Open Science Grid

Workflows: from Development to Automated Production

Friday morning, 10:30 am

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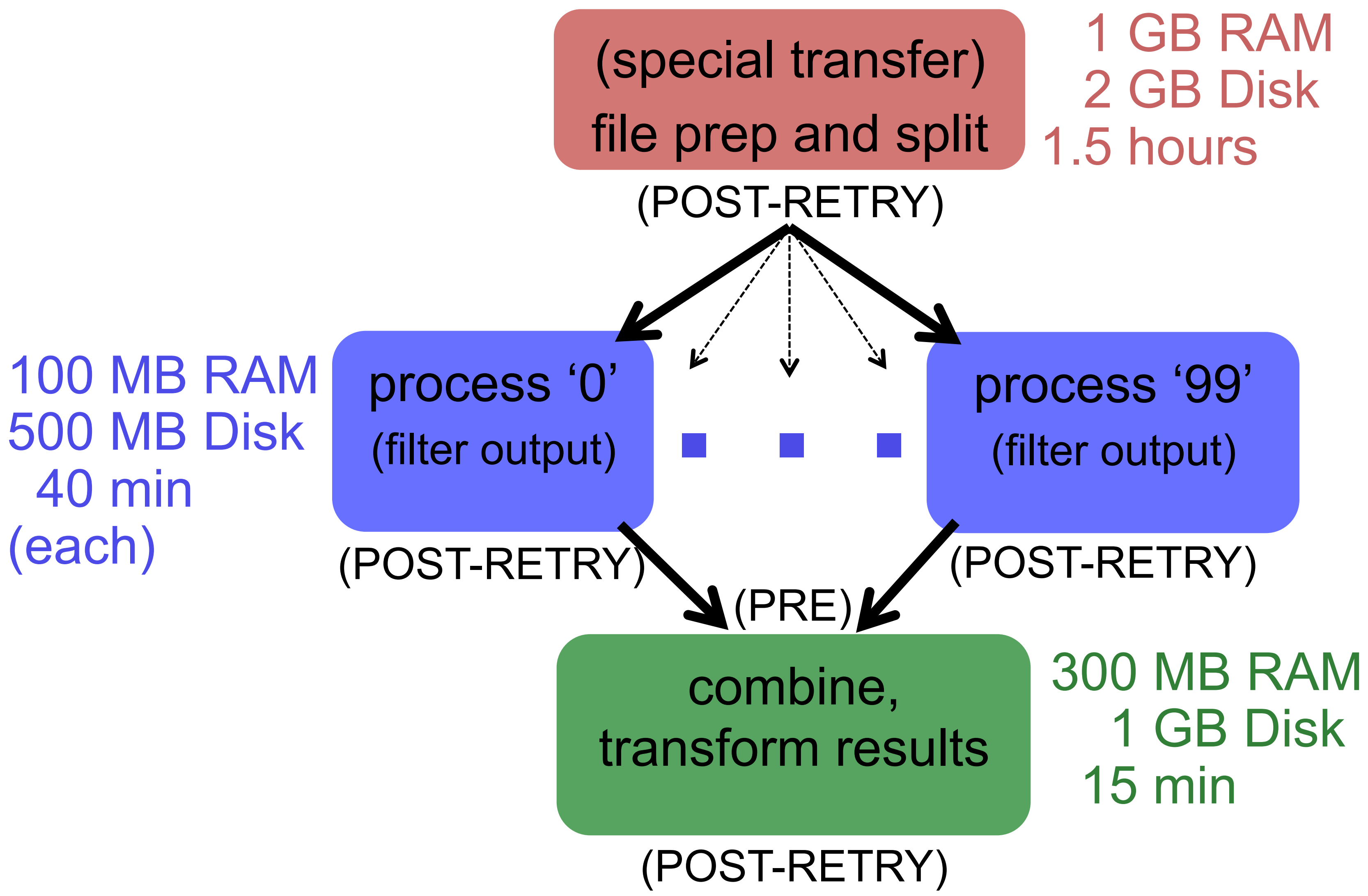
OR, GETTING THE MOST OUT OF WORKFLOWS, PART 2

Building a Good Workflow

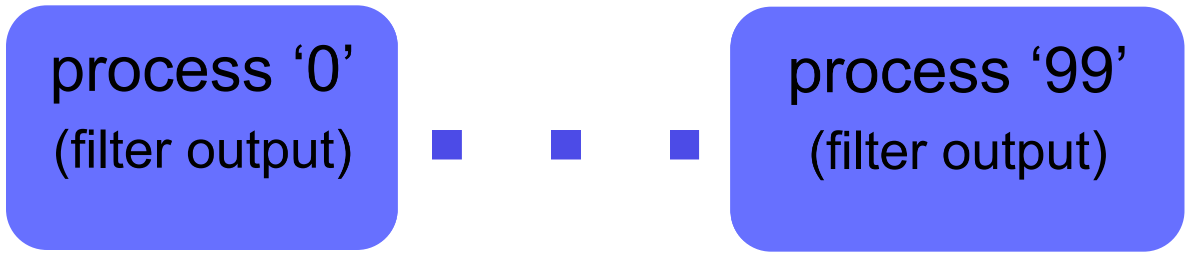
1. Draw out the *general* workflow
2. Define details (test ‘pieces’ with HTCondor jobs)
   - divide or consolidate ‘pieces’
   - determine resource requirements
   - identify steps to be automated or checked
3. **Build it modularly; test and optimize**
4. Scale-up gradually
5. Make it work consistently
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)
(POST-RETRY)
process '99'
(filter output)
(POST-RETRY)
(PRE)
combine, transform results
300 MB RAM
1 GB Disk
15 min
(POST-RETRY)

start with the HTC "step" in the DAG…



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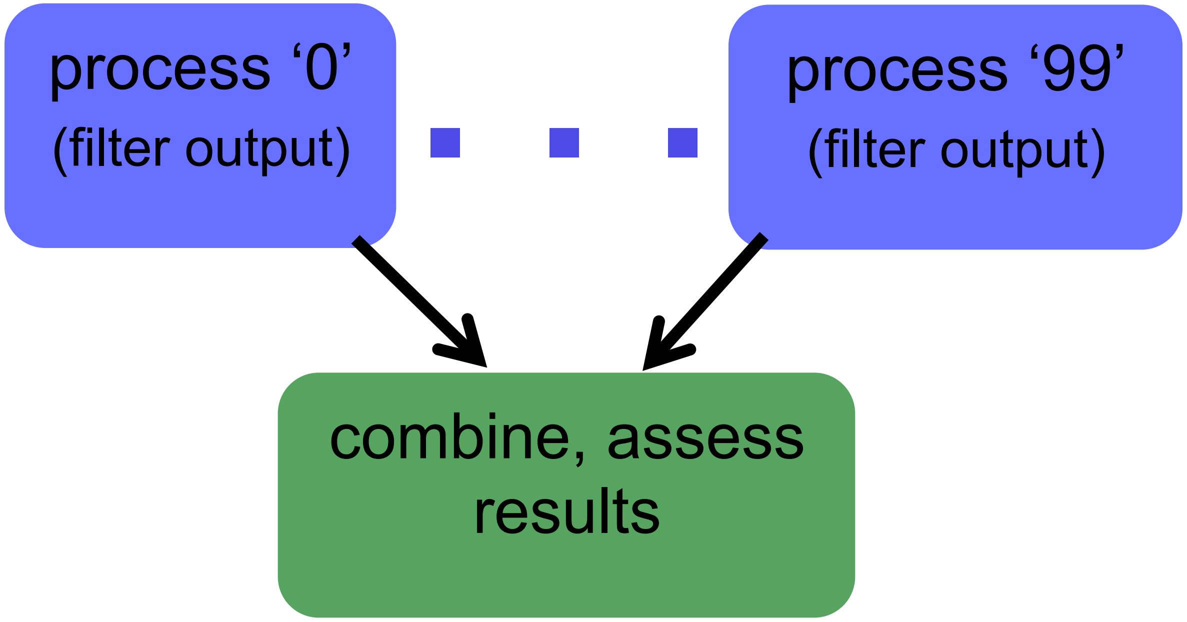
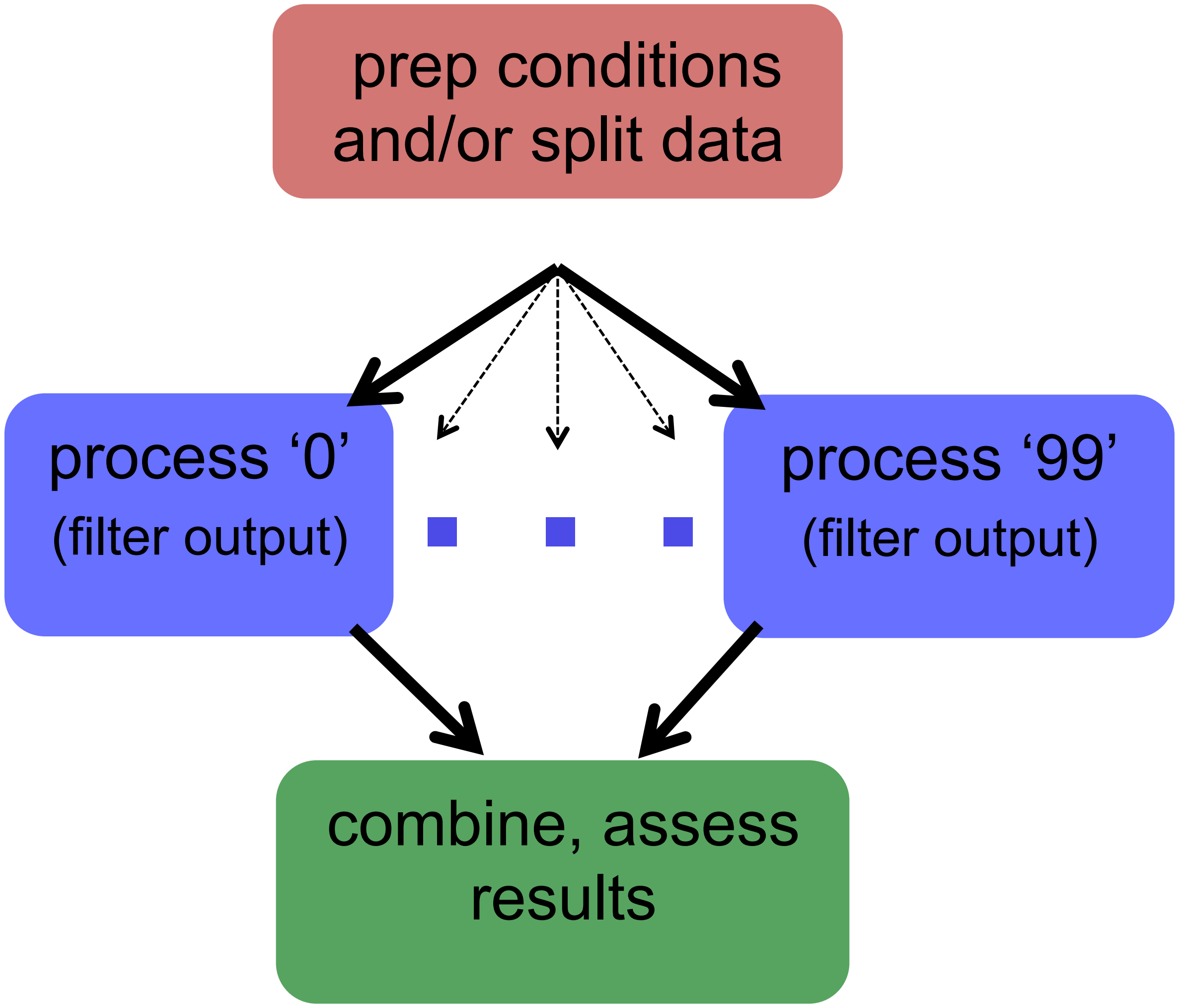
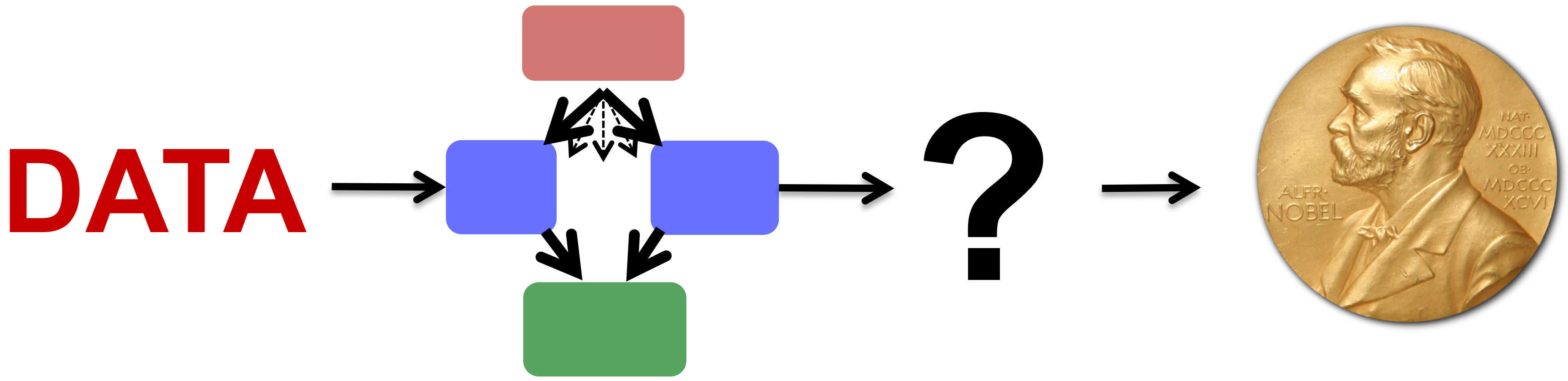
… then add in another step …



… and another step …


prep conditions and/or split data
process '0' (filter output)
process '99' (filter output)
combine, assess results

and End Up with This?



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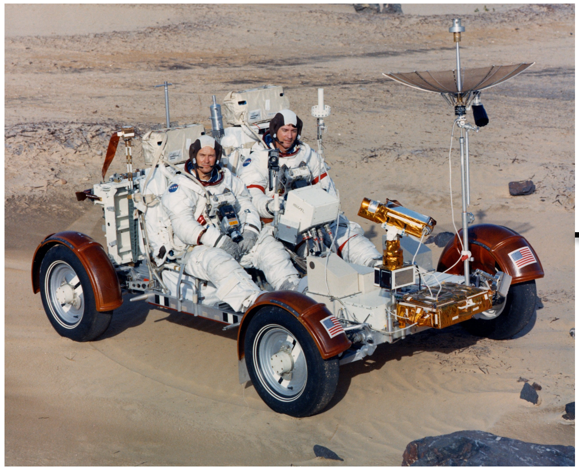
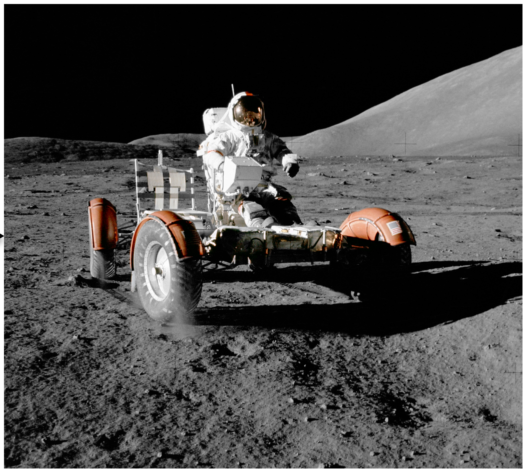
Scaling Workflows

- 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")
- Add more resiliency measures
  - "RETRY" (works per-submit file)
  - "SCRIPT POST" (use $RETURN, check output)
- Use SPLICE, VAR, and DIR for modularity/organization

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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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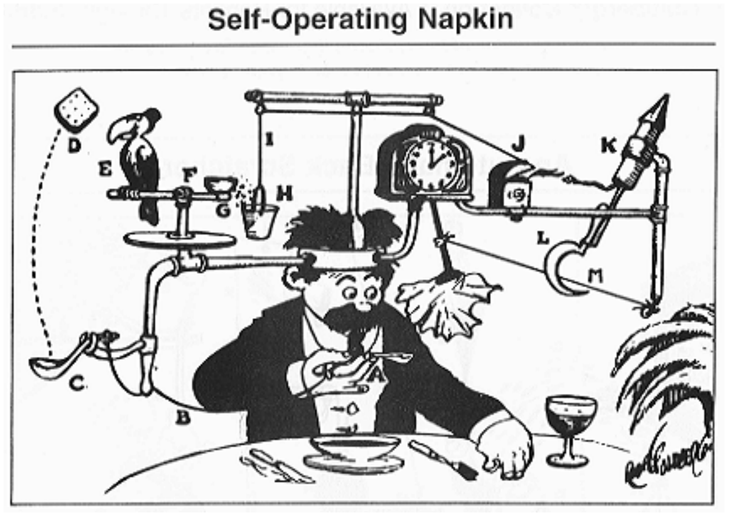
Robust Workflows

- 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*



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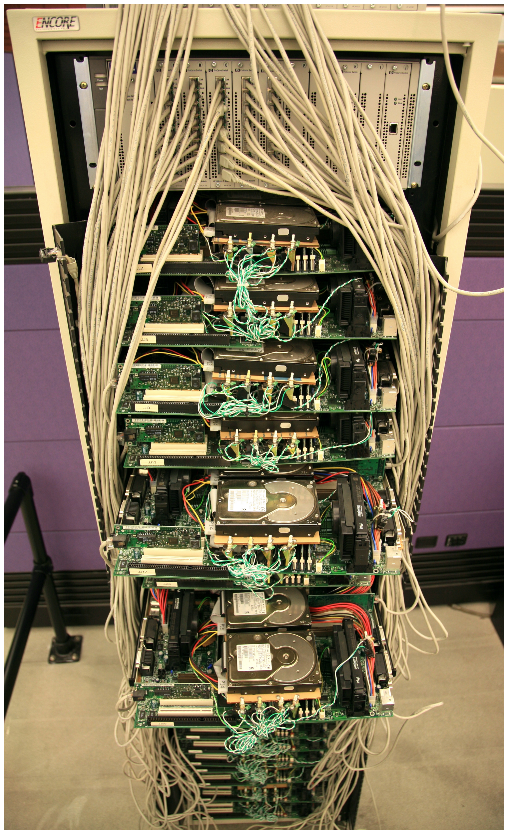
Make It Run Everywhere

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



The expanding onion

- 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

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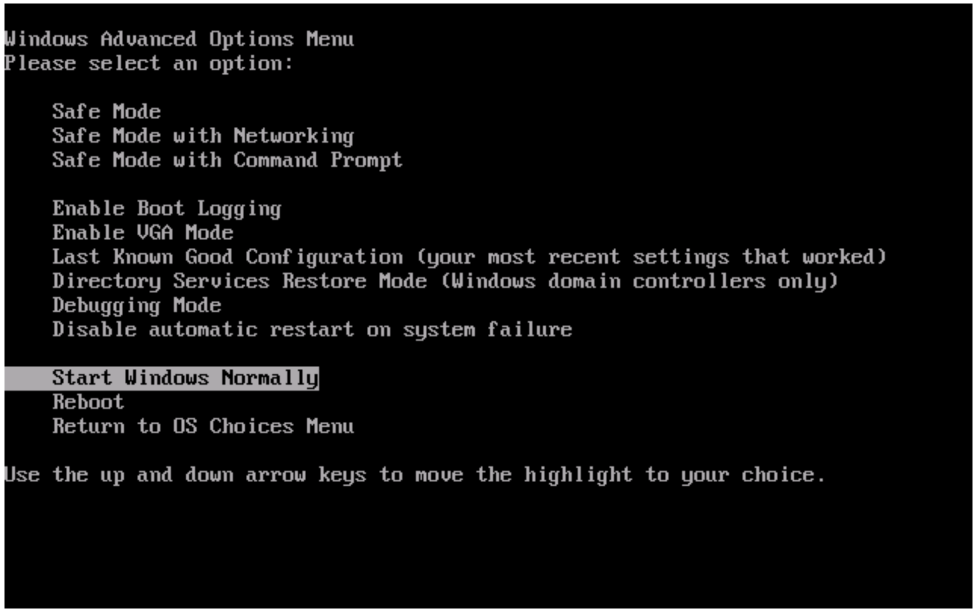
Error Checks Are Essential

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

What to do if a check fails

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



```
Windows Advanced Options Menu
Please select an option:

    Safe Mode
    Safe Mode with Networking
    Safe Mode with Command Prompt

    Enable Boot Logging
    Enable VGA Mode
    Last Known Good Configuration (your most recent settings that worked)
    Directory Services Restore Mode (Windows domain controllers only)
    Debugging Mode
    Disable automatic restart on system failure

    Start Windows Normally
    Reboot
    Return to OS Choices Menu

Use the up and down arrow keys to move the highlight to your choice.
```

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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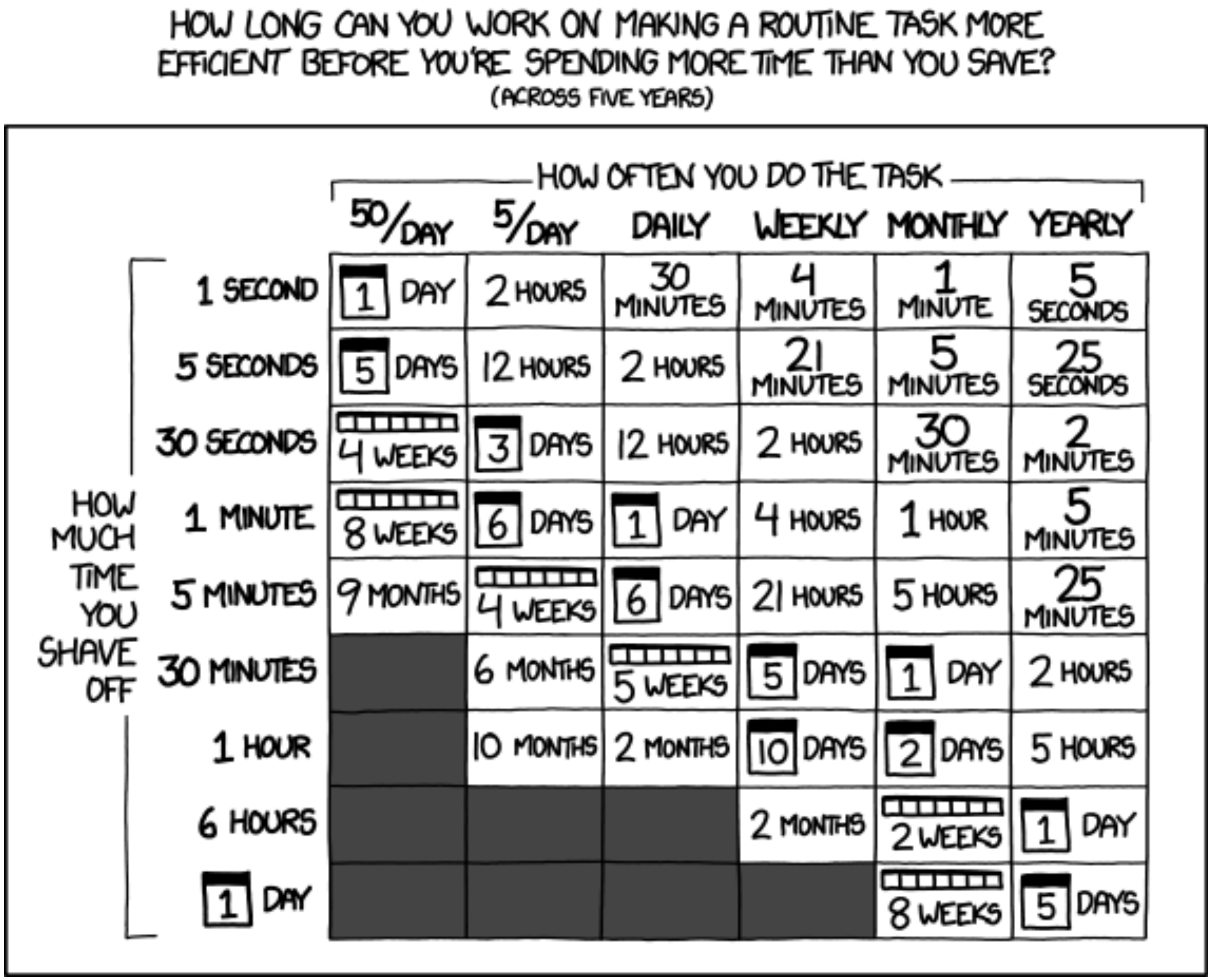
Automate *All* The Things

- 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



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/

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

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PARTING THOUGHTS

Make It Run Faster? Maybe.

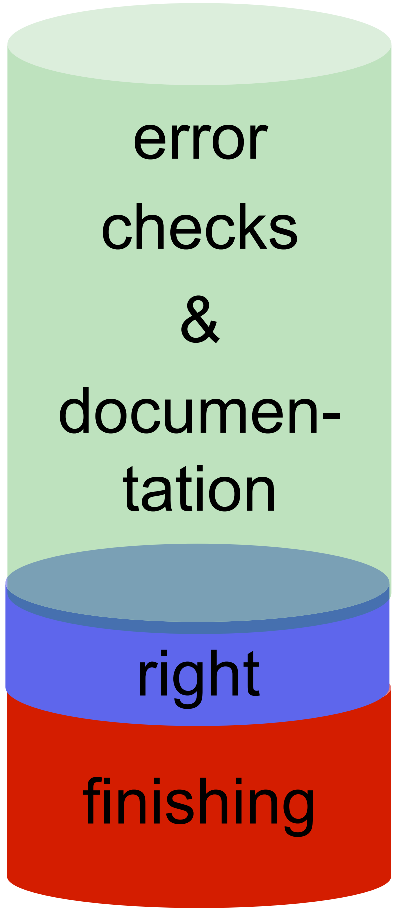
- Throughput, throughput, throughput
  - Resource reductions (match more slots!)
  - Wall-time reductions
    - if significant *per workflow*
    - Why not *per job*?
- Think in orders of magnitude:
  - Say you have 1000 hour-long jobs that are matched at a rate of 100 per hour …

Waste the computer's time, not yours.

If HTC workflows were a test…

- 20 points for finishing at all
- 10 points for the right answer
- 1 point for every error check
- 1 point per documentation line

Out of 100 points? 200 points?



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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

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Questions?

- Now: Exercises 2.1 (2.2 Bonus)
- Next:
  - HTC Showcase!