Open Science Grid

Getting the Most out of HTC with Workflows

Friday

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Why are we here?

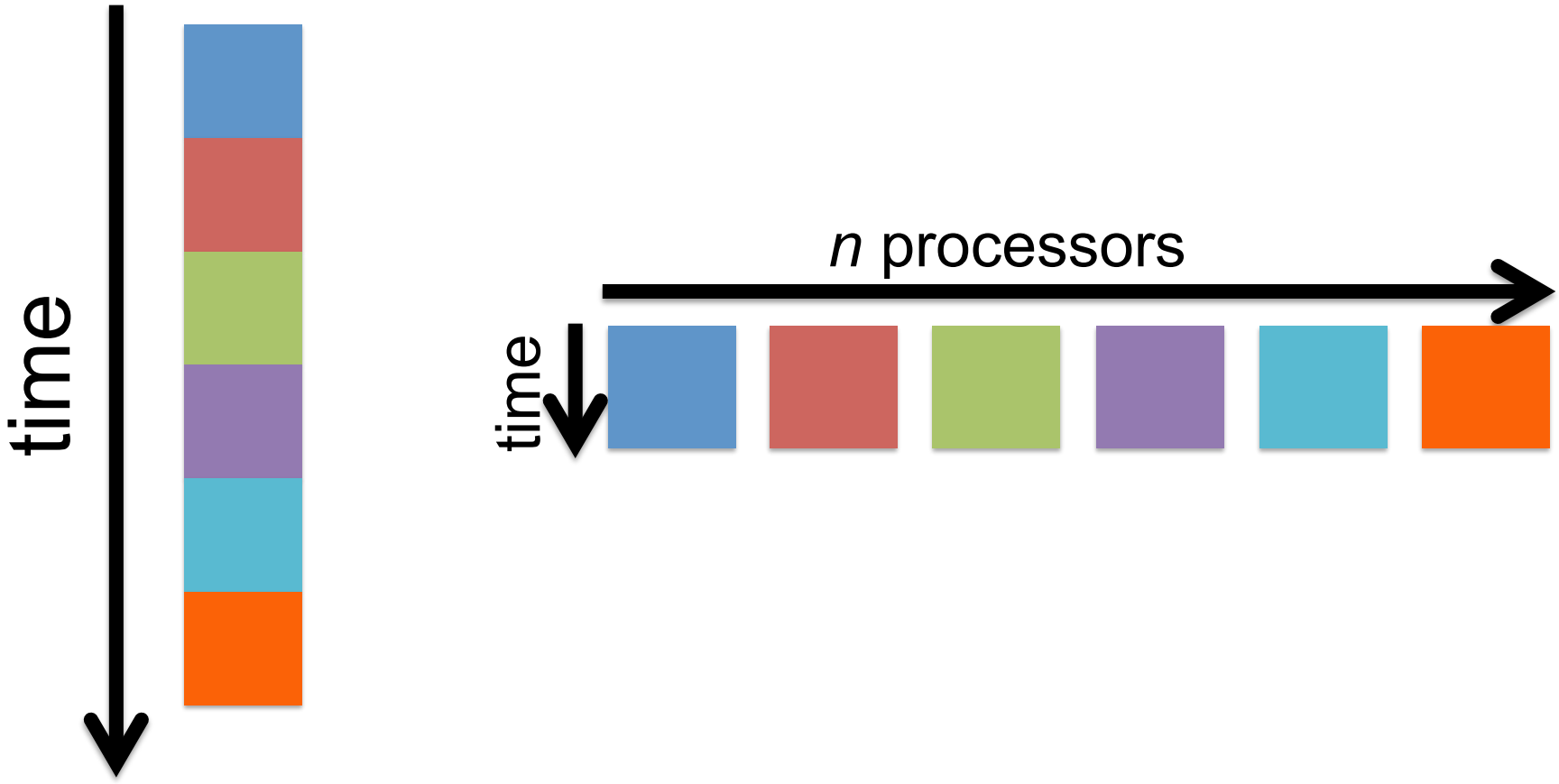
Why are we here?

To do SCIENCE!!!

- A lot of science is best-done with computing – sometimes, LOTS of computing
- Science needs to be reproducible
- And, we'd really like science to happen FAST(er)

HTC Payoffs

For science with *MANY* independent calculations…



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Focus on Throughput

What is *throughput* in computing?

- time from *submission* to *overall completion*

What is *High Throughput* Computing?

- many 'smaller' independent tasks
- optimizing time-to-completion
  - including automation of HTC and non-HTC steps within an overall "*workflow*"

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What is not HTC?

- fewer numbers of jobs
- jobs individually requiring significant resources
  - RAM, Data/Disk, # CPUs, time

  (though, “significant” depends on the HTC compute system you use)
- restrictive licensing

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Typical HTC Problems

- batches of similar program runs (>10)
- “loops” over independent tasks
- others you might not think of …
  - programs/functions that
    - process files that are already separate
    - process columns or rows, separately
    - iterate over a parameter space
  - *a lot* or programs/functions that use multiple CPUs on the same server

Ultimately: Can you break it up?

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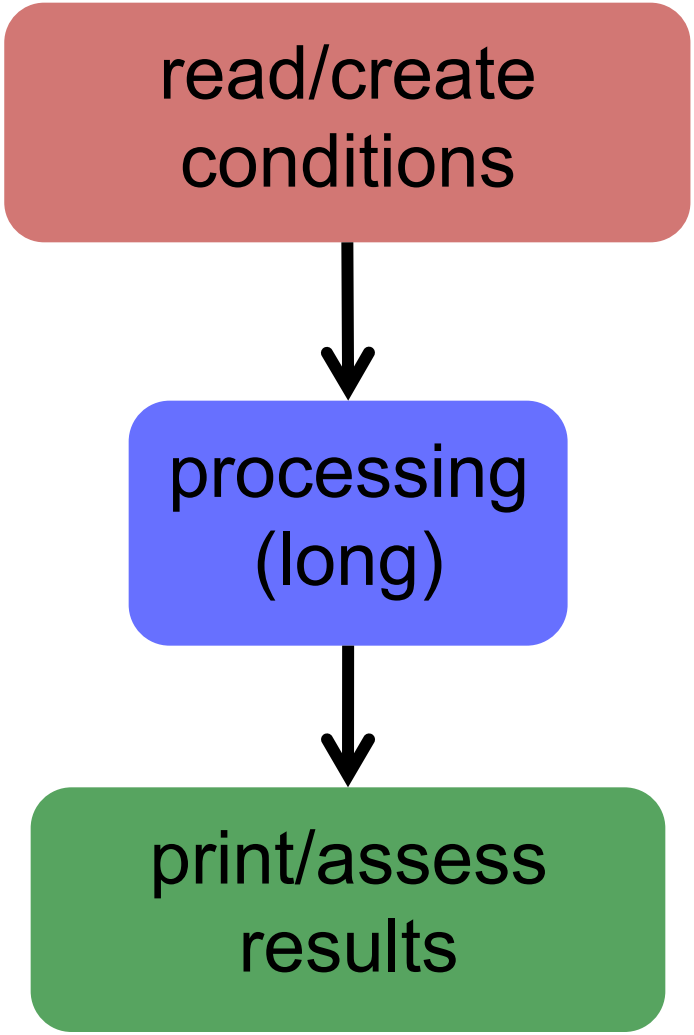
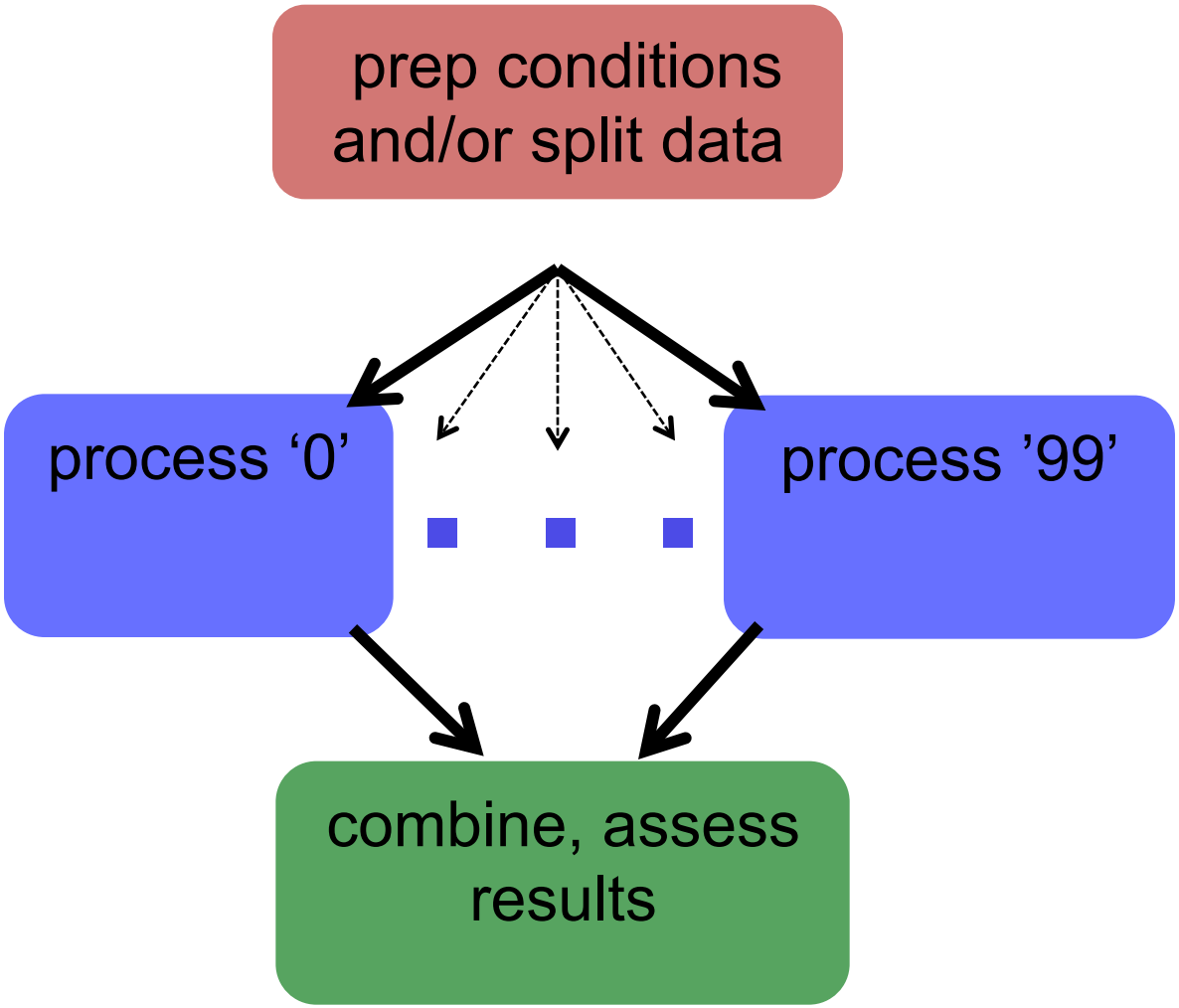
Many programs



with HTC!


prep conditions
and/or split data
process ‘0’
process ’99’
combine, assess
results

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Key HTC Tactics

1. Increase Overall Throughput
2. Utilize Resources Efficiently!
3. Bring Dependencies With You
4. Automate As Many Steps As Possible
5. Scale Gradually, Testing Generously

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Know and Optimize Job Use of Resources!

- **CPUs** ("1" is best for matching; essential for OSG)
  - restrict, if necessary/possible
  - software that uses all available CPUs is BAD!
- **CPU Time**

  > ~5 min, < ~1 day; **Ideal: 1-2 hours**
- **RAM** (not always easily modified)
- **Disk** per-job (execute) and in-total (submit)
- **Network Bandwidth**
  - minimize transfer: filter/trim/delete, compress

The job log shows all

```
005 (2576205.000.000) 06/07 14:12:55 Job terminated.
        (1) Normal termination (return value 0)
                Usr 0 00:00:00, Sys 0 00:00:00  -  Run Remote Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Run Local Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Total Remote Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Total Local Usage
        5  -  Run Bytes Sent By Job
        104857640  -  Run Bytes Received By Job
        5  -  Total Bytes Sent By Job
        104857640  -  Total Bytes Received By Job
        Partitionable Resources :    Usage  Request Allocated
           Cpus                 :                1         1
           Disk (KB)            :   122358   125000  13869733
           Memory (MB)          :       30      100       100
```

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Breaking up is hard to do…

- Ideally into parallel (separate) jobs
  - reduced job requirements = more matches
  - not always easy or possible
- Strategies
  - break HTC-able steps out of a single program
  - break up loops
  - break up input
- Self-checkpointing if jobs are too long

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Batching (Merging) is easy

- A single job can
  - execute multiple independent tasks
  - execute multiple short, sequential steps
  - avoid transfer of intermediate files
- Use scripts!
  - need adequate error reporting for each "step"
  - easily handle multiple commands and arguments

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Bring *What* with You?

- Software (that was Wednesday)
- Parameters and random numbers
  - create a single, standard executable, responsive to:
    - arguments
    - input files (better)
  - generate and record ahead of time
    - reproducibility!
    - perhaps in an earlier DAG job
- What else?

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Wrapper Scripts are Essential

- Before task execution (bring it with you!)
  - transfer/prepare files and directories
  - setup/configure software environment and other dependencies
- Task execution
  - prepare complex commands and arguments
  - batch together many ‘small’ tasks
- After task execution
  - filter/combine/compress files and directories
  - check for and report on errors

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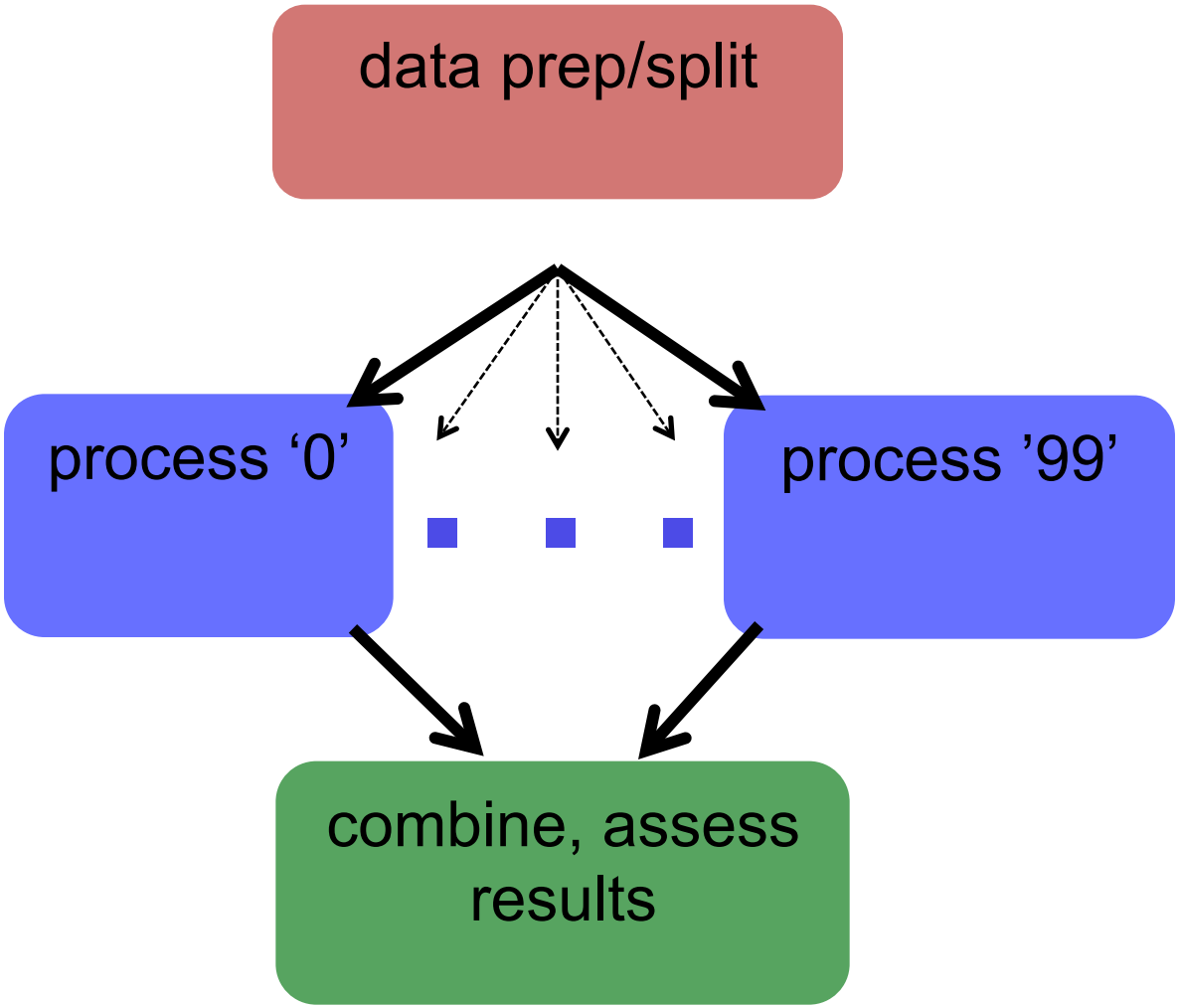
DAGs Automate Workflows!



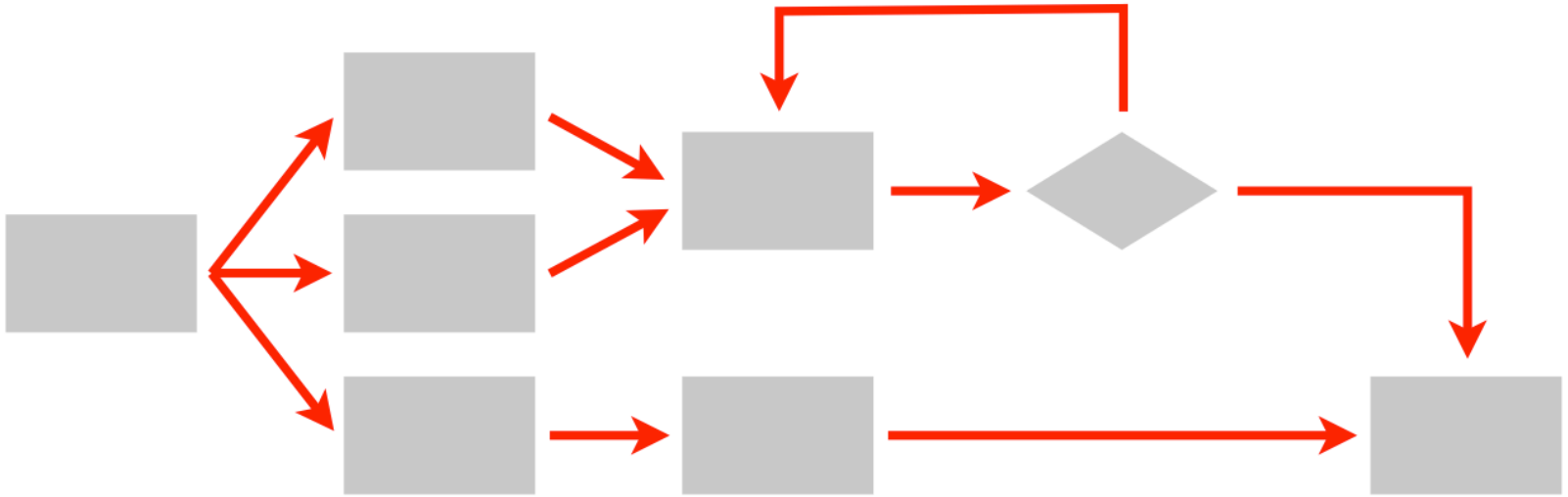
Workflows *Should* Make ~~Life~~ Science Easier

- non-computing "workflows" are all around you … especially in science
  - instrument setup
  - experimental procedures

- when planned/documented, workflows help with:
  - organizing and managing processes
  - saving time with **automation**
  - objectivity, reliability, and reproducibility (THE TENENTS OF GOOD SCIENCE!)

Workflows are like Computing Algorithms

- Steps
- Connections
- (Metadata)



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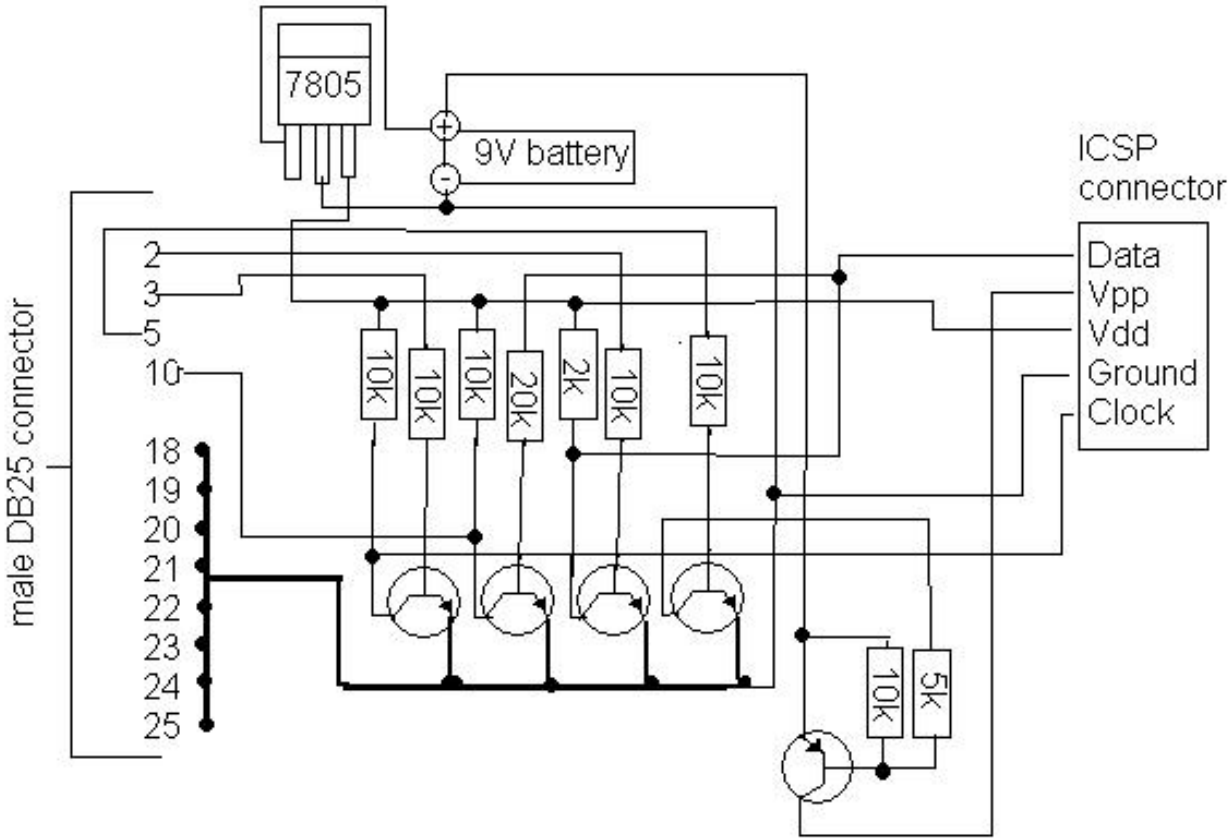
Building a Good Workflow

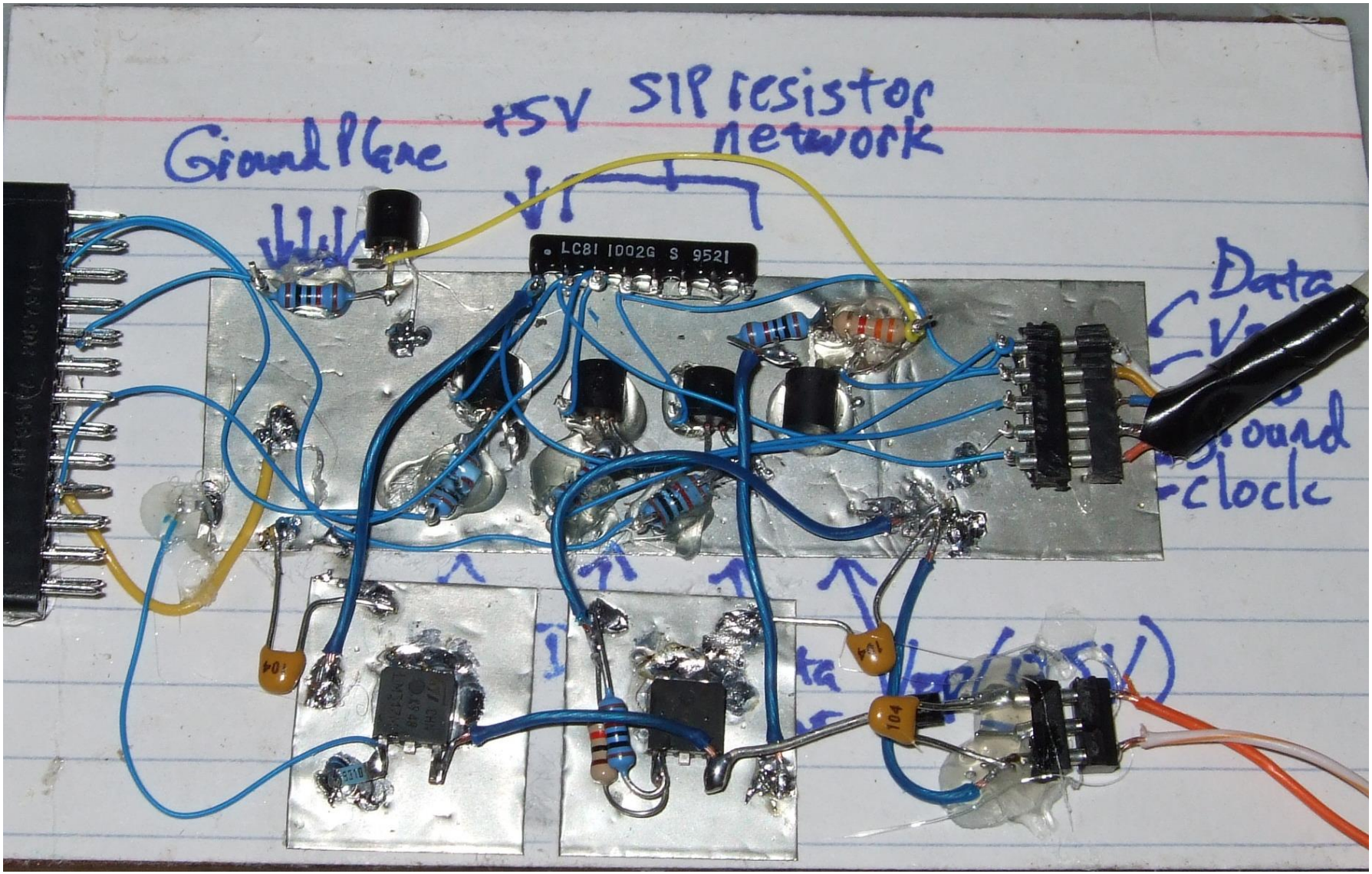
1. Draw out the *general* workflow
2. Define details (test 'pieces' with HTCondor jobs)
   - divide or consolidate 'pieces'
   - determine resource requirements
   - identify steps to be automated or checked
3. Build it modularly; test and optimize
4. Scale-up gradually
5. What more can you automate or error-check?

(And remember to document!)

From schematics…



… to the real world



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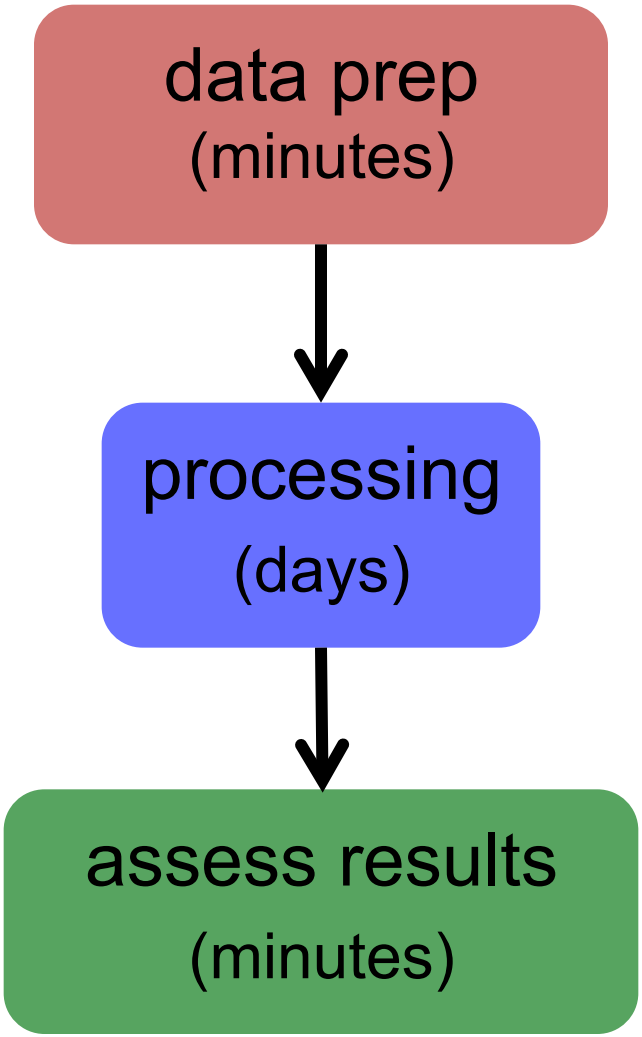
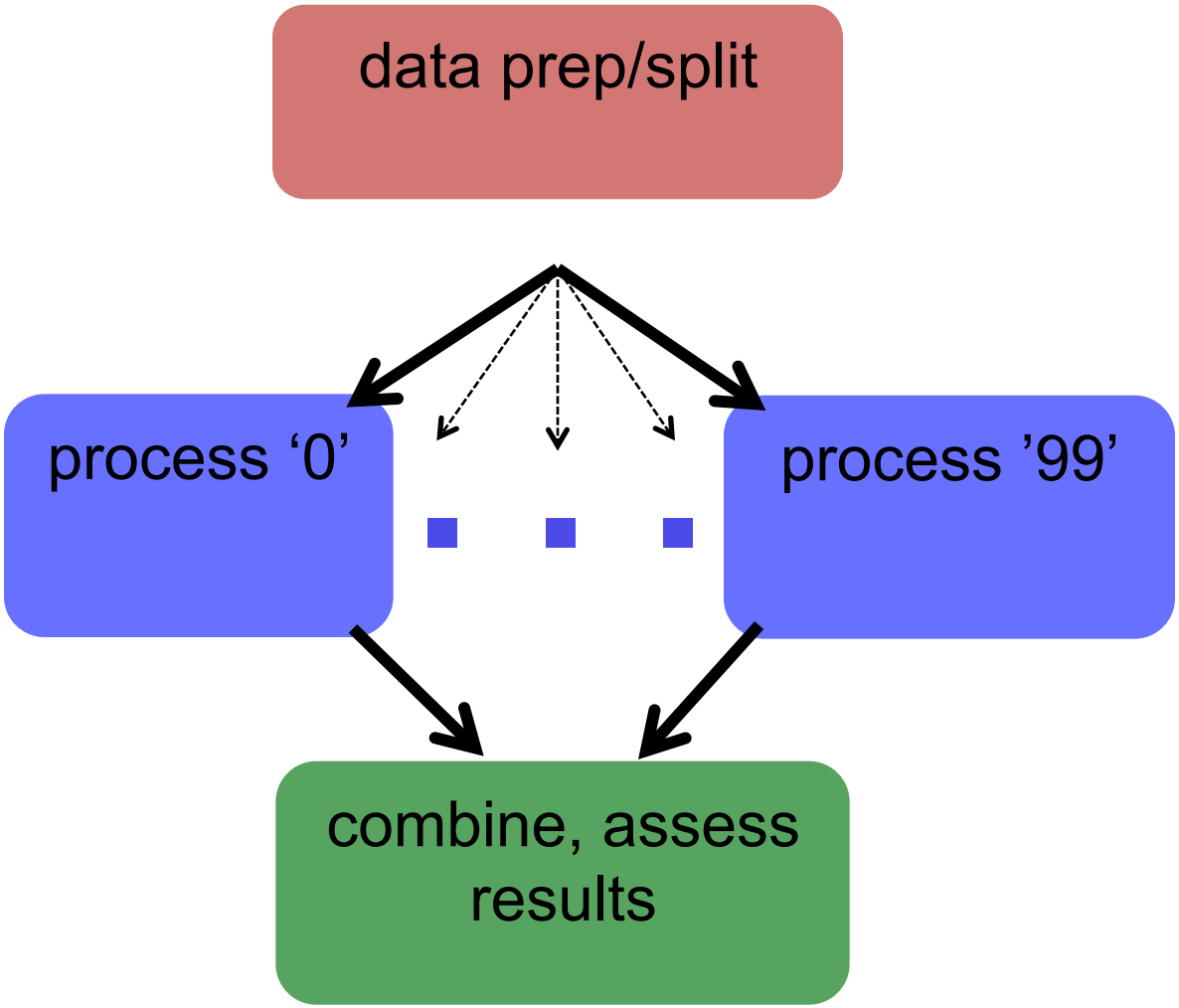
Start with This



Parallelize with HTC Splitting



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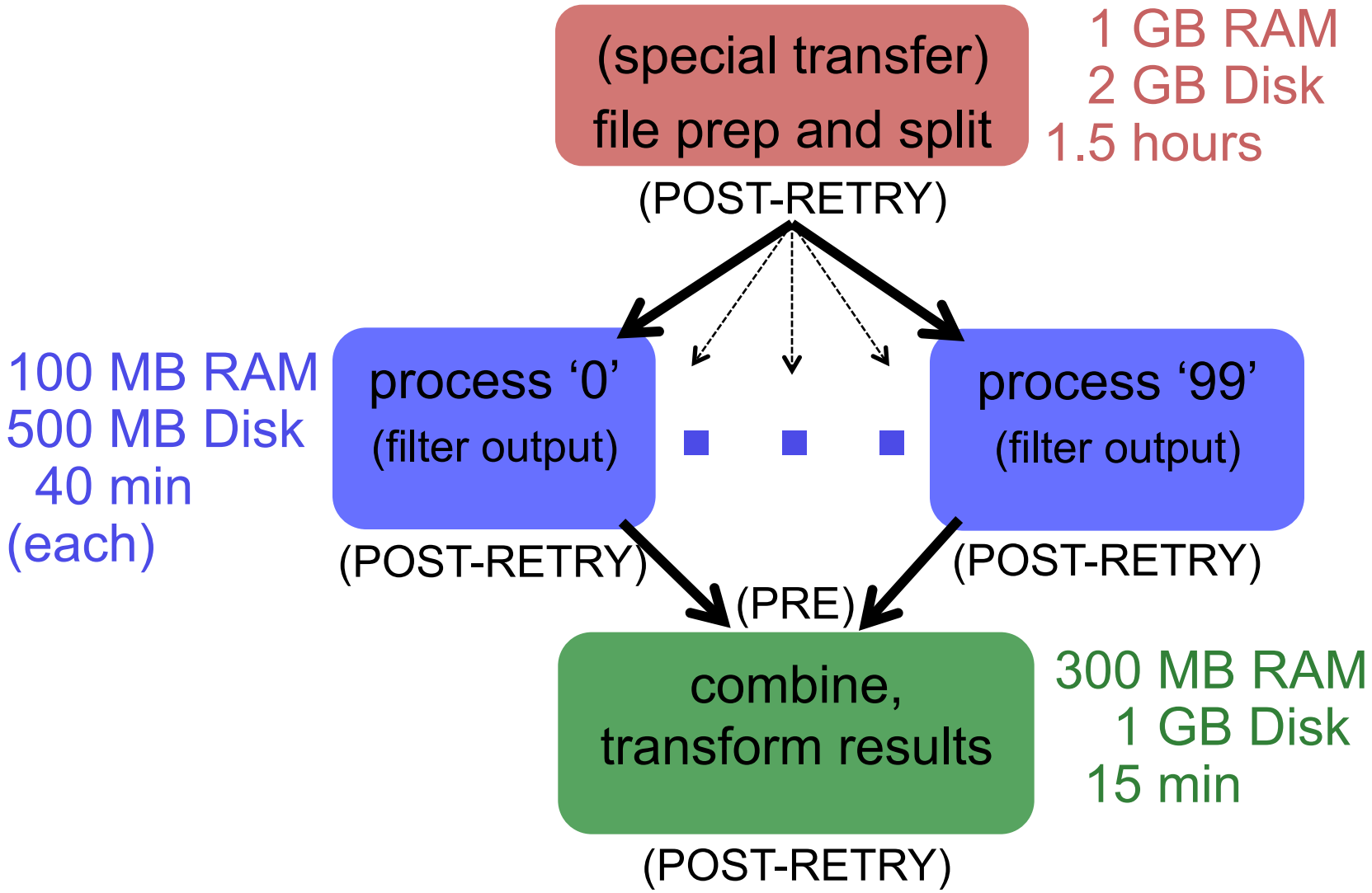
Determine Resource Usage

- Run locally first
- Then get one job running remotely
  - (on execute machine, not submit machine)!
  - get the logistics correct! (HTCondor submission, file and software setup, etc.)
- Once working, run a couple of times
  - If big variance in resource needs, should you take the…

    Average? Median? Worst case?

End Up with This



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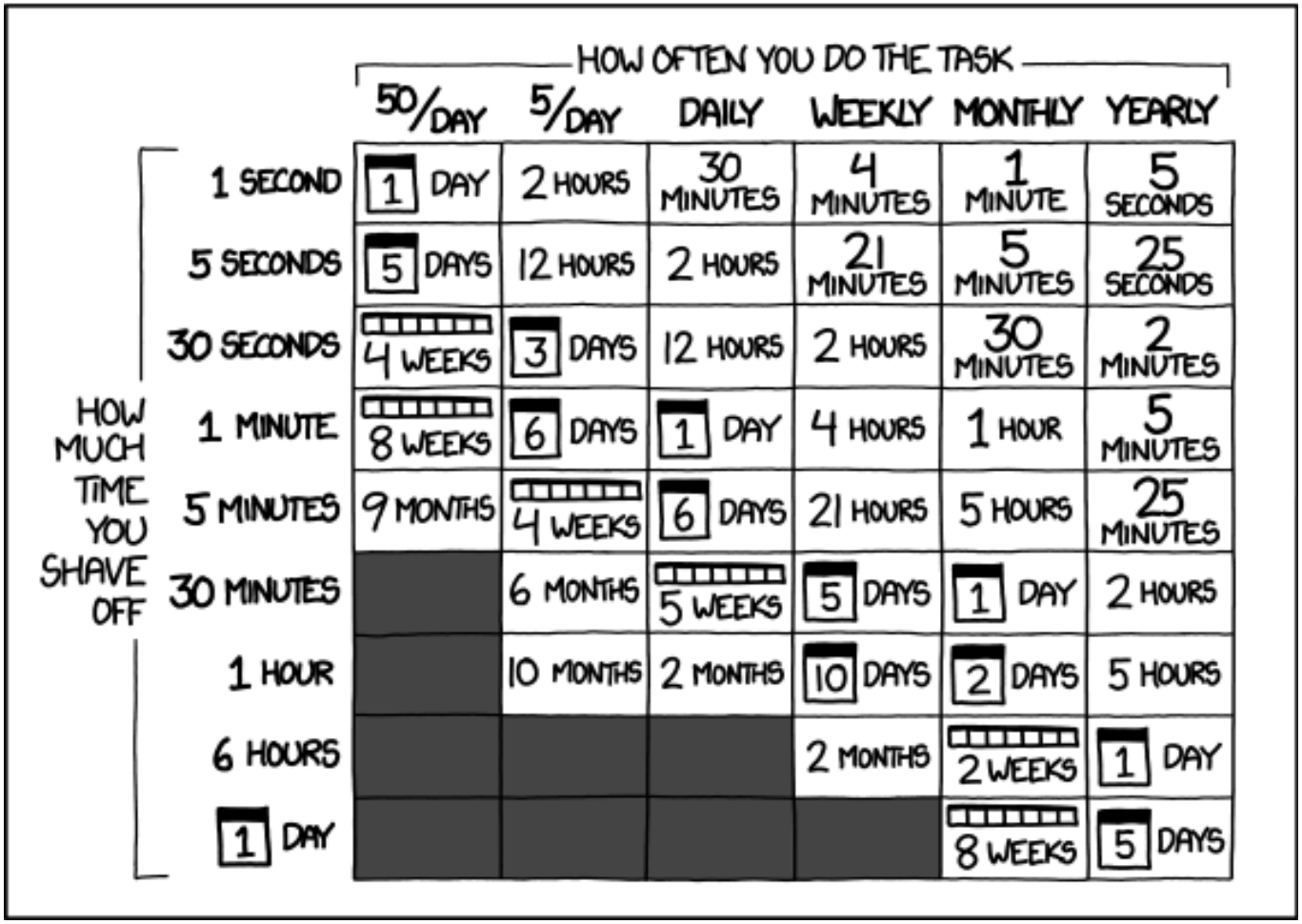
Automation Trade-offs!

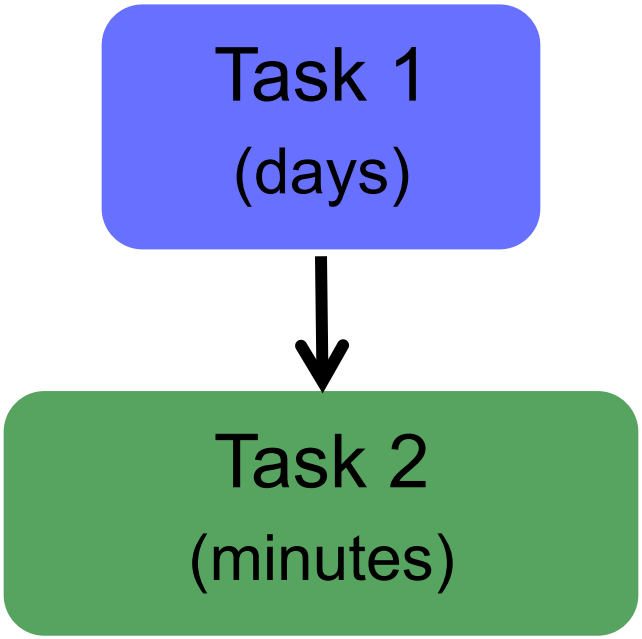


http://xkcd.com/1205/

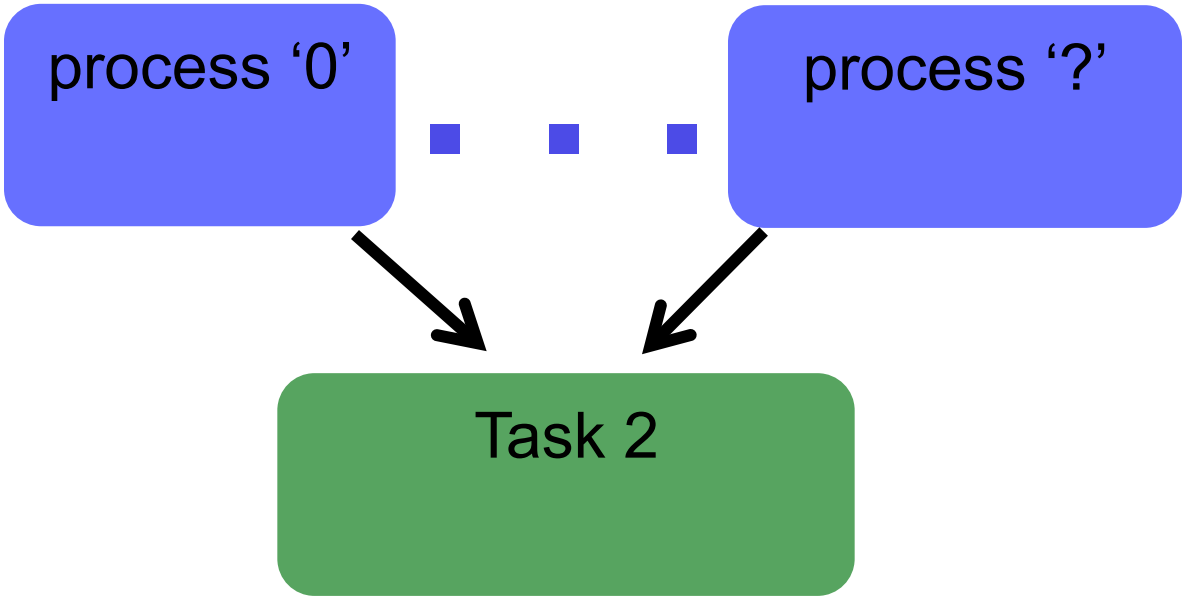
… but there are even more benefits of automating workflows!!

- Reproducibility!!
- Building knowledge and experience
- New ability to imagine greater scale, functionality, possibilities, and better SCIENCE!!

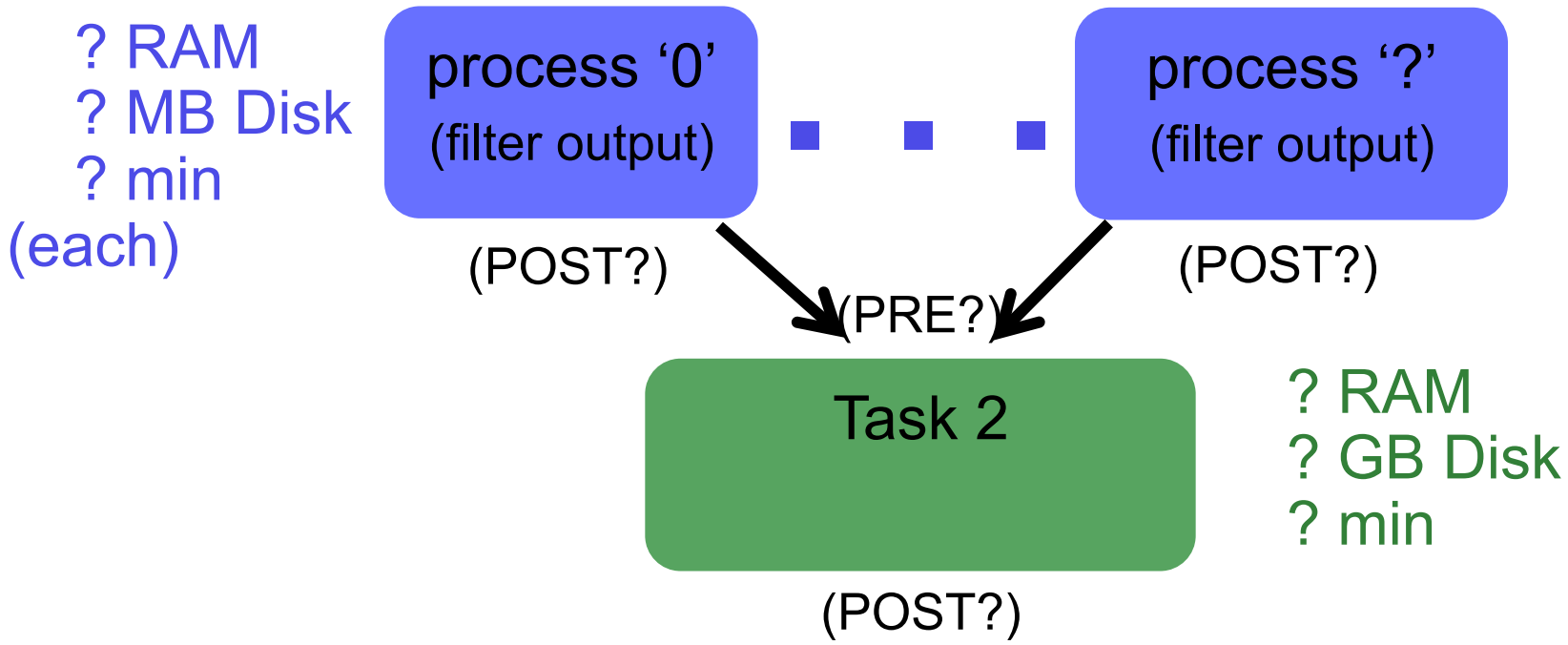
Exercise 1



Exercise 1



Exercise 2


? RAM
? MB Disk
? min
(each)
process '0'
(filter output)
process '?'
(filter output)
(POST?)
(POST?)
(PRE?)
Task 2
? RAM
? GB Disk
? min
(POST?)

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Questions?

- Feel free to contact me:
  - lmichael@wisc.edu
- Now: “Joe’s Workflow” Exercise 1.1,1.2
  - In groups of 2-3
- Later:
  - Lecture: From Workflow to Production
  - Exercises 1.3, 1.4