

Setting up and running a full pipeline on the Peregrine computer cluster

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<https://github.com/richelbilderbeek/Peregrine>

What, Why, Mastery

- I will show how to set up a pipeline that is easy to run and runs multiple jobs in parallel
- Starting each step manually is tedious and might lead to irreproducible research
- You can create a pipeline that is started with a single command and runs multiple jobs in parallel

Overview

- bash #1
- Job without dependencies
- bash #2
- Sequential jobs
- Parallel 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

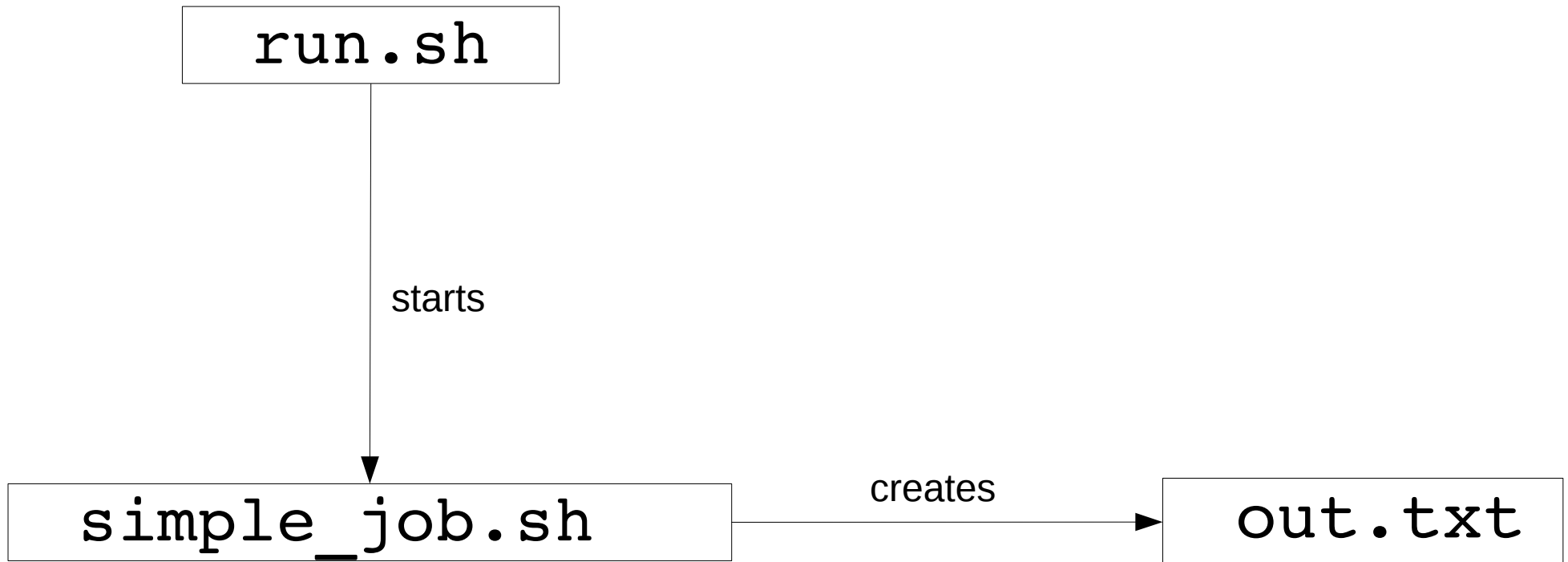
```
cat tmp.txt
```

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

```
echo "Hello world" | cut -d " " -f 1 > tmp.txt
```

Pipe the words 'Hello world' to cut.

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

```
echo "Hello world" | cut -d " " -f 2 >> tmp.txt
```

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
```

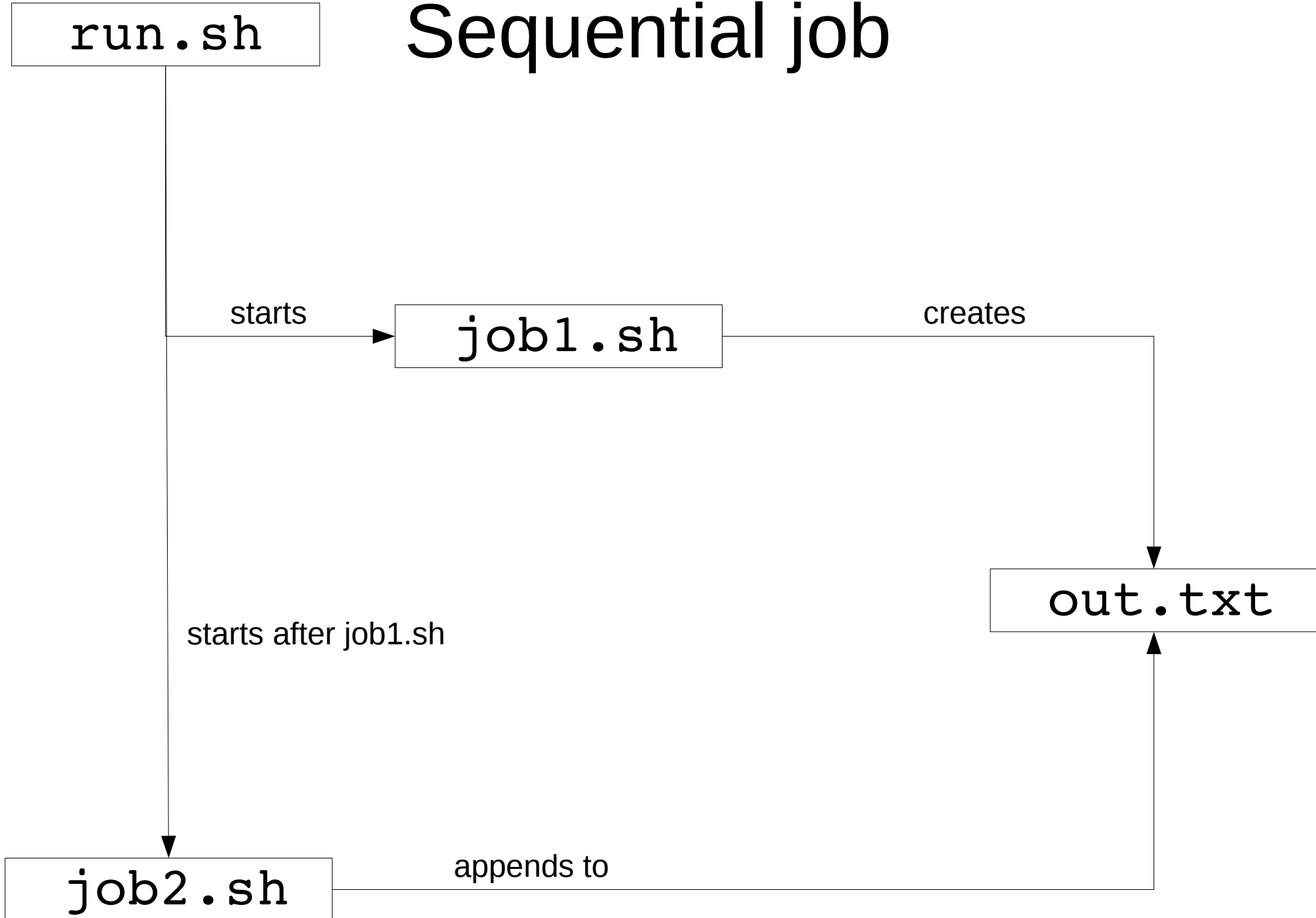
Pipe the words 'Hello world' to cut.

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

Store this result in the variable called 'hi'

Display the content of the variable 'hi'

Sequential job



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

# Start job1, store job ID
jobid=`sbatch job1.sh | cut -d ' ' -f 4`

# Start 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
```

Parallel jobs

run.sh

starts

job1_master.sh

creates

starts

job1_slave.sh

appends

starts

job1_slave.sh

starts

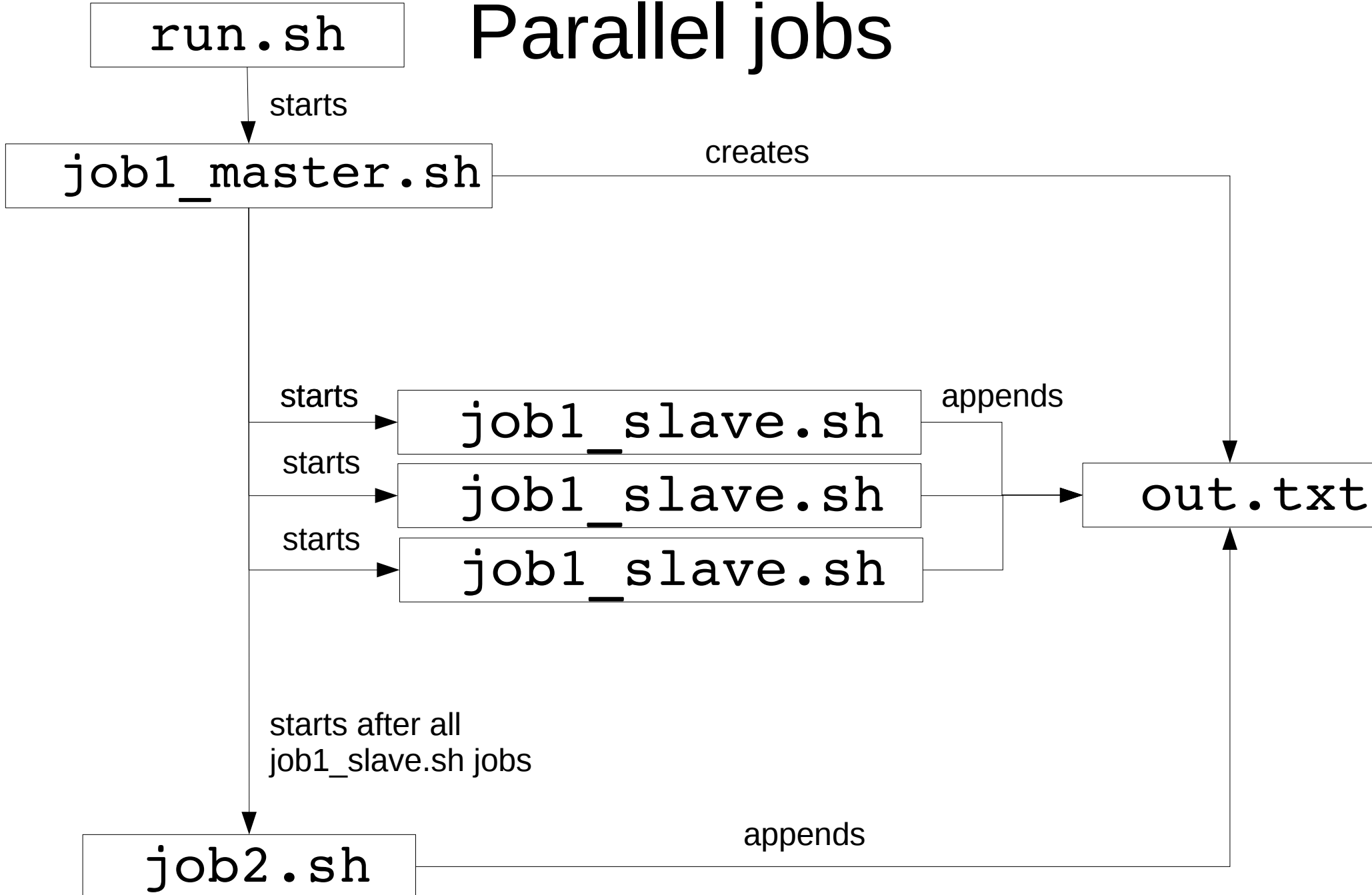
job1_slave.sh

starts after all
job1_slave.sh jobs

job2.sh

appends

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

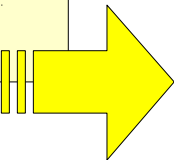
```
#!/bin/bash
```

```
sbatch job1_master.sh
```

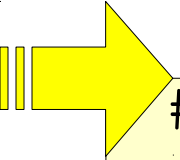
job1_master.sh 1/2

```
#!/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
echo "Created by job1 master" > out.txt
```



job1_master.sh 2/2



```
# Start 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}

# Start 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'

```
egrep -iR "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