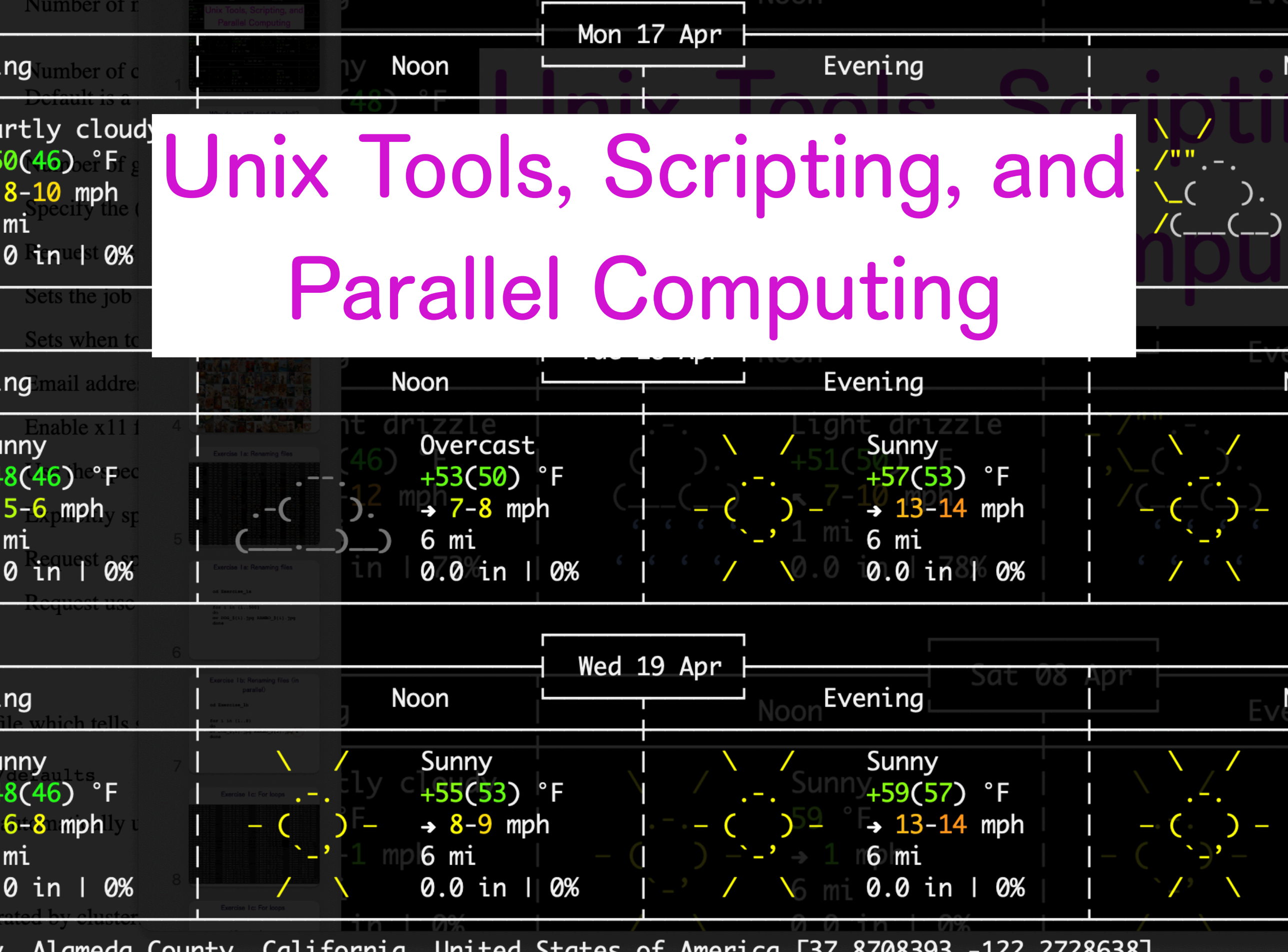
Unix Tools, Scripting, and Parallel Computing



Why do we still need the shell? (Psst… the command line is 50 years old)

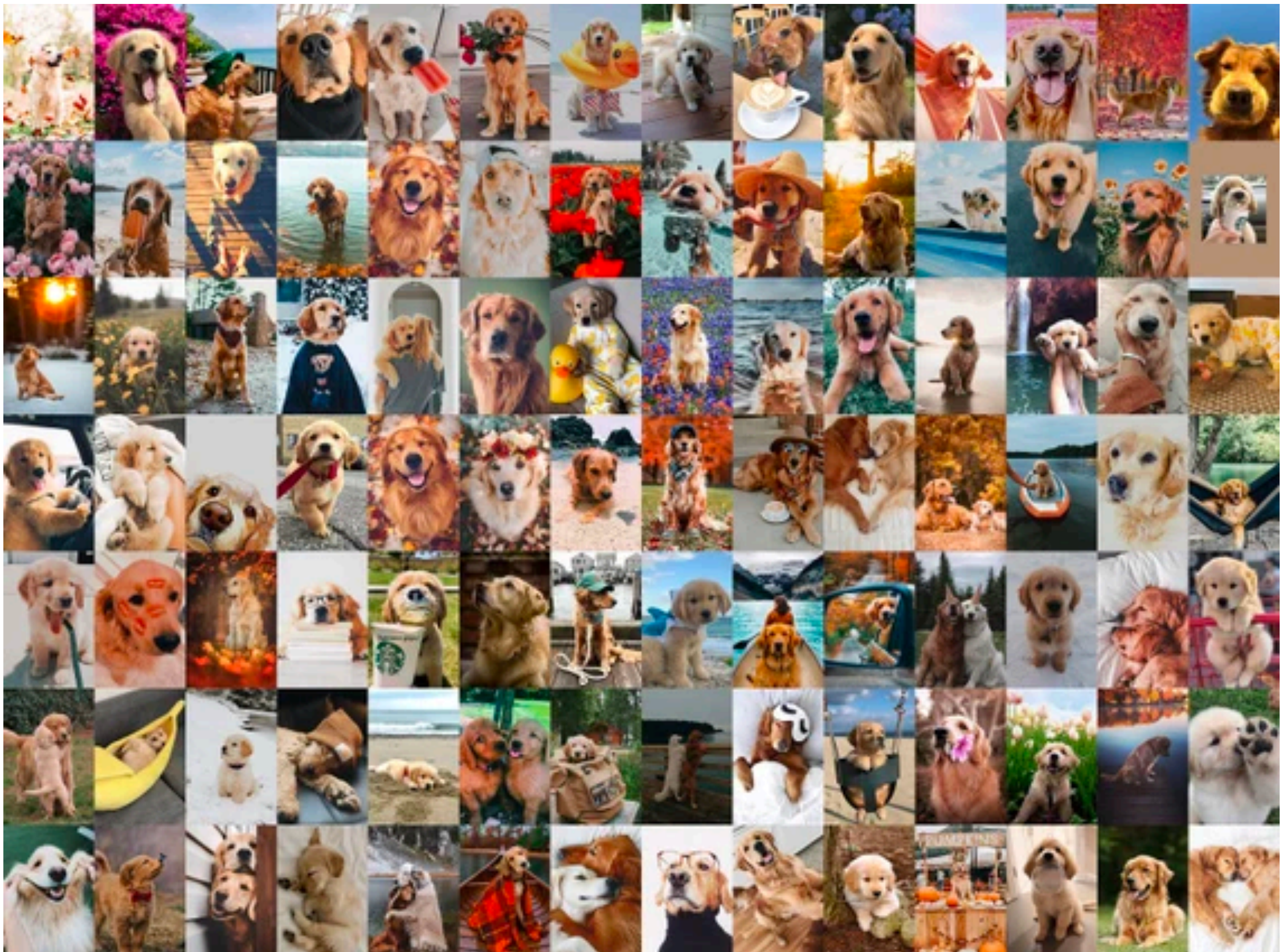
- Scripting and automation
  - Everything you can do in a GUI, you can do in a CLI
- Very old, very new, or very simple programs
  - all designed to be chained together
- low-overhead, no-frills system access
  - It's super fast!

To follow along interactively git clone the workshop repository

```
git clone https://github.com/lpipes/unix_workshop.git

brew install parallel
```

Exercise 1a: Renaming files



Exercise 1a: Renaming files

DOG_125.jpg DOG_182.jpg DOG_239.jpg DOG_296.jpg DOG_352.jpg DOG_409.jpg DOG_466.jpg
DOG_126.jpg DOG_183.jpg DOG_24.jpg DOG_297.jpg DOG_353.jpg DOG_41.jpg DOG_467.jpg
DOG_127.jpg DOG_184.jpg DOG_240.jpg DOG_298.jpg DOG_354.jpg DOG_410.jpg DOG_468.jpg
DOG_128.jpg DOG_185.jpg DOG_241.jpg DOG_299.jpg DOG_355.jpg DOG_411.jpg DOG_469.jpg
DOG_129.jpg DOG_186.jpg DOG_242.jpg DOG_3.jpg DOG_356.jpg DOG_412.jpg DOG_47.jpg
DOG_13.jpg DOG_187.jpg DOG_243.jpg DOG_30.jpg DOG_357.jpg DOG_413.jpg DOG_470.jpg
DOG_130.jpg DOG_188.jpg DOG_244.jpg DOG_300.jpg DOG_358.jpg DOG_414.jpg DOG_471.jpg
DOG_131.jpg DOG_189.jpg DOG_245.jpg DOG_301.jpg DOG_359.jpg DOG_415.jpg DOG_472.jpg
DOG_132.jpg DOG_19.jpg DOG_246.jpg DOG_302.jpg DOG_36.jpg DOG_416.jpg DOG_473.jpg
DOG_133.jpg DOG_190.jpg DOG_247.jpg DOG_303.jpg DOG_360.jpg DOG_417.jpg DOG_474.jpg
DOG_134.jpg DOG_191.jpg DOG_248.jpg DOG_304.jpg DOG_361.jpg DOG_418.jpg DOG_475.jpg
DOG_135.jpg DOG_192.jpg DOG_249.jpg DOG_305.jpg DOG_362.jpg DOG_419.jpg DOG_476.jpg
DOG_136.jpg DOG_193.jpg DOG_25.jpg DOG_306.jpg DOG_363.jpg DOG_42.jpg DOG_477.jpg
DOG_137.jpg DOG_194.jpg DOG_250.jpg DOG_307.jpg DOG_364.jpg DOG_420.jpg DOG_478.jpg
DOG_138.jpg DOG_195.jpg DOG_251.jpg DOG_308.jpg DOG_365.jpg DOG_421.jpg DOG_479.jpg
DOG_139.jpg DOG_196.jpg DOG_252.jpg DOG_309.jpg DOG_366.jpg DOG_422.jpg DOG_48.jpg
DOG_14.jpg DOG_197.jpg DOG_253.jpg DOG_31.jpg DOG_367.jpg DOG_423.jpg DOG_480.jpg
DOG_140.jpg DOG_198.jpg DOG_254.jpg DOG_310.jpg DOG_368.jpg DOG_424.jpg DOG_481.jpg
DOG_141.jpg DOG_199.jpg DOG_255.jpg DOG_311.jpg DOG_369.jpg DOG_425.jpg DOG_482.jpg
DOG_142.jpg DOG_2.jpg DOG_256.jpg DOG_312.jpg DOG_37.jpg DOG_426.jpg DOG_483.jpg
DOG_143.jpg DOG_20.jpg DOG_257.jpg DOG_313.jpg DOG_370.jpg DOG_427.jpg DOG_484.jpg
DOG_144.jpg DOG_200.jpg DOG_258.jpg DOG_314.jpg DOG_371.jpg DOG_428.jpg DOG_485.jpg
DOG_145.jpg DOG_201.jpg DOG_259.jpg DOG_315.jpg DOG_372.jpg DOG_429.jpg DOG_486.jpg
DOG_146.jpg DOG_202.jpg DOG_26.jpg DOG_316.jpg DOG_373.jpg DOG_43.jpg DOG_487.jpg
DOG_147.jpg DOG_203.jpg DOG_260.jpg DOG_317.jpg DOG_374.jpg DOG_430.jpg DOG_488.jpg
DOG_148.jpg DOG_204.jpg DOG_261.jpg DOG_318.jpg DOG_375.jpg DOG_431.jpg DOG_489.jpg
DOG_149.jpg DOG_205.jpg DOG_262.jpg DOG_319.jpg DOG_376.jpg DOG_432.jpg DOG_49.jpg
DOG_15.jpg DOG_206.jpg DOG_263.jpg DOG_32.jpg DOG_377.jpg DOG_433.jpg DOG_490.jpg
DOG_150.jpg DOG_207.jpg DOG_264.jpg DOG_320.jpg DOG_378.jpg DOG_434.jpg DOG_491.jpg
DOG_151.jpg DOG_208.jpg DOG_265.jpg DOG_321.jpg DOG_379.jpg DOG_435.jpg DOG_492.jpg
DOG_152.jpg DOG_209.jpg DOG_266.jpg DOG_322.jpg DOG_38.jpg DOG_436.jpg DOG_493.jpg

Exercise 1a: Renaming files

```
cd unix_workshop
cd Exercise_1a
```

```
for i in {1..500}
do
mv DOG_${i}.jpg RAMBO_${i}.jpg
done
```

Exercise 1b: Renaming files (in parallel)

```
cd ../Exercise_1b


for i in {1..8}
do
mv DOG_${i}.jpg RAMBO_${i}.jpg &
done
```

Exercise 1c: For loops

```
16S_K1354-G5-S47_R1.fastq
16S_K1354-G5-S47_R2.fastq
16S_K1354-K6-S50_R1.fastq
16S_K1354-K6-S50_R2.fastq
16S_K1354-M8-S63_R1.fastq
16S_K1354-M8-S63_R2.fastq
16S_K1355-A1-S58_R1.fastq
16S_K1355-A1-S58_R2.fastq
16S_K1355-C3-S84_R1.fastq
16S_K1355-C3-S84_R2.fastq
16S_K1355-E4-S78_R1.fastq
16S_K1355-E4-S78_R2.fastq
16S_K1355-G5-S71_R1.fastq
16S_K1355-G5-S71_R2.fastq
16S_K1355-K6-S56_R1.fastq
16S_K1355-K6-S56_R2.fastq
16S_K1355-L7-S59_R1.fastq
16S_K1355-L7-S59_R2.fastq
16S_K1355-M8-S66_R1.fastq
16S_K1355-M8-S66_R2.fastq
16S_K1355-T9-S48_R1.fastq
16S_K1355-T9-S48_R2.fastq
16S_K1356-A1-S80_R1.fastq
16S_K1356-A1-S80_R2.fastq
16S_K1356-B2-S62_R1.fastq
16S_K1356-B2-S62_R2.fastq
16S_K1356-C3-S61_R1.fastq
16S_K1356-C3-S61_R2.fastq
16S_K1356-E4-S51_R1.fastq
16S_K1356-E4-S51_R2.fastq
16S_K1356-G5-S55_R1.fastq
16S_K1356-G5-S55_R2.fastq
16S_K1356-K6-S60_R1.fastq
16S_K1356-K6-S60_R2.fastq
16S_K1481-T9-S76_R1.fastq
16S_K1481-T9-S76_R2.fastq
16S_K1482-A1-S86_R1.fastq
16S_K1482-A1-S86_R2.fastq
16S_K1482-B2-S79_R1.fastq
16S_K1482-B2-S79_R2.fastq
16S_K1482-C3-S85_R1.fastq
16S_K1482-C3-S85_R2.fastq
16S_K1482-E4-S74_R1.fastq
16S_K1482-E4-S74_R2.fastq
16S_K1482-K6-S65_R1.fastq
16S_K1482-K6-S65_R2.fastq
16S_K1482-M8-S82_R1.fastq
16S_K1482-M8-S82_R2.fastq
16S_K1482-T9-S81_R1.fastq
16S_K1482-T9-S81_R2.fastq
16S_K1495-A1-S54_R1.fastq
16S_K1495-A1-S54_R2.fastq
16S_K1495-B2-S72_R1.fastq
16S_K1495-B2-S72_R2.fastq
16S_K1495-C3-S67_R1.fastq
16S_K1495-C3-S67_R2.fastq
16S_K1495-E4-S64_R1.fastq
16S_K1495-E4-S64_R2.fastq
16S_K1495-G5-S77_R1.fastq
16S_K1495-G5-S77_R2.fastq
16S_K1495-K6-S70_R1.fastq
16S_K1495-K6-S70_R2.fastq
16S_WK1159-C3-S21_R1.fastq
16S_WK1159-C3-S21_R2.fastq
16S_WK1160-E4-S22_R1.fastq
16S_WK1160-E4-S22_R2.fastq
16S_WK1354-B2-S39_R1.fastq
16S_WK1354-B2-S39_R2.fastq
16S_WK1355-C3-S4_R1.fastq
16S_WK1355-C3-S4_R2.fastq
16S_WK1355-E4-S19_R1.fastq
16S_WK1355-E4-S19_R2.fastq
16S_WK1355-G5-S28_R1.fastq
16S_WK1355-G5-S28_R2.fastq
16S_WK1355-K6-S32_R1.fastq
16S_WK1355-K6-S32_R2.fastq
16S_WK1355-L7-S37_R1.fastq
16S_WK1355-L7-S37_R2.fastq
16S_WK1355-M8-S31_R1.fastq
16S_WK1355-M8-S31_R2.fastq
16S_WK1355-T9-S3_R1.fastq
16S_WK1355-T9-S3_R2.fastq
16S_WK1356-A1-S7_R1.fastq
16S_WK1356-A1-S7_R2.fastq
16S_WK1356-B2-S1_R1.fastq
16S_WK1356-B2-S1_R2.fastq
16S_WK1356-E4-S33_R1.fastq
16S_WK1356-E4-S33_R2.fastq
16S_WK1356-G5-S35_R1.fastq
16S_WK1356-G5-S35_R2.fastq
16S_WK1356-K6-S2_R1.fastq
16S_WK1356-K6-S2_R2.fastq
16S_WK1356-L7-S25_R1.fastq
16S_WK1356-L7-S25_R2.fastq
16S_WK1356-M8-S34_R1.fastq
16S_WK1356-M8-S34_R2.fastq
16S_WK1481-L7-S9_R1.fastq
16S_WK1481-L7-S9_R2.fastq
16S_WK1481-M8-S10_R1.fastq
16S_WK1481-M8-S10_R2.fastq
16S_WK1481-T9-S18_R1.fastq
16S_WK1481-T9-S18_R2.fastq
16S_WK1482-K6-S23_R1.fastq
16S_WK1482-K6-S23_R2.fastq
16S_WK1482-M8-S11_R1.fastq
16S_WK1482-M8-S11_R2.fastq
16S_WK1482-T9-S12_R1.fastq
16S_WK1482-T9-S12_R2.fastq
16S_WK1495-A1-S36_R1.fastq
16S_WK1495-A1-S36_R2.fastq
16S_WK1495-B2-S24_R1.fastq
16S_WK1495-B2-S24_R2.fastq
16S_WK1495-E4-S30_R1.fastq
16S_WK1495-E4-S30_R2.fastq
16S_WK1495-G5-S16_R1.fastq
16S_WK1495-G5-S16_R2.fastq
16S_WK1495-K6-S26_R1.fastq
16S_WK1495-K6-S26_R2.fastq
16S_blank-1-S5_R1.fastq
16S_blank-1-S5_R2.fastq
16S_blank-2-S17_R1.fastq
16S_blank-2-S17_R2.fastq
16S_blank-3-S44_R1.fastq
16S_blank-3-S44_R2.fastq
16S_blank-4-S53_R1.fastq
16S_blank-4-S53_R2.fastq
16S_blank-5-S75_R1.fastq
16S_blank-5-S75_R2.fastq
16S_blank-6-S89_R1.fastq
16S_blank-6-S89_R2.fastq
16S_blank-7-S90_R1.fastq
16S_blank-7-S90_R2.fastq
16S_blank-8-S91_R1.fastq
16S_blank-8-S91_R2.fastq
16S_pcr-blank-1-S92_R1.fastq
16S_pcr-blank-1-S92_R2.fastq
```

Exercise 1c: For loops

```
cd ../Exercise_1c

for file in *.fastq
do
gzip ${file}
done
```

Exercise 1c: Using `find`

```
for file in *.fastq.gz
do
gunzip ${file}
done
```

```
find . -name “*.fastq” | xargs -I {}
gzip {}
```

Exercise 1c: Using `find` and `parallel`

```
find . -name “*.fastq.gz” | parallel
-j 4 “gunzip {}”

find . -name “*.fastq” | sed ’s/\.\///g’
| parallel -j 4 “gzip {}”

find . -name “*.fastq.gz” | sed 's/\.
\///g' | sed ’s/\.fastq\.gz//g' |
parallel -j 4 "gunzip {}.fastq.gz &> {}
_resultslog”
cd ..
```

Exercise 1d: Writing a bash script (Exercise_1d.sh) for benchmarking

```
#!/bin/bash

file=$1
name=`basename ${file} .fastq`
logFile="$name""_runlog"
timeLog=Exercise_1d/"$name""_time.out"
cp Exercise_1c/${file} Exercise_1d
/usr/bin/time -o ${timeLog} -p bash -c
"gzip Exercise_1d/${file} &>
Exercise_1d/${logFile}"
```

Exercise 1d: Wrapping up your bash script (Exercise_1d_wrapper.sh)

```
#!/bin/bash

find Exercise_1c -name "*.fastq" | sed
's/Exercise_1c\///g' | parallel -j 4
"./Exercise_1d.sh {}"
```

```
./Exercise_1d_wrapper.sh
```

Exercise 1e: Multiple arguments using `parallel`

Exercise_1e.txt (made with change_case.py):

```
16S_K1356-L7-S69_R2.fastq       k1356-l7-s69_r2
16S_K1482-A1-S86_R2.fastq       k1482-a1-s86_r2
16S_WK1481-M8-S10_R2.fastq      wk1481-m8-s10_r2
16S_WK1354-E4-S6_R1.fastq       wk1354-e4-s6_r1
16S_pcr-blank-1-S92_R2.fastq    pcr-blank-1-s92_r2
16S_K1354-C3-S52_R1.fastq       k1354-c3-s52_r1
16S_K1355-A1-S58_R2.fastq       k1355-a1-s58_r2
16S_WK1482-C3-S20_R1.fastq      wk1482-c3-s20_r1
16S_WK1354-M8-S42_R1.fastq      wk1354-m8-s42_r1
16S_K1354-E4-S57_R1.fastq       k1354-e4-s57_r1
```

Exercise 1e: Multiple arguments using `parallel`

```
parallel -j 4 –colsep '\t' -a
Exercise_1e.txt ./Exercise_1e.sh {1}
{2}
```

Now that you can run parallel jobs on your computer, let's move on to running parallel jobs on an HPC cluster

Logging on to Savio

```
ssh [USERNAME]@hpc.brc.berkeley.edu
sftp [USERNAME]@dtn.brc.berkeley.edu
```

Scratch directory

```
cd /global/scratch/users/lpipes

git clone https://github.com/lpipes/
unix_workshop.git

cd unix_workshop
```

Writing a slurm script (test.slurm)

```
#!/bin/bash
#SBATCH –job-name=[TEST]
#SBATCH –account=[ACCOUNT_NAME]
#SBATCH –partition=[PARTITION_NAME]
#SBATCH –time=00:00:30

echo “hello world”
```

Savio partitions (https://docs-research-it.berkeley.edu/services/high-performance-computing/user-guide/hardware-config/)

Partition	Nodes	Node Features	Nodes shared?	SU/core hour ratio
savio	132	savio	exclusive	0.75
savio_bigmem	4	savio_bigmem or savio_m512	exclusive	1.67
savio2	163	savio2 or savio2_c24 or savio2_c28	exclusive	1.00
savio2_bigmem	36	savio2_bigmem or savio2_m128	exclusive	1.20
savio2_htc	20	savio2_htc	shared	1.20
savio2_gpu	17	savio2_gpu	shared	2.67 (5.12 / GPU)
savio2_1080ti	8	savio2_1080ti	shared	1.67 (3.34 / GPU)
savio2_knl	28	savio2_knl	exclusive	0.40
savio3	184	savio3 or savio3_c40	exclusive	1.00
savio3_bigmem	20	savio3_bigmem or savio3_m384	exclusive	2.67
savio3_htc	24	savio3_htc or savio3_c40	shared	2.67
savio3_xlmem	4	savio3_xlmem or savio3_c52	exclusive	TBD
savio3_gpu	2	savio3_gpu (2x V100)	shared	TBD
savio3_gpu	9	4rtx (4x GTX)	shared	TBD
savio3_gpu	10	8rtx, 8a5k (8 GPU)	shared	TBD
savio3_gpu	16	a40 (2 GPU)	shared	TBD
savio4_htc	32	savio4_m256 or savio4_m512	shared	TBD

Writing a slurm script (test.slurm) with more directives

```
#!/bin/bash
#SBATCH –job-name=[TEST]
#SBATCH –account=[ACCOUNT_NAME]
#SBATCH –partition=[PARTITION_NAME]
#SBATCH –time=00:00:30
#SBATCH –nodes=[# NODES]
#SBATCH –ntasks-per-node=[# TASKS/NODE]
#SBATCH –cpus-per-task=[# CPUS/TASK]
#SBATCH –mail-type=START,END,FAIL
#SBATCH –mail-user=[YOUR EMAIL]

echo “hello world”
```

Run generate_job_scripts.py

```
./generate_job_scripts.py 40

cd Exercise_2_slurm

for file in {0..3}
do
sbatch ${i}.slurm
done
```

Thank you!

Please email me if you have any feedback or have any questions:
lpipes@berkeley.edu