

# Profiling Applications to Choose the Right Computing Infrastructure plus Batch Management with HTCondor

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# Follow Along at:

<https://github.com/CODATA-RDA-DataScienceSchools/Materials/tree/master/docs/DataTrieste2023AdvancedWorkshop/HighThroughput>



# 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 me 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

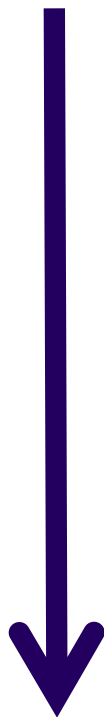
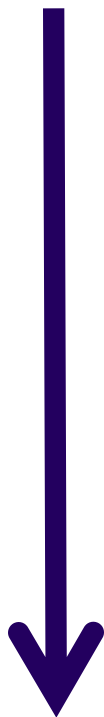
- Profiling your application
- Picking the appropriate resources
- Understand the basics of HTCondor



# Let's take one step at a time

Small

Local



Large

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 in the school



# 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



# Large Jobs

- Let's assume you have a 'large job'
  - What factors could make it large?
- Large Data Input or Output or both
- Needs to do heavy calculation
- Needs a lot of memory
- Needs to communicate with other jobs (whether required or not)
- Reads and writes a lot of data/files
- Heavy graphics processing
- Any combination of any of the above

# There is no “One Size Fits All Solution”

- But some solutions are more “Open” than others.
  - Local Laptop/Desktop
  - Local Cluster
  - HPC System
  - Shared HTC Resources
  - Clouds



# 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!)



# Surprise!

## HTCondor does this (and more)

- Methods to:
  - Submit/Cancel job. `condor_submit/condor_rm`
  - Check on state of job. `condor_q`
  - Check on state of avail. computers. `condor_status`
- Processes to:
  - Reliably track set of submitted jobs. `schedd`
  - Reliably track set of avail. computers. `collector`
  - Decide which job runs on where. `negotiator`
  - Manage a single computer `startd`
  - Start up a single job `starter`

# But not only Condor

- You can use other systems:
  - PBS/Torque
  - Oracle Grid Engine (né Sun Grid Engine)
  - LSF
  - SLURM
  - ...
- But I won't cover them.
  - My experience is with Condor
  - My bias is with Condor
  - Overlays exist
- What should you learn at the school?
  - How do you think about Computing Resources?
  - How can you do your science with HTC?
  - ... For now, learn it with Condor, but you can apply it to other systems.



# A brief introduction to Condor

- Please note, we will only scratch the surface of Condor:
  - We won't cover MPI, Master-Worker, advanced policies, site administration, security mechanisms, submission to other batch systems, virtual machines, cron, high-availability, computing on demand, containers.



# Quick Terminology

- **Cluster**: A dedicated set of computers not for interactive use
- **Pool**: A collection of computers used by Condor
  - May be dedicated
  - May be interactive
- **Remember**:
  - Condor can manage a cluster in a machine room
  - Condor can use desktop computers
  - Condor can access remote computers
  - HTC uses all available resources

# Matchmaking

- Matchmaking is fundamental to Condor
- Matchmaking is two-way
  - Job describes what it requires:  
I need Linux && 8 GB of RAM
  - Machine describes what it requires:  
I will only run jobs from the Physics department
- Matchmaking allows preferences
  - I **need** Linux, and I **prefer** machines with more memory but will run on any machine you provide me





# Why Two-way Matching?

- Condor conceptually divides people into three groups:
    - Job submitters
    - Computer owners
    - Pool (cluster) administrator
- } May or may not be the same people
- All three of these groups have preferences



- ClassAds state facts
  - My job's executable is analysis.exe
  - My machine's load average is 5.6
- ClassAds state preferences
  - I require a computer with Linux
- ClassAds are extensible
  - They say whatever you want them to say



# Example ClassAd

```
MyType           = "Job"      ← String
TargetType       = "Machine"
ClusterId        = 1377      ← Number
Owner            = "roy"
Cmd              = "analysis.exe"
Requirements     =           ← Expression
    (Arch == "INTEL")
    && (OpSys == "LINUX")
    && (Disk >= DiskUsage)
    && ((Memory * 1024) >= ImageSize)
...
```



# Schema-free ClassAds

- Condor imposes some schema
  - Owner is a string, ClusterID is a number...
- But users **can extend it however they like**, for jobs or machines
  - `AnalysisJobType = "simulation"`
  - `HasJava_1_6 = TRUE`
  - `ShoeLength = 10`
- Matchmaking can use these attributes
  - `Requirements = OpSys == "LINUX"`  
`&& HasJava_1_6 == TRUE`



# Don't worry

- You won't write ClassAds (usually)
  - You'll create a simple *submit file*
  - Condor will write the ClassAd
  - You can extend the ClassAd if you want to
- You won't write requirements (usually)
  - Condor writes them for you
  - You can extend them
  - In some environments you provide attributes instead of requirements expressions

# Why do jobs fail?

- The computer running the job fails
  - Or the network, or the disk, or the OS, or...
- Your job might be *preempted*:
  - Condor decides your job is less important than another, so your job is stopped and another started.
  - Not a “failure” per se, but it may feel like it to you.



# Reliability

- When a job fails or is preempted:
  - It stays in the queue (on the schedd)
  - A note is written to the job log file
  - It reverts to “idle” state
  - It is eligible to be matched again
- Relax! Condor will run your job again



# Access to data in Condor

- Option #1: Shared filesystem
  - Simple to use, but make sure your filesystem can handle the load
- Option #2: Condor's file transfer
  - Can automatically send back changed files
  - Atomic transfer of multiple files
  - Can be encrypted over the wire
  - Most common for small applications and data
- Option #3: Remote I/O





# Condor File Transfer

- `ShouldTransferFiles = YES`
  - Always transfer files to execution site
- `ShouldTransferFiles = NO`
  - Rely on a shared filesystem
- `ShouldTransferFiles = IF_NEEDED`
  - Will automatically transfer the files if needed

```
Universe      = vanilla
Executable    = my_job
Log           = my_job.log
ShouldTransferFiles = YES
Transfer_input_files = dataset$(Process), common.data
Queue 600
```

# Condor File Transfer with URLs

- Transfer\_input\_files can be a URL  
For example:

```
transfer_input_files = http://www.example.com/input.data
```



# Not Only Programming Languages

- You ran a C program this morning
- You can also run scripting languages such as bash, python, and perl
- You can also executing programs via the command like R



# Wrap Up Notes

- There are several different computing environments
- There is a very diverse set of computing jobs
- Matching jobs to resources is key to not wasting resources
- Not all of the available environments are open environments
- Research Computing is Complex

# Quick UNIX Refresher Before We Start

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- \$
- nano, vi, emacs, cat >, etc.
- source, module, chmod, ls



# That was a whirlwind tour!

- Enough with the presentation: let's use HTCondor!
- Goal: Extend the diversity of our jobs and add some data to the mix.



# Questions?

- Questions? Comments?
  - Feel free to ask me questions now or later:  
Rob Quick [rquick@iu.edu](mailto:rquick@iu.edu)
- Exercises are here:  
<https://github.com/CODATA-RDA-DataScienceSchools/Materials/blob/master/docs/DataSanJose2019/CI/Materials.md>

Presentations are also available from this  
URL.