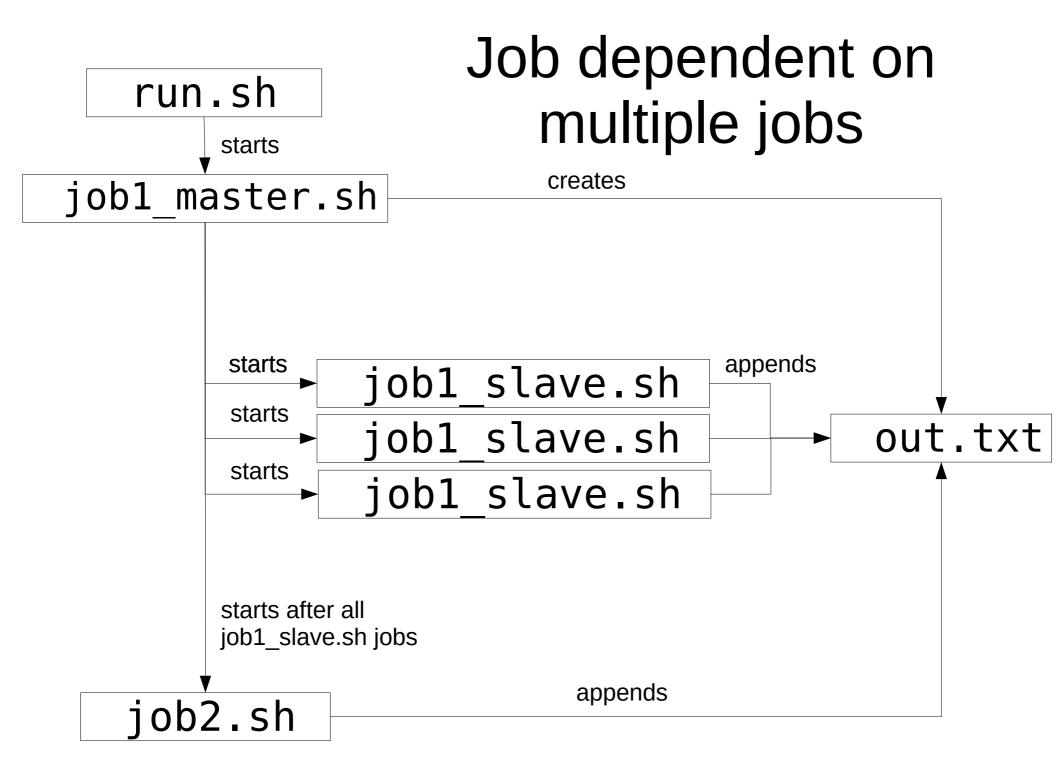
Submitted batch job 7144425

job1.sh

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH --job-name=job1
#SBATCH --output=job1.log
echo "Created by job1.sh" > out.txt
```

job2.sh

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH -- job-name=job2
#SBATCH --output=job2.log
echo "Appended by job2.sh" >> out.txt
```



Run and check it

```
p230198@pg-login:jobs_in_parallel ./run.sh
Submitted batch job 7144527
```

```
p230198@pg-login:jobs_in_parallel cat out.txt
Created by job1 master

Added by job1 slave number 2

Added by job1 slave number 1

Added by job1 slave number 3

Appended by job2
```

run.sh

```
#!/bin/bash
sbatch job1_master.sh
```

job1_master.sh 1/2

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH --job-name=job1 master
#SBATCH --output=job1 master.log
# Start file creation
# (may create race condition)
echo "Created by job1 master" > out.txt
```

job1_master.sh 2/2

```
# Submit all jobs, while collecting the job IDs
jobids=()
for i in {1..3}
do
  cmd="sbatch job1 slave.sh $i"
  jobids+=$($cmd | cut -d ' ' -f 4)
done
# Convert array of job IDs to colon-seperated string
txt=$(printf ":%s" "${jobids[@]}")
txt=${txt:1}
# Submit job2 after all previous jobs have finished
sbatch --dependency=afterok:$txt job2.sh
```

job1_slave.sh

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH --job-name=job1 slave
#SBATCH --output=job1 slave %j.log
echo "Added by job1 slave number "$1 >> out.txt
# To be sure the output file is created before the
next step
sleep 1
```

job2.sh

```
#!/bin/bash
#SBATCH --time=0:01:00
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --ntasks=1
#SBATCH --mem=1M
#SBATCH -- job-name=job2
#SBATCH --output=job2.log
echo "Appended by job2" >> out.txt
```

bash #3

egrep -R "error"

Searches all files in folders and subfolders for the regex 'error'

Searches all files in folders and subfolders for the regex 'error', case insensitively

```
egrep -iR "error" --include=*.log
```

Searches all files with a .log file extension in folders and subfolders for the regex 'error', case insensitively

```
scp p230198@peregrine.hpc.rug.nl:/home/p230198/any_folder/
*.* ~/any_other_folder
```

Securely copy all files from a Peregrine folder to a folder in your LWP home

```
echo "alias q='squeue -u $USER'" >> ~/.bashrc
```

Use the command 'q' to show your jobs in the queue (after a restart)

Conclusion

- Setting up linear and parallel jobs is doable
- Some knowledge of bash is useful
 - especially when something goes wrong