Open Science Grid

RDA RESEARCH DATA ALLIANCE U.S.

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

DOSAR

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Follow Along at:

opensciencegrid.org/dosar/ASP2022/ASP2022_Materials/

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"

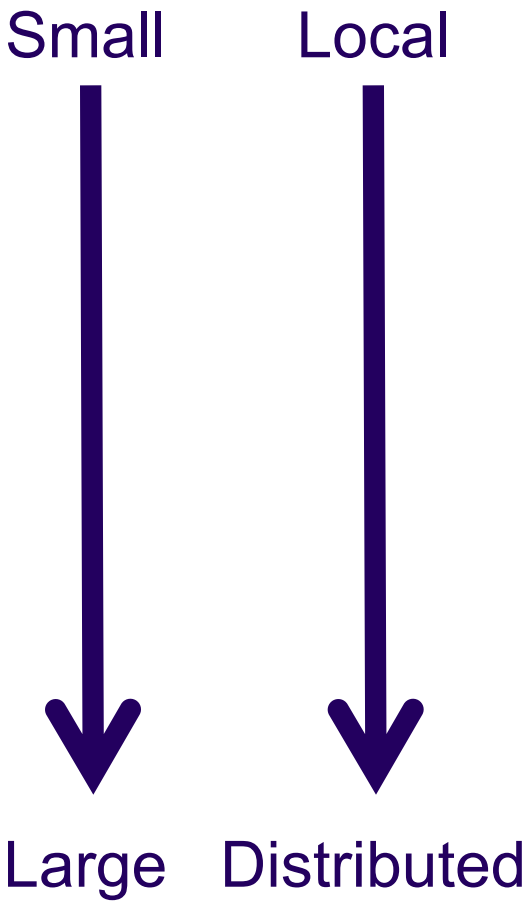
Most important!

- Please ask us questions!
  - …during the lectures
  - …during the exercises
  - …during the breaks
  - …during the meals
  - …over dinner
  - …via email after we depart (hs@ou.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



- 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

Gedankenexperiment

- 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

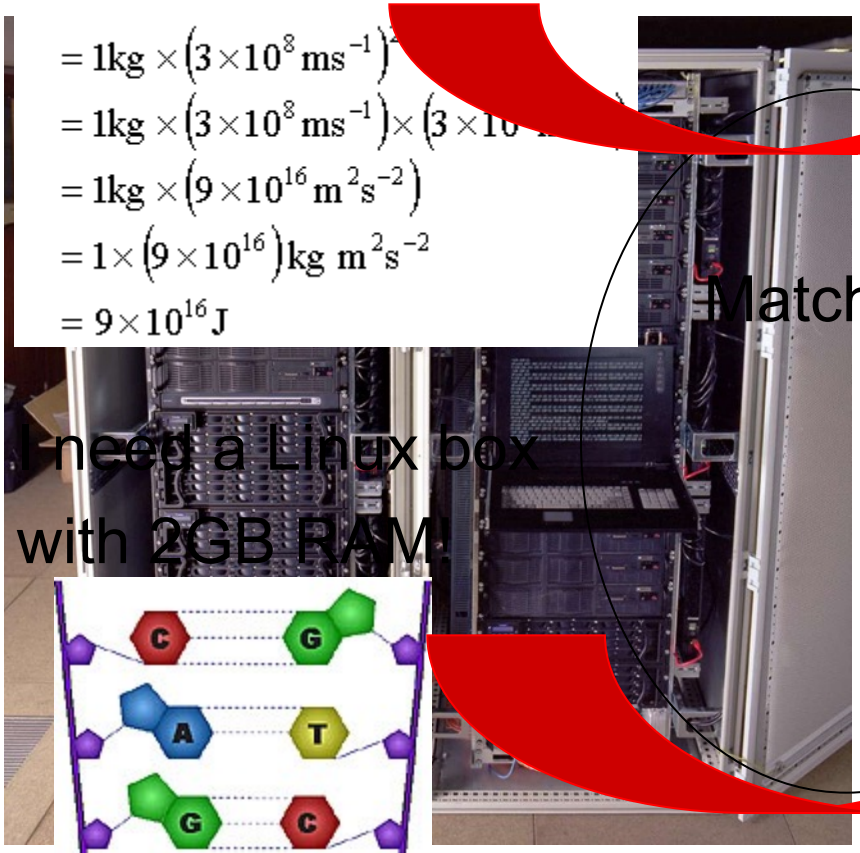
- Please note, we will only scratch the surface of Condor:
  - We won't cover MPI, Master-Worker, advanced policies, site administration, security mechanisms, submission to other batch systems, virtual machines, cron, high-availability, computing on demand, containers.

Condor Takes Computers… And matches them

I need a Mac!

Desktop Computers

$$E = mc^2$$
$$= 1\text{kg} \times \left(3 \times 10^8 \text{ms}^{-1}\right)^2$$
$$= 1\text{kg} \times \left(3 \times 10^8 \text{ms}^{-1}\right) \times \left(3 \times 10^8 \text{ms}^{-1}\right)$$
$$= 1\text{kg} \times \left(9 \times 10^{16} \text{m}^2\text{s}^{-2}\right)$$
$$= 1 \times \left(9 \times 10^{16}\right)\text{kg m}^2\text{s}^{-2}$$
$$= 9 \times 10^{16}\text{J}$$



I need a Linux box with 2GB RAM!

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

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ClassAds

- 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)
…
```

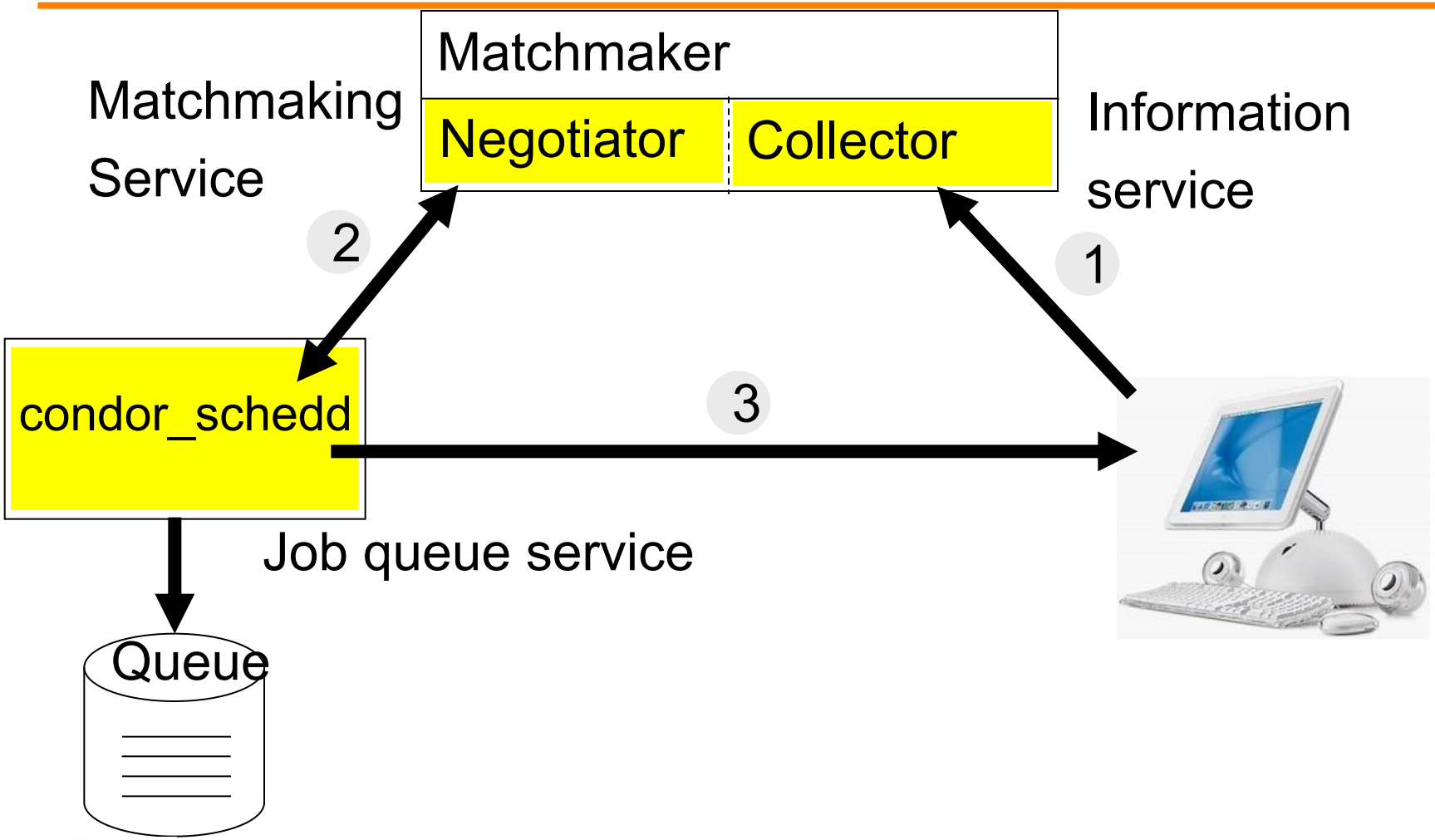
Schema-free ClassAds

- 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

Matchmaking diagram



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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
```

Clusters & Processes

- One submit file can describe lots of jobs
  - All the jobs in a submit file are a *cluster* of jobs
  - Yeah, same term as a cluster of computers
- Each cluster has a unique "cluster number"
- Each job in a cluster is called a "process"
- A Condor "job ID" is the cluster number, a period, and the process number ("20.1")
- A cluster is allowed to have one or more processes.
  - There is always a cluster for every job

The $(Process) macro

- The initial directory for each job can be specified as run_$(Process), and instead of submitting a single job, we use “Queue 600” to submit 600 jobs at once
- The $(Process) macro will be expanded to the process number for each job in the cluster (0 - 599), so we’ll have “run_0”, “run_1”, … “run_599” directories
- All the input/output files will be in different directories!

Example of $(Process)

```
# Example condor_submit input file that defines
# a cluster of 600 jobs with different directories
Universe   = vanilla
Executable = my_job
Log        = my_job.log
Arguments  = -arg1 -arg2
Input      = my_job.stdin
Output     = my_job.stdout
Error      = my_job.stderr
InitialDir = run_$(Process)
Queue 600
```

run_0 … run_599
Creates job 3.0 … 3.599

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More $(Process)

- You can use $(Process) anywhere:

```
Universe   = vanilla
Executable = my_job
Log        = my_job.$(Process).log
Arguments  = -randomseed $(Process)
Input      = my_job.stdin
Output     = my_job.stdout
Error      = my_job.stderr
InitialDir = run_$(Process)
Queue 600
```

Sharing a directory

- You don't have to use separate directories.
- $(Cluster) will help distinguish runs

```
Universe   = vanilla
Executable = my_job
Arguments  = -randomseed $(Process)
Input      = my_job.input.$(Process)
Output     = my_job.stdout.$(Cluster).$(Process)
Error      = my_job.stderr.$(Cluster).$(Process)
Log        = my_job.$(Cluster).$(Process).log
Queue 600
```

Not Only Programming Language

- 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

Day One 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 us questions now or later:
  - Jae Yu jaehoonyu1@gmail.com
  - Horst Severini severini@ou.edu
  - Pat Skubic pskubic@ou.edu

  Exercises start here:

  opensciencegrid.org/dosar/ASP2022/ASP2022_Materials/

  Presentations are also available from this URL.