Practical Coding Series: Elzar Batch Analysis

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Schedule

Jan 6	John Hover	Elzar Batch System Usage
Jan o	JOHITTIOVEI	Lizar Datch System Osage
Feb 3	Hannah Meyer	Snakemake
Mar 3	Ammar	Python packages
April 7	Batuhan	Optimizing for performance/speed (Matlab, Python)
May 5	Rohit	Github workflow
June 2	Shaina	Personal Web dev
July 7	Amber	TensorFlow

Note: This session is being recorded.



Logistics

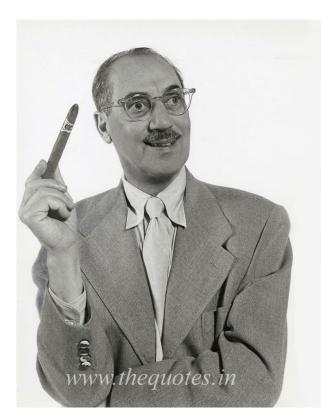
- All materials will be available afterwards on Github.
- Please feel free to interrupt--intended to be interactive!
- We are catering to many levels, so if you have further questions afterward feel free to contact us

https://github.com/juliawang22/CSHLPracticalCoding

Outline

- General Batch Principles
 - Why use Elzar? When not to. Pros/Cons
 - Principles, Process, Layout
 - Software Environment and Data Management
- Elzar/UGE Basics
 - Work process overview
 - Job assessment
 - Submission, resource specification
 - Testing, monitoring, debugging
- Elzar Usage Examples
 - Array Jobs, GPU requests
 - Snakemake Intro

Batch Principles/ Best Practices



Those are my principles, and if you don't like them... well, I have others.

Groucho Marx

Caveats & Omissions

No MPI discussion.

All of these hints/approaches are things that have worked for me.

But not gospel! Feel free to accept or reject.

No substitute for figuring out what works for your own work...

Question 0: Why? Can I even benefit from using batch for an analysis?

- Is the work iterative with frequent tweaks? Ad-hoc analysis at each step?
 No
- Is it very small-scale (size/number files, resources, runtime, space) -> No
- Will you need to (re)do the same analysis with new/additional input? ->
 Maybe
- Does the analysis need to be refined enough for public consumption/publication? -> Probably.
 - o If it needs to be polished and validated anyway, why not batch?

Question 0 (cont)

- Do you need to do a multi-dimensional parameter sweep (e.g. all against all?) -> Probably.
- Does the analysis involve a large number of files, where some step exceeds your server/desktop memory/ cores/ local storage capacity? -> Yes
- Does the analysis require GPUs, high performance? -> Yes

Batch Pros/Cons

Pros:

- Safe, long-running computing.
- Resources! E.g. on Elzar...
 - o 34 nodes
 - 768GB/ 3TB memory
 - GPUs 32GB
 - Fast distributed filesystem, with lots of storage.
 - GPFS: TBs depending on your group's quota.
 - vs. non-distributed FS

Cons:

- Requires a more structured approach to effectively run on HPC.
- Requires more up-front effort to automate.
- ... at least if the unavoidable extra work is not to be lost.
- Requires learning SGE/UGE basics and probably 1 additional utility.

Principles

- Rigorous common sense.
- Take stuff you (maybe) already do and formalize it.
- Pay attention to portability.
- 99% automatic = manual.

Standardization **limits complexity** to let you deal with the underlying task...

Cost effort up front. Reduces mental effort after. Eases later **re-entry.**..

- Work Process
 - Develop
 - Test
 - Run, Iterate
 - Archive
- Portability
 - Consistent Layout
 - Symlinks
 - Modularity/DRY
 - Software versioning
- Automation
 - Nomenclature
 - Consistency

Standardization -> Reproducibility

Project Work/Code/Data Layout

Directory	Usage	Comment	Tape?
~/data/genomes /GTEx /CoCoCoNet	External data (re-downloadable) Long term local data (usable by others)	Symlink to global /data area.	No
~/git/cshlwork/ <proj1> /<proj2></proj2></proj1>	Project-specific code/scripts. Snakemake file		Yes (github)
~/project/ <proj1></proj1>	Working dir. ad-hoc one-off scripts? Snakemake -> ~/git/ <proj>/Snakemake. Jupyter notebooks.</proj>	On home partition.	Yes
~/work/ <proj1></proj1>	Global project-specific working area. Possibly cleared after each run.	On data partition. Symlink to ~/data/work	No
~/data/ <proj1>/</proj1>	Intermediate data worth keeping. Final output data location.		Yes

Software Environments

- Won't talk modules...
 - o Fine on HPC, but not available on desktops (or laptops). Use Conda
- Hierarchy:
 - OS-level Local Installs
 - OS-level RPMs
 - User-level local installs
 - Module system (optional)
 - Conda

 Modularize software at this level

 Python

 R

 CRAN installations.

 Java tools.

 3rd party tarball software

 Your custom software.
- Don't install/use modules (except maybe compilers) at OS level!
- Create script to re-create environment, e.g...

```
For werner1 project.
                                                      labelled gatk.
Script serves as
                                 samtools-1.11
record of
                                 bedtools-2.29.2
                                 gatk-4.1.9.0
dependencies.
                                 igvtools-2.8.9
                                 STAR 2.7.2a (tied to genome dir version)
                              set -x
Hard to fully
automate on
                              # Conda
                              conda create -y -n gatk python=3.8
multiple platforms,
                              conda activate gatk
but close is OK.
                              # Conda available packages
                              conda install -y pandas numpy scipy seaborn matplotlib plotly h5py
                              conda install -c conda-forge -c bioconda snakemake
Note use of
                              # Tarball installs
$CONDA PREFIX with
                                 Samtools 1.11
                              wget https://github.com/samtools/samtools/releases/download/1.11/samtools-1.11.ta
tarball/make.
                              tar -xvjf samtools-1.11.tar.bz2
                              cd samtools-1.11
                              ./configure --prefix=$CONDA_PREFIX
                              make
pip install also
                              make install
good here.
                              cd ..
                              rm -rf samtools-1.11.tar.bz2 samtools-1.11
                                 bedtools
```

#!/bin/bash -l

Nomenclature & Style

Suggestions:

Directory names should be short, lowercase, no spaces.

For files, pick underscore or hyphen and stick with it.

Script names should be specific, descriptive, versioned. E.g.

final_filter_script.sh vs.remove_bam_snp_dupes_v13.sh

... (see Style and Organization session from the Practical Coding Series.)

Data Management

Disk usage on batch systems is measured. You/ your group have a limited quota. Always calculate disk usage for analyses:

```
# jobs * (input + temp + output)
```

If temp >> input + output, and you run 1000 jobs at once...

Think explicitly about data lifecycle...

- What to copy in (don't pull anything directly from the internet)
- What to keep during processing (until correctness is confirmed).
- What to keep for potential followup investigations.
- What to copy back to external storage.

Benefits of Portability

Even if you don't develop on a desktop/laptop, and don't intend to move work between platforms, it is still worth working *as if you might*.

If you have a complete snapshot of software and versions, paths, input data, etc. and can easily establish the same environment on another host (and especially another OS), then your confidence in the correctness of the answers it produces should be very high.

Portability -> Reproducibility

Reproducibility -> Confidence

Work Process: Develop locally

- Create software environment, preferably with script, versions.
- Define cut-down input data. < 5 minute run.
- Get simple end-to-end bash script working. Initial sanity-checking.
- Assess...
 - core/memory requirements,
 - step runtime
 - temp,intermediate and final storage usage.
- Decide batch strategy. Create git repo for project handling...
 - ad-hoc: just submit individual jobs from the command line.
 - unix/bash: use an array job to launch a large set of jobs
 - Snakemake: create a rule, or longer pipeline.

Work Process: Test/Assess on Batch

To run on batch, you must know exact core/memory usage for each tool.

- Test small/medium input batch (~5 jobs), but with full-size data, on cluster.
- Core usage control requires you to tell the tool. Many will take all...
- May use UGE to test memory usage. Run with high request, then check actual usage, e.g.

```
qacct -j <jobid> | grep maxvmem
```

- Confirm/check success and output. Check file validity.
- Don't test intensive or long-running processes on bamdev1|2.
 - a. You'll get warning. Use interactive mode...

Aside: Batch vs. Interactive

Elzar is primarily a batch resource, oriented toward multiple, automated jobs submitted from a head node. But it is also a very large, standard resource, usable interactively.

qrsh -1 m_mem_free=1024G -pe threads 48 -1 gpu=1

Gives out local login with more resources than a rugen. But, you may get

Your "qrsh" request could not be scheduled, try again later.

So, copy data from your local server, login to bamdev, qrsh, run, copy back.

Work Process: Run at scale and monitor

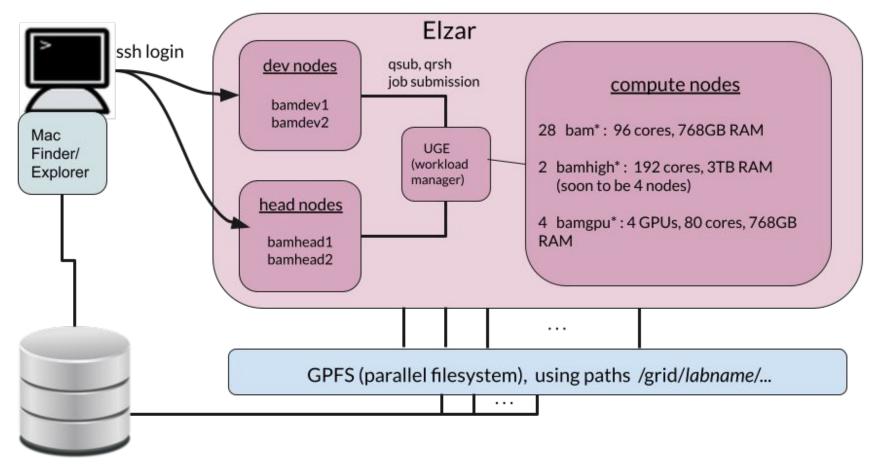
- Very rarely will large numbers of jobs all run perfectly.
- Check job exit status, file output, etc.
- If something goes wrong, consider aborting run.
- Debug the inevitable failures. Discard bad cases? Re-run.
- Sanity check/validation of intermediate and final results.

After confirmed successful run:

- Copy/move important data to final location.
- Cleanup unneeded intermediate/temp data!

Elzar/SGE/UGE Basics





DDN storage system

SGE/UGE commands

```
qhost, status: information about current cluster state (nodes, queued jobs..)
```

qsub <script>: run a script non-interactively on a worker node

qrsh: get an interactive shell on a worker node

qstat: information about running jobs.

qdel: remove running/queued jobs

qacct: retrospective info about finished jobs.

Will touch on most of these as we go along...

GPFS Storage Space

Appears to be 4.3 Petabytes.

Currently \$29/TB/year. First 30TB free.

You can see filesets (which map to directories) with

findmnt

Then you can you can check your quota on those directories, e.g.

```
/usr/lpp/mmfs/bin/mmlsquota -j gillis_hpc_data grid
/usr/lpp/mmfs/bin/mmlsquota -j gillis_hpc_home grid
```

Submission, resource specification

Pseudo variables usable within job script.

```
#$ -o ~/project/$JOB_NAME/logs/$JOB_NAME.o$JOB_ID.$TASK_ID
#$ -e ~/project/$JOB_NAME/logs/$JOB_NAME.e$JOB_ID.$TASK_ID
```

Interpolated at job execution time, not at submit.

Submission, resource specification (cont)

qsubbed jobs run on the remote worker...

- Under your user account
- From whatever working directory you submit from (unless altered).
- Under the same shell environment. (E.g conda env).

Default resources are 1 core, 2048M memory.

Logging/debugging

- Logs placed wherever you specified from -o / -e locations in submit script.
- I always direct mine in submit script, to:

```
~/project/<name>/logs/<job_name>.[e|o]<job_id>.<task_id>
```

- Or, they get dropped into your home directory with default name:
 <job name>.[e|o]<job id>.<task id>
- .o is standard out of running job. .e is standard error. Contents depend on executables. Different tools write to different places.
- Always useful to emit full command lines, and exit statuses to stdout.

Testing/Debugging

Do not run analysis commands on bamdev1|2! Go interactive...

Get interactive session on worker node. Specify resources as in submission. e.g.,

qrsh -N werner2 -pe threads 8 -1 m_mem_free=5760M

Within the session you can run tools to confirm they work. Or to manually test a previously failed job.

This is where printing *interpolated command lines* in your code is crucial, so you can cut-and-paste specific examples upon failure.

Monitoring/ Post-run Checking

During run check job progress with qstat ...

Once some jobs have finished, this

will give you key-value pair lists of all jobs you have completed in the last day, which can be used to check exit statuses, e.g.

```
qacct -j -d 1 -o hover | grep exit_status
```

If things look bad and you need to abort:

Both qstat and qacct have -j <jobid> args, which outputs key-value pairs for a particular job.

Miscellaneous Gotchas/Hints

- Memory usage can depend on input size. For testing I usually run 3 jobs,
 1 with largest input, 1 with smallest, 1 from middle.
- Java JVM tricky to limit CPU usage. E.g,
 - --java-options '-XX:ActiveProcessorCount=8 ' Java >JDK 8u191
- Screen messes up scrolling from Mac terminal...
 - # ~.screenrc
 # Enable mouse scrolling and scroll bar history scrolling
 termcapinfo xterm* ti@:te@

Miscellaneous Gotchas/Hints (cont)

- qstat and qacct produce key-value pair output one per line, with jobs separated by bar.
- Not very useful if you're interested in lots of jobs. I wrote a quick script that formats it one job per line:

https://raw.githubusercontent.com/jhover/elzar-example/master/bin/qhist

qhist | head

Gives one job per line output: jobid, name, taskid, start, end, wallclock, cores, memory, and exit status.

Array jobs: GoFocus

Array jobs

You provide an argument to qsub e.g.

```
qsub -t 1-478 [...] jobscript.sh
```

and UGE will set an environment variable within each job, e.g.:

Your runscript must check it, and index into some list to make each job do something different, like handle a different file (or use a different set of parameters).

Array Job Example: Gofocus (Pytorch ML model)

This will be an array job, where we want to run against each file in an input directory. For this we'll just use Bash scripts...

- Simple one-step processing.
- Consumes species-specific FASTA (multi-) protein sequence file.
- Makes many GOTerm predictions, w/ probabilities, for each, to one file.
- Needs GPU.

Array Job Example (cont)

Prerequisites..

- File with base labels for all files to be processed:
 ~/project/jones/baselist.txt
- Gofocus script: ~/git/gofocus/pytorch_goterm_pred.py
- Setup source script: ~/project/jones/setup.sh
- Common shell functions file: ~/git/elzar-example/lib/common.sh
- Execution script to be submitted: ~/git/cshlwork/jones/rungofocus.sh

Gofocus Python program:

This part of a software package provided to us by David Jones at UCL.

```
(pytorch) [hover@bamdev2 ~]$ ~/git/gofocus/gofocus/pytorch_goterm_pred.py
usage: pytorch_goterm_pred.py [-h] [-d] [-v] [-c CONFFILE] fastafile outfile
pytorch_goterm_pred.py: error: the following arguments are required: fastafile, outfile
```

So we just need the fasta input file and prediction out file.

Create a base list, check length...

```
(pytorch) [hover@bamdev2 jones]$ ls ~/data/cococonet/sequences/ | grep 'dog\|tomato' | awk -F _ '{print $1}'
    > testlist.txt
(pytorch) [hover@bamdev2 jones]$ cat testlist.txt | wc -l
2
```

This length will be used to create the job array. We will need to explicitly specify it on the command line.

setup.sh Source file

Optional as long as you're not using modules.

Triggered from within the run script.

```
. ~/.bash_profile
# module load Java/11.0.2
conda activate pytorch
```

As long as you have established the required Conda environment the job will run with the same shell environment.

Common shell functions

Collecting info about the host.

Getting the Task id, with a default.

```
prelude() {
   echo "*******************************
   date
nodeinfo() {
   echo "*******************************
   hostname -f
   cat /etc/redhat-release
   NPROC=`cat /proc/cpuinfo
                           | grep processor | wc -l'
   echo "Processors: $NPROC "
   KMEM=`cat /proc/meminfo
                            grep MemTotal | awk '{print $2}'`
   MBMEM='expr $KMEM / 1000'
   echo "Memory MB: $MBMEM"
   NPROC=`cat /proc/cpuinfo
                            grep processor | wc -l'
   echo "Processors: $NPROC "
   KMEM=`cat /proc/meminfo
                            grep MemTotal | awk '{print $2}'`
   MBMEM='expr $KMEM / 1000'
   echo "Memory MB: $MBMEM"
taskid(){
   if [ -z ${SGE TASK ID} ]; then
       SGE TASK ID=1
   fi
   echo $SGE TASK ID
postlude() {
   date
```

Run script (1)

Args embedded, with usage of pseudo-vars.

Constants up front.

Ready for manual usage.

Name positional args for clarity.

```
#!/bin/bash
    Usage: rungofocus.sh <setup> <basefile> <inputdir> <outputdir>
#$ -N jones
#$ -wd $HOME/project/$10B NAME
#$ -pe threads 8
   -l m mem free=5G
#$ -l qpu=1
#$ -o $HOME/project/$JOB NAME/logs/$JOB NAME.o$JOB ID.$TASK ID
#$ -e $HOME/project/$JOB NAME/logs/$JOB NAME.e$JOB ID.$TASK ID
COMMON=~/git/elzar-example/lib/common.sh
CMD=~/git/gofocus/gofocus/pytorch_goterm_pred.py
NUMARGS=4
# Check for arg count...
if [ $# -ne $NUMARGS ]; then
    echo "Incorrect number of arguments."
    echo "Usage: rungofocus.sh <setup> <basefile> <indir> <outdir>"
    exit 1
fi
# Source common functions.
$COMMON
# Normalize args.
setup=$1
basefile=$2
inputdir=$3
outputdir=$4
```

Run script (cont.)

Sources env setup.

Gets taskid to choose entry from list of base labels.

Prints info.

Runs the command.

Ensures that the underlying command exit code is propagated.

```
echo "Running setup from $1"
$setup
# $SGE_TASK_ID
taskid=$(gettaskid)
echo "taskid is $taskid"
filebase=`head -$taskid test $basefile | tail -1 `
echo "filebase is $filebase"
infile="$inputdir/${filebase} hiprio.tfa "
outfile="$outputdir/${filebase} hiprio.predout"
echo "$infile -> $outfile"
nodeinfo
prelude
echo $CMD -v $infile $outfile
time $CMD -v $infile $outfile
RET=$?
if [ $RET -ne 0 ] ; then
    exit $RET
fi
echo "Job command Return code was $RET"
postlude
exit $RET
```

Pseudo environment vars for runscript header.

Get interpolated from script directives on a per-job basis:

r coddo on vandolo	2 dddiiption
\$USER	User name of the submitting user
\$HOME	Home directory of the submitting user
\$JOB_ID	ID of the job

Description

\$HOSTNAME Hostname of the execution host

Name of the job

\$SGE_TASK_ID ID of the array task

Pseudo env variable

\$JOB_NAME

Launch w/ indices. Check GPU usage once running

```
(pytorch) [hover@bamdev2 jones]$ qsub -t 1-2 ~/git/cshlwork/project/jones/rungofocus.sh]
~/project/jones/setup.sh ~/project/jones/testlist.txt ~/data/cococonet/sequences ~/wor
k/jones/
Your job-array 763646.1-2:1 ("jones") has been submitted
(pytorch) [hover@bamdev2 jones]$ qstat
job-ID
          prior
                  name
                                           state submit/start at
                              user
                                                                     queue
             jclass
                                            slots ja-task-ID
   763646 0.50866 jones
                                                 12/05/2020 13:58:18 gpu.q@bamgpu03
                              hover
                                                8 1
   763646 0.50866 jones
                              hover
                                                 12/05/2020 13:58:18 gpu.q@bamgpu04
                                                8 2
(pytorch) [hover@bamdev2 jones]$ gpustats | grep hover
(pytorch) [hover@bamdev2 jones]$ gpustats | grep hover
[1] Tesla V100-SXM2-32GB | 36'C, 40 % |
                                          4192 / 32510 MB | hover:python(4189M)
                                                            hover:python(2873M)
[0] Tesla V100-SXM2-32GB | 49'C, 56 % |
                                          2876 / 32510 MB |
```

Record jobids! Not easy to get after completion.

```
#!/bin/bash
# gpustats per Heywood
tail -n 5 /grid/it/data/elzar/gpustat/bamgpu0*.log
```

Check for completion. Stats...

```
(pytorch) [hover@bamdev2 ~]$ qstat
(pytorch) [hover@bamdev2 ~]$ qacct -j 763646 | grep ^wallclock
wallclock
            60.936
wallclock 108.350
(pytorch) [hover@bamdev2 ~]$ qacct -j 763646 | grep maxvmem
            12.564G
maxvmem
            11.184G
maxvmem
(pytorch) [hover@bamdev2 ~]$ qacct -j 763646 | grep slots
slots
            8
slots
            8
(pytorch) [hover@bamdev2 ~]$ qacct -j 763646 | grep failed
failed
            0
failed
            0
```

Snakemake: (Very) Brief Introduction



Snakemake

A framework for reproducible data analysis

https://snakemake.github.io/

Basic concept is simple: A set of rules, each with defined:

- input(s)
- 2. output(s)
- 3. shell/script/wrapper to create outputs from inputs.

Rules go in a Snakefile.

User executes snakemake and it processes the Snakefile, resolving rules.

Snakemake (cont.)

Basic tool runs locally--not particuarly tied to clusters/batch analyis. Focussed on running pipelines and/or complex workflow DAGs.

Has a -cluster "qsub" arg to submit to various batch systems.

Snakefiles are slightly tweaked Python syntax, so arbitrary Python code will execute within them.

```
import os
                       homedir = os.path.expanduser("~/")
Complete
                       (SAMPLES,) = glob_wildcards(homedir + "data/cococonet/sequences/{sample}_hiprio.tfa")
                                                                                                                 1. list of
implementation of
                                                                                                                 labels.
previous array job.
                       wildcard_constraints:
                          sample = ' \mid w+'
Added in post-prediction
                       rule all:
sorting step.
                           input:
                                                                                                      2. list of final
                               expand(homedir + "work/jones/{sample}_hiprio.pred", sample=SAMPLES)
                                                                                                      output.
Way easier.
                       rule aofocus:
                                                                                                      Where's input?
                           input:
                               homedir + "data/cococonet/sequences/{sample} hiprio.tfa"
                           output:
                                                                                         4. gofocus output = sorted input.
                               homedir + "work/jones/{sample}_hiprio.predout"
                                                                                          Input exists?
                           resources:
                               gpu=1, mem_mb=5120
                                                                                         Yes (first input) -> run shell.
                           threads: 4
                           shell:
                               homedir + "git/gofocus/gofocus/pytorch goterm pred.py -v {input} {output} "
                       rule sorted:
                           input:
                               homedir + "work/jones/{sample}_hiprio.predout"
                           output:
                                                                                     3. 'sorted' rule output matches
                               homedir + "work/jones/{sample}_hiprio.pred"
                                                                                     rule 'all' input.
                           resources:
                               gpu=0 , mem_mb=2048
                                                                                     Input exists?
                           threads: 1
                                                                                     yes -> run shell
                           shell:
                               "cat {input} | sort -k 1,1 -k 3,3rn > {output} "
                                                                                     no -> find input.
```

Desktop/Laptop submit command

Snakemake useful outside of a batch context as well.

Although gofocus uses GPUs, it can run (slowly) on a desktop/server.

```
cd cd conda activate pytorch
snakemake --cores 16 -l gpu=0 --resources mem_mb=81920
```

The --cores and --resources args tell Snakemake how much system resources to allow for **all** processes, based on rule threads and resources directive values.

"Mini"- batch system...

So, e.g. no more than 2 simultaneous jobs will run, since each uses 8 cores. Snakemake will fill in unused resources, with various rule jobs, as long as dependencies are satisfied.

Snakemake Submit

Submit command on Elzar is a bit longer, since we need to pass args through to qsub (since they can't be embedded in a script).

```
cd <project directory>
conda activate pytorch
snakemake --jobs 50 --cluster "qsub -N jones -cwd -pe
threads {threads} -l m_mem_free={resources.mem_mb}M -l
gpu={resources.gpu} "
```

The specified variables will be filled in for each job by the values in the rule that generated it.

Snakemake Summary

- Excellent for automating file-driven analysis.
- Very natural for Python programmers.
 - But can execute arbitrary programs.
- Well supported. Large community.
- Nicely moves between desktop/laptop/server and batch cluster.
- Integrated Conda software management (not covered).
- Nice reporting/visualization tools (not covered).

Just barely scratched surface of functionality...

- Conda environment specification-> automatic install within job
- Cluster profiles
- Tool wrappers.

Overall Summary

- Batch Principles
 - Automation and encapsulation required for reliable batch usage.
 - But extra effort for standardization minimizes error, allows re-use, and eases picking up old work -> reproducible, high-confidence results

Good for science.

Elzar/UGE

- Large, complex HPC installation, but useable with a small command set.
- Don't worry about using modules. Just use Conda.
- Interactive use to get access to very large cores/memory, GPUs.

Don't have to use batch.

- Snakemake. My new favorite thing...
 - Use it locally for anything even slightly "pipeline-like", very easy to get going.
 - Can be a "mini" batch system, throttling by resource availability.

Good stepping stone to batch.

Questions/Discussion?

Resources/ References

Software Carpentry Analysis pipelines with Python (draft).

Covers basic local use of Snakemake, cluster usage with Slurm:

https://hpc-carpentry.github.io/hpc-python/

CSHL Practical Coding Series:

https://github.com/juliawang22/CSHLPracticalCoding

Heywood Elzar Tutorial/ Docs:

https://docs.google.com/presentation/d/1MHGlb9kF7SsBnmVL98e8OodBCP

PHtjXqcFPWuRkjd U/

https://www.youtube.com/watch?v=D3wfhM cQPY

Wiki: http://intranet.cshl.edu/administration/information-technology/hpcc/elzar

Slack Workspace: https://elzarusers.slack.com/