An Introduction to High-Throughput Computing

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Some Content Contributed by the University of Wisconsin Condor Team and Scot Kronenfeld

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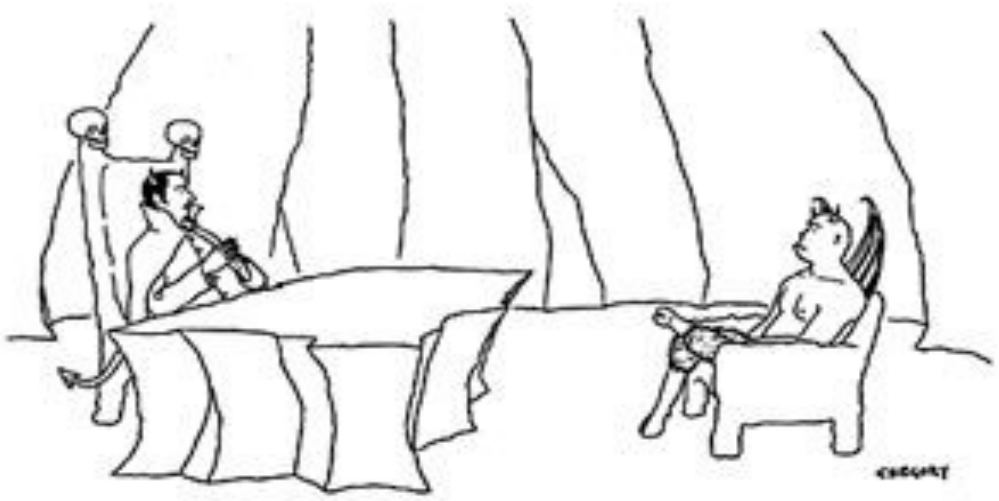
Who Am I?

- Manager High Throughput Computing Indiana University
- Chief Operations Officer of the Open Science Grid – 8 years
- Institutional OSG PI
- Co-PI International Science Grid This Week
- External Advisor to European Grid Infrastructure

Overview of day

- Lectures alternating with exercises
  - Emphasis on lots of exercises
  - Hopefully overcome PowerPoint fatigue & help you understand better



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

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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"

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Most important!

- Please ask me questions!
  - …during the lectures
  - …during the exercises
  - …during the breaks
  - …during the meals
  - …over dinner
  - …the rest of the week
- If I don't know, I'll find the right person to answer your question.

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Goals for this session

- Understand basics of high-throughput computing
- Understand the basics of Condor
- Run a basic Condor job

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The setup: You have a problem

- Your science computing is complex!
  - Monte carlo, 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: 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?

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Option 2: 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**

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What is 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
    - That slow four-year old cluster down the hall? Use it!

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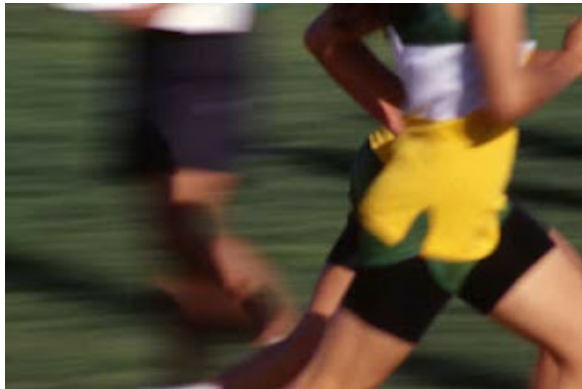
Think about a race

- Assume you can run a four minute mile
- Does that mean you can run a 104 minute marathon?
- The challenges in sustained computation are different than achieving peak in computation speed
  - Our focus is sustained computation



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HTC is not for all problems

- Do you need real time results?
- Do you need to minimize latency to results?
- Do you have very parallel code with lots of communication between modules?

- You might need HPC instead

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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
- We'll try out BLAST later today

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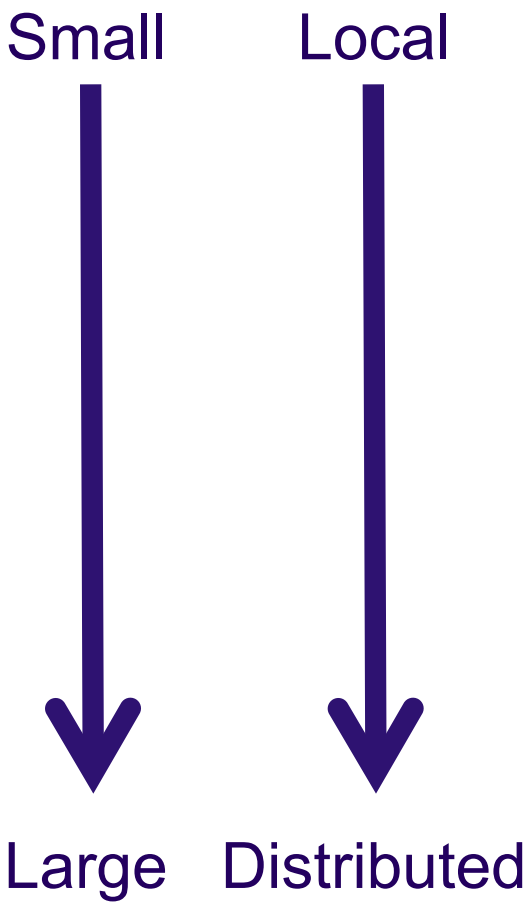
Why is HTC hard?

- 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



- Can you run one job on one computer?
- Can you run one job on another local computer?
- Can you run 10 jobs on a set of local computers?
- Can you run 1 job on a remote computer?
- Can you run 10 jobs at a remote site?
- Can you run a mix of jobs here and remotely?

This is the path we'll take in the school this week

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Discussion

- For 5 minutes, talk to a neighbor: If you want to run one job in a local cluster of computers:
  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.

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Rob's answer: 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

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Rob's answer: 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

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Surprise! Condor 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`

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But not only Condor

- You can use other systems:
  - PBS/Torque
  - Oracle Grid Engine (né Sun Grid Engine)
  - LSF
  - ...
- But I won't cover them.
  - Our expertise is with Condor
  - Our bias is with Condor
- What should you learn at the school?
  - How do you think about HTC?
  - 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, Condor-C, submission to other batch systems, virtual machines, cron, high-availability, computing on demand, anything with the word cloud (though concepts are the same) …
- Why?

Condor Takes Computers…

…And jobs matches them

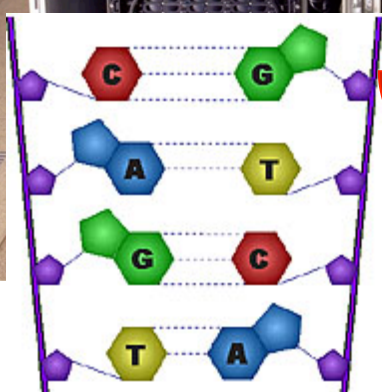
I need a Mac!

Desktop Computers

$$
\begin{aligned}
E &= mc^2 \\
&= 1\text{kg} \times \left(3\times10^8\,\text{ms}^{-1}\right)^2 \\
&= 1\text{kg} \times \left(3\times10^8\,\text{ms}^{-1}\right)\times\left(3\times10\right. \\
&= 1\text{kg} \times \left(9\times10^{16}\,\text{m}^2\text{s}^{-2}\right) \\
&= 1\times\left(9\times10^{16}\right)\text{kg m}^2\text{s}^{-2} \\
&= 9\times10^{16}\,\text{J}
\end{aligned}
$$

Match

I need a Linux box with 2GB RAM!



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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 for all available resources

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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

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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)
…
```

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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_4 = TRUE`
  - `ShoeLength = 7`
- Matchmaking can use these attributes
  - `Requirements = OpSys == "LINUX"`
    `&& HasJava_1_4 == TRUE`

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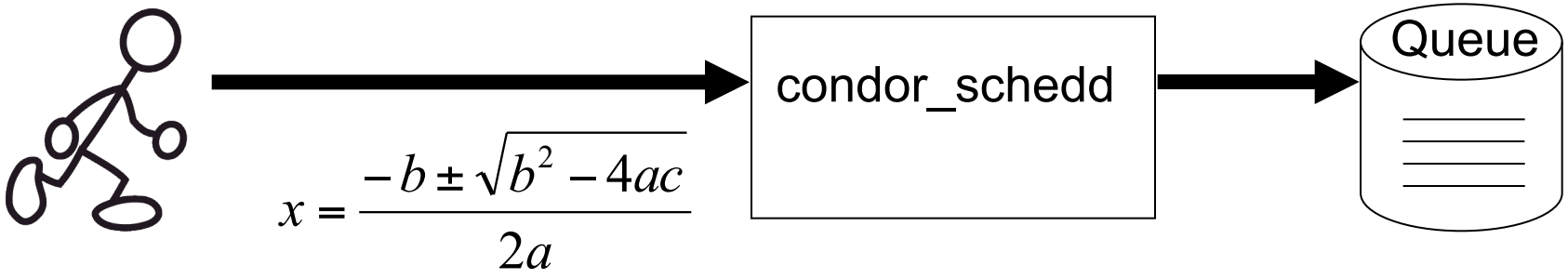
Don't worry

- 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

Submitting jobs: condor_schedd

- Users submit jobs from a computer
  - Jobs described as ClassAds
  - Each submission computer has a queue
  - Queues are not centralized
  - Submission computer watches over queue
  - Can have multiple submission computers
  - Submission handled by *condor_schedd*



Advertising computers

- Machine owners describe computers
  - Configuration file extends ClassAd
  - ClassAd has dynamic features
    - Load Average
    - Free Memory
    - …
  - ClassAds are sent to Matchmaker by *condor_startd* on computer

ClassAd

`Type = "Machine"`

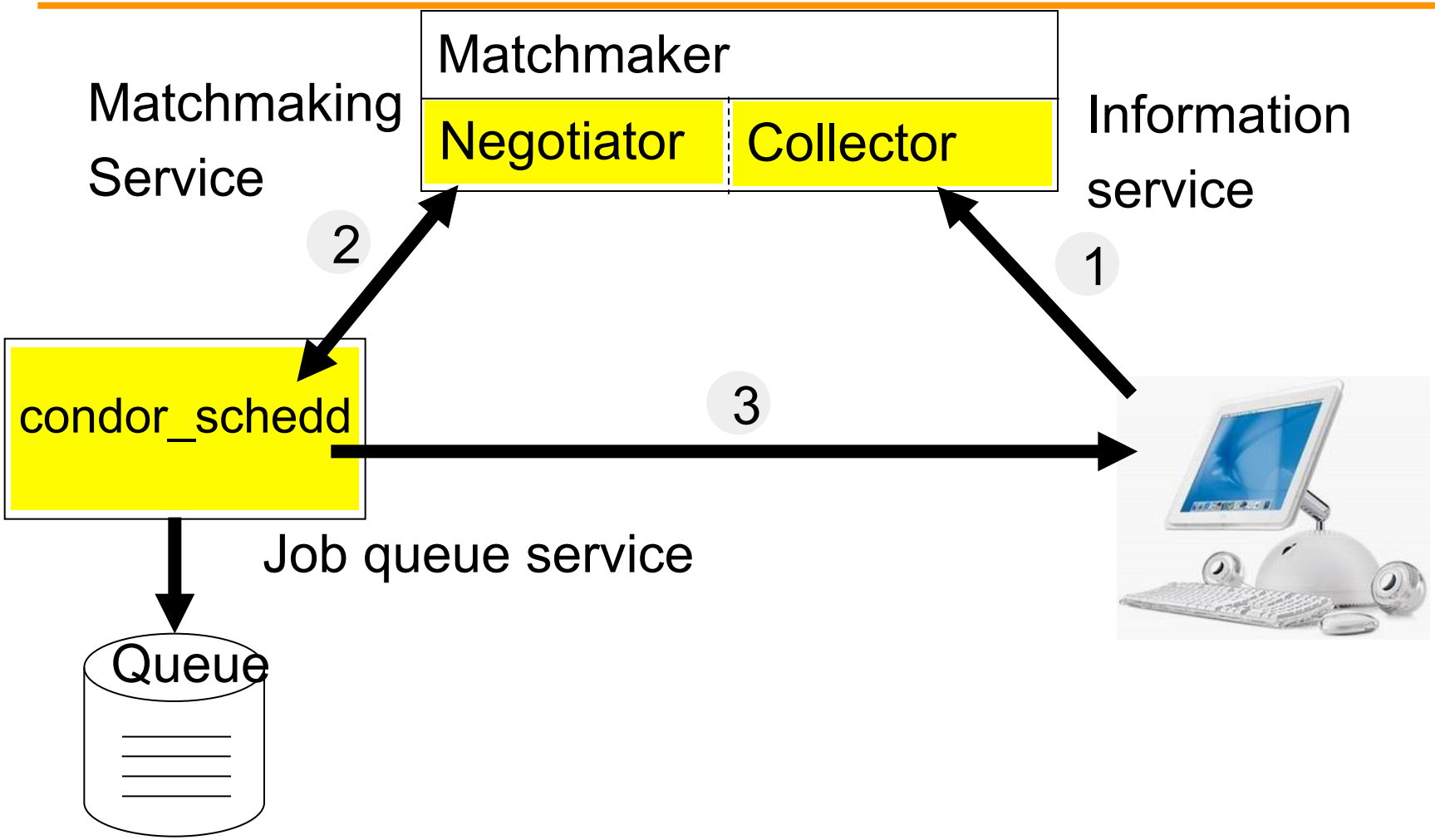
`Requirements = "…"`

Matchmaker (Collector)

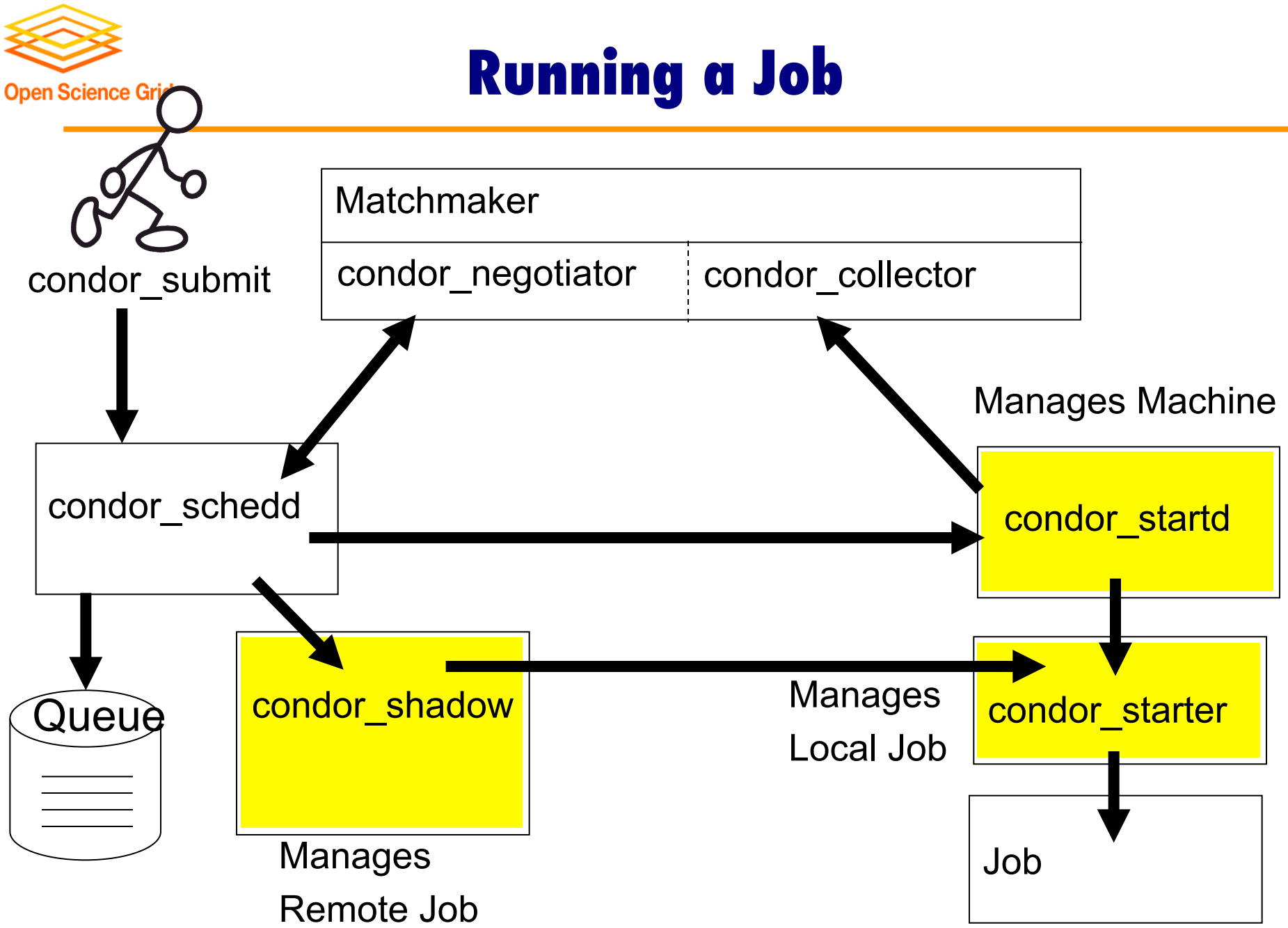
Matchmaking

- Negotiator collects list of computers
- Negotiator contacts each schedd
  - What jobs do you have to run?
- Negotiator compares each job to each computer
  - Evaluate requirements of job & machine
  - If both are satisfied, there is a match
- Upon match, schedd contacts execution computer to run job

Matchmaking diagram



Running a Job



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Condor processes

Process	Function
Master	Takes care of other processes
Collector	Stores ClassAds
Negotiator	Performs Matchmaking
Schedd	Manages job queue
Shadow	Manages job (submit side)
Startd	Manages computer
Starter	Manages job (execution side)

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If you forget most of these remember two (for other lectures)

Process	Function
Master	Takes care of other processes
Collector	Stores ClassAds
Negotiator	Performs Matchmaking
Schedd	**Manages job queue**
Shadow	Manages job (submit side)
Startd	**Manages computer**
Starter	Manages job (execution side)

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Some notes

- One negotiator/collector per pool
  (Perhaps extras for reliability)
- Can have many schedds (submitters)
- Can have many startds (computers)
- A machine can play multiple roles
  - E.g. Can have both schedd & startd

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Today's Condor setup

- One submit computer
  - One schedd/queue for everyone
  - osg-ss-submit.chtc.wisc.edu
- Will use local Condor pool
  - Have dedicated subset
- Tomorrow we will expand the setup

That was a whirlwind tour!

- Enough with the theory: let's use Condor!
- Goal: Check out our installation, run some basic jobs.

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Questions?

- Questions? Comments?
  - Feel free to ask me questions later:

    Rob Quick <rquick@iu.edu>