Open Science Grid

Getting the Most out of HTC with Workflows

Friday morning, 9:00 am

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Why are we here?

Why are we here?

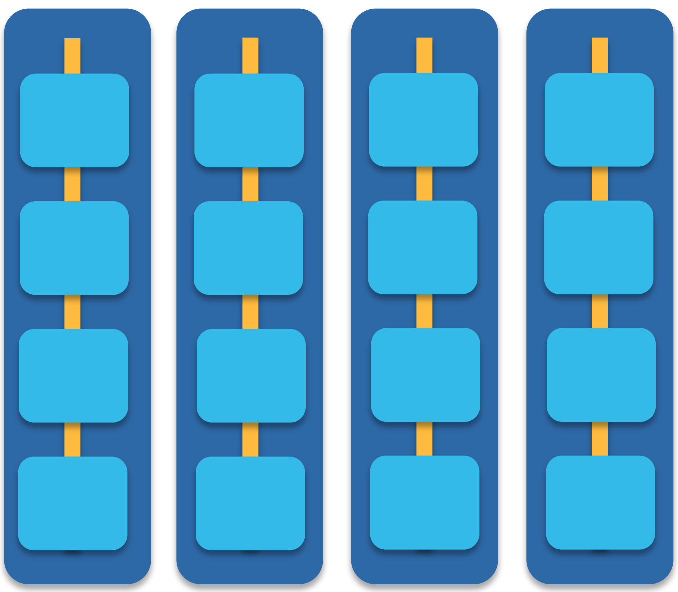
To do SCIENCE!!!

- 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)

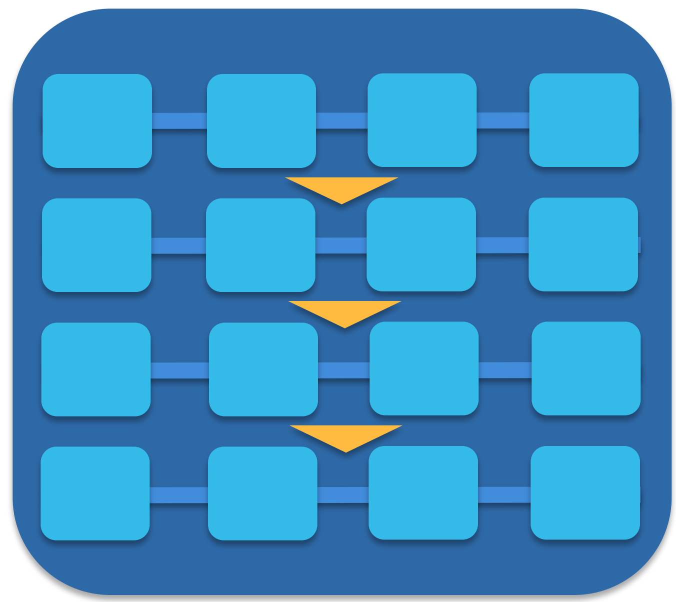
GETTING THE MOST OUT OF COMPUTING (FOR RESEARCH)

Computing types

- At the beginning of the week, we talked about two different approaches for tackling large compute tasks...



high-throughput



high-performance (e.g.MPI)

Two Strategies

High Throughput

Focus: Workflows with many *small*, *largely independent* compute tasks

Optimize: *throughput*, or time from *submission* to *overall completion*

High Performance

- Focus: Workflows with *large, highly coupled* tasks
- Optimize: *individual tasks*, software, communication between processes

Making Good Choices

- How do you choose the best approach?
- Guiding question:

Is your problem “HTC-able”?

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* of programs/functions that use multiple CPUs on the same server

Ultimately: Can you break it up?

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

The Real World

- However, it's not just about finding the right computing approach to your problem.
- These approaches will be *most* effective if they're running on appropriate compute systems.

The Real World

- Not all compute systems are created equal.

- Two questions to ask:

What resources are available to me?

Which one is the best match for the kind of computing I want to do?

Campus Resources

- Start with your local campus compute system
- Some considerations:
  - Who has access? Are there allocations?
  - What kind of system? What is it optimized for?
- An HPC cluster may not handle lots of jobs well, in the same way that an HTC system has limited multicore capabilities - be aware of how a system matches/doesn’t match your computation strategy.
- Ask questions! Be a good citizen!
- If local resources are limited, explore other options.

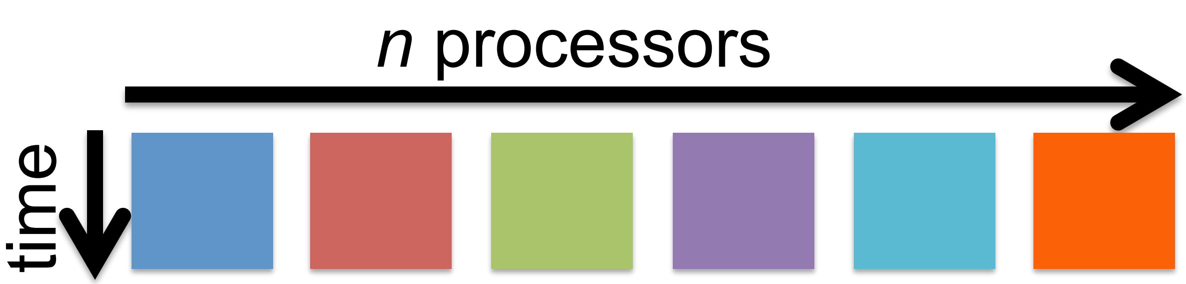
Beyond your campus

- Open Science Grid!
  - This afternoon, Tim will talk about ways to access OSG after the school is over

- Other grids
  - European Grid Infrastructure
  - Other national and regional grids
  - Commercial cloud systems

The payoff

- HTC is, beyond everything, scalable
  - If you can run 10 jobs, you can run 10,000, maybe even 10 million
- Worth pursuing the right kind of resources (if you can) for the right kind of problem.



GETTING THE MOST OUT OF HTC

Key HTC Tactics

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

Throughput, revisited

- In HTC, we optimize *throughput*: time from submission to overall completion

Instead of making individual jobs as fast as possible...

...optimize how long it takes for *all* jobs to finish

- We do this by breaking large processes into smaller pieces

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
- Use self-checkpointing if jobs are too long

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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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

Use the job log

```
001 (2576205.000.000) 06/07 11:57:57 Job executing on host:
<128.104.101.248:9618>
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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Bring *What* with You?

- Software (covered Wednesday)
- Data and other input files
  - Parameters and random numbers: generate and record ahead of time (for reproducibility)

- What else?

Wrapper Scripts are Essential

- Before task execution
  - 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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Testing, testing, testing!

- Will be a major focus of our exercises today.
- Allows you to optimize resource use (see HTC tactic #2)
- Just because it worked for 10 jobs, doesn't mean it will work for 10,000 jobs (scaling issues)
  - Data transfer (in and out)
  - Discover site-specific problems

Key HTC Tactics

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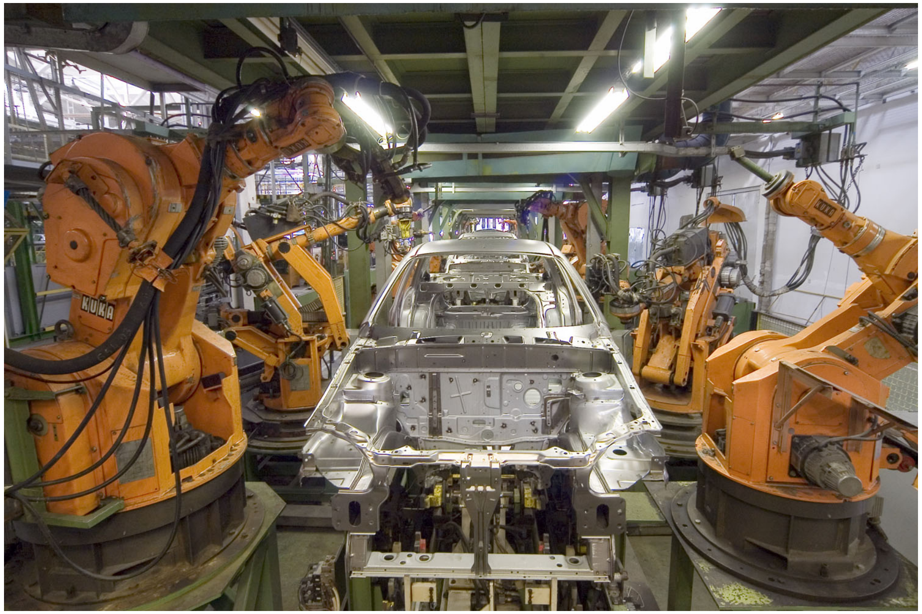
Open Science Grid

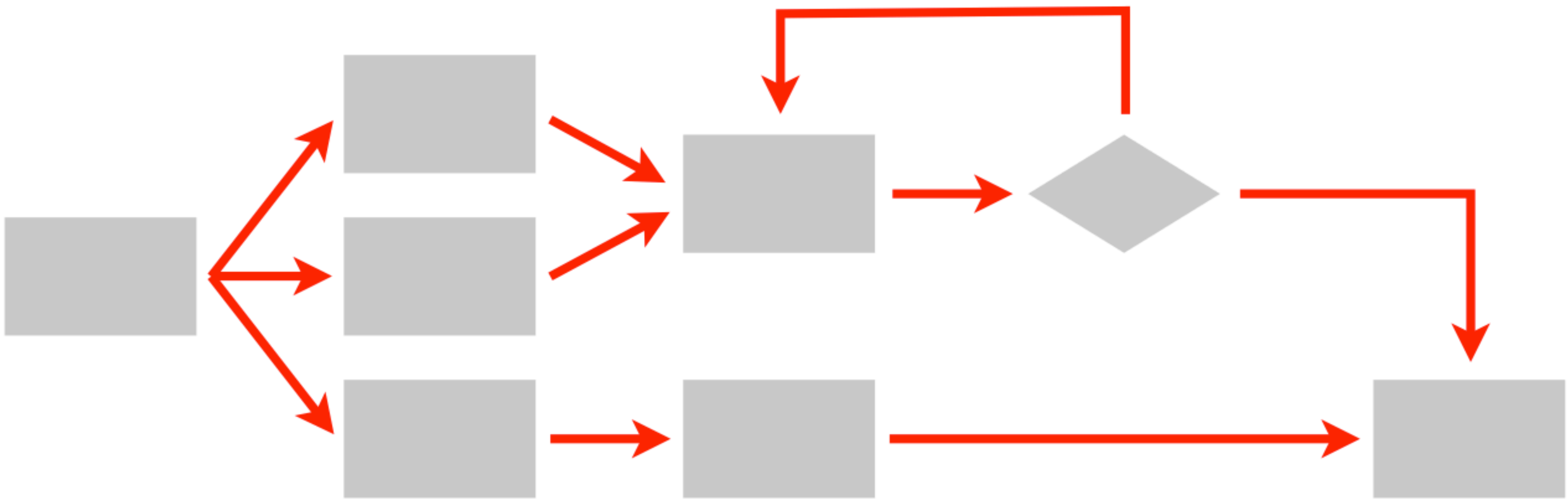
What to Automate?

- Submitting many jobs (using HTCondor)
- Writing submit files using scripts
- Running a series of jobs, or workflow



What is a workflow?

- A series of ordered steps
  - Steps
  - Connections
  - (Metadata)



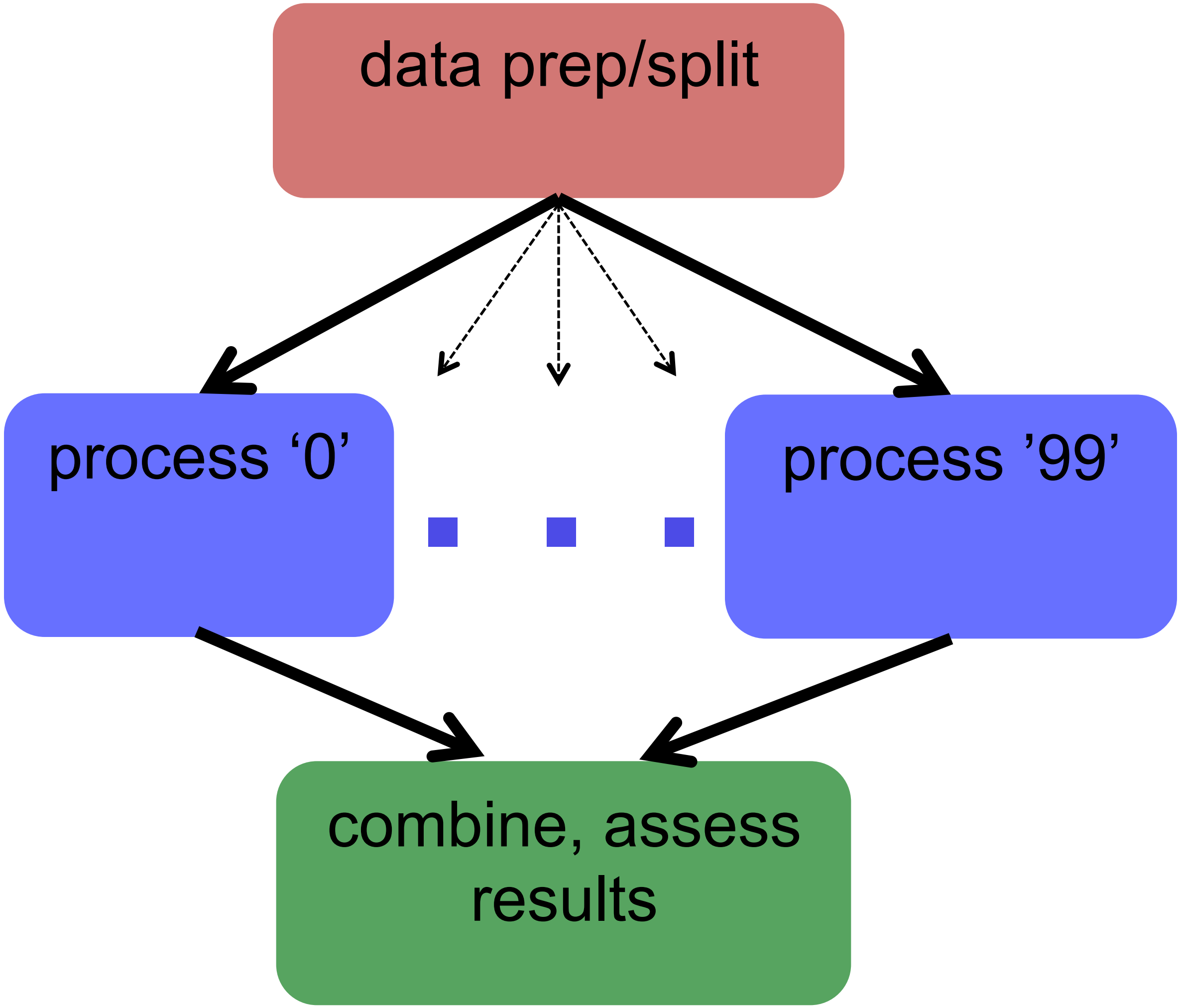
We ❤ workflows

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

- when planned/documented, workflows help with:
  - organizing and managing processes
  - saving time with **automation**
  - objectivity, reliability, and reproducibility

    (THE TENETS OF GOOD SCIENCE!)

DAGs Automate Workflows



Automating workflows can save you time...

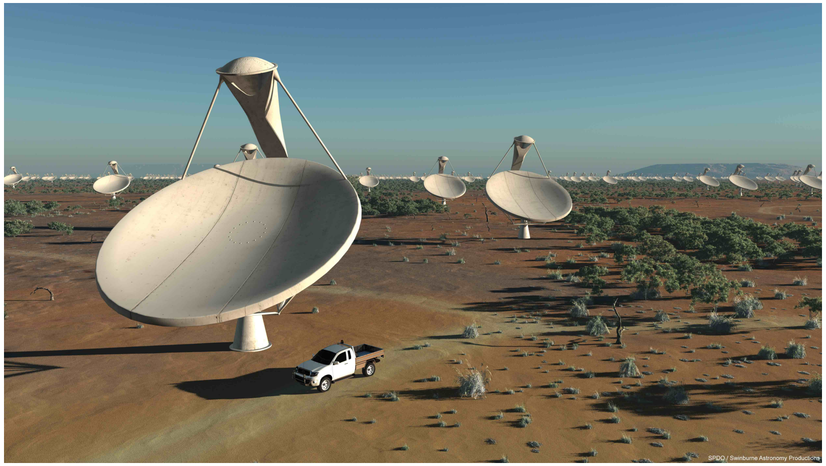
HOW LONG CAN YOU WORK ON MAKING A ROUTINE TASK MORE EFFICIENT BEFORE YOU'RE SPENDING MORE TIME THAN YOU SAVE?
(ACROSS FIVE YEARS)

HOW MUCH TIME YOU SHAVE OFF	HOW OFTEN YOU DO THE TASK: 50/DAY	5/DAY	DAILY	WEEKLY	MONTHLY	YEARLY
1 SECOND	1 DAY	2 HOURS	30 MINUTES	4 MINUTES	1 MINUTE	5 SECONDS
5 SECONDS	5 DAYS	12 HOURS	2 HOURS	21 MINUTES	5 MINUTES	25 SECONDS
30 SECONDS	4 WEEKS	3 DAYS	12 HOURS	2 HOURS	30 MINUTES	2 MINUTES
1 MINUTE	8 WEEKS	6 DAYS	1 DAY	4 HOURS	1 HOUR	5 MINUTES
5 MINUTES	9 MONTHS	4 WEEKS	6 DAYS	21 HOURS	5 HOURS	25 MINUTES
30 MINUTES		6 MONTHS	5 WEEKS	5 DAYS	1 DAY	2 HOURS
1 HOUR		10 MONTHS	2 MONTHS	10 DAYS	2 DAYS	5 HOURS
6 HOURS				2 MONTHS	2 WEEKS	1 DAY
1 DAY					8 WEEKS	5 DAYS

http://xkcd.com/1205/

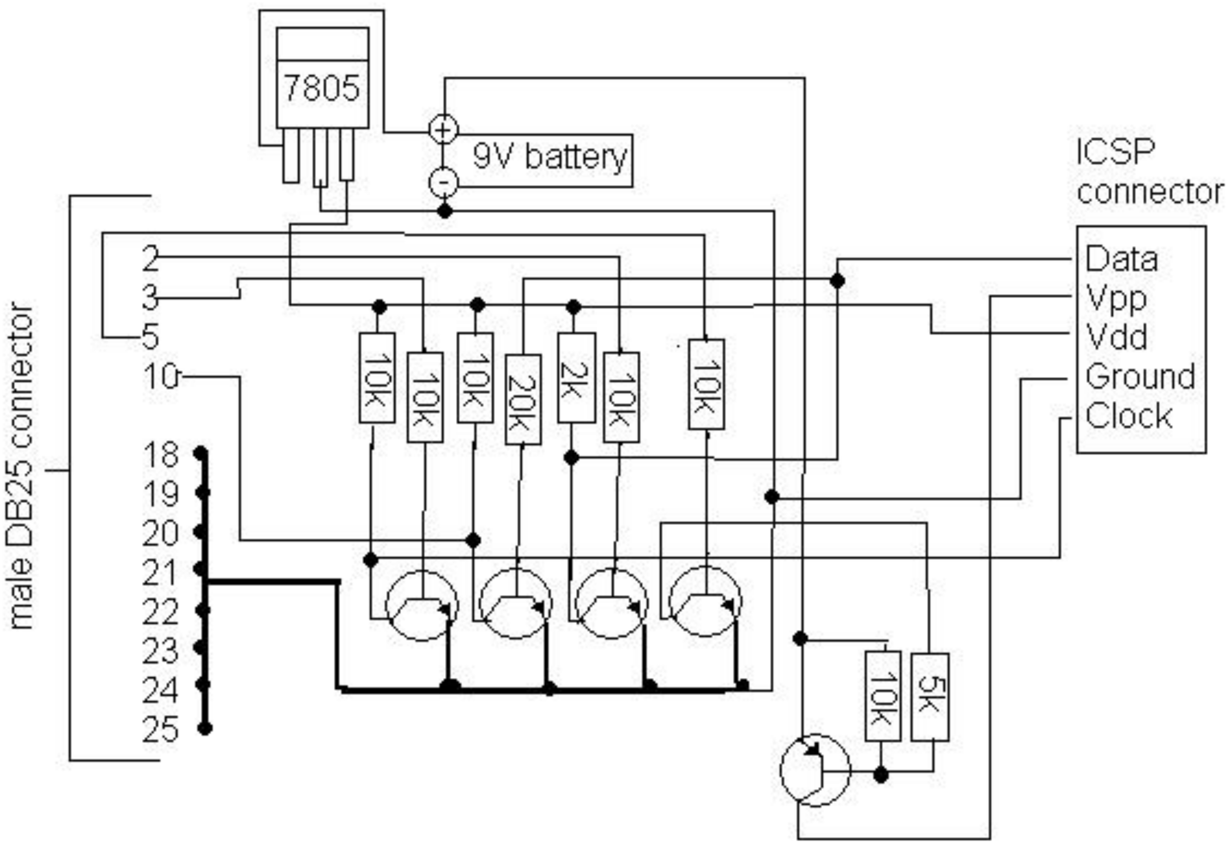
… but there are even more benefits of automating workflows

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

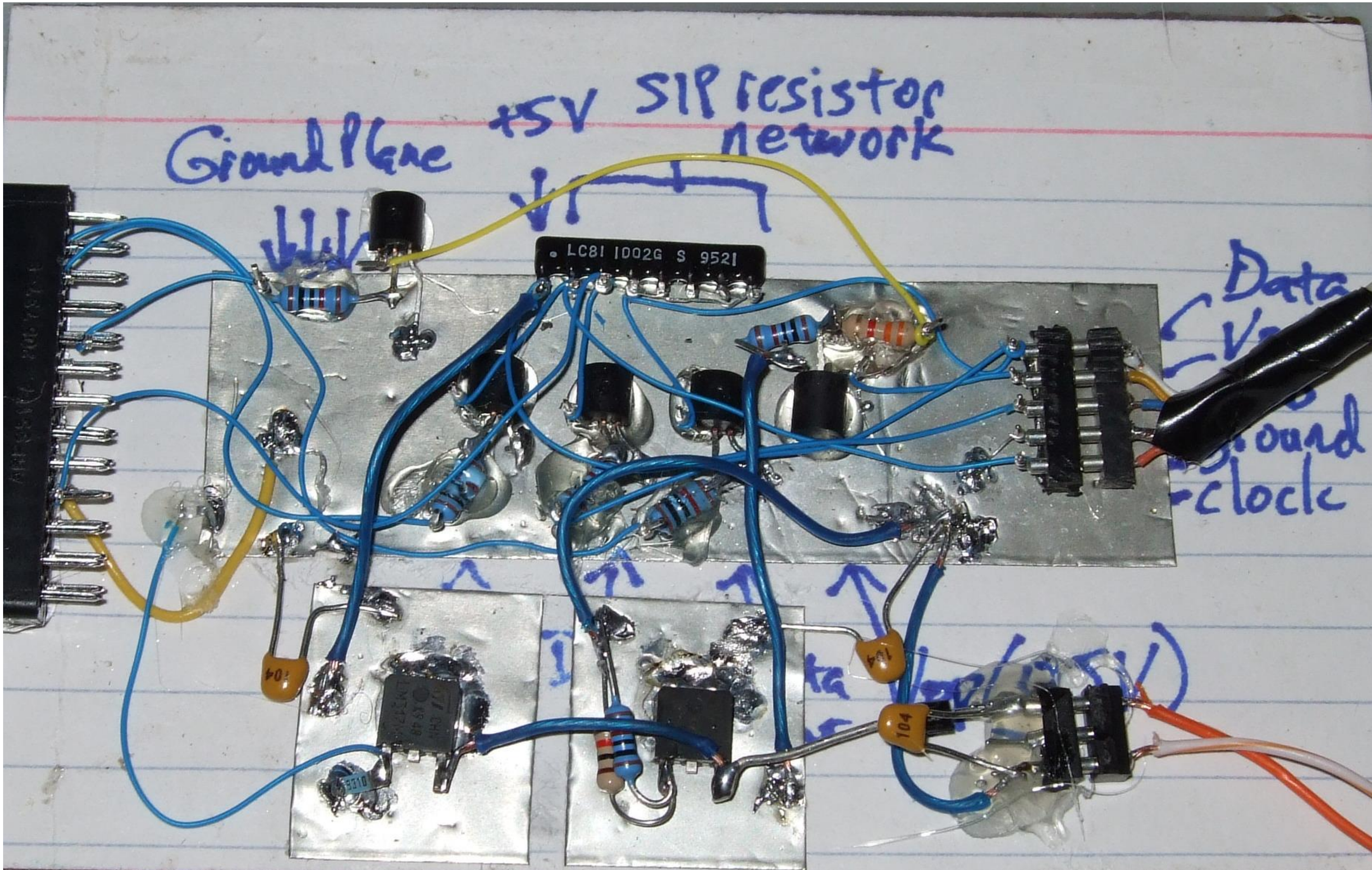


GETTING THE MOST OUT OF WORKFLOWS, PART 1

From schematics…



… to the real world

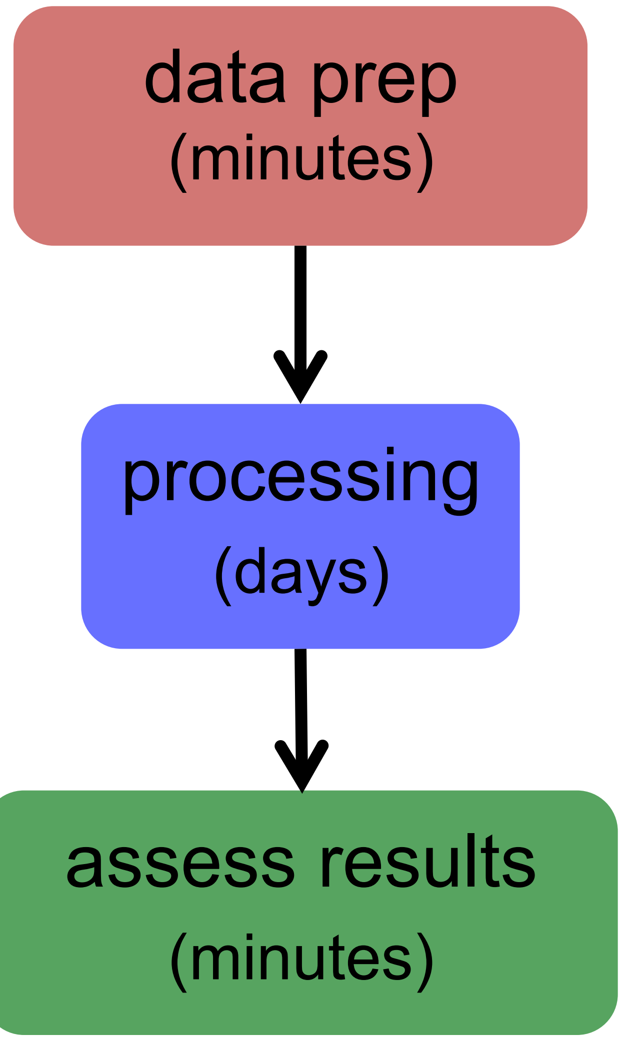


Building a Good Workflow

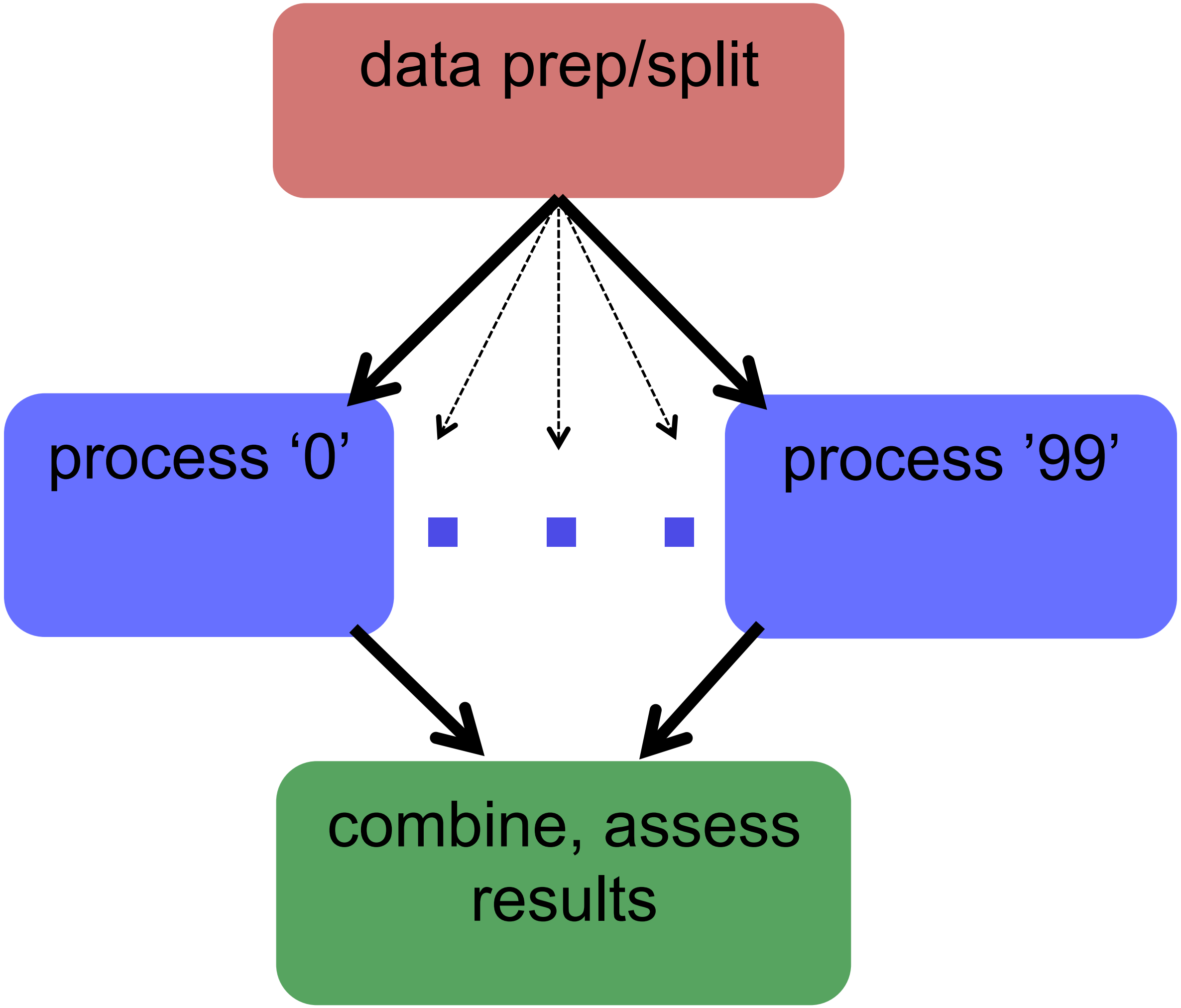
1. **Draw out the *general* workflow**
2. Define details (test ‘pieces’ with HTCondor jobs)
   - divide or consolidate ‘pieces’
   - determine resource requirements
   - identify steps to be automated or checked
3. Build it modularly; test and optimize
4. Scale-up gradually
5. Make it work consistently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

(And remember to document!)

Workflow, version 1



Workflow, version 2 (HTC)



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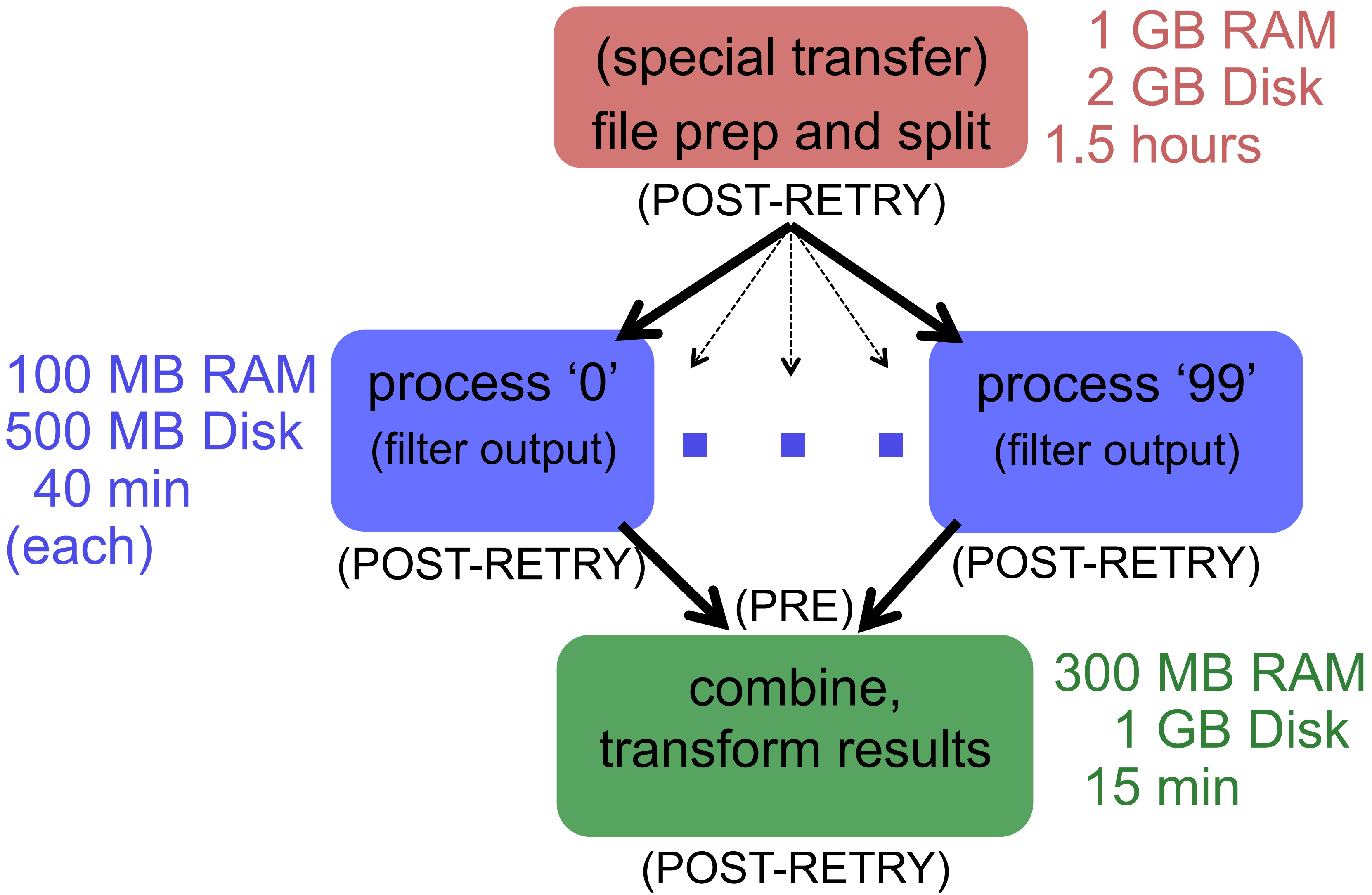
Determine Resource Usage

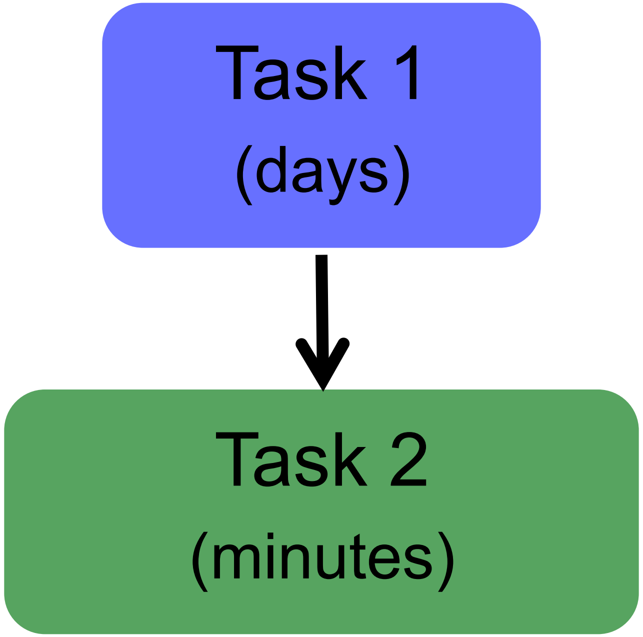
- Run locally first
- Then get one job running remotely
  - (on execute machine, not submit machine)!
  - get the logistics correct! (HTCondor submission, file and software setup, etc.)
- Once working, run a couple of times
  - If big variance in resource needs, should you take the…

    Average? Median? Worst case?

End Up with This



Exercise 1.1



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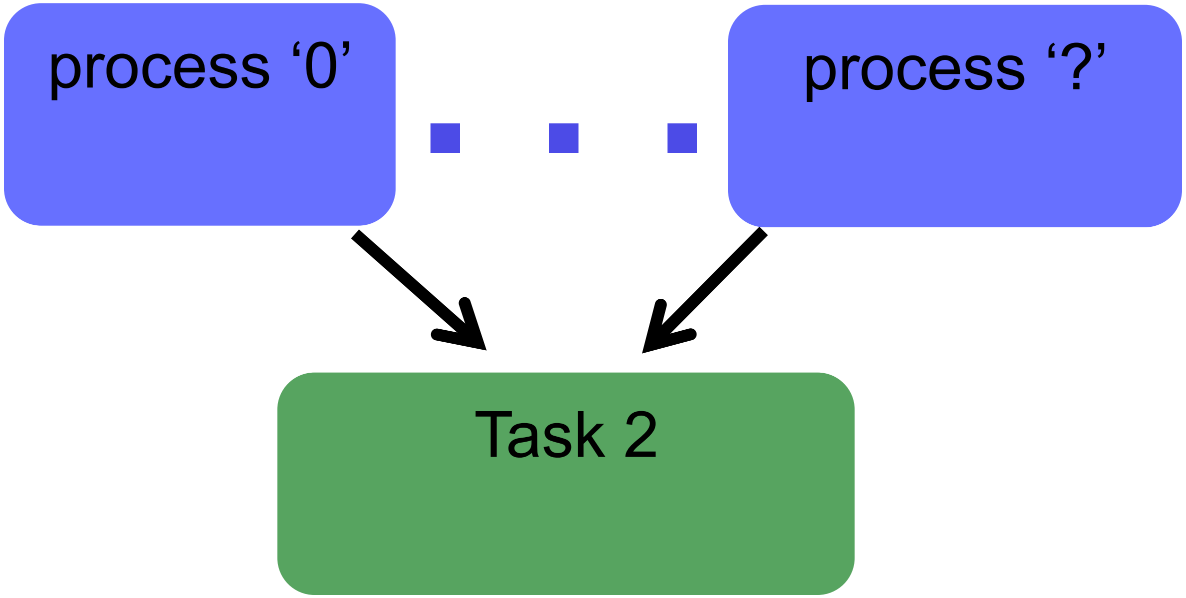
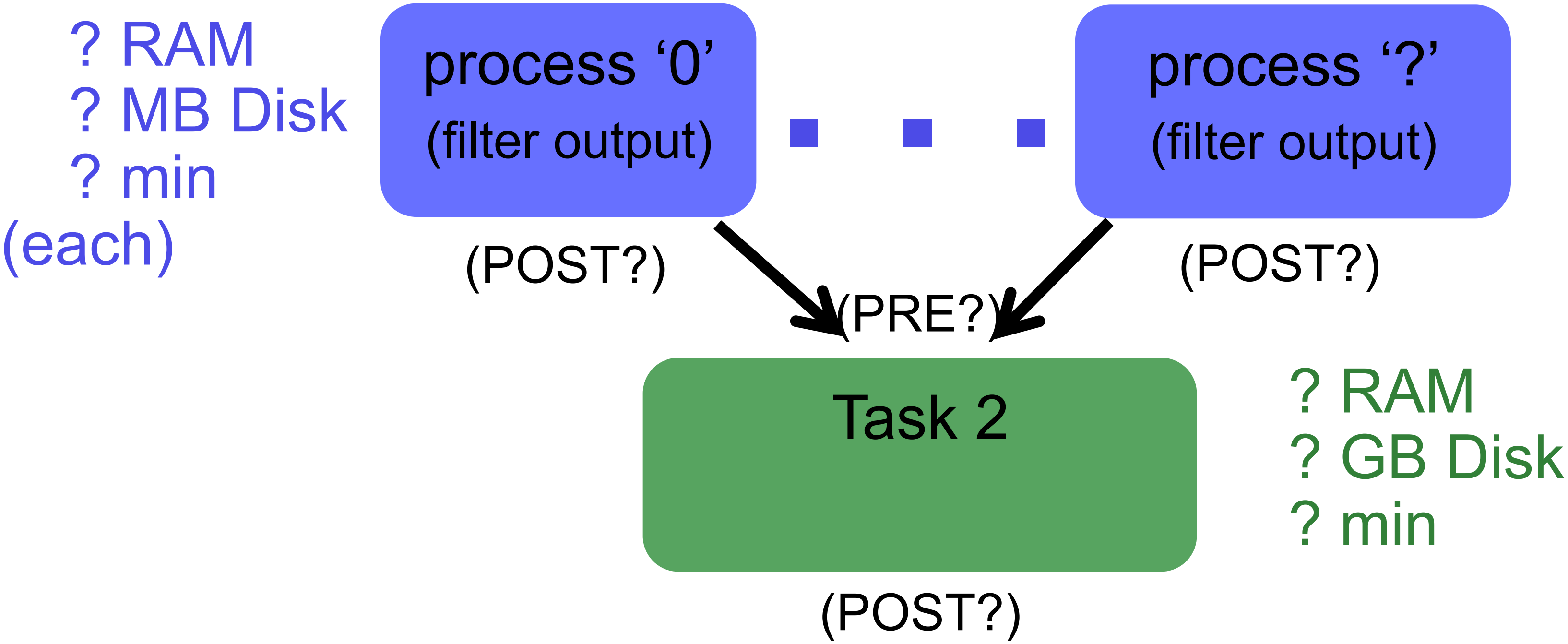


Exercise 1.2


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

Questions?

- Now: “Joe’s Workflow” Exercise 1.1,1.2
  - In groups of 2-3
  - Read carefully!
- Later:
  - Lecture: From Workflow to Production
  - Exercises 2.1, 2.2