Dynamically optimize your jobs' RAM and run time requests with SmartSlurm

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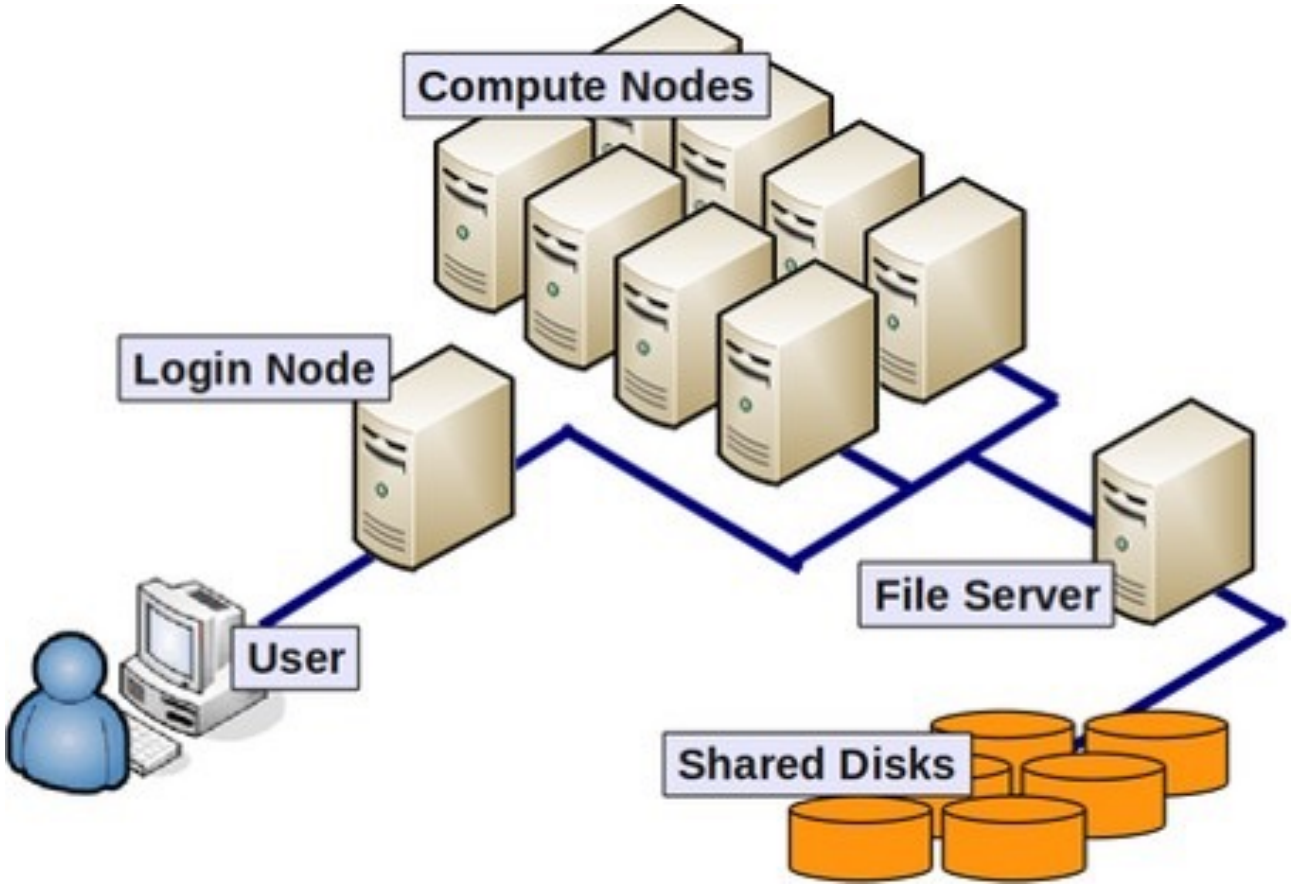
Generic Cluster Architecture



What is Slurm scheduler

- Allocates exclusive and/or non-exclusive access to resources (compute nodes) to users for some duration of time so they can perform work.
- Provides a framework for starting, executing, and monitoring work (normally parallel jobs) on the set of allocated nodes.
- Arbitrates contention for resources by managing a queue of pending work.

-- from: https://slurm.schedmd.com/overview.html

Slurm scheduler

- Sbatch command to submit jobs:

```
sbatch --mem 2G -t 2:0:0 cmd
```

- Job dependency:

```
sbatch --mem 2G -t 2:0:0 \
   -d afterok:123:321 cmd
```

HMS RC O2 Cluster

- O2 runs wildly diverse software and each software has unique resource requirement
- Same software run on different data set can have different specs
- The software x reqs x dataset combination space is huge. Impossible to efficiently assign static resources
- Number of jobs also very large, not possible to manually manage

Issues to resolve

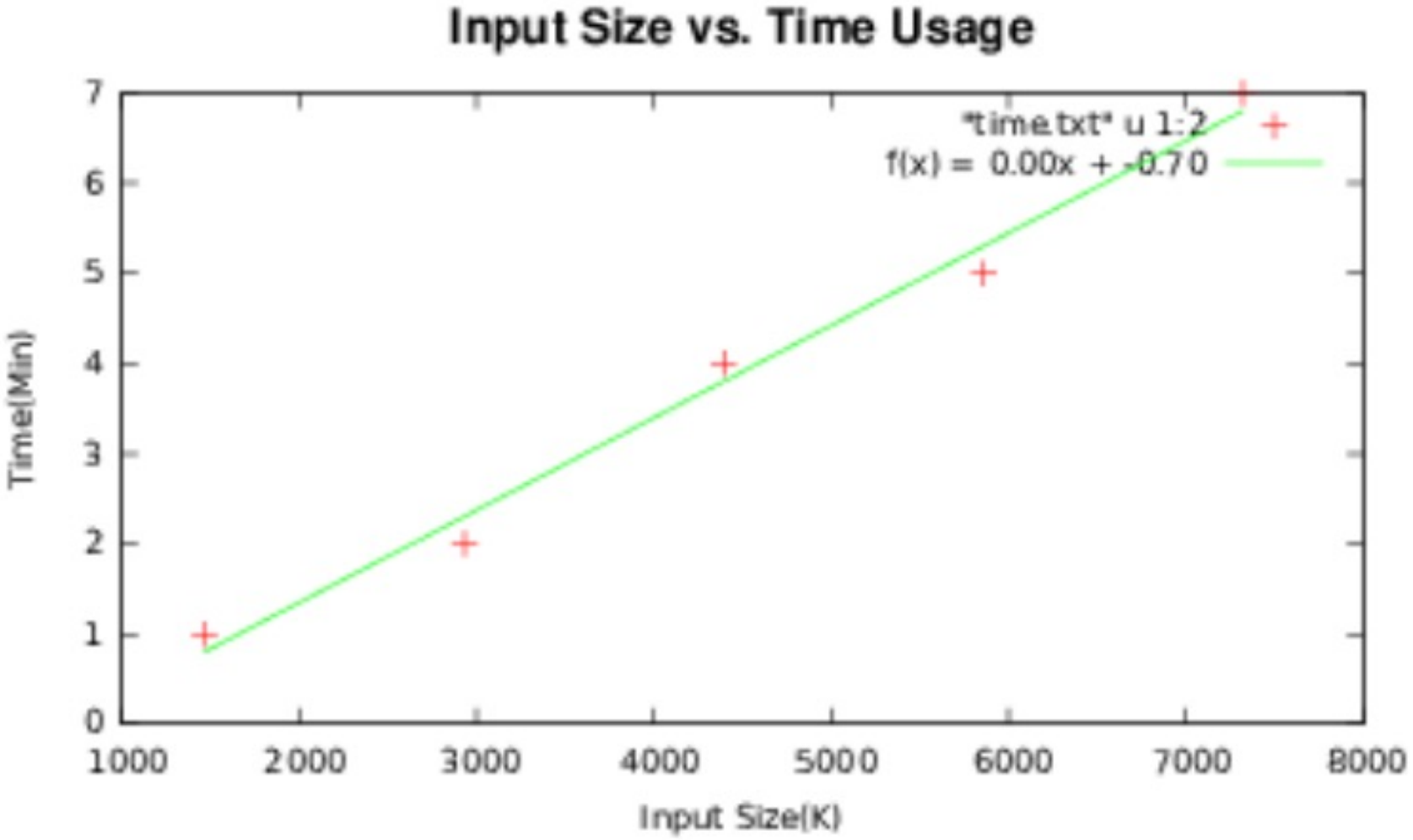
Jobs reserve excessive resources

- Jobs succeed
- Wasted resources unavailable to other users

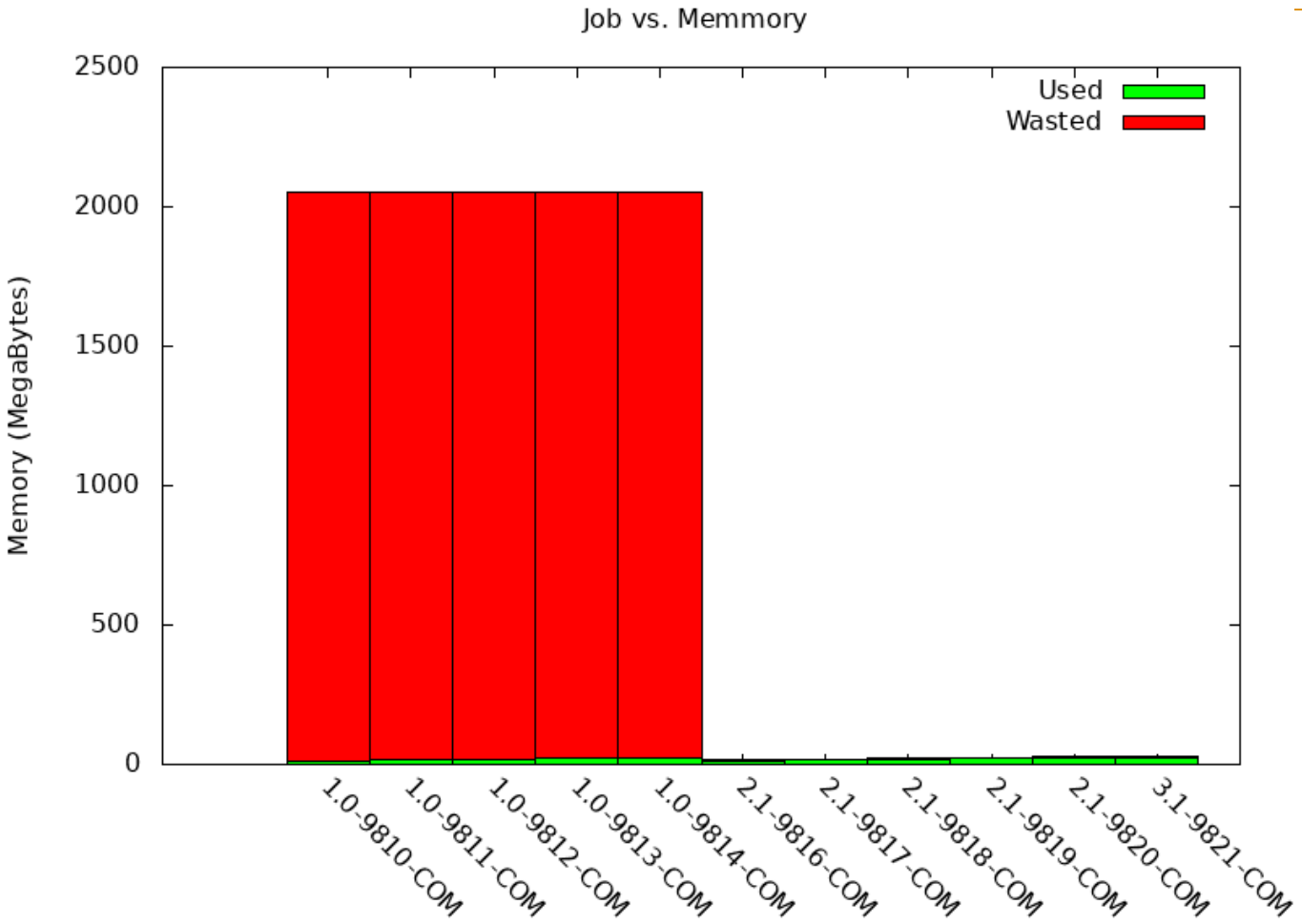
Jobs reserve insufficient resources

- Jobs fail
- Jobs must be manually rerun with more resources
- Wastes user time. Delays results

Ideal solution



Ideal solution

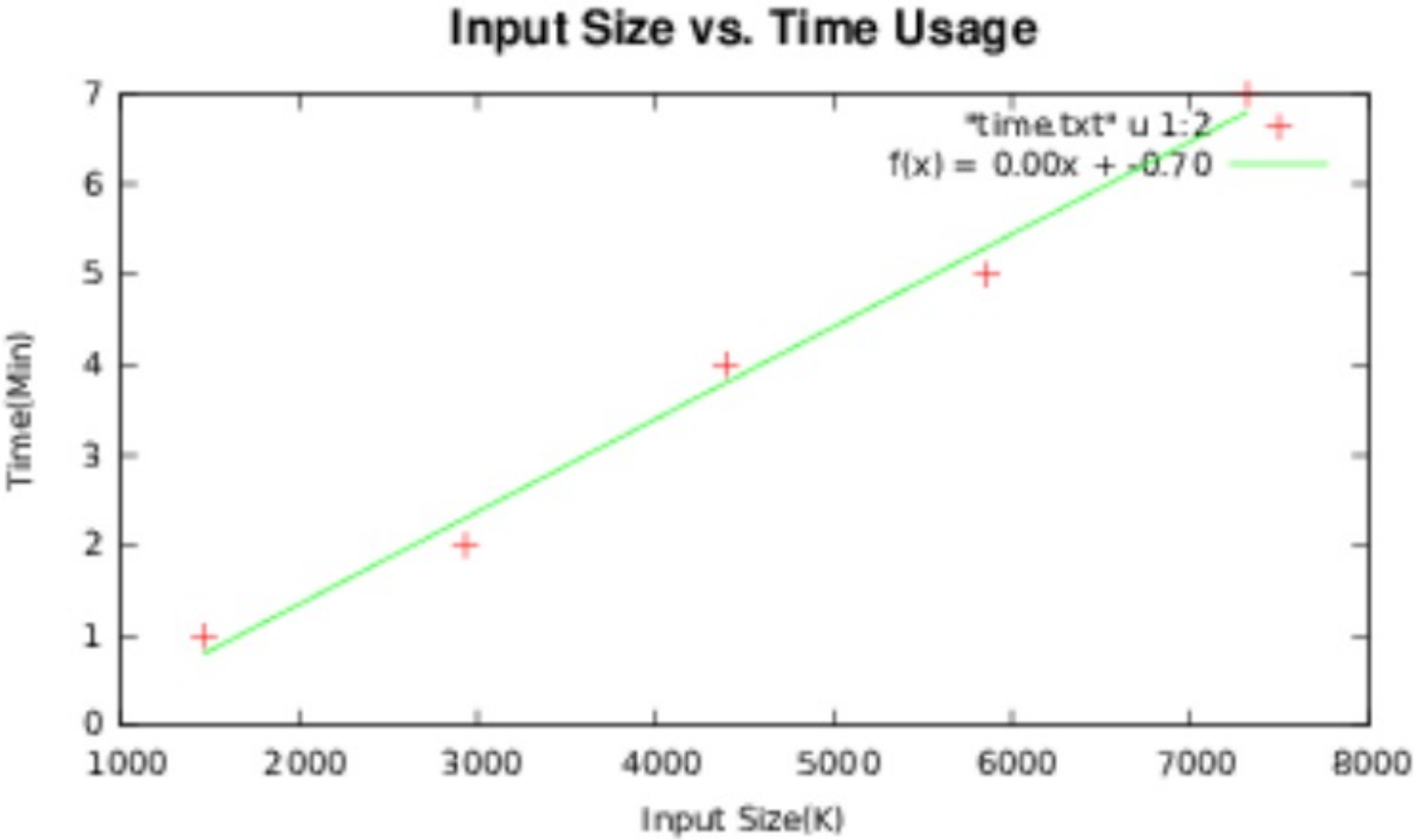


Smart Slurm

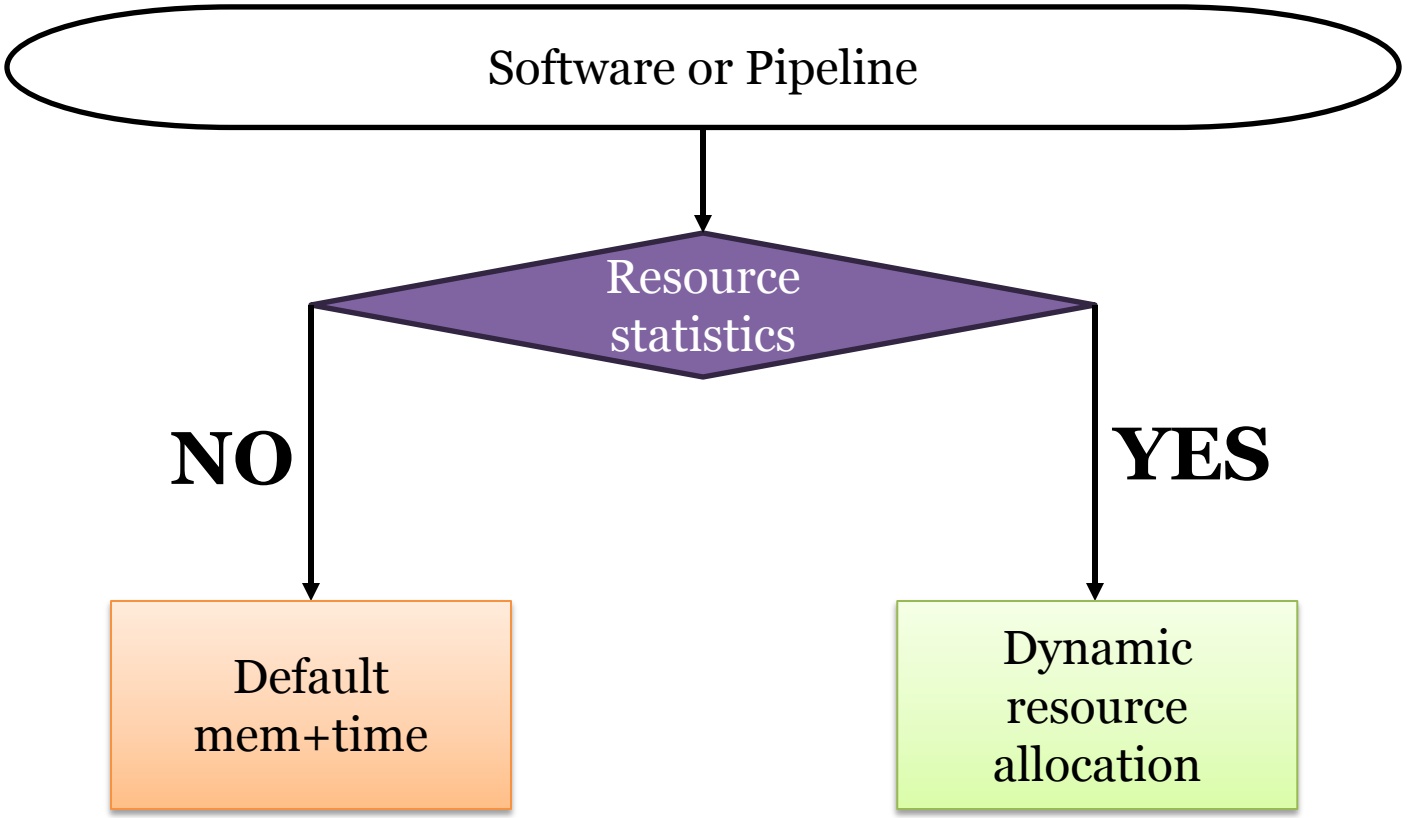
- ssbatch, which is a sbatch wrapper:
  - Check job was finished successfully or not
  - Estimate memory RAM and time based on several factors (i.e., program type, input size, previous job records)
  - Submit job
  - Monitor and log memory and time usage by the job
  - Re-run OOT/OOM job and send detailed email notifications
- runAsPipeline: It parses special bash script to find user defined commands and call ssbatch to submit jobs to Slurm. It take care of job dependency.

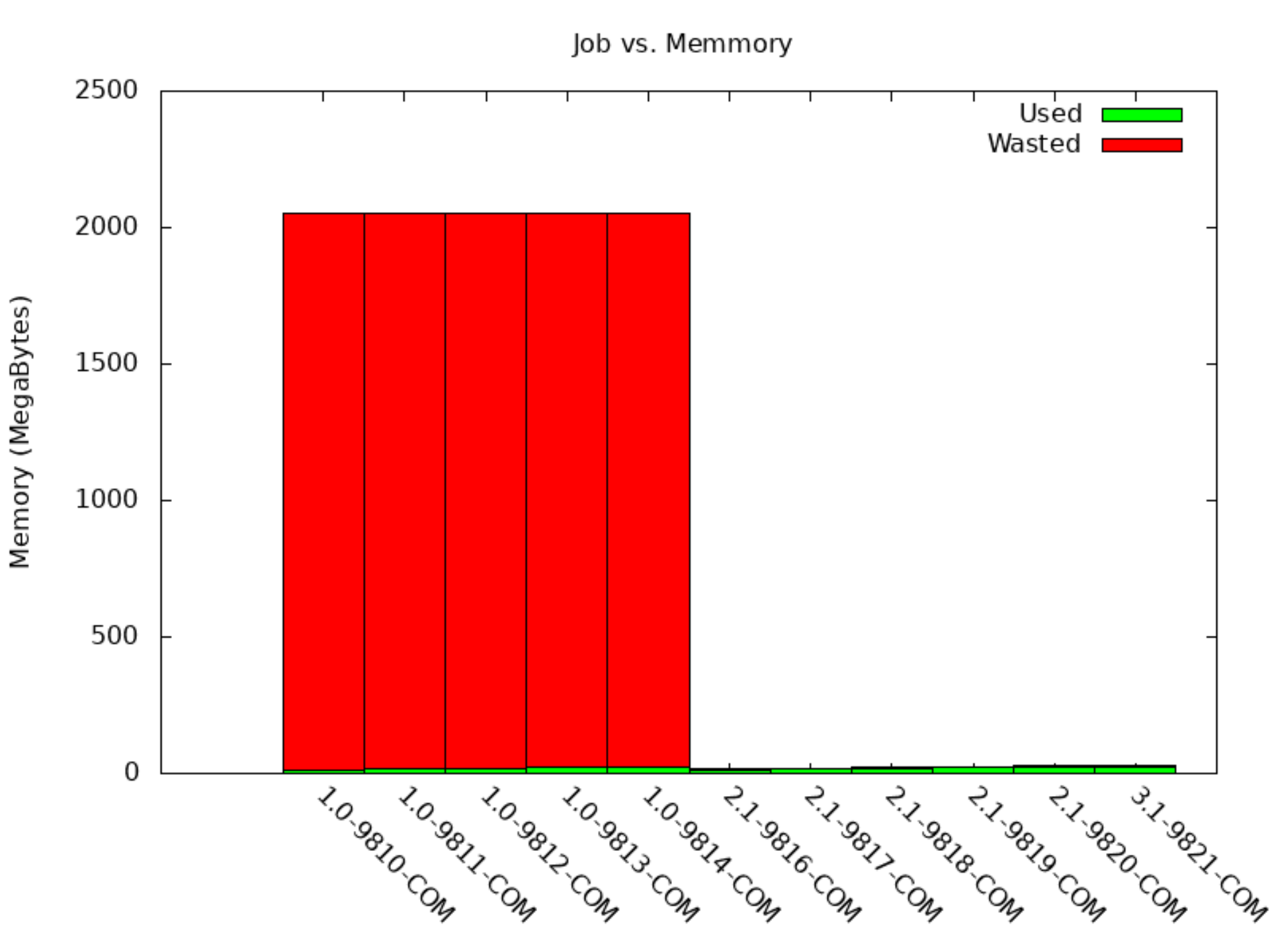
ssbatch

```
$ ssbatch           \
    -P program \
    -R reference   \
    -I input.txt     \
   -F uniqueJobFlag  \
    --mem 2G -t 2:0:0 -p short cmd
```


Input Size vs. Time Usage
"time.txt" u 1:2
f(x) = 0.00x + -0.70
Time(Min)
Input Size(K)
0
1
2
3
4
5
6
7
1000
2000
3000
4000
5000
6000
7000
8000

ssbatch logic




Job vs. Memmory
Memory (MegaBytes)
2500
2000
1500
1000
500
0
Used
Wasted
1.0-9810-COM
1.0-9811-COM
1.0-9812-COM
1.0-9813-COM
1.0-9814-COM
2.1-9816-COM
2.1-9817-COM
2.1-9818-COM
2.1-9819-COM
2.1-9820-COM
3.1-9821-COM

Inside each job

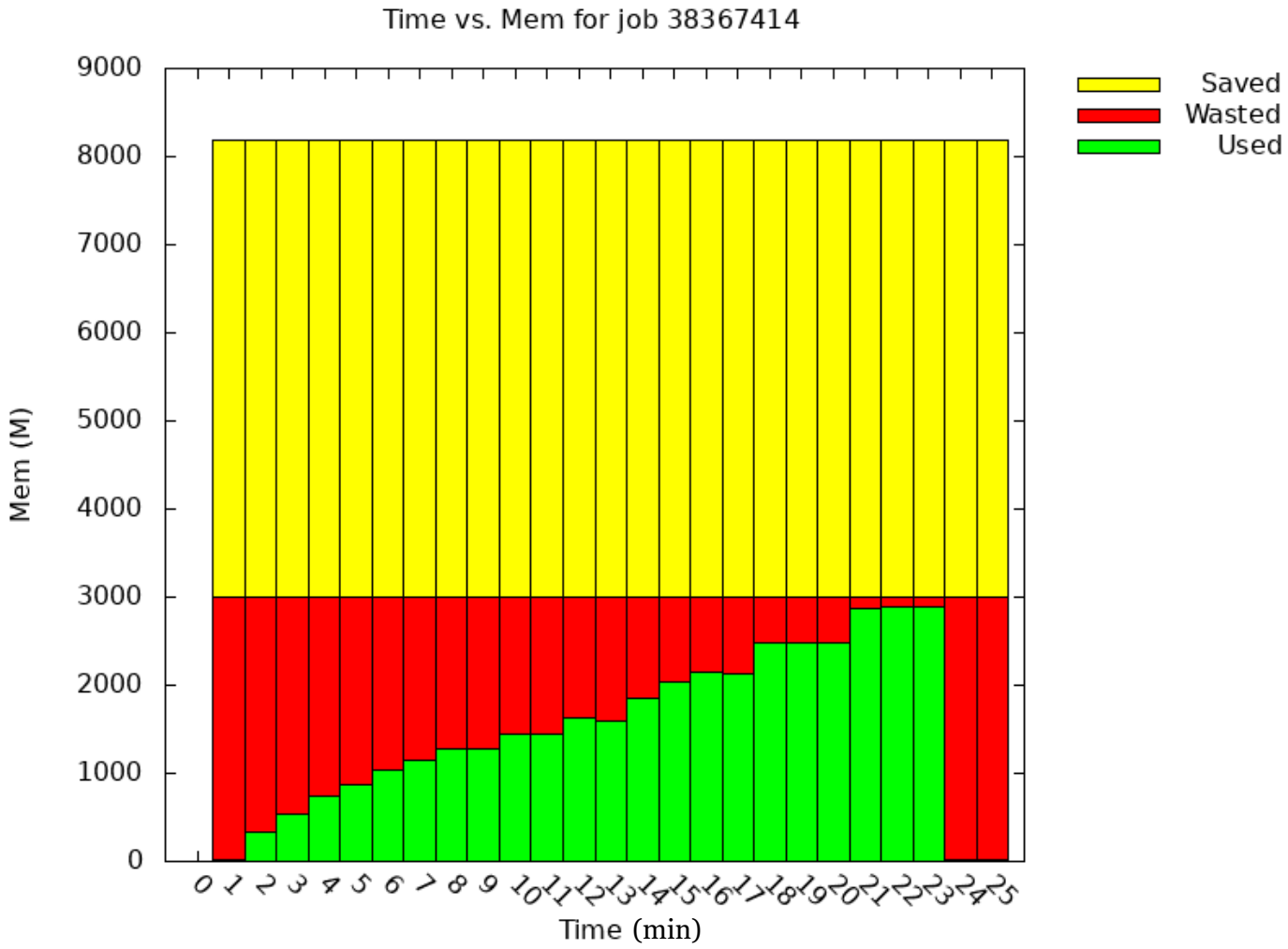
- Monitor real-time mem/CPU usage
- When job finishes, send email notification
- If job succeeds, keep a log of max mem and time
- Otherwise
  1. OOM ==> re-submit with more memory
  2. OOT ==> re-submit with more time
  3. Fail: save error message to output file
- Send user notification email
- Manage pending/downstream jobs

Scripts

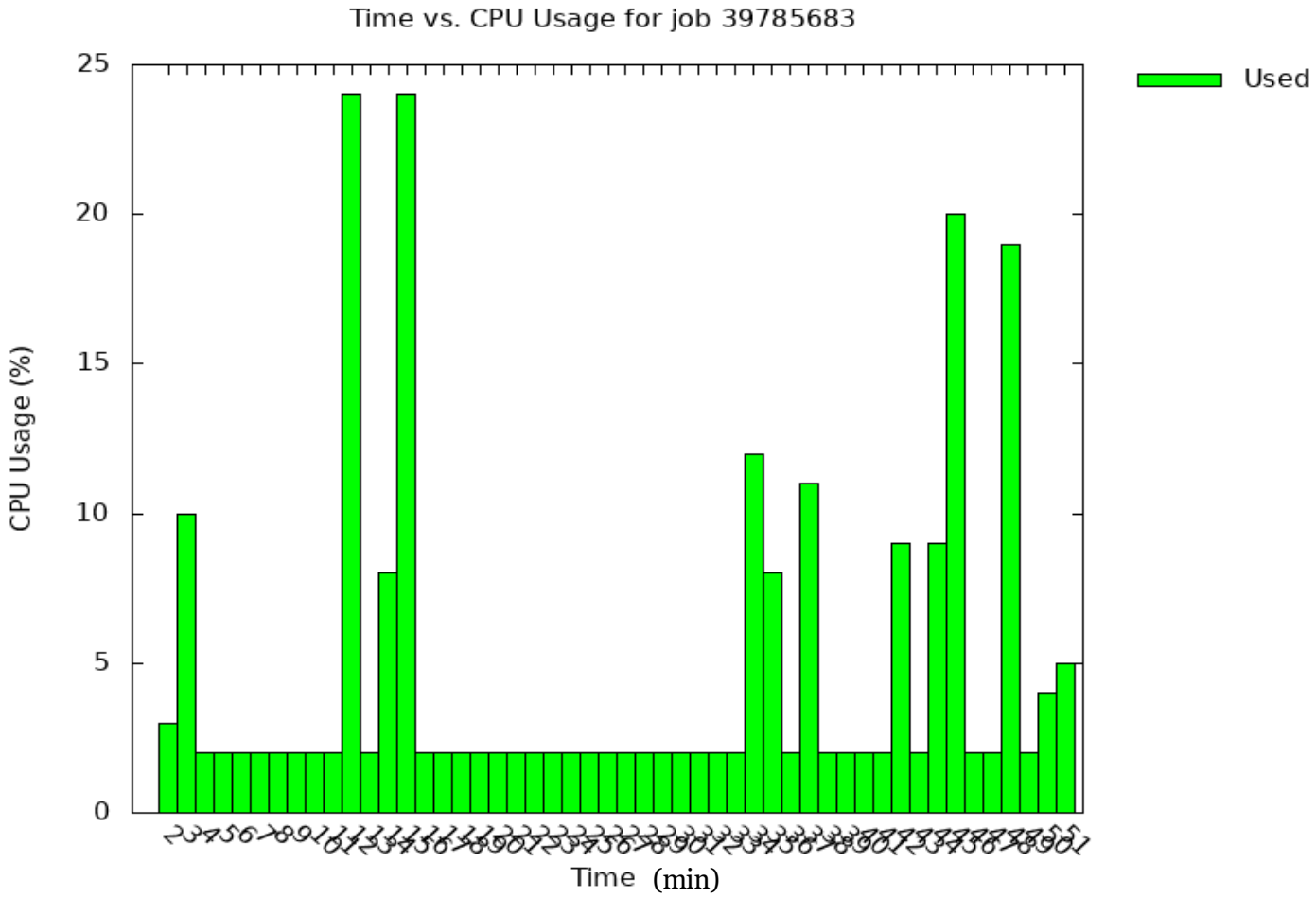
```
jid=$(checkIfItIsDone.sh &&   \
     estimateMemTime.sh &&   \
   sbatch -t $mT --mem $mMem \
      -o jobx.out -e jobx.err
      --wrap "monitorResource.sh & \
      someCmd && touch jobx.success;\
      cleanUp.sh;")
```

What the red scripts do?

Memory usage report



CPU usage report



Smart Slurm

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A simple pipeline in bash

```
$ cat bashScript.sh

for i in {1..5}; do

    input=numbers$i.txt

    grep 123 $input > number.$i.txt

Done

cat number.*.txt > all.txt

$ sbatch –mem 25G –t 20-0:0 bashScript.sh
```

Converting to Slurm pipeline

```
for i in {1..5}; do
    input=numbers$i.txt

   id=$(sbatch -p short -t 5 --wrap "grep 123 \
        $input > number$i.txt")
done

sbatch -p short -t 5 -d afterok:$id --wrap "cat \
       number.*.txt > all.txt"
```

Converting to Slurm pipeline

```
deps=afterok
for i in {1..5}; do
   input=numbers$i.txt

    id=$(sbatch -p short -t 5 --wrap "grep 123 \
        $input > number$i.txt")
   deps=$deps:$id
done

sbatch -p short -t 5 -d $deps --wrap "cat \
   number.*.txt > all.txt"
```

Can we automate it?

```
for i in {1..5}; do
   input=numbers$i.txt

   #@ Please submit as job with 1G memory,
   #@ with 5 minute and 1 CPU without pending.
   grep 123 $input > number.$i.txt

Done

#@ Please submit as job with 2G memory,
#@ with 5 minute and 1 CPU and wait for the other 5 jobs
cat number.*.txt > all.txt
```

Smart Slurm decorator syntax

```
#@1,0,find,none,input,sbatch -t 5 --mem 1G
find.sh 123 $input > number.$i.txt

#@    → This row is a decorator for runAsPipeline to parse
1     → Step ID

0     → The step IDs this step depends on
find   → Step name.

None   -> Reference
Input.  -> input for the step.

sbatch → default sbatch command to use
```

Can we automate it?

```
$ cat specialBashScript.sh

for i in {1..5}; do
   input=numbers$i.txt

   #@1,0,find,,input,sbatch -t 5 --mem 1G
   grep 123 $input > number.$i.txt

Done

#@2,1,merge
cat number.*.txt > all.txt
```

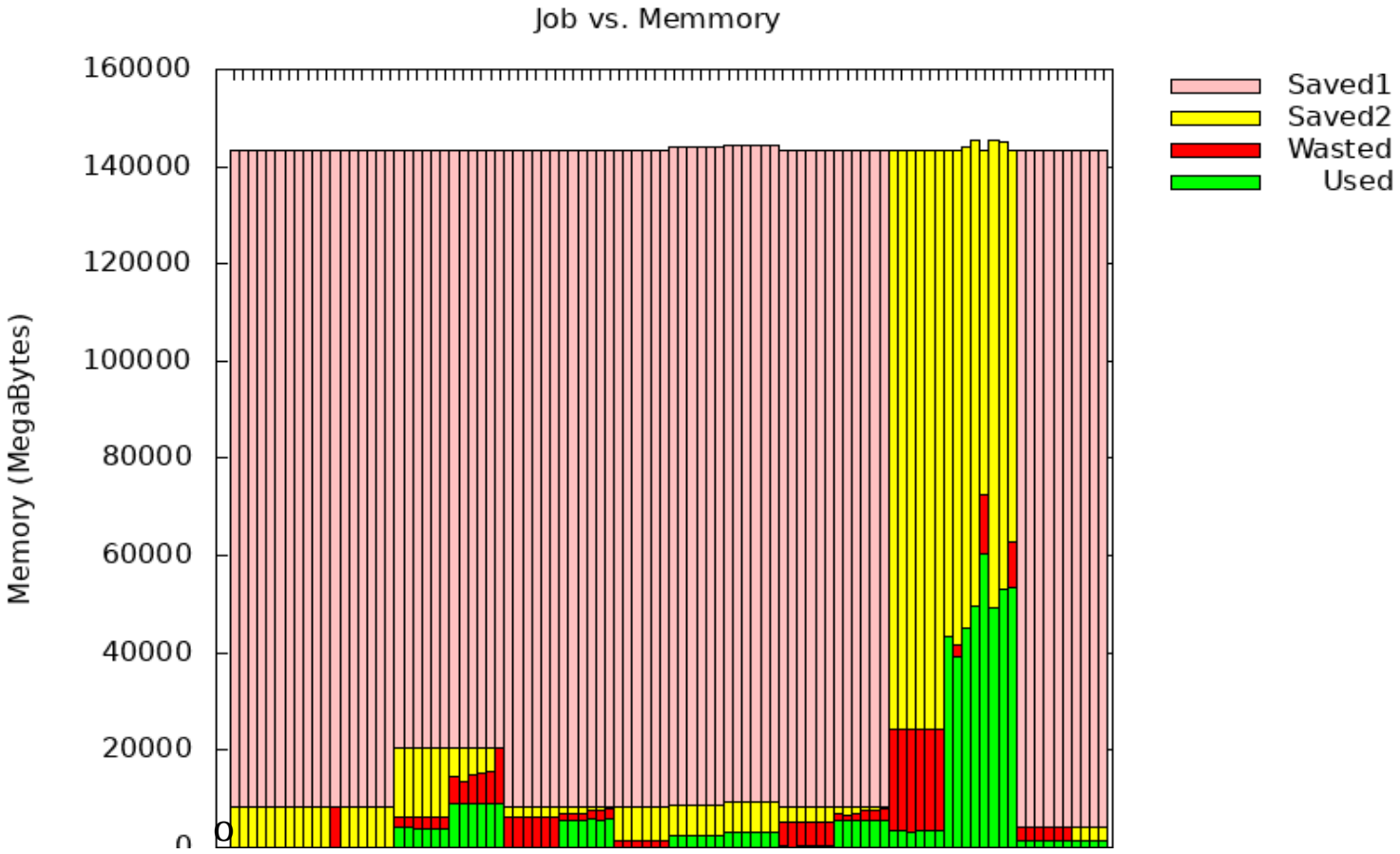
runAsPipeline

```
$ runAsPipeline                    \
specialBashScript.sh               \
“sbatch --mem 2G -t 2:0:0” \
useTmp/noTmp [run]
```

Other tools

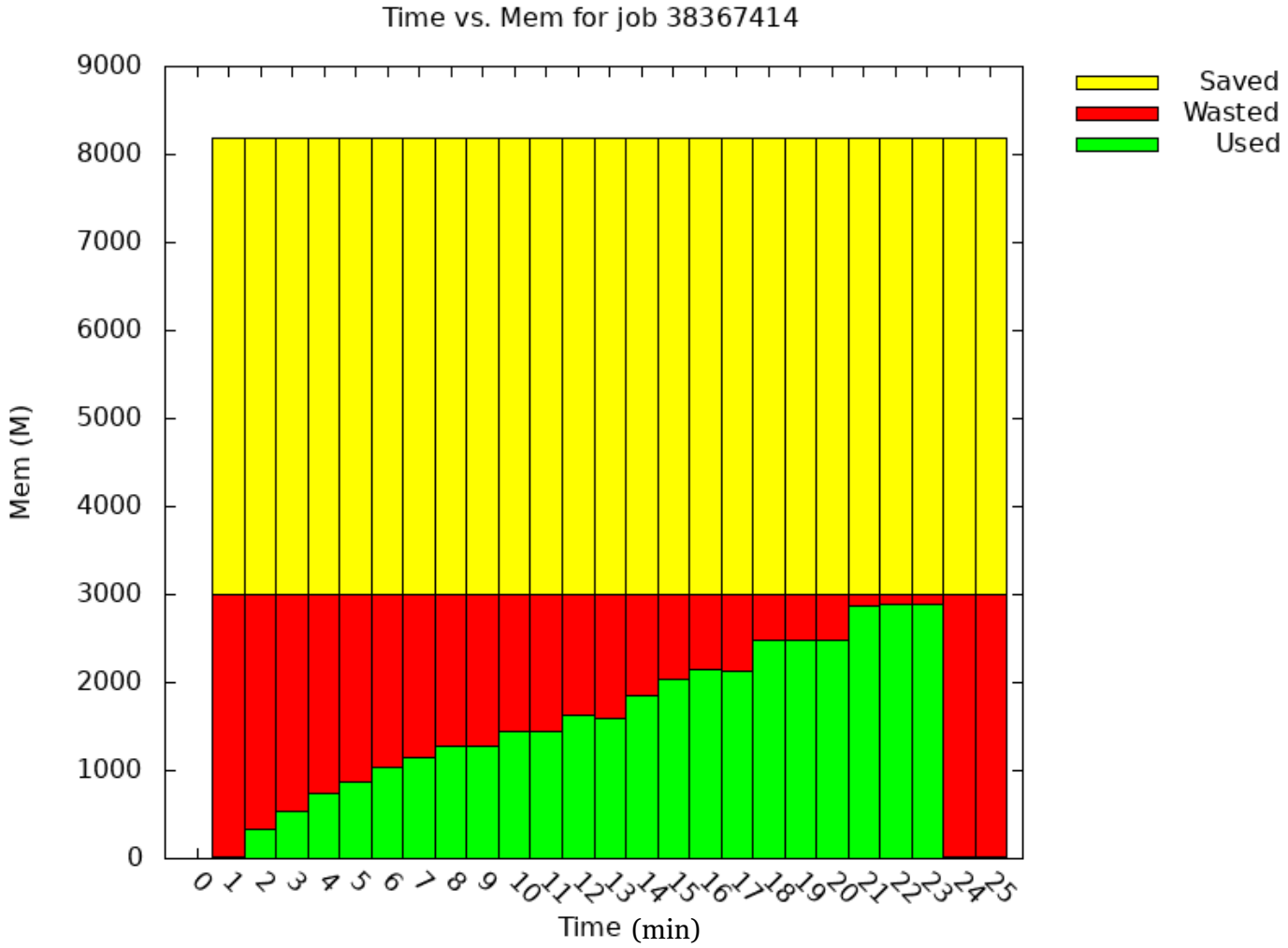
```
$ checkRun
Available log folders or log file:
1 folder: log
2 file:   .smartSlurm.log
3 folder: log.2024-05-30.10-06-18
4 file:   .smartSlurm.log.2024-05-30.10-06-15
Please select the log or folder you want to
check or type q to quit:


$ cancelAllJobs
```

Case study(Nascent Transcriptomics Core @ HMS)

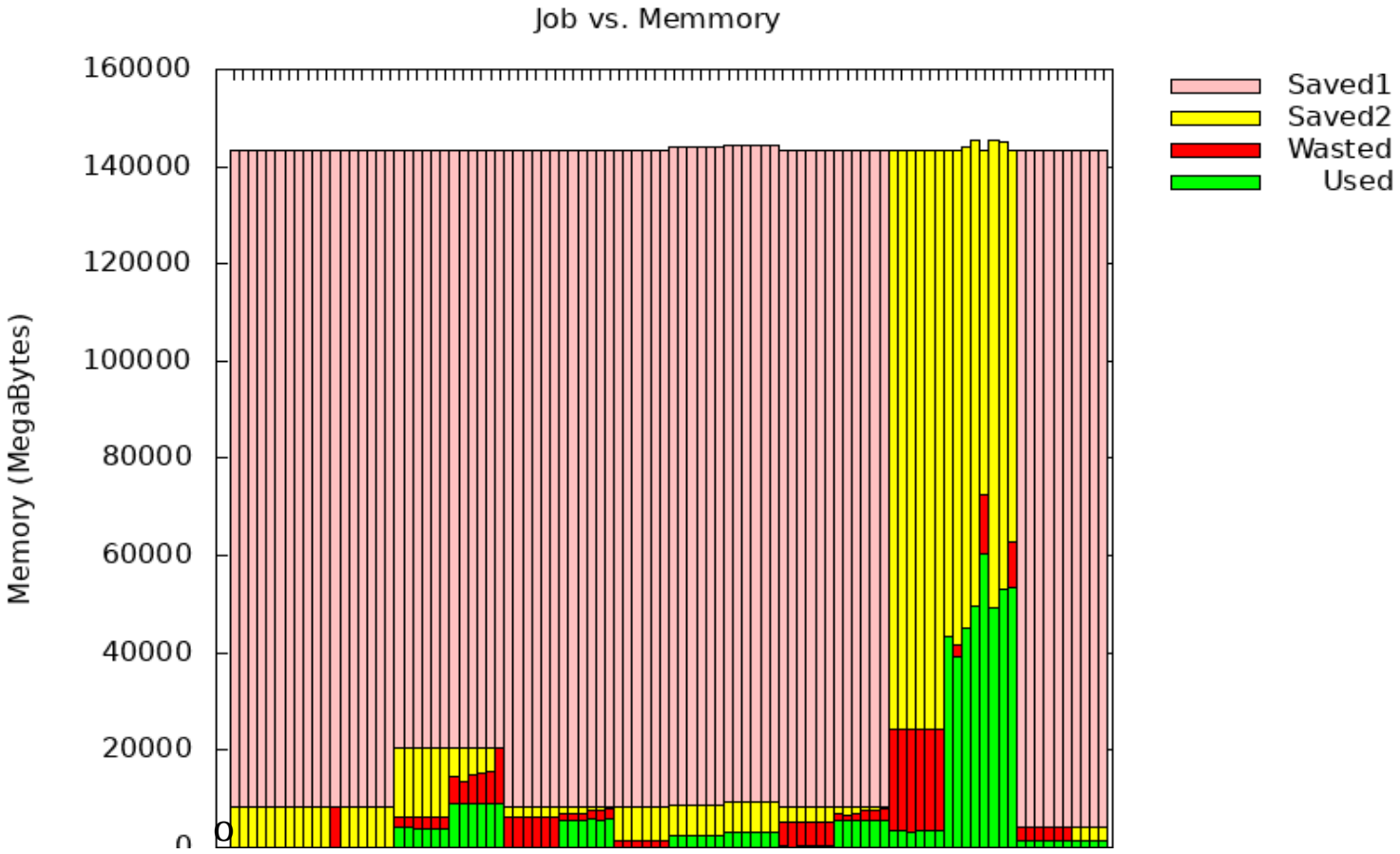


Jobs (each bar is a job)

Future 1: Breakpoint support



Future 2: Auto split workflow



Jobs (each bar is a job)

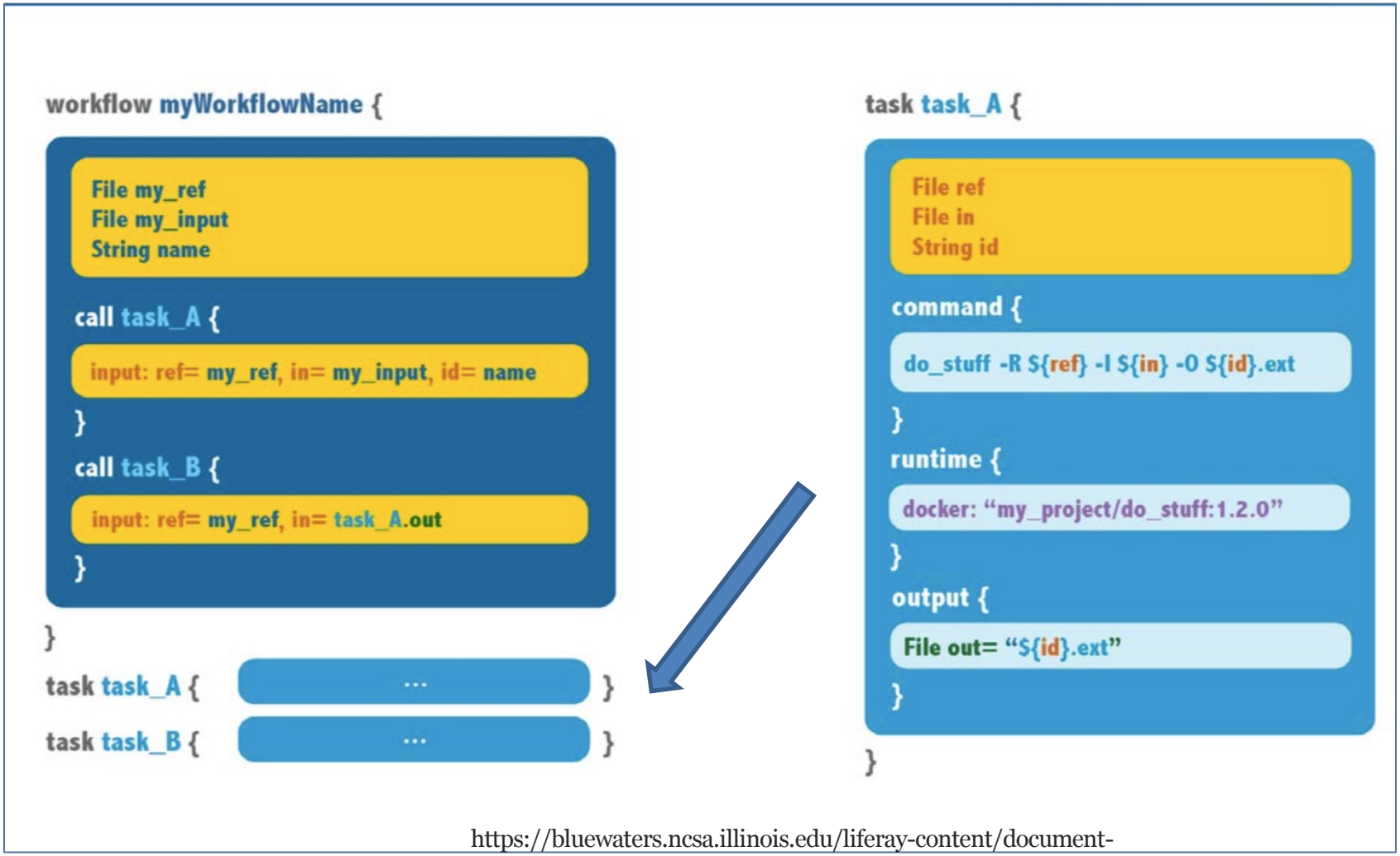
How do I access Smart Slurm?

- https://github.com/ld32/SmartSlurm

- Git clone https://github.com/ld32/smartSlurm

- `export PATH=$PWD/SmartSlurm/bin:$PATH`

Solution 1: Cromwell using 'CWL' file



https://bluewaters.ncsa.illinois.edu/liferay-content/document-library/content/Ruchi%20Munshi.%20Blue%20Waters%20webinar.%20Cromwell%20and%20WDL.pdf

Solution 2: BCBio using 'yaml/CWL' file

```
upload:
  dir: ../final
details:
  - files: [../input/NA12878-NGv3-LAB1360-A_1.fastq.gz, ..
    description: NA12878
    metadata:
      sex: female
    analysis: variant2
    genome_build: hg38
    algorithm:
      aligner: bwa
      variantcaller: gatk-haplotype
      validate: giab-NA12878/truth_small_variants.vcf.gz
      validate_regions: giab-NA12878/truth_regions.bed
      variant_regions: capture_regions/Exome-NGv3
```

bcbio_nextgen.py config/NA12878-exome-methodcmp.yaml -n 8

https://bcbio-nextgen.readthedocs.io/en/latest/contents/intro.html#workflow

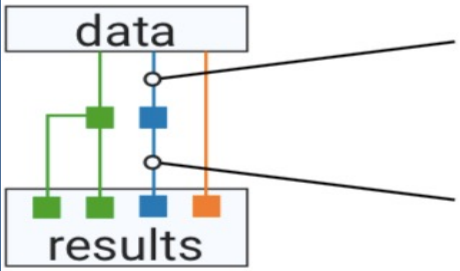
Solution 3: NextFlow script

```
#!/usr/bin/env nextflow

params.in = "$baseDir/data/sample.fa"

/*
 * split a fasta file in multiple files
 */
process splitSequences {

    input:
    path 'input.fa' from params.in

    output:
    path 'seq_*' into records

    """
    awk '/^>/{f="seq_"++d} {print > f}' < input.fa
    """
}
```

https://www.nextflow.io/example1.html

Solution 4: Snakemake using makefile

Dependencies are implicit and 'backwards'




```
rule a:
    input: "start/{sample}.txt"
    output: "mid/{sample}.txt"
    shell: "sort {input} > {output}"
rule b:
    input: "mid/{sample}.txt"
    output: "final/{ABC}.summary"
    shell: "uniq -c {input} > {output}"
```

```
$ snakemake final/ABC.summary
```

https://hpc.nih.gov/training/handouts/180221_snakemake_class_web.pdf

For more direction

- **Email:** rchelp@hms.harvard.edu
- **O2 wiki**: https://harvardmed.atlassian.net/wiki/spaces/O2/overview
- **Website**: http://rc.hms.harvard.edu
- **RC Office Hours**: Wed 1-3p Gordon Hall 500
  - https://rc.hms.harvard.edu/office-hours/ for Zoom web conferencing during remote work