Workflows: from Development to Automated Production

Friday morning, 10:30 am

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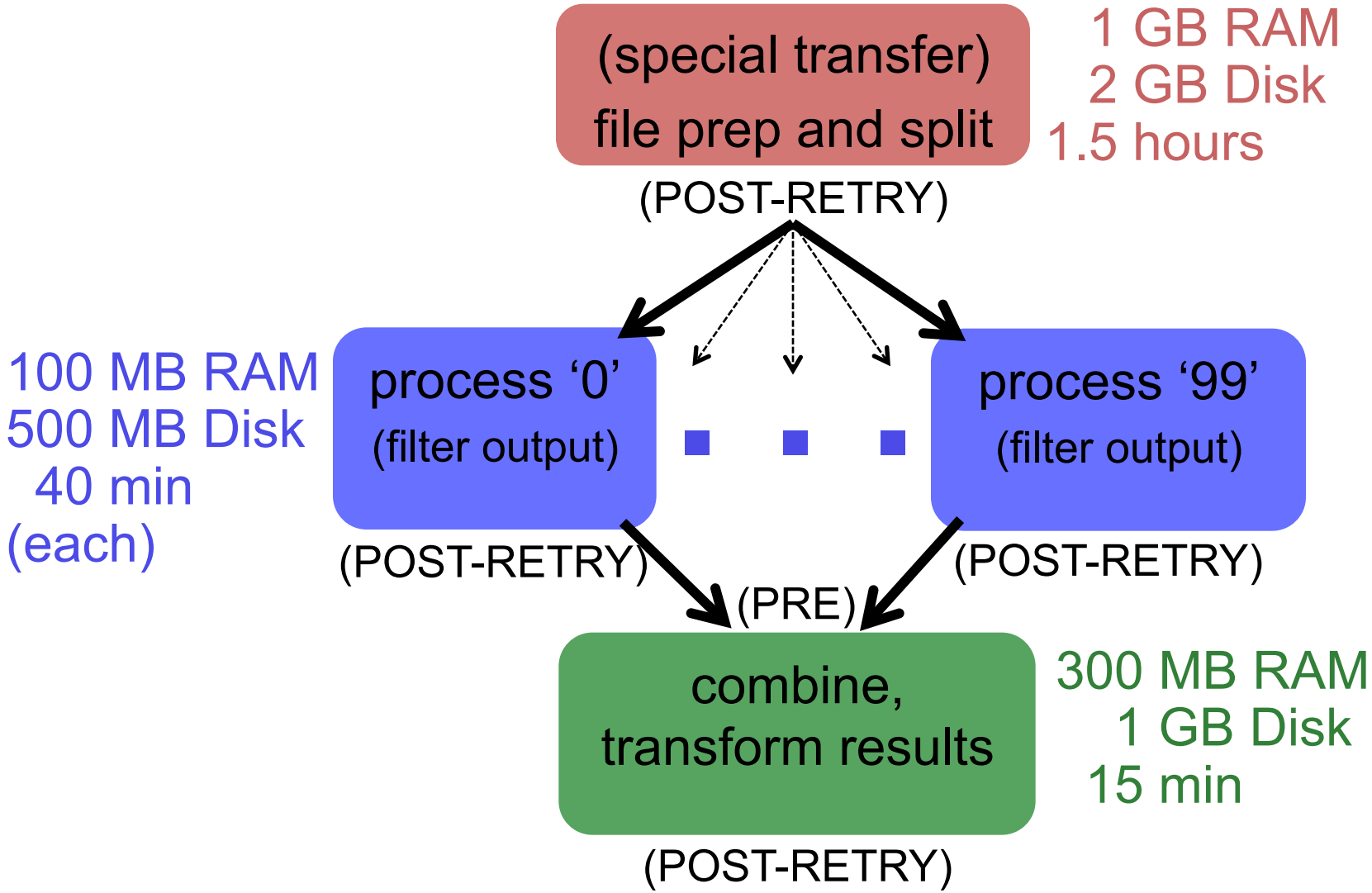
OR, GETTING THE MOST OUT OF WORKFLOWS, PART 2

Building a Good Workflow

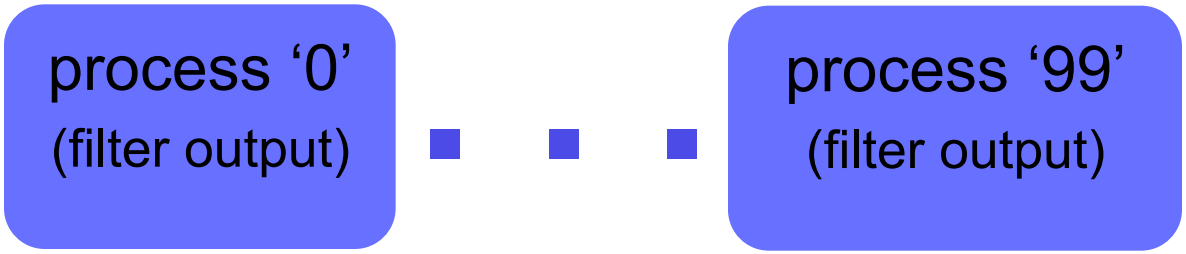
1. Draw out the *general* workflow
2. Define details (test 'pieces' with HTCondor jobs)
   - divide or consolidate 'pieces'
   - determine resource requirements
   - identify steps to be automated or checked
3. **Build it modularly; test and optimize**
4. Scale-up gradually
5. Make it work consistently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

(And remember to document!)

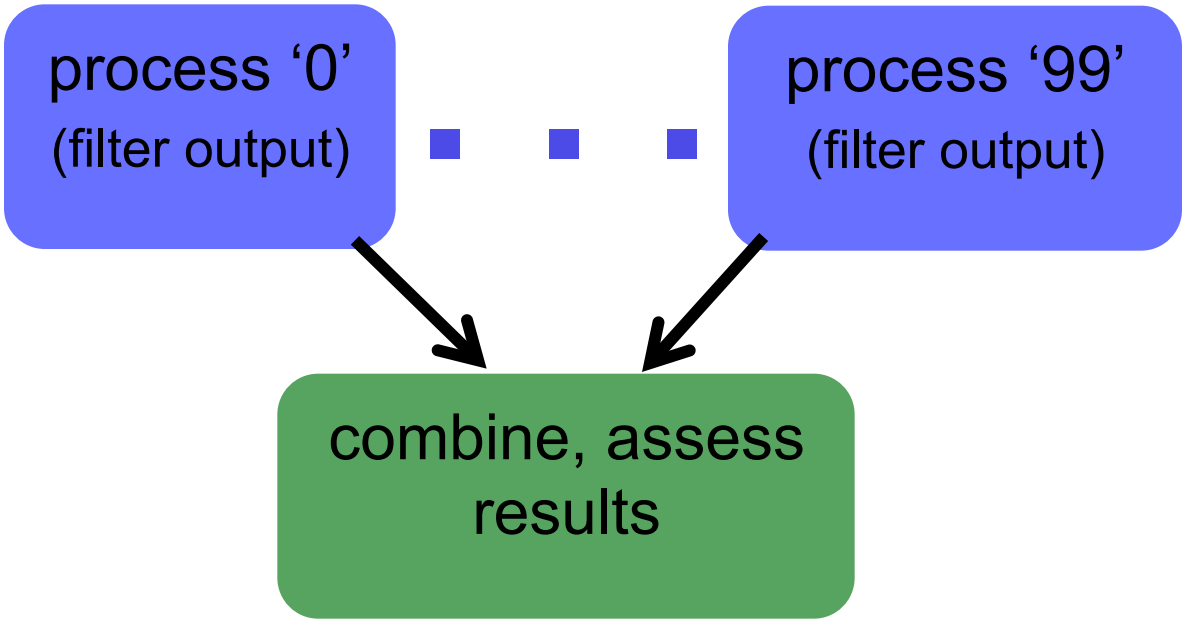
To Get Here …


(special transfer)
file prep and split
1 GB RAM
2 GB Disk
1.5 hours
(POST-RETRY)
100 MB RAM
500 MB Disk
40 min
(each)
process ‘0’
(filter output)
process ‘99’
(filter output)
(POST-RETRY)
(POST-RETRY)
(PRE)
combine,
transform results
300 MB RAM
1 GB Disk
15 min
(POST-RETRY)

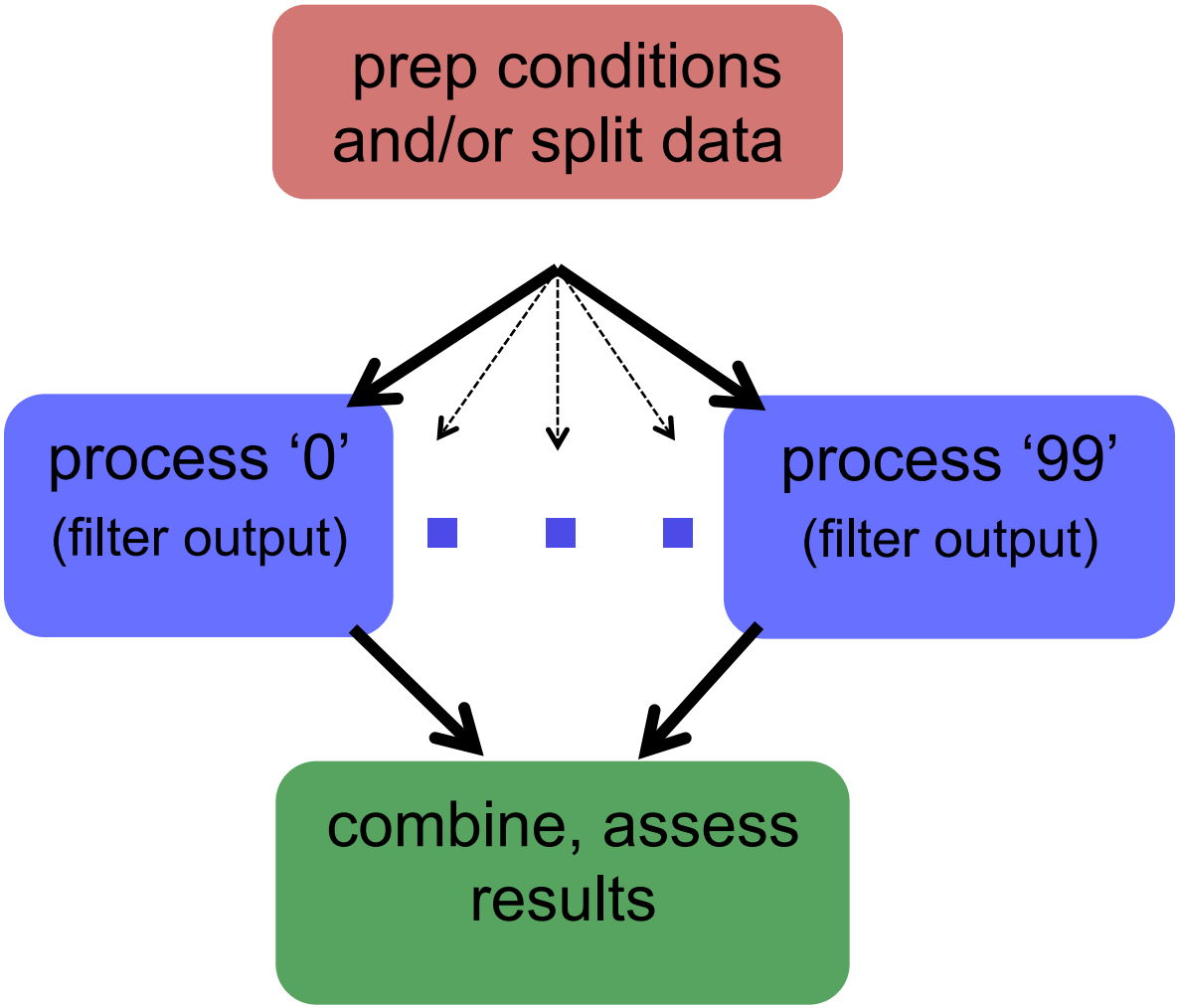
Start Here



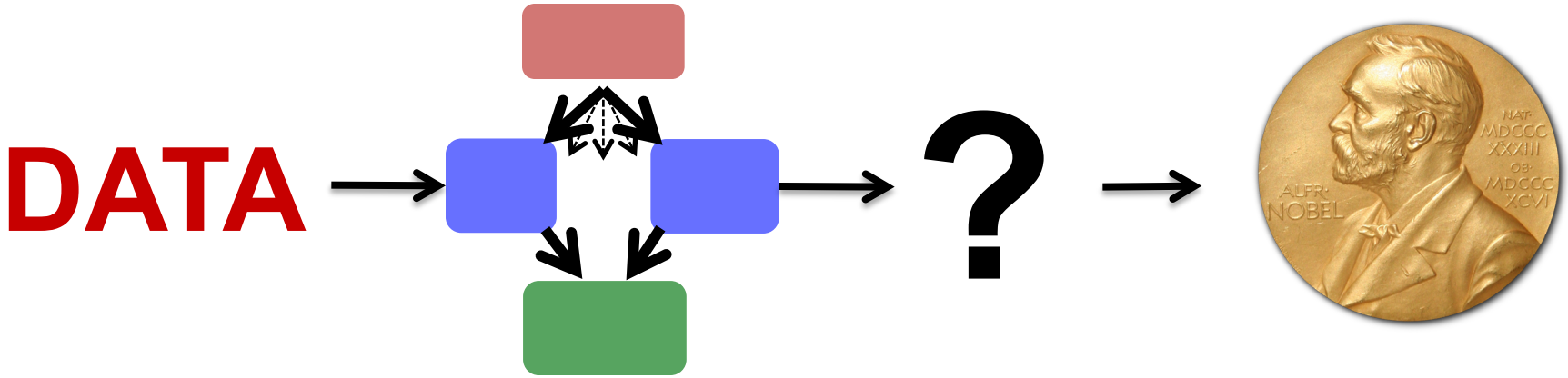
Add a Step


process ‘0’
(filter output)
process ‘99’
(filter output)
combine, assess results

And Another Step



End Up With This?



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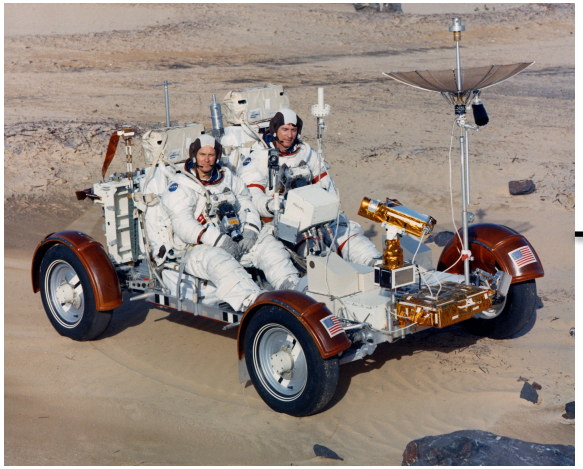
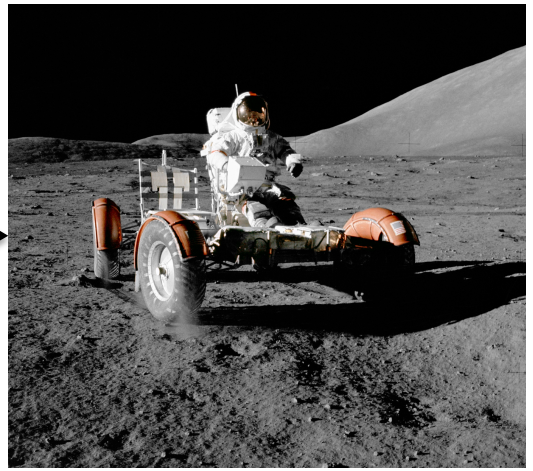
Scaling Workflows

- Your ("small") DAG runs! Now what?
  - Need to make it run *full scale*



to the moon!



Scaling Up: OSG Rules of Thumb

- CPU (single-threaded)
  - Best jobs run between **10 min** and **10 hrs**
    (Upper limit somewhat soft)
- Data (disk and network)
  - Keep scratch working space < 20 GB
  - Intermediate needs (/tmp?)
  - Use alternative data transfer appropriately
- Memory
  - Closer to 1 GB than 8 GB

Testing, Testing, 1-2-3 …

- ALWAYS test a subset after making changes
  - How big of a change needs retesting?
- Scale up gradually
- Avoid making problems for others (and for yourself)

Scaling Up - Things to Think About

- More jobs:
  - 100-MB per input files may be fine for 10 or 100 jobs, but not for 1000 jobs. Why?
  - most submit queues will falter beyond ~10,000 total jobs
- Larger files:
  - more disk space, perhaps more memory
  - potentially more transfer and compute time

Be kind to your submit and execute nodes and to fellow users!

Solutions for More Jobs

- Use a DAG to throttle the number of idle or queued jobs ("max-idle" and/or "DAGMAN CONFIG")
  - new HTCondor options to do this in a submit file as well
- Add more resiliency measures
  - "RETRY" (works per-submit file)
  - "SCRIPT POST" (use $RETURN, check output)
- Use SPLICE, VAR, and DIR for modularity/organization

Solutions for Larger Files

- File manipulations
  - split input files to **send minimal data** with each job
  - **filter** input *and* output files to transfer only essential data
  - use compression/decompression

- Follow file delivery methods from yesterday for files that are still “large”

Self-Checkpointing

Solution for long jobs and “shish-kebabs”

1. Changes to your code
   - Periodically save information about progress to a new file (every hour?)
   - At the beginning of script:
     - If progress file exists, read it and start from where the program (or script) left off
     - Otherwise, start from the beginning
2. Change to submit file:

```
when_to_transfer_output = ON_EXIT_OR_EVICT
```

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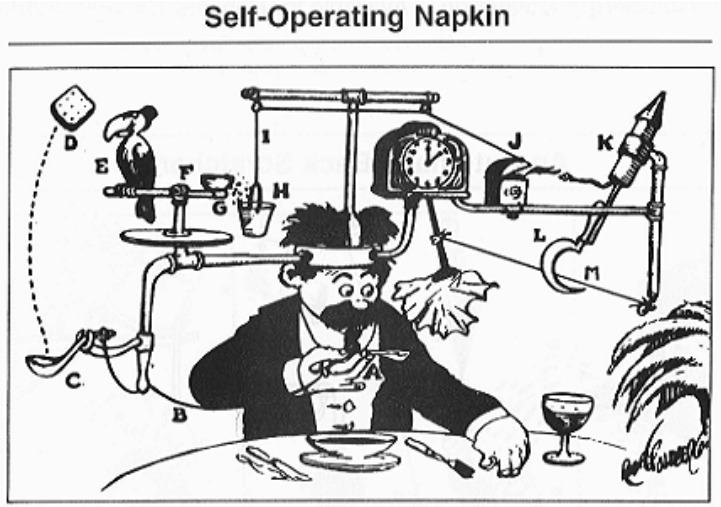
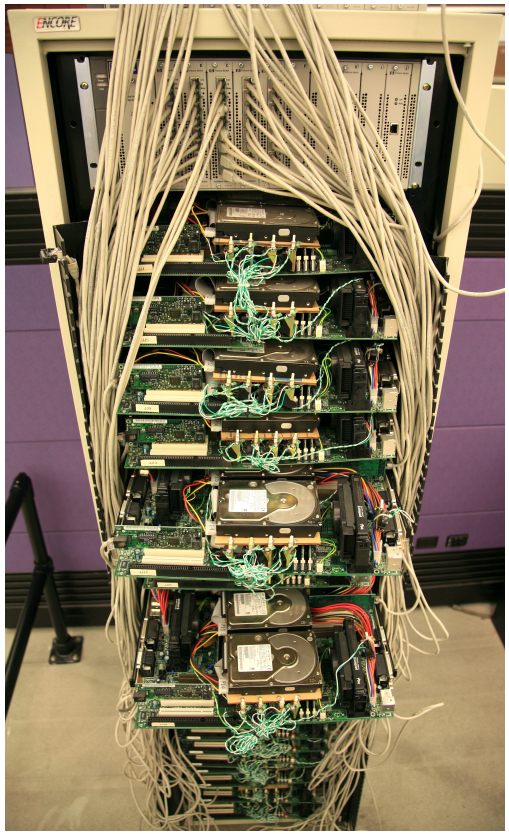
Robust Workflows

- Your DAG runs at scale! Now what?
  - Need to make it run *everywhere, everytime*
  - Need to make it run *unattended*
  - Need to make it run *when someone else tries*



Make It Run Everywhere

- What does an OSG machine have?
  - Prepare for very little
- Bring as much as possible with you, including:
  - executable
  - likely, more of the "environment"



Open Science Grid

The Spectrum

- Laptop (1 machine)
  - You control everything!
- Local cluster (1000 cores)
  - You can ask an admin nicely
- Campus (5000 cores)
  - It better be important/generalizable
- OSG (50,000 cores)
  - Good luck finding the pool admins

Make It Work Everytime

- What could possibly go wrong?
  - Eviction
  - Non-existent dependencies
  - File corruption
  - Performance surprises
    - Network
    - Disk
    - …
  - *Maybe* even a bug in your code

Performance Surprises

One bad node can ruin your whole day

- **"Black Hole" machines**
  - Depending on the error, email OSG!
- ***REALLY* slow machines**
  - use periodic_hold / periodic_release

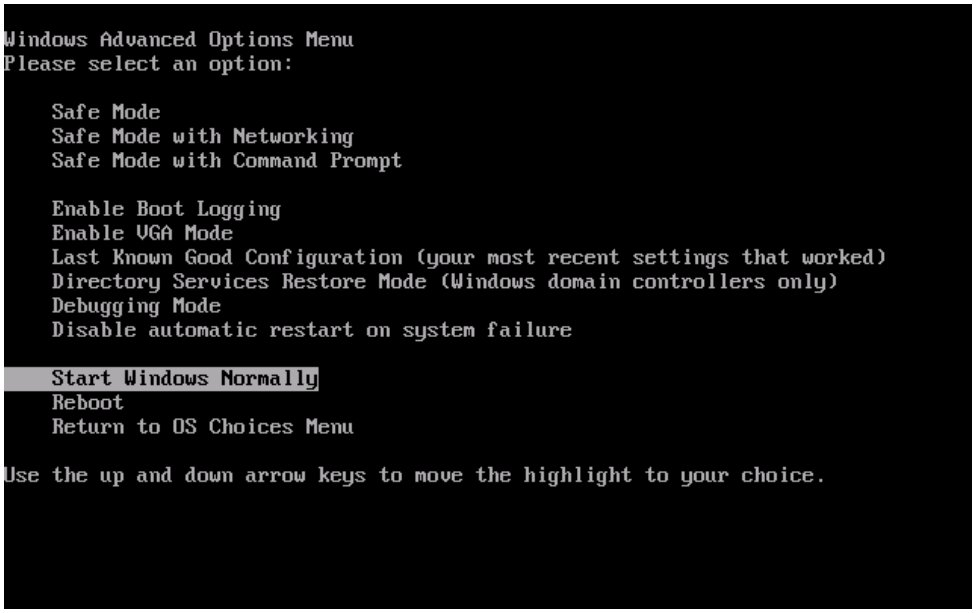
Error Checks Are Essential

If you don't check, it will happen…

- Check expected file existence, and repeat with a finite loop or number of retries
  - better yet, check *rough* file size too
- Advanced:
  - RETRY for *specific* error codes from wrapper
  - "periodic_release" for specific hold reasons

Handling Failures

- Understand something about failure
- Use DAG “RETRY”, when useful
- Let the rescue dag continue…



Make It Run(-able) for Someone Else

- Automation is a step towards making your research reproducible by someone else
  - Work hard to make this happen.
  - It's *their* throughput, too.
- Can benefit those who want to do similar work

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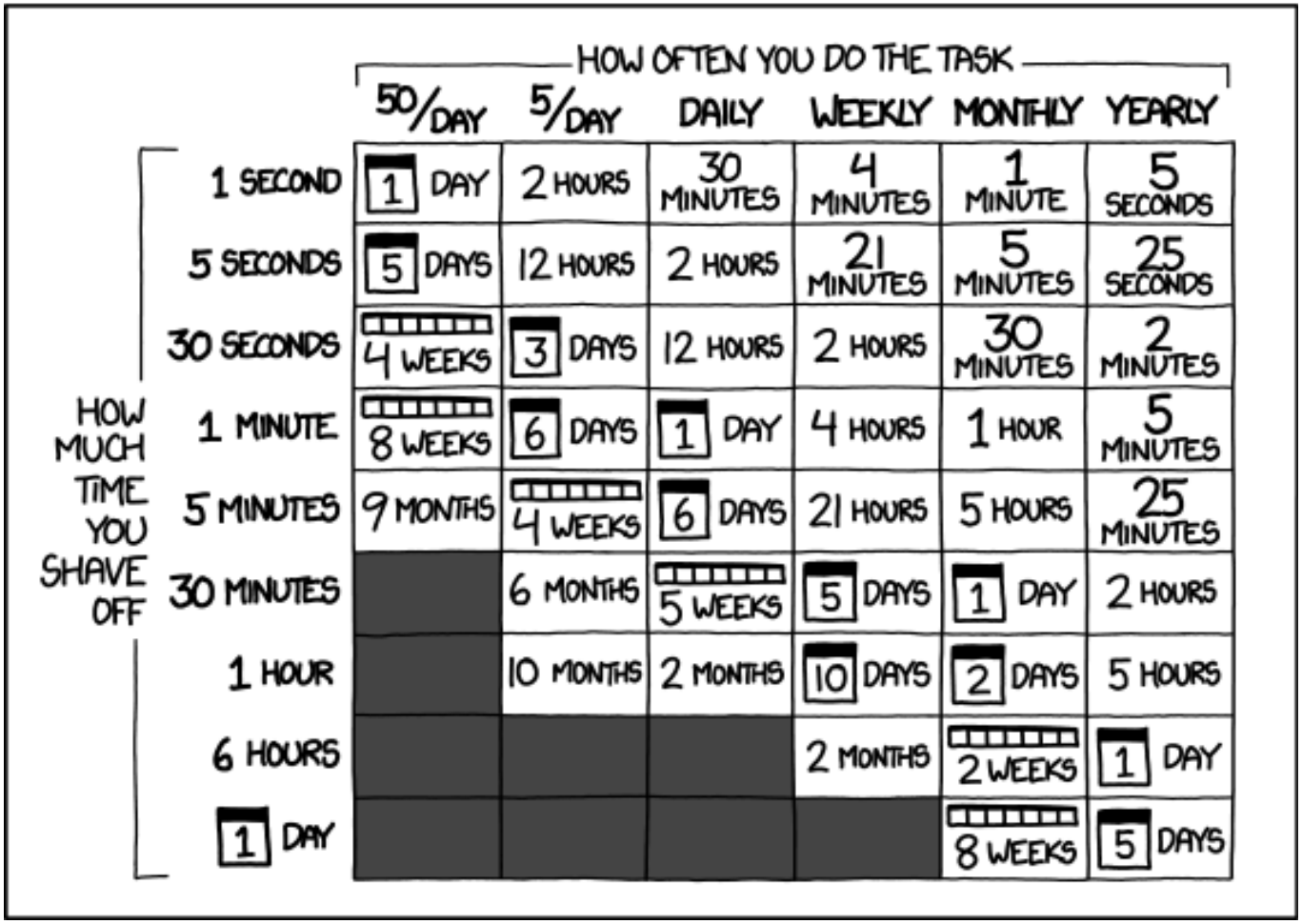
Open Science Grid

Automate *All* The Things?

- Well, not really, but kind of …
- Really: What is the minimal number of manual steps necessary?

  even 1 might be too many; zero is perfect!
- Consider what you get out of automation
  - time savings (including less 'babysitting' time)
  - reliability and reproducibility

Automation Trade-offs



http://xkcd.com/1205/

Make It Work Unattended

- Remember the ultimate goal:

  Automation! Time savings!

- Potential things to automate:
  - Data collection
  - Data preparation and staging
  - Submission (condor cron)
  - Analysis and verification
  - LaTeX and paper submission ☺

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Documentation at Multiple Levels

- In job files: comment lines
  - submit files, wrapper scripts, executables
- In README files
  - describe file purposes
  - define overall workflow, justifications
- In a document!
  - draw the workflow, explain the big picture

PARTING THOUGHTS

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Getting Research Done

- End goal: getting the research done
- Hopefully you now have the tools to get the most out of:
  - **Computing**: which approach and set of resources suit your problem?
  - **High Throughput computing**: optimize throughput, use portable data and software
  - **Workflows**: test, automate and scale

Questions?

- Now: Exercises 2.1 (2.2 Bonus)
- Next:
  - Lunch
  - Discovery Tour + Group Photo
  - HTC Showcase!