Open Science Grid

RESEARCH DATA ALLIANCE U.S.

The Landscape of Academic Research Computing

The African School of Fundamental Physics 2022

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Some Slides Contributed by the University of Wisconsin HTCondor Team and Scot Kronenfeld

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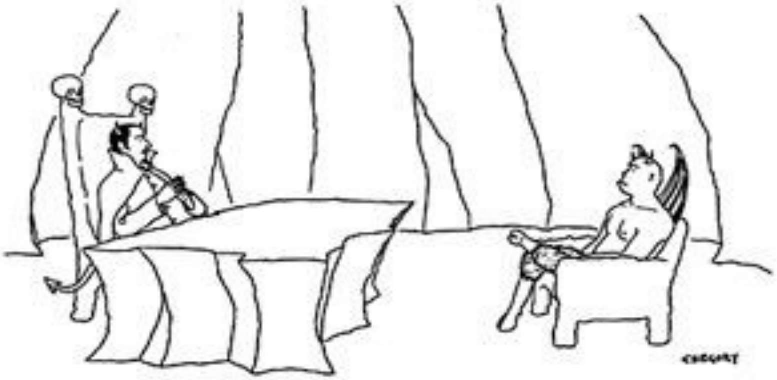
Follow Along at:

https://osg-htc.org/dosar/ASP2022/ASP2022_Materials/

DOSAR: Distributed Organization for Scientific & Academic Research

Overview of day

- Lectures alternating with exercises
  - Emphasis on lots of hands-on exercises
  - Hopefully overcome PowerPoint fatigue
- Note: Power Shedding expected to start at noon ➔ We go for an early lunch and return by 1:45pm.



"I need someone well versed in the art of torture—do you know PowerPoint?"

Some thoughts on the exercises

- It's okay to move ahead on exercises if you have time
- It's okay to take longer on them if you need to
- If you move along quickly, try the "On Your Own" sections and "Challenges"

Most important!

- Please ask questions!

  …during the lectures

  …during the exercises

  …during the breaks

  …during the meals

  …via email after we depart

  If we don't know the answers, we'll find the right people to answer your questions.

Goals for this lecture

- Define Local, Clustered, High Throughput Computing (HTC), High Performance Computing (HPC), and Cloud Computing (XaaS – Anything as a Service)
- Shared, Allocated, and Purchased resources
- What is HTCondor? And why are we using it in this school?

The setup: You have a problem

- Your science computing is complex!
  - Monte Carlo simulations, image analysis, genetic algorithm, simulation…
- It will take a year to get the results on your laptop, but the conference is in a week.
- What do you do?

Option 1: Wait a year

Option 2: Local Clustered Computing

- Easy access to additional nodes
- Local support for porting to environment (maybe)
- Often a single type of resource
- Often running at capacity

Option 3: Use a "supercomputer" aka High Performance Computing(HPC)

- "Clearly, I need the best, fastest computer to help me out"
- Maybe you do…
  - Do you have a highly parallel program?
    - i.e. individual modules must communicate
  - Do you require the fastest network/ disk/ memory?
- Are you willing to:
  - Port your code to a special environment?
  - Request and wait for an allocation?

Option 4: Use lots of commodity computers

- Instead of the fastest computer, lots of individual computers
- May not be fastest network/disk/memory, but you have a lot of them
- Job can be broken down into separate, independent pieces
  - If I give you more computers, you run more jobs
  - You care more about **total quantity** of results than instantaneous speed of computation
- This is **high-throughput computing (HTC)**

Option 5: Buy (or Borrow) some computing from a Cloud Provider

- Unlimited resources (if you can afford them)
- Full administrative access to OS of the resources you 'buy'
- Specialized VM images reducing effort in porting
- XaaS Business Model

These are All Valid Options

- Remember the problem you have one month to publish results for your conference
  - Option 1: You WILL miss your deadline
  - Option 2: You might miss your deadline – But if your lucky you'll make it (or if you know the admin)
  - Option 3: If you have parallelized code and can get an allocation you have a good chance
  - Option 4: If you can serialize your work-flow you have a good chance
  - Option 5: You can meet your deadline for a price. Though some efforts are underway to enable academic clouds

Computing Infrastructure

- Local Laptop/Desktop – Short jobs with small data
- Local Cluster – Larger jobs and larger data but subject to availability
- HPC – Prime performance with parallelized code
- HTC – Sustained computing over a long period for serialized workflow
- Cloud – Need deeper permission on an OS and have deeper pockets

Why focus on high-throughput computing? (HTC)

- An approach to distributed computing that focuses on long-term throughput, not instantaneous computing power
  - We don't care about operations per second
  - We care about operations per year
- Implications:
  - Focus on reliability
  - Use all available resources
    - Any Linux based machine can participate

Think about a race

- Assume you can run a 2-minute km
- Does that mean you can run a 80 minute marathon?
- The challenges in sustained computation are different than achieving peak in computation speed

An example problem: BLAST

- A scientist has:
  - Question: Does a protein sequence occur in other organisms?
  - Data: lots of protein sequences from various organisms
  - Parameters: how to search the database.
- More throughput means
  - More protein sequences queried
  - Larger/more protein data bases examined
  - More parameter variation

Why is HTC hard?

- The HTC system has to keep track of:
  - Individual tasks (a.k.a. jobs) & their inputs
  - Computers that are available
- The system has to recover from failures
  - There will be failures! Distributed computers means more chances for failures.
- You have to share computers
  - Sharing can be within an organization, or between orgs
  - So you have to worry about security
  - And you have to worry about policies on how you share
- If you use a lot of computers, you have to handle variety:
  - Different kinds of computers (arch, OS, speed, etc..)
  - Different kinds of storage (access methodology, size, speed, etc…)
  - Different networks interacting (network problems are hard to debug!)

Let's take one step at a time

Small → Large

Local → Distributed

- Can you run one job on one computer?
- Can you run one job on another computer?
- Can you run 10 jobs on a set of computers?
- Can you run a multiple job workflow?
- How do we put this all together?

This is the path we'll take

Discussion

- For 5 minutes, talk to a neighbor: If you want to run a multi-job workflow in a distributed environment:
  1) What do you (the user) need to provide so a single job can be run?
  2) What does the system need to provide so your single job can be run?
     - Think of this as a set of processes: what needs to happen when the job is given? A "process" could be a computer process, or just an abstract task.

What does the user provide?

- A "headless job"
  - Not interactive/no GUI: how could you interact with 1000 simultaneous jobs?
- A set of input files
- A set of output files
- A set of parameters (command-line arguments)
- Requirements:
  - Ex: My job requires at least 2GB of RAM
  - Ex: My job requires Linux
- Control/Policy:
  - Ex: Send me email when the job is done
  - Ex: Job 2 is more important than Job 1
  - Ex: Kill my job if it runs for more than 6 hours

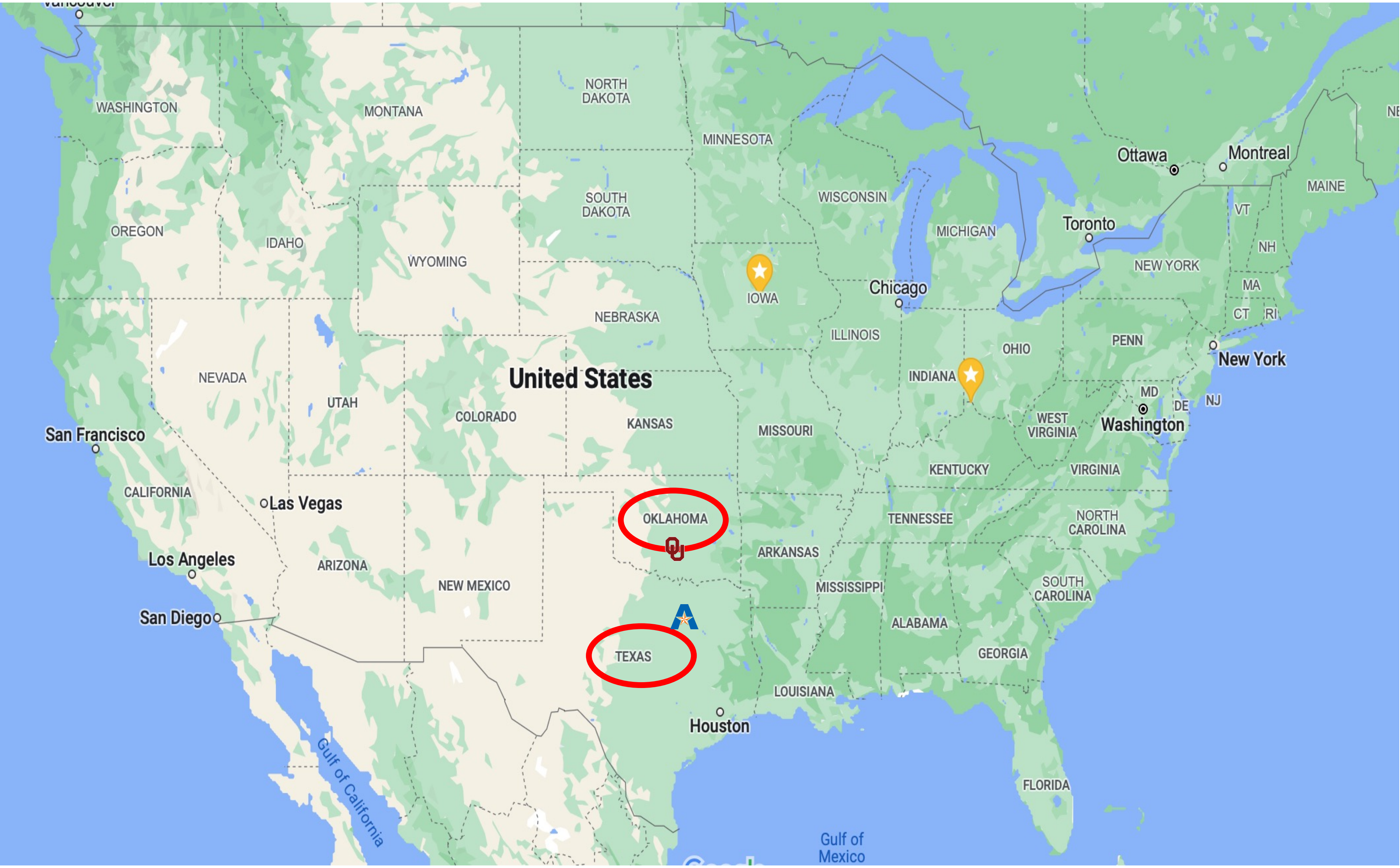
What does the system provide?

- Methods to:
  - Submit/Cancel job
  - Check on state of job
  - Check on state of available computers
- Processes to:
  - Reliably track set of submitted jobs
  - Reliably track set of available computers
  - Decide which job runs on which computer
  - Manage a single computer
  - Start up a single job

Quick UNIX Refresher Before We Start

- **$** #This symbolizes the prompt.
- **nano**, vi, emacs, cat >, etc.
- **which, rpm, ps,** mkdir, cd, **gcc,** ls
- A variety of condor_* commands

Where are your lecturers from?



Questions?

- Questions? Comments?
  - Feel free to ask us questions now or later:
  - Jaehoon Yu jaehoonyu1@gmail.com
  - Horst Severini hs@nhn.ou.edu
  - Pat Skubic pskubic@ou.edu

  Exercises start here:

  https://osg-htc.org/dosar/ASP2022/ASP2022_Materials/

  Presentations are also available from this URL.