Running Jobs on the Open Science Grid

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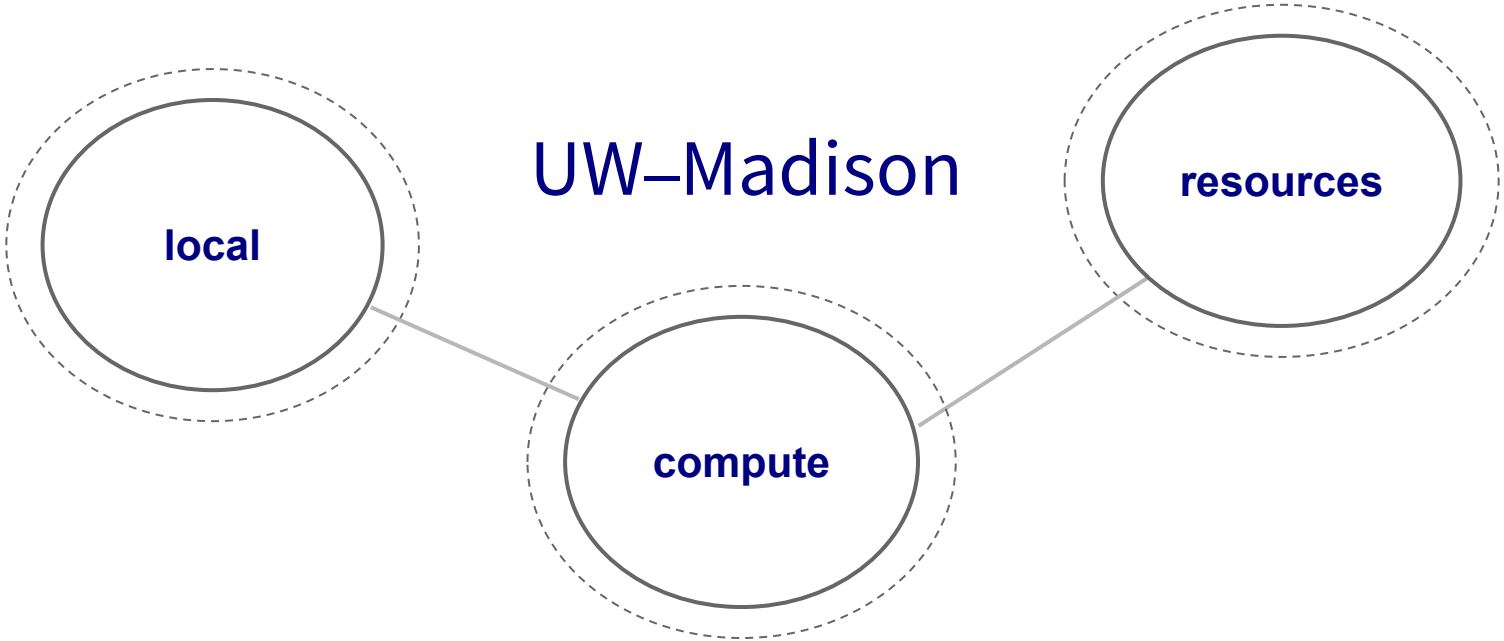
Local High Throughput Computing



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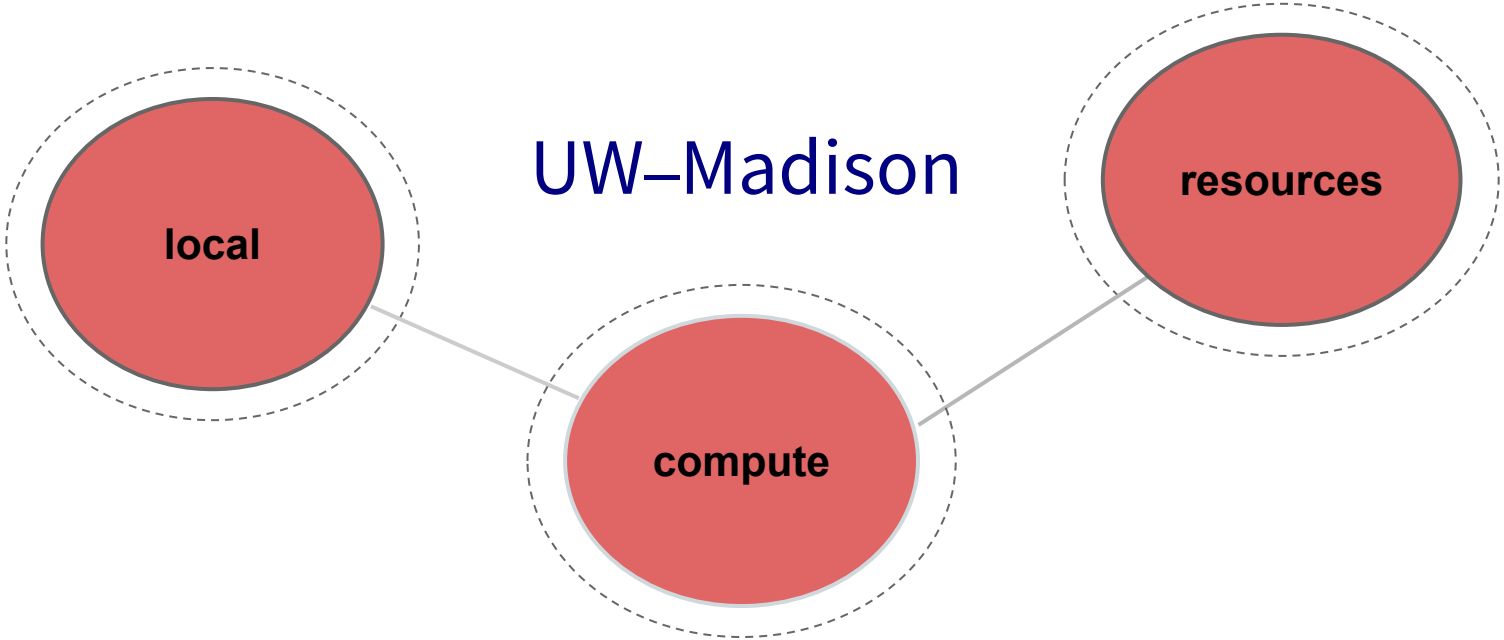


How do you get more computing resources?

#1: Buy Hardware

- Great for specific hardware/privacy requirements
- Costs $$$
  - Initial cost
  - Maintenance
  - Management
  - Power and cooling
- Rack/floor space
- Obsolescence
- Plan for peak usage, pay for all usage
- Delivery and installation takes time

#2: Use the Cloud - Pay per cycle

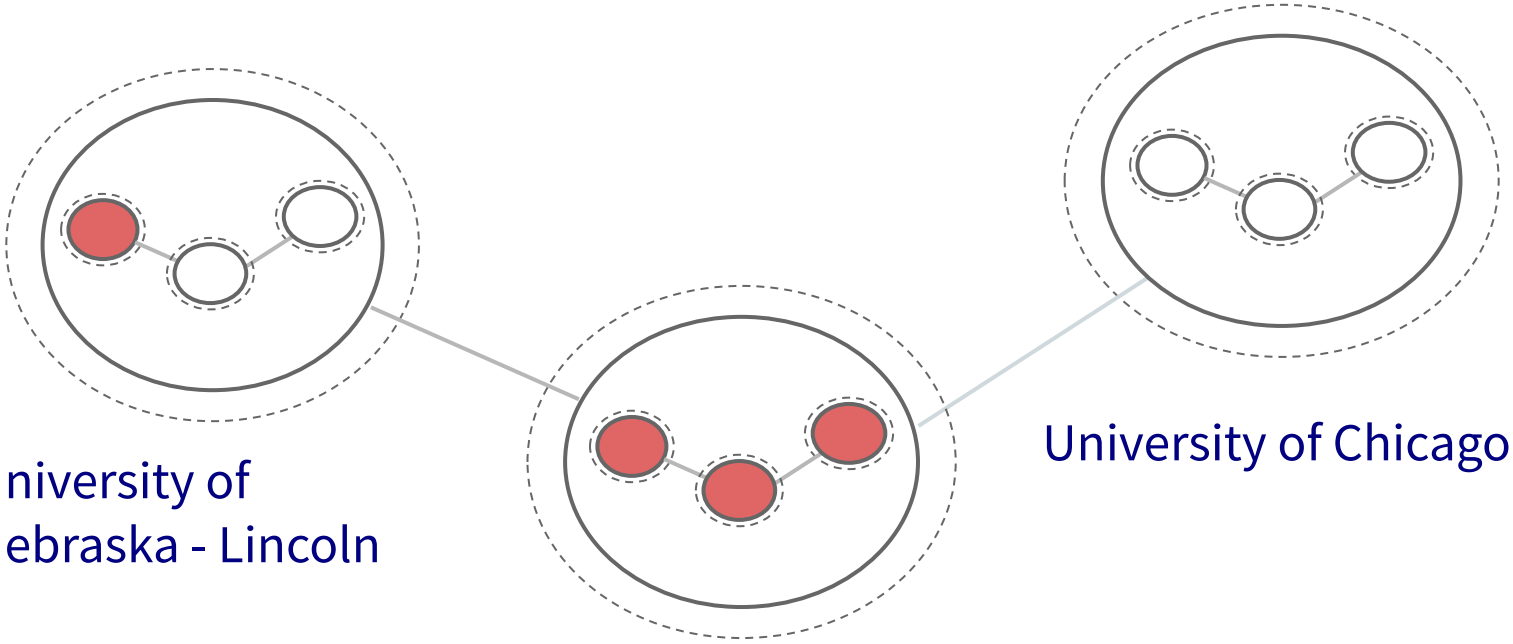
- Amazon Web Services, Google Compute Engine, Microsoft Azure, etc.
- Fast start-up
- Costs $$$
- Still needs expertise + management
  - Easier than in the past with the `condor_annex` tool
- Does payment fit with your institutional or grant policies?

#2: Use the Cloud - 'Managed' clouds

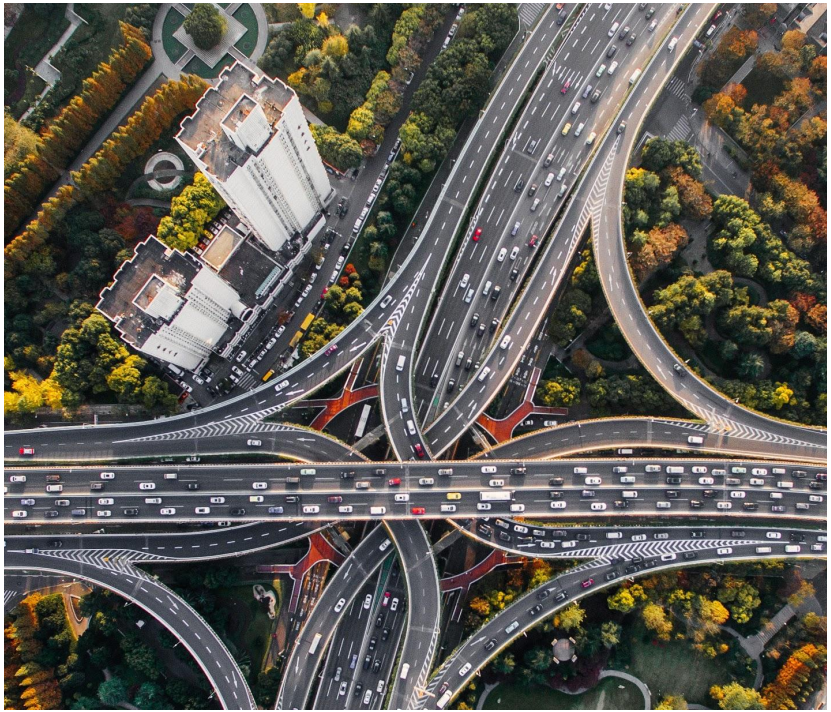
- Cycle Computing, Globus Genomics
- Pay someone to manage your cloud resources — still costs $$$
- Researchers and industry have used this to great success
  - Using Docker, HTCondor, and AWS for EDA Model Development
  - Optimizations in running large-scale Genomics workloads in Globus Genomics using HTCondor
  - HTCondor in the enterprise
  - HTCondor at Cycle Computing: Better Answers. Faster.

#3: *Distributed* High Throughput Computing (dHTC)

#3: Share Resources - Distributed HTC



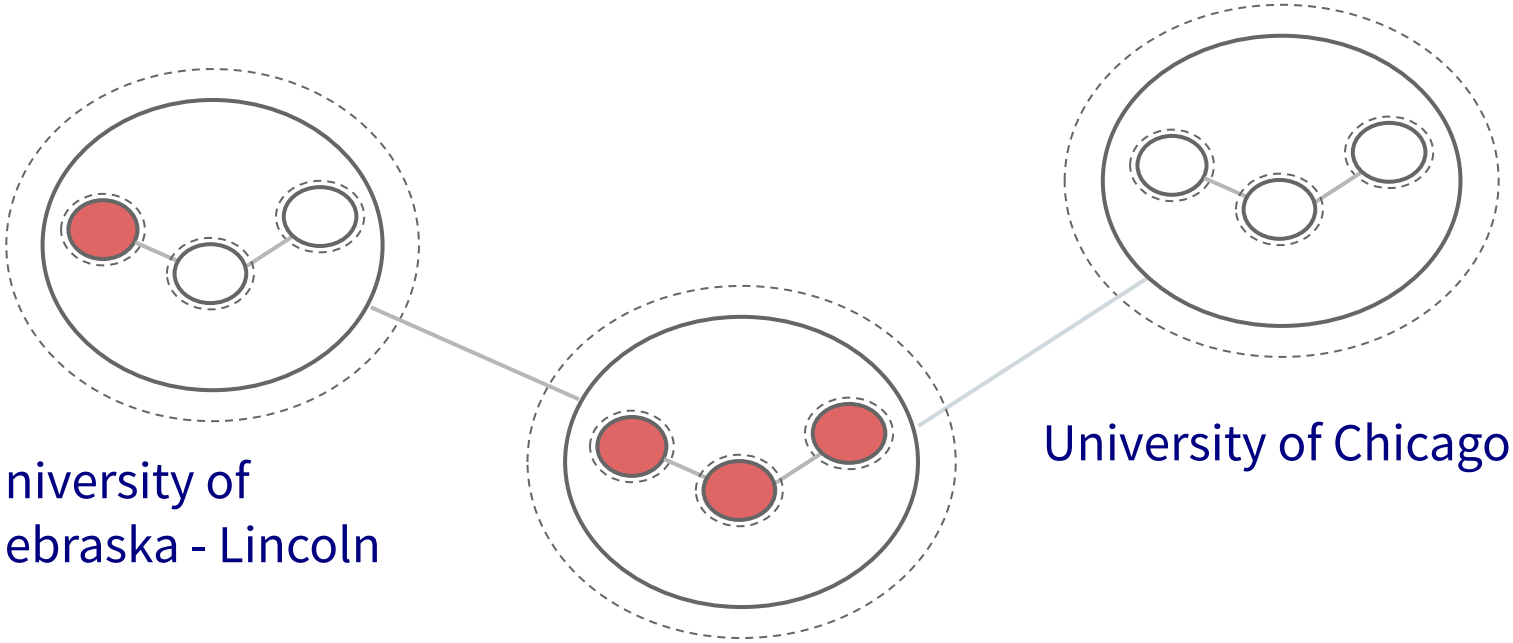
Manual Job Division



- Obtain login access
- Query each cluster for idle resources
- Divide and submit jobs based on resource availability

Photo by Denys Nevozhai on Unsplash

#3: Share Resources - Distributed HTC



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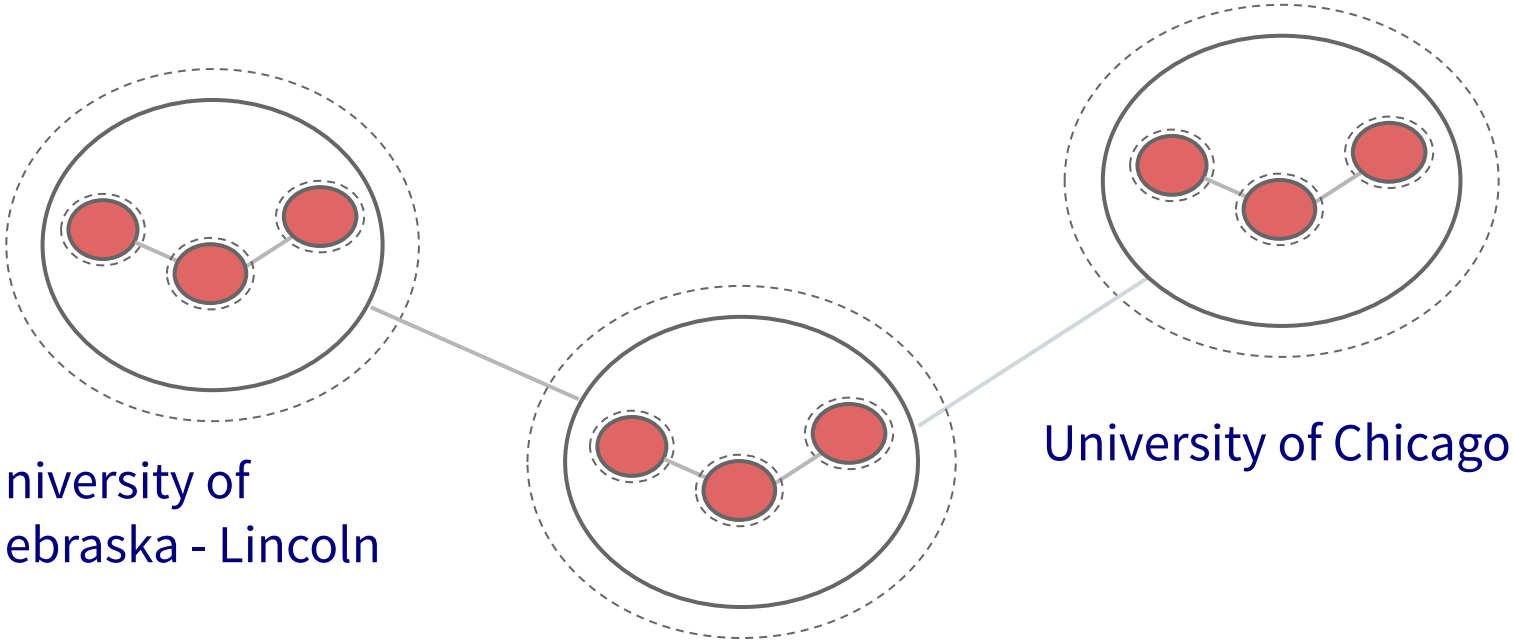


Manual Job Division - Shortcomings

- Fewer logins = fewer potential resources, more logins = more account management
- How will you get accounts?
- Not all clusters use HTCondor — other job schedulers e.g., Slurm, PBS/Torque, etc.
- Querying clusters and dividing jobs is tedious and inaccurate

Automatic Job Division - Shortcomings

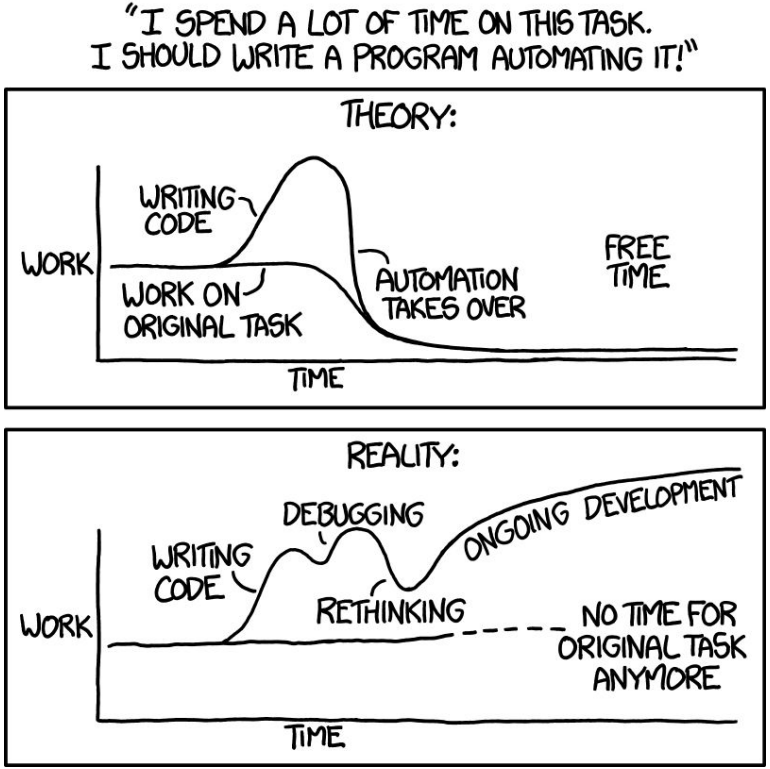
Homer: Kids: there's three ways to do things; the right way, the wrong way and the Max Power way!

Bart: Isn't that the wrong way?

Homer: Yeah, but faster!

Groening, M (Writer), Michels, P. (Director) . (1999). Homer to the Max [Television Series Episode]. In Scully, M. (Executive Producer), *The Simpsons.* Los Angeles, CA: Gracie Films

Automatic Job Division - Shortcomings

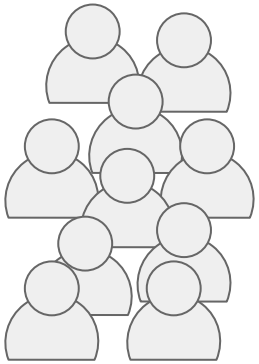


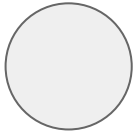
Source: https://xkcd.com/1319/

#3: Share Resources - Requirements

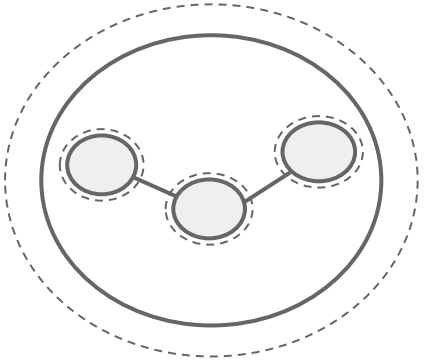
- Minimal account management
- No job division
- HTCondor only!
- No resource contribution requirements

The OSG Model



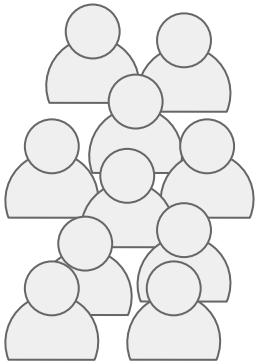


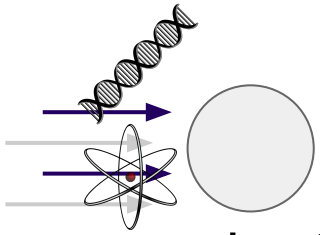
OSG Submit and CM



Cluster

The OSG Model





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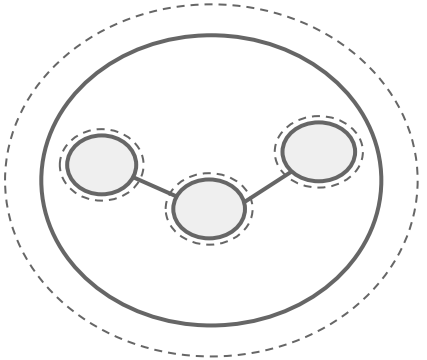

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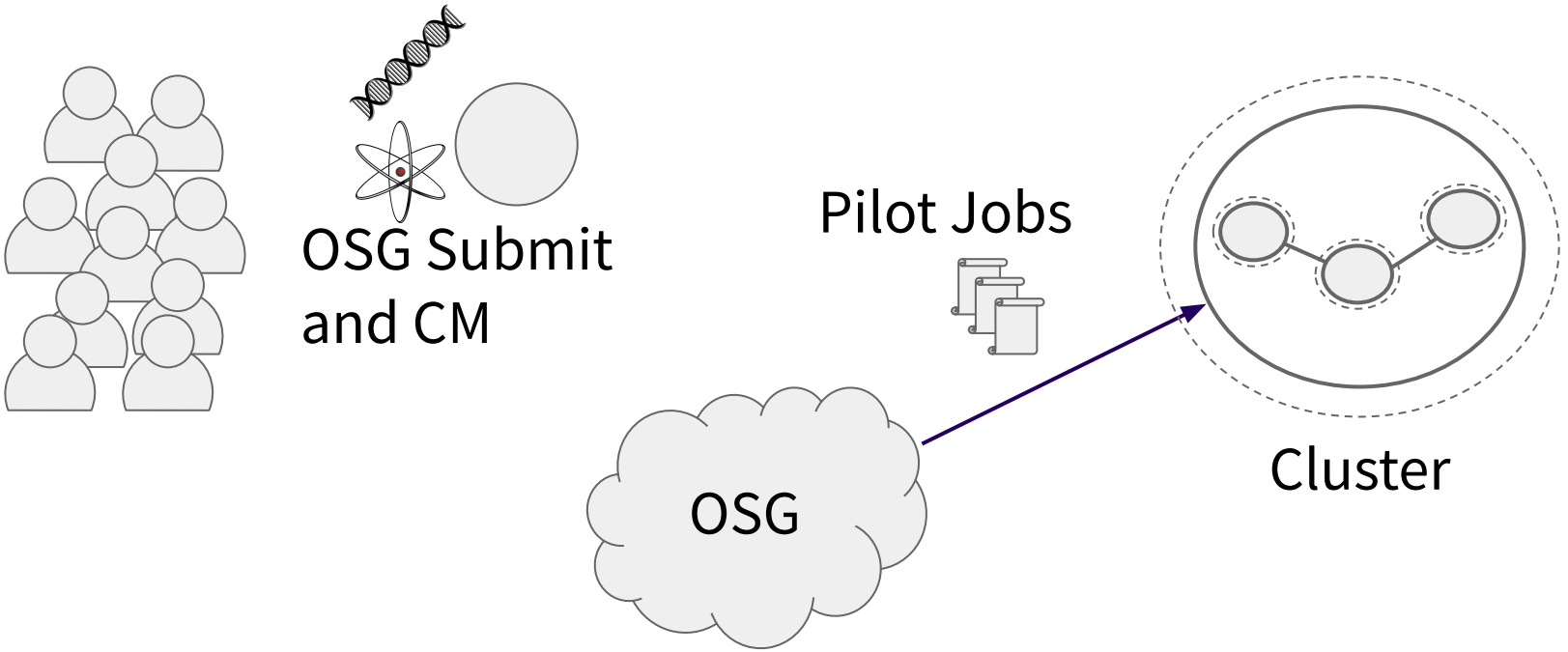

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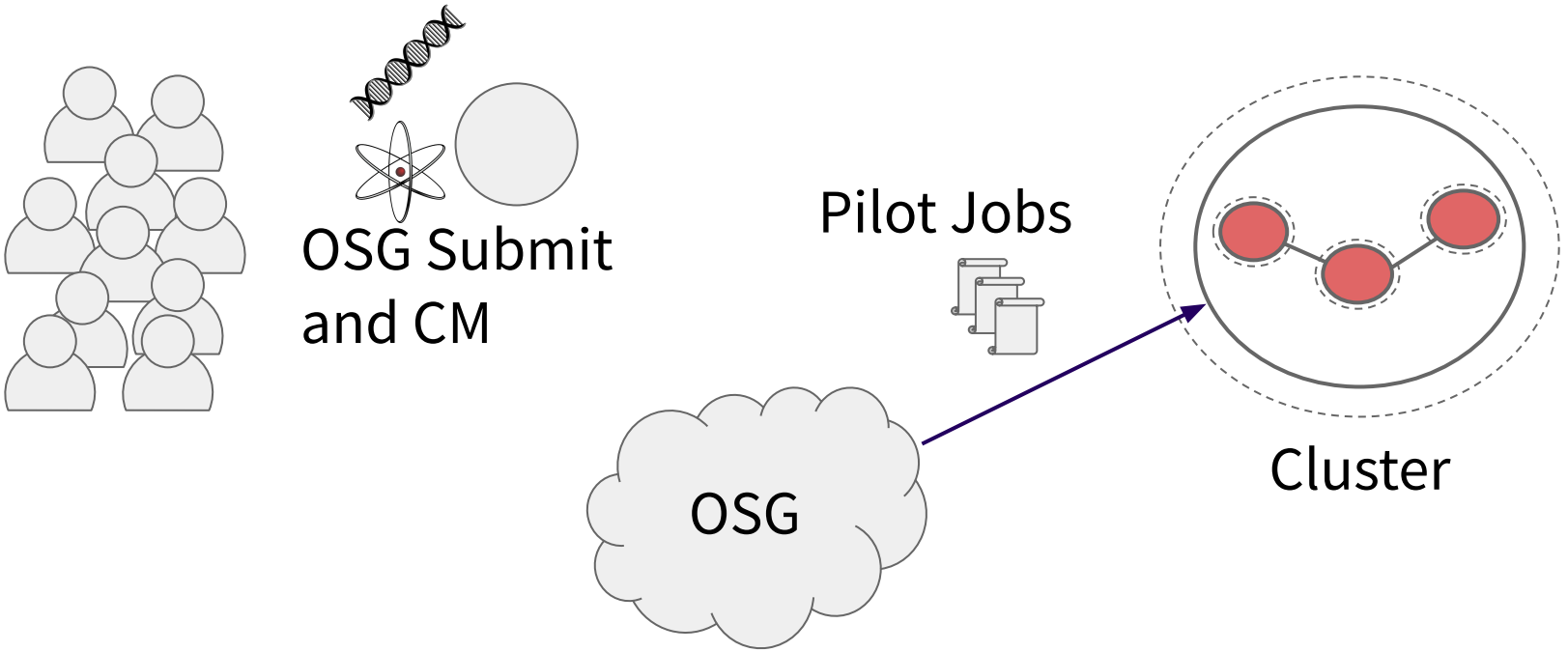
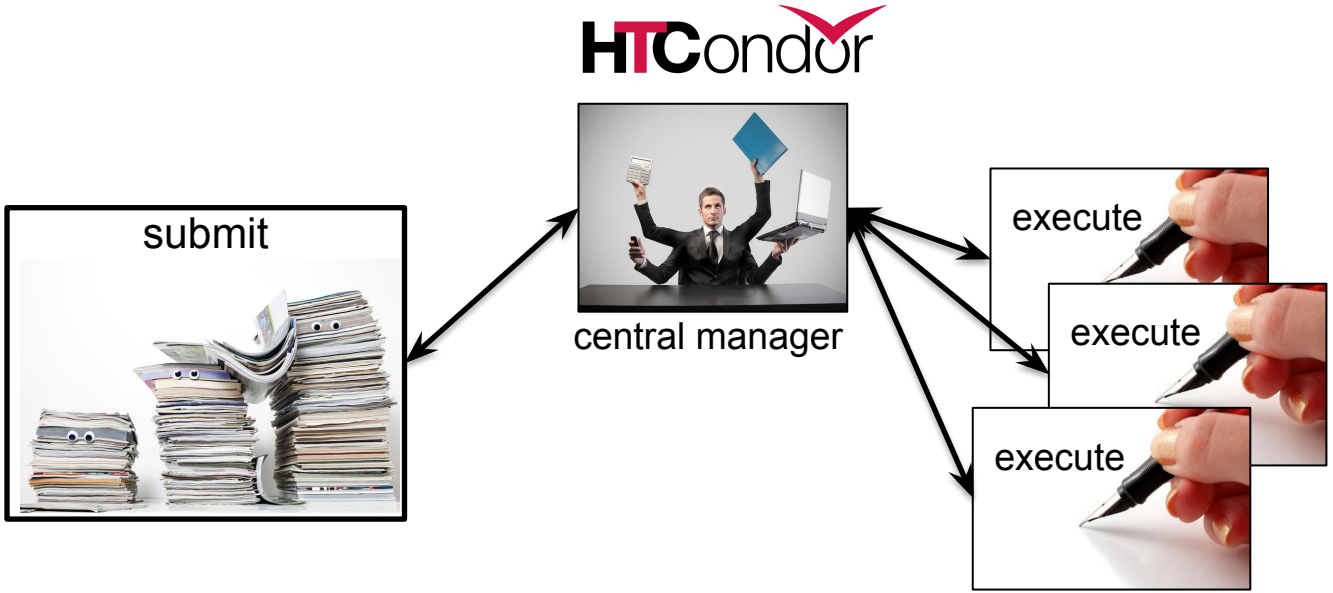


Job Matching

- On a regular basis, the central manager reviews Job and Machine attributes and matches jobs to slots.



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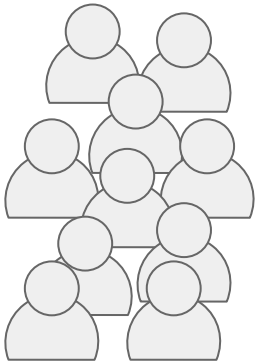

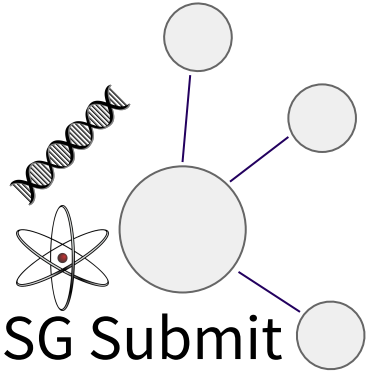

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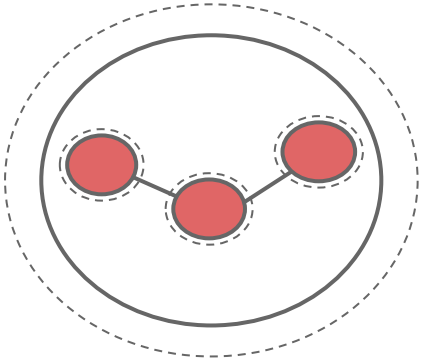

Cluster

The OSG Model - Jobs in Jobs

Photo Credit: Shereen M, Untitled, Flickr https://www.flickr.com/photos/shereen84/2511071028/ (CC BY-NC-ND 2.0)

The OSG Model - Details

- Pilot jobs (or pilots) are special jobs
- Pilots are sent to clusters with idle resources
- Pilot payload = HTCondor execute server software
- Execute server reports to the Open Science pool
- Pilots lease resources from OSG clusters:
  - Lease expires after a set amount of time or lack of demand
  - Leases can be revoked!
- On average, the Open Science pool has 10k total cores and most users get 500+ cores at a time!

#3: Share Resources - Requirements

- Minimal account management: only one submit server
- No job division: only one HTCondor pool
- HTCondor only: pilots report back as HTCondor slots, you'll be using an HTCondor submit server
- No resource contribution requirements: the OSG doesn't require that users "pay into" the OSG. Approved researchers can use OSG for free!

The OSG Model - Collection of Pools

- Your jobs will run in the Open Science pool (open to individual researchers and campuses)
- The Open Science pool is one of many!
- Separate pools for each Virtual Organization (VO)

Photo by Martin Sanchez on Unsplash

The OSG Model - Collection of Pools

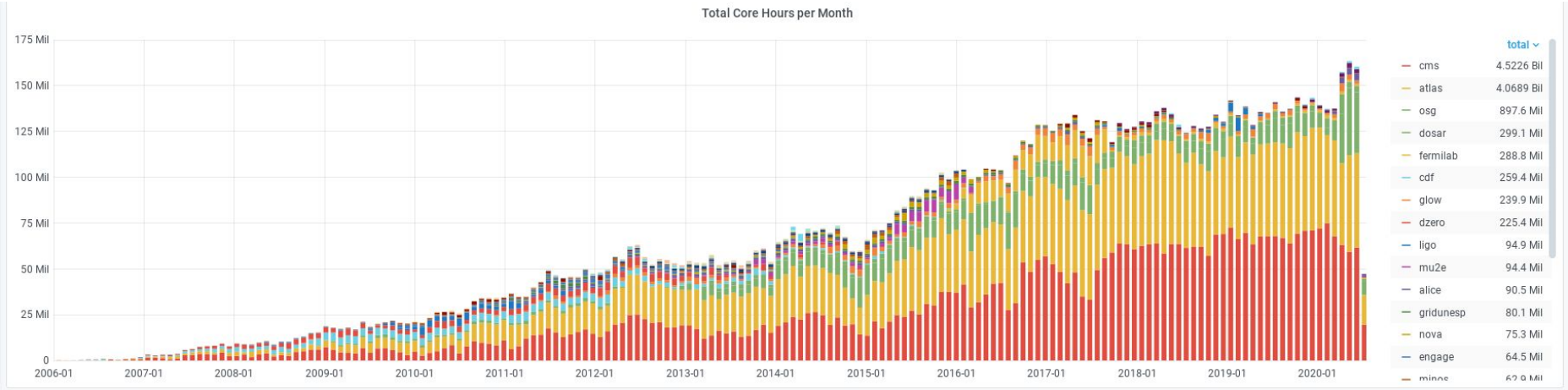

Photo by Martin Sanchez on Unsplash

Pilot jobs are awesome!

Photo by Zachary Nelson on Unsplash

What's the Catch?

dHTC requires complex machinery but OSG manages the hard bits so you don't have to!

#1: Heterogenous Resources

Accounting for differences between the
OSG and your local cluster

Clusters of the OSG

Source: http://display.opensciencegrid.org/

Het. Resources - Software

- Different variants of Linux (Red Hat based)
- Varying software versions (e.g., at least Python 2.6)
- Varying software availability (e.g., no BLAST*)

Solution: Make your jobs more portable (more in tomorrow's talk and exercises)

Het. Resources - Hardware

- CPU: Mostly single core
- RAM: Mostly < 8GB
- GPU: Limited #s but more being added
- Disk: No shared file system (more next Tuesday)

Solution: Where possible, split up your workflow to make your jobs more high throughput!

#2: With Great Power Comes Great Responsibility

How to be a good netizen

Resources You Don’t Own

- Primary resource owners can kick you off for any reason (generally if your job is using too many resources)
- No local relationships
- No sensitive data!

Photo by Nathan Dumlao on Unsplash

Be a Good Netizen!

- Use of shared resources is a privilege
- Only use the resources that you request
- Be nice to your submit servers

Solution: Test jobs on local resources with `condor_submit -i` (covered in tomorrow's exercises)

#3: Slower Ramp Up

Leasing resources takes time!

Slower Ramp Up

- Adding slots: pilot process in the OSG
  vs slots already in your local pool
- Not a lot of time (~minutes) compared to most job runtimes (~hours)
  - Small trade-off for increased availability
  - Tip: If your jobs only run for < 10min each, consider combining them so each job runs for at least 30min

Job Robustification

- Test small, test often
- Specify `output`, `error`, and `log` files at least while you develop your workflow
- In your own code:
  - Storing intermediate results (i.e., self checkpointing)
  - Defensive troubleshooting (`hostname`, `ls -l`, `pwd`, `condor_version` in your wrapper script)
  - Add simple logging (e.g. print, echo, etc). Be strategic and don't fill your disk with logs!

#4: dHTC Security

The internet can be a scary place!

dHTC Security

- OSG does its best but security is a game of risk mitigation, not perfection
  - OSG uses secure technologies to verify the identities of distributed servers
  - OSG Security Team tracks software vulnerabilities and responds to security incidents
- Not just any old cluster or user can join the OSG! VOs approve users, cluster owners verify servers, and OSG verifies clusters
- But there are thousands of servers and users!

So What Can You Do?

- You are using a shared computer that you don't own so take basic precautions!
- Protect your data:
  - No files that can be overwritten by other users (i.e., not world writable)
  - No private data or software
- Protect your account
  - Do not share your account
  - Use good passwords (and a password manager)
  - Use SSH keys wherever possible

Questions?

Coming next:

- Grid exercises: https://opensciencegrid.org/virtual-school-pilot-2020/#materials/#grid
  - New submit host: login04.osgconnect.net
  - Set a default project for your login04 account:
    ```
    $ connect project
    ```
- Tomorrow: Working with real software
- Bonus topic next Wednesday: more grid!