

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

Rob Quick <rquick@iu.edu>

Associate Director Science Gateways Research Center
Indiana University

Follow Along at:

<https://github.com/CODATA-RDA-DataScienceSchools/Materials/blob/master/docs/DataSanJose2019/CI/Materials.md>



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

- `$`
- `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
- Exercises are here:
<https://github.com/CODATA-RDA-DataScienceSchools/Materials/blob/master/docs/DataSanJose2019/CI/Materials.md>

Presentations are also available from this
URL.