

## PIPELINES WITH SLURM

Bio Code club end-of-semester event

### BASH AND SLURM

#### Conventional script:

> bash scriptname.bash

script is executed

#### On HPC:

- > sbatch scriptname.bash
- 1)resources requested, job queued
- 2)job allocated on compute node
- 3)script is executed



Compute cluster

### SCALING UP ON HPC

#### **Benefits**

- More time
- More memory
- Larger/more datasets

#### Requirements

- Say you want to scale from 10 input files to 50 or 100
- But you have a complex pipelines (branching, multiple steps)
- Learning Workflow tools like Nextflow are a whole new system
- $\blacksquare$  Basic  $\rightarrow$  intermediate level scripting might be enough to do the coordination

#### This talk

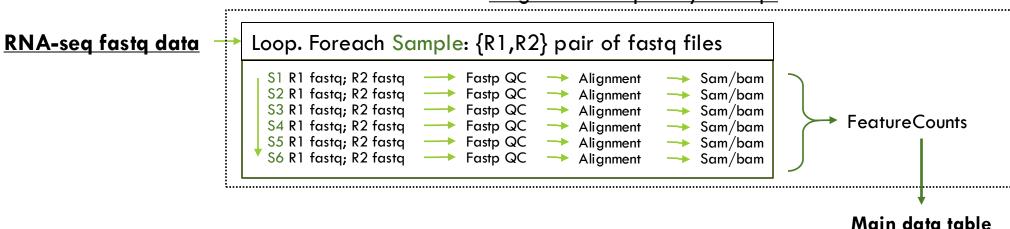
- Introduce some features in SLURM to parallelize and coordinate scripts
- Talk about some debugging techniques
- Tools and Templates



Compute cluster

### All data processed in single script, single job

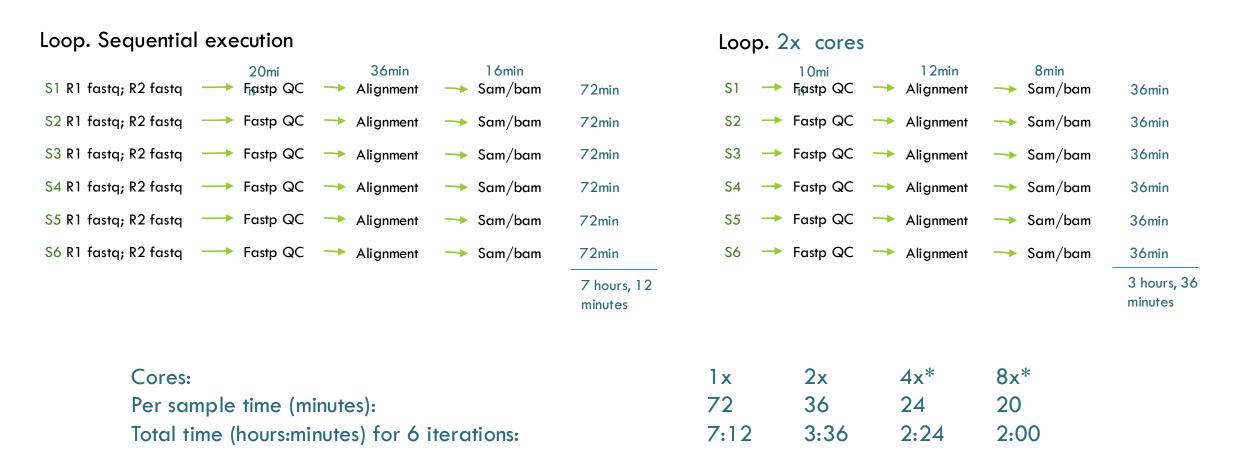
#### Single RNA-seq Analysis script



#### Pipeline synopsis

- Several steps per input file set \$1...\$6
- Loop iteration contains bulk of work, but ...
- ...not parallelized: doesn't scale well to large/many files
- Final step FeatureCounts run after loop has completed

### All data processed in single script, single job



\*diminishing return

## ALL DATA PROCESSED SEQUENTIALLY



\*diminishing return

### PARALLEL TIMING

		72min	36min	24min	20min
S6 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
S5 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
S4 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
S3 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
S2 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
S1 R1 fastq; R2 fastq	→ Fastp QC → Alignment → Sam/bam	72min	36min	24min	20min
		Ix	2x	4x	8x

- Put independent work in independent jobs:
  - Riviera: 40 Nodes, 7912 cores
  - Alpine: 696 Nodes, 40,200 cores
  - HPC!!!

- Parallelization
  - In a bash script: distribute jobs across cores
  - Scaling up:
    - Total run time is largest individual job, not sum of jobs
    - Dependent on queue- resources/priority

### Using sbatch with the array argument

\$ sbatch --array=1-6 main.sh <- hit enter Submitted job with ID 9223918 SLURM ARRAY TASK ID=1 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK\_ID=2 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=3 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=4 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=5 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=6

S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam

Launches Main RNA-seq Analysis script 6 times; sets SLURM\_ARRAY\_TASK\_ID to different values: (1,2,3,4,5,6)

```
JOBID PARTITION NAME USER ST
                                   TIME NODES NODELIST(REASON)
25736 1 short-cpu rna-seq dking R
                                   0:04
                                         1 node001
25736 2 short-cpu rna-seq dking R
                                  0:04
                                         1 node001
25736 3 short-cpu rna-seq dking R
                                  0:04
                                         1 node001
25736 4 short-cpu rna-seq dking R
                                  0:01
                                         1 node001
25736 5 short-cpu rna-seq dking R
                                  0:01
                                         1 node001
25736 6 short-cpu rna-seq dking R
                                  0:01
                                         1 node001
```

### Using sbatch with the array argument

\$ sbatch --array=1-6 main.sh <- hit enter Submitted job with ID 9223918 SLURM ARRAY TASK ID=1 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=2 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=3 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=4 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=5 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam SLURM ARRAY TASK ID=6 S■ R1 fastq; R2 fastq → Fastp QC → Alignment → Sam/bam

Launches Main RNA-seq Analysis script 6 times; sets SLURM ARRAY TASK ID to different values: (1,2,3,4,5,6) S■ R1 fastq; R2 fastq What's this? Base input filenames on SLURM ARRAY TASK ID e.g.: R1=S\${SLURM ARRAY TASK ID} R1.fastq R2=S\${SLURM ARRAY TASK ID} R2.fastq fastp -i \$R1 -I \$R2 SLURM\_ARRAY\_TASK\_ID=3 R1=S3 R1.fastq R2=S3 R2.fastq

fastp -i S3 R1.fastq -I S3 R2.fastq

# Features of array jobs: monitoring with squeue

```
$ squeue -u $USER
                                            TIME NODES NODELIST(REASON)
      JOBID PARTITION
                         NAME
                                 USER ST
      25736 1 short-cpu rna-seq
                                dking R
                                           0:04
                                                  1 node001
      25736_2 short-cpu rna-seq
                                           0:04
                                dking R
                                                  1 node001
      25736 3 short-cpu rna-seq
                                dking R
                                           0:04
                                                  1 node001
                                dking R
      25736_4 short-cpu rna-seq
                                           0:01
                                                  1 node001
                                dking R
      25736 5 short-cpu rna-seq
                                           0:01
                                                  1 node001
                                dking R
      25736 6 short-cpu rna-seq
                                           0:01
                                                  1 node001
```

Run as a group,
Share JOB\_ID
Number after '\_' is array job ID.

Might be staggered due to resource/priority

### Features of array jobs: Specifying log file names

### Single job script

```
#!/usr/bin/env bash
#SBATCH ...
#SBATCH --job-name=rna-seq
#SBATCH --output=%x.%j.log
#SBATCH ...
...
```

### Log file:

```
rna-seq.25736.log %x %i
```

### Array job script

```
#!/usr/bin/env bash
#SBATCH ...
#SBATCH --job-name=rna-seq
#SBATCH --output=%x.%A_%a.log
#SBATCH ...
...
```

```
rna-seq.25736_1.log
rna-seq.25736_2.log
rna-seq.25736_3.log
rna-seq.25736_4.log
rna-seq.25736_5.log
rna-seq.25736_6.log
%x %A %q
```

### Features of array jobs: filename patterns for logs

#### **FILENAME PATTERN**

**sbatch** allows for a filename pattern to contain one or more replacement symbols, which are a percent sign "%" followed by a letter (e.g. %j).

```
%A Job array's master job allocation number.
```

%a Job array ID (index) number.

**%j** jobid of the running job.

%x Job name.

--From "sbatch" help page

```
rna-seq.25736.log

%x %i

rna-seq.25736_1.log
rna-seq.25736_2.log
rna-seq.25736_3.log
rna-seq.25736_4.log
rna-seq.25736_5.log
rna-seq.25736_6.log
%x %A %a
```

### SUBMISSION SCRIPT VERSUS ARRAY

submit.sh

```
#!/usr/bin/env bash
# run as `bash submit.sh`

for inputfile in *.R1.fastq
do
    sbatch single_rnaseq_analyzer.sh $inputfile
done
```

Simpler script, but no longer tied to a shared job id.

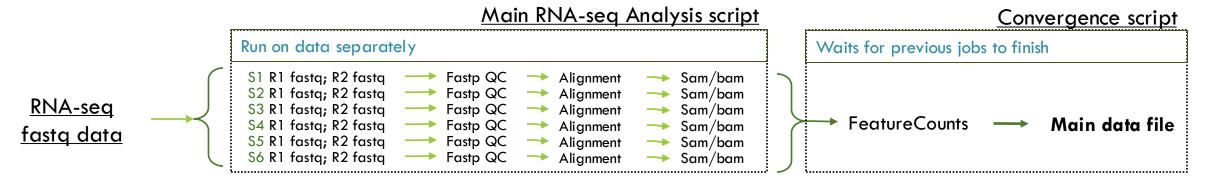
Harder to track, coordinate with other jobs



## JOB COORDINATION

Converge after array job

### Parallel workflow → Convergence



#### How?

\$ sbatch --array=1-6 main.sh Submitted job with ID 9223918 \$ sbatch --dependency=afterok:9223918 converge.sh Submitted job with ID 9223925

### Capture job id

\$ jobid=\$(sbatch -p --array=1-6 main.sh)
\$ sbatch --dependency=afterok:\$(jobid) converge.sh
Submitted job with ID 9223925

### SLURM DEPENDENCIES

\$ jobid=\$(sbatch -p --array=1-6 main.sh)



```
$ sbatch --dependency=afterok:$(jobid) converge.sh

Submitted job with ID 31033

$ squeue -u $USER

JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)

31033 short-cpu converge dking PD 0:00 1 (Dependency)

31032_1 short-cpu rnaseq dking R 0:01 1 node001

31032_2 short-cpu rnaseq dking R 0:01 1 node001

31032_3 short-cpu rnaseq dking R 0:01 1 node001
```

• • •

### SLURM DEPENDENCIES

- -d, --dependency=<<u>dependency\_list</u>>
- Defer the start of this job until the specified dependencies have been satisfied.
- <dependency list</p>is of the form

afterok:job\_id -Job with job\_id must complete successfully

**afternotok:job\_id** -Job with job\_id failed: (non-zero exit code, node failure, timed out, etc). *Cleanup/error* script?

**afterany:job\_id** – Job with job\_id completes for any reason

See shatch documentation for more complex forms

### SIMPLE PIPELINE WITH DEPENDENCIES

\$ sbatch sleep10.sh

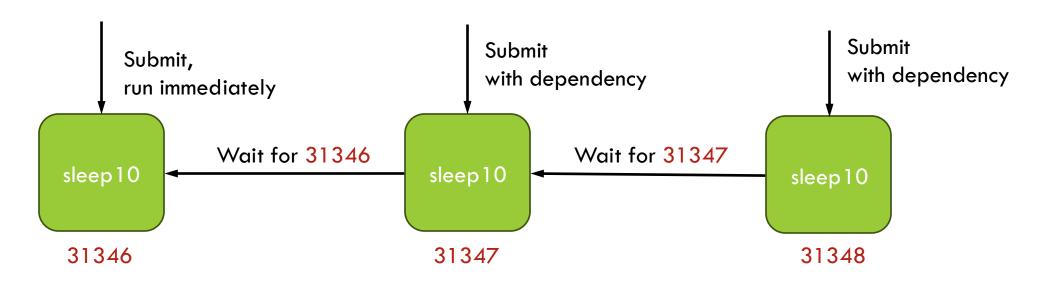
Submitted job id 31346

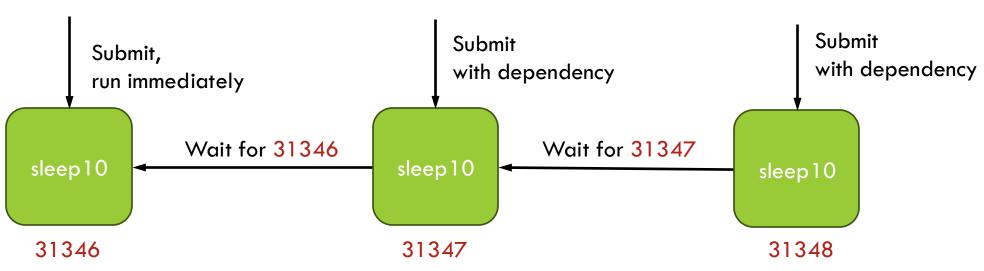
\$ sbatch --dependency=afterok:31346 sleep10.sh

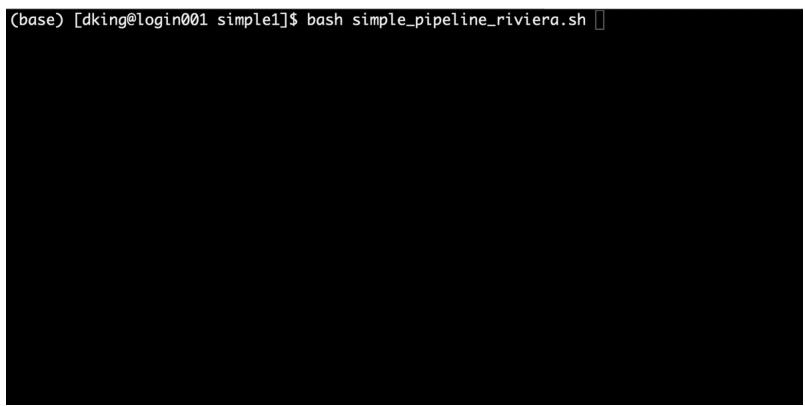
Submitted job id 31347

\$ sbatch --dependency=afterok:31347 sleep10.sh

Submitted job id 31348

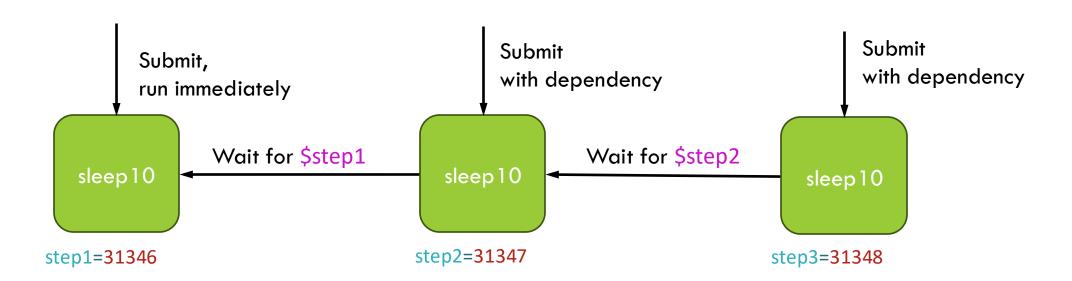






### SCRIPTABLE PIPELINE

```
step1=$(sbatch --parsable sleep10.sh)
step2=$(sbatch --parsable --dependency=afterok:$step1 sleep10.sh)
step3=$(sbatch --parsable --dependency=afterok:$step2 sleep10.sh)
```



### ARRAY WITH CONVERGENCE

#### **Array Script**

#### 

#### Convergence script

```
Waits for all array jobs to finish

cat $SLURM_ARRAY_JOB_ID/*.txt
```

slept 15 seconds slept 11 seconds slept 16 seconds slept 14 seconds

### 

3 echo "slept \$rand seconds 
\$SLURM\_ARRAY\_JOB\_ID/\$SLURM\_ARRAY\_TASK\_ID.txt

4 echo "slept \$rand seconds 
\$\infty\$ \$\text{\$\sum\_ARRAY\_JOB\_ID}\\$\$\text{\$\sum\_ARRAY\_TASK\_ID.txt}\$

Waits for all array jobs to finish

cat \$SLURM\_ARRAY\_JOB\_ID/\*.txt

```
job_monitor.sh 31588,31589
                                       squeue -u dking -j 31588,31589
                                                      TIME NODES NODELIST(REASON)
                      JOBID PARTITION
                                            USER ST
                                                      0:00
                                                              1 (None)
                31588_[1-10] short-cpu
                                           dking PD
                                    array
                      31589 short-cpu converge
                                                              1 (Dependency)
                                           dking PD
                                                      0:00
                                         sacct -X -j 31588,31589
                                           State Elapsed Timelimit
                   JobID
                          JobName AllocCPU
                                                                 Start
                                                                         End
                                                                                     Reason
             CTRL-C to quit.
```

## ARRAY/CONVERGENCE LAUNCHER SCRIPT

```
#!/usr/bin/env bash
array_job_id=$(sbatch --parsable --array=1-10 array.sbatch)
converge_job_id=$(sbatch --parsable --dependency=afterok:${array_job_id} converge.sbatch $array_job_id)
```

\*This script is run with `bash` not `sbatch`



## **EXAMPLES: LOOPS TO ARRAYS**

Some examples of how to modify your scripts to go from sequential to array

Three ways to modify/remove loops

- 1. Arguments on the command line
- 2. Already looping over an array
- 3. Reading a file, use sed to select specific line

1. Arguments on the command line

#### Original: script loops over '\$@'

```
for arg in "$@"; do
progname $arg
...
done
```

#### New version:

- convert command line to array
- Set loop variable from array and \$SLURM\_ARRAY\_TASK\_ID
- Remove loop

```
args=($@)
arg=${args[$SLURM_ARRAY_TASK_ID]}

#for arg in "$@"; do
progname $arg
...

#done

args=($@)
args=($@)
arg=${args[$SLURM_ARRAY_TASK_ID]}
progname $arg
...
```

2. Already looping over an array in main script

```
Original: '@' expands to full array
```

```
# Loop through each subdirectory

for folder_name in "${subdirectories[@]}"; do

# Verify if the folder contains exactly two files: .dv and its reference file

dv_files=($(find "$folder_name" -maxdepth 1 -type f -name "*.dv" | sort))

...

...

done
```

#### New version: Keep the loop, replace with \$SLURM\_ARRAY\_TASK\_ID

```
# Loop through each subdirectory

for folder_name in "${subdirectories[$SLURM_ARRAY_TASK_ID]}"; do

# Verify if the folder contains exactly two files: .dv and its reference file

dv_files=($(find "$folder_name" -maxdepth 1 -type f -name "*.dv" | sort))

...

...

done
```

3. Select a line of a file for input with sed

### Original: while loop through file

```
while read -a line; do
    arg1=${line[0]}
    arg2=${line[1]}
    arg3=${line[2]}
    cmd $arg1 $arg2 $arg3
done < metadata.txt</pre>
```

### New version: Pass \$SLURM\_ARRAY\_TASK\_ID to sed

```
line=( $(sed -n "${SLURM_ARRAY_TASK_ID}p" metadata.txt) )
arg1=${line[0]}
arg2=${line[1]}
arg3=${line[2]}
cmd $arg1 $arg2 $arg3
```



## DEBUGGING WITH EXIT TRAP

Cool stuff

## DEBUGGING/COOL STUFF

script	Output/log if succe		
#!/usr/bin/env bash			
echo " <job \$(date)="" on="" started="">"</job>	<job dec<="" fri="" on="" started="" td=""></job>		
cmd1	[cmd1 output]		
	[ cmd2 output ]		

cmd2

cmd3

cmd4

echo "<job finished on \$(date)>"

essful

6 13:25>

[ cmd3 output ]

[cmd4 output]

<job finished on Fri Dec 6 15:25>

An error early on

<job started on Fri Dec 6 13:25>

[cmd1 output]

cmd2 error output cmd2 error cmd2 err or output cmd2 error output cmd3 error output cmd3 error cmd3 err or output cmd3 error output cmd4 error output cmd4 error cmd4 err or output cmd4 error output

## DEBUGGING/COOL STUFF — USING BASH SETTINGS

#### script

```
#!/usr/bin/env bash
set -e # quit on error
set -o pipefail # detect error in pipe
echo "<job started on $(date)>"
```

cmd1

cmd2

cmd3

cmd4

echo "<job finished on \$(date)>"

An error early on

<job started on Fri Dec 6 13:25>

[cmd1 output]

cmd2 error output cmd2 error cmd2 error output cmd2 error output

## DEBUGGING/COOL STUFF — THE EXIT SIGNAL

#### script

#!/usr/bin/env bash
set -e # quit on error
set -o pipefail # detect error in pipe
echo "<job started on \$(date)>"
cmd1
cmd2
cmd3
cmd4
echo "<job finished on \$(date)>"

An error early on

<job started on Fri Dec 6 13:25>

[cmd1 output]

cmd2 error output cmd2 error cmd2 error output cmd2 error output

<job FAILED on Fri Dec 6 13:26>

## DEBUGGING/COOL STUFF — TRAPPING SIGNALS

Signals can be sent to any process on linux to interrupt, cancel jobs, among other things

Some signals can be handled "trapped" and given code to run

#### Syntax:

trap code\_to\_run SIGNAL

#### **Example:**

Script says "have a nice day" when user CTRL-C's their script:

trap 'echo "have a nice day"; exit 0' SIGINT

## DEBUGGING/COOL STUFF — THE EXIT TRAP

script

```
#!/usr/bin/env bash
set -e # quit on error
set -o pipefail # detect error in pipe
echo "<job started on $(date)>"
trap 'echo "Job ended at $(date) "' EXIT
cmd1
cmd2
cmd3
cmd4
echo "<job finished on $(date)>"
```

An error early on

<job started on Fri Dec 6 13:25>

[cmd1 output]

cmd2 error output cmd2 error cmd2 error output cmd2 error output

<job ended at Fri Dec 6 13:26>

## DEBUGGING/COOL STUFF — THE EXIT TRAP

script

Output/log if successful

```
#!/usr/bin/env bash
                                                                           <job started on Fri Dec 6 13:25>
set -e # quit on error
set -o pipefail # detect error in pipe
                                                                           [cmd1 output]
echo "<job started on $(date)>"
                                                                           [ cmd2 output ]
trap 'echo "Job ended at $(date) "' EXIT
                                                                           [ cmd3 output ]
cmd1
                                                                           [ cmd4 output ]
cmd2
cmd3
                                                                           <job finished on Fri Dec 6 15:25>
cmd4
                                                                           <job ended at Fri Dec 6 15:25>
echo "<job finished on $(date)>"
```

### EXIT TRAP WITH HANDLING FUNCTION

```
"<<<< Script started at $(date) >>>>>"
JOBSTEP=SETUP
davidsExitFunc()
   exitcode=$1
   if [ -z "$exitcode" ] || [ $exitcode -eq 0 ] # wasn't provided or is 0
       echo "<<<<< Script reached $JOBSTEP successfully at $(date) >>>>>"
       echo "<<<< Script failed at $JOBSTEP with exit code $exitcode at $(date) >>>>>"
rap 'davidsExitFunc $?' EXIT
OBSTEP=STEP1
OBSTEP=STEP2
OBSTEP=STEP3
exit 1 # uncomment to exit in controlled manner
JOBSTEP=STEP4
exit 0
IOBSTEP=END
```

#### # quits at exit 1 under JOBSTEP=STEP3

\$ bash cleanup\_function.sh
<<<<< Script started at Mon Dec 9 11:51 >>>>>
<<<<< Script failed at STEP3 with exit code 1 at Mon Dec 9 11:51:49
>>>>>>

#### # delete the '4' under JOBSTEP=STEP2 (syntax error)

\$ bash cleanup\_function.sh

<<<< Script started at Mon Dec 9 11:53 >>>>>

cleanup\_function.sh: line 25: [: 1: unary operator expected

<<<< Script failed at STEP2 with exit code 2 at Mon Dec 9 11:53:42

>>>>>>

#### # replace the 4 and comment out exit statements

### EXIT TRAP WITH HANDLING FUNCTION

#### Other uses:

- Close connections, free resources
- Ex: Close Amazon machine instance (charges MONEY \$\$\$)

```
#!/bin/bash

# define the base AMI ID somehow
ami=$1

function finish {
   ec2-terminate-instances "$ami"
}

trap finish EXIT
ec2-run-instances "$ami"
```

Simplified from: http://redsymbol.net/articles/bash-exit-traps/

## REPO FOR THIS TALK AND SLURM TOOLS

https://github.com/Colorado-State-University-CMB/slurm-scripting-pipelines

- Use: git clone https://github.com/Colorado-State-University-CMB/slurm-scripting-pipelines on alpine or riviera
- Do bash INSTALL.sh to install job\_monitor.sh, which is used in the pipeline examples
- The subdirectories contain the examples used in this presentation