

The Landscape of Academic Research Computing

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Director Cyberinfrastructure Integration Research Center

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



Who Am I?

- Director Cyberinfrastructure Integration Research Center
- NSF PI – A Gateway for the Event Horizon Telescope
- NSF Co-PI – Cyberwater – Interop of hydrology, biology, environmental engineering and climate datasets.
- NIH Co-PI - Informing mechanistic rules of agent-based models with single-cell multi-omics
- Co-chair CODATA/RDA School of Research Data Science Initiative
- Co-chair of the Technical and Organizational Advisory Boards for RDA
- Steering Committee FAIR Digital Object Forum
- 12+ Years - Chief Operations Officer of the Open Science Grid and the Software Assurance Marketplace
- Ph.D. Candidate – Luddy School of Informatics, Computing, and Engineering
- Lecturer – Fairbanks School of Public Health

Infrastructure

- What is infrastructure?
- What are some examples?
- What is Cyberinfrastructure?
- What are some examples?
- What would this week have looked like without CI?












Protein Docking Project at the IU School of Medicine

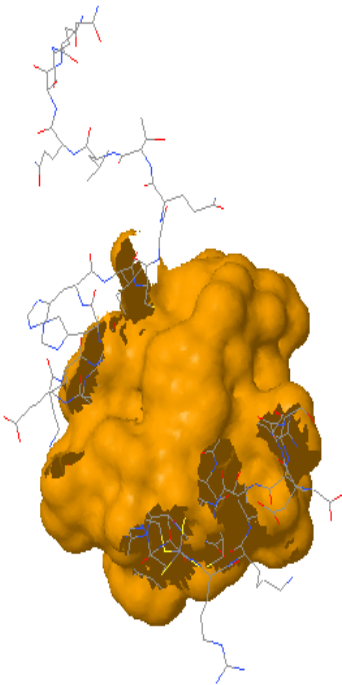
- SPLINTER - Structural Protein-Ligand Interactome
- Used autodock-vina – “...open-source program for drug discovery, molecular docking and virtual screening...”
- First run - docked ~3900 Proteins with 5000 Ligands for a total of ~19M docked pairs.
- Submitted via command line to Condor using Pegasus on the OSG-XSEDE submission node
- Infrastructure is set and new runs can be easily started
- To date more than 6.3B dockings completed



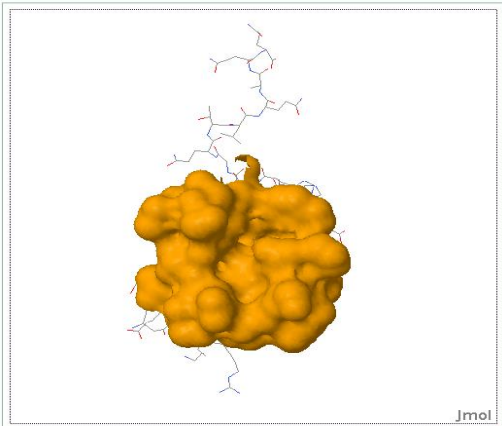


•Various rotations of Protein CBFA2T1 (Cyclin-D-related protein) (Eight twenty one protein) (Protein ETO) (Protein MTG8) (Zinc finger MYND domain-containing protein 2)

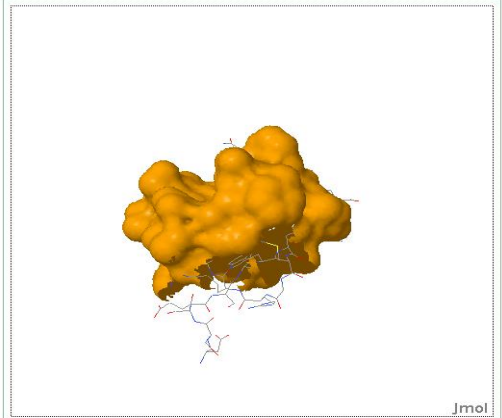
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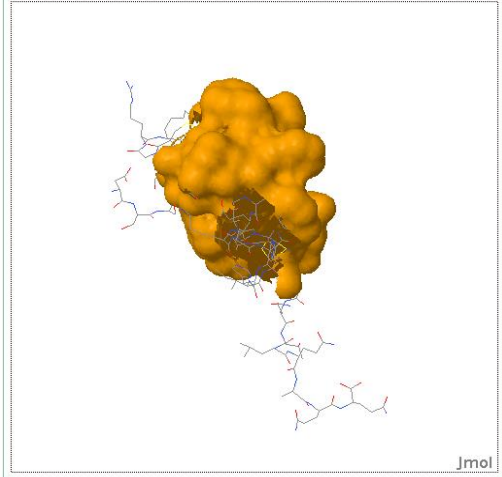
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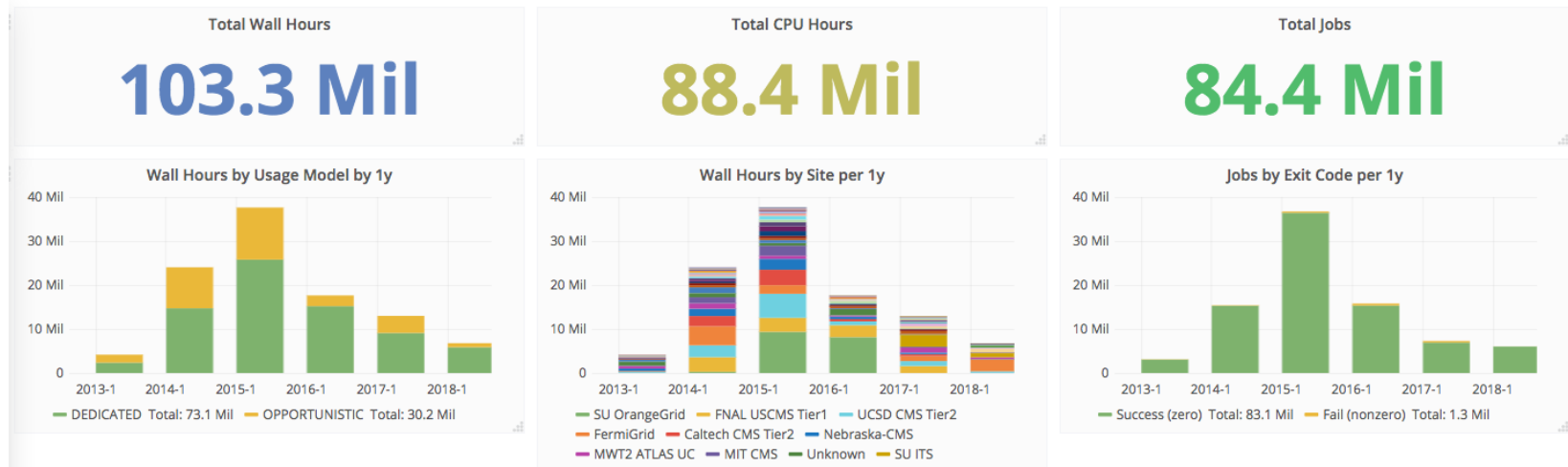
Jmol



Jmol



Jmol



- Amazon EC2 Computing \$0.046/hour
- \$4.066M Compute Only
- Data Transfer and Storage Not Included

Follow Along at:

<https://github.com/CODATA-RDA-DataScienceSchools/Materials/tree/master/docs/DataTrieste2023/CI>

Some thoughts on the exercise

- 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
 - ...over dinner
 - ...via email after we depart (rquick@iu.edu)
- If I don't know, I'll find the right person to answer your question.

Goals for this session

- Define Local, Clustered, High Throughput Computing (HTC), High Performance Computing (HPC), Cloud Computing (XaaS), and Containers
- Shared, Allocated, and Purchased

The setup: You have a problem

- Your science computing is complex!
 - Monte carlo, image analysis, genetic algorithm, simulation, ML or AI algorithms...
- It will take a year (CPU time) to get the results on your laptop, but your paper is due 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 can access 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**





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 week 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 workflow you have a good chance
 - Option 5: You can meet your deadline for a price. Though academic clouds are becoming more available.

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



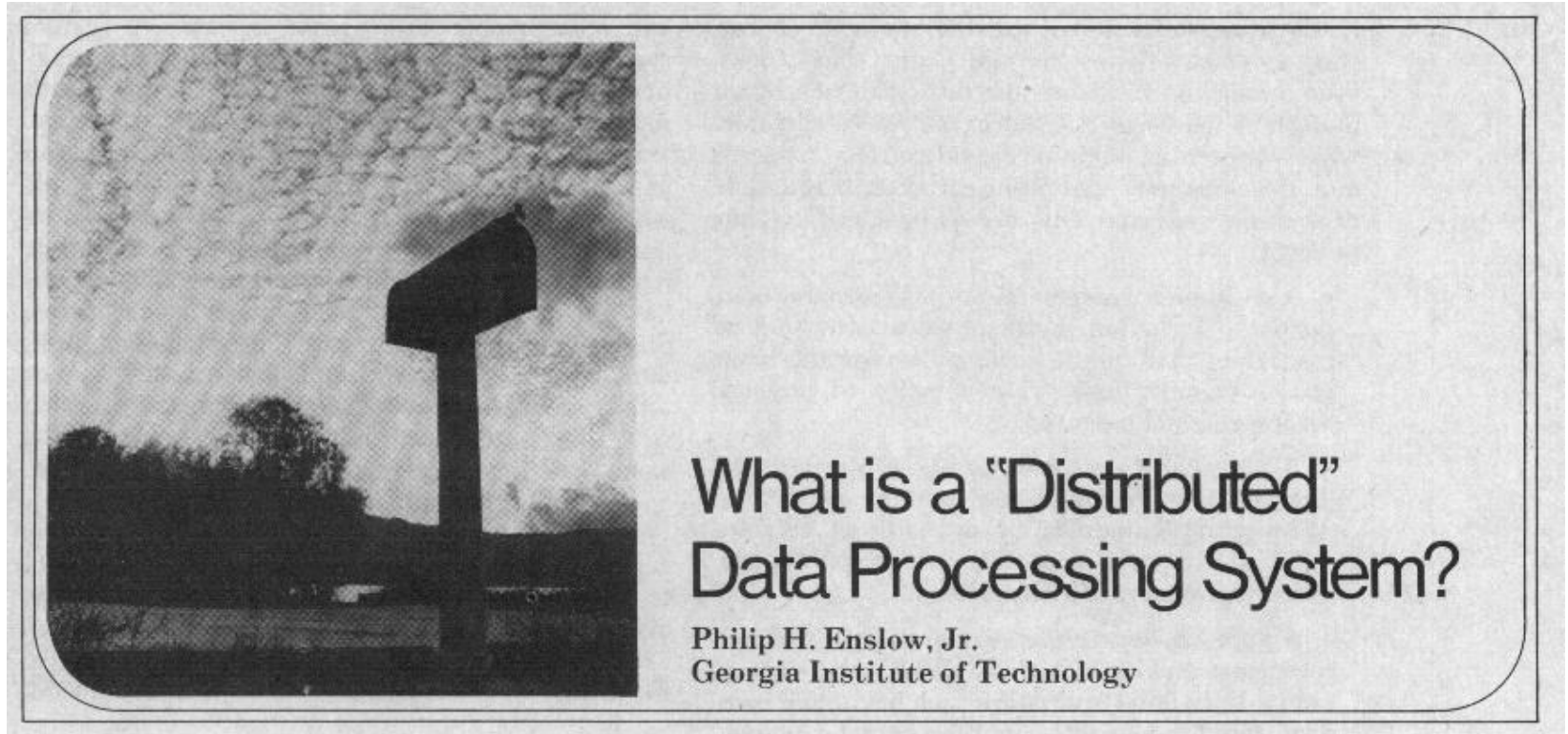
Why focus on high-throughput computing? (HTC)

- An approach to distributed computing that focuses on long-term throughput, not instantaneous computing power
- The lessons learned in HTC environments and HTCCondor are easily applied to other clustered or HPC systems
- We have access to an international HTC system to show the power of distributed computing



*Only that shall happen
Which has happened,
Only that occur
Which has occurred;
There is nothing new
Beneath the sun!*

Ecclesiastes Chapter 1 verse 9

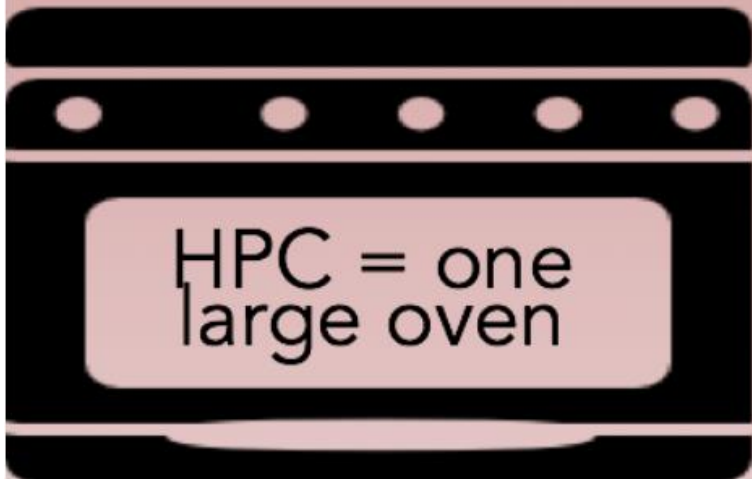


HPC vs HTC

- You've decided you want to bake a cake large enough to break the World's Record for wedding cakes.
- Currently WR 6.818 tonnes (15,032 lb)
- You could approach this two ways...



The HPC Approach



A special oven

Expensive to build & maintain

Scheduling use



The HTC Approach



High throughput
Many ovens working
independently,
outputs assembled
afterwards



- For 5 minutes, talk to a neighbor: If you want to run a 100 job parameter sweep in a local 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 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 scheme of output
- A set of parameters (command-line arguments)
- Requirements:
 - Ex: My job requires at least 2GB of RAM
 - Ex: My job requires 2 CPUs
- 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 resources
- Processes to:
 - Reliably track set of submitted jobs
 - Reliably track set of available resources
 - Decide which job runs on which resource
 - Manage a single computer
 - Start up a set of jobs

Questions?

- Questions? Comments?
 - Feel free to ask me questions now or later:
Rob Quick rquick@iu.edu

Exercises start here:

<https://github.com/CODATA-RDA-DataScienceSchools/Materials/blob/master/docs/DataTrieste2024/CI/>

Slides are also available from this URL.

SoRDS Community Map

<http://bit.ly/SoRDS-Trieste>

