Open Science Grid

Optimizing Your Computing

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Why Are We Here?

Why Are We Here?

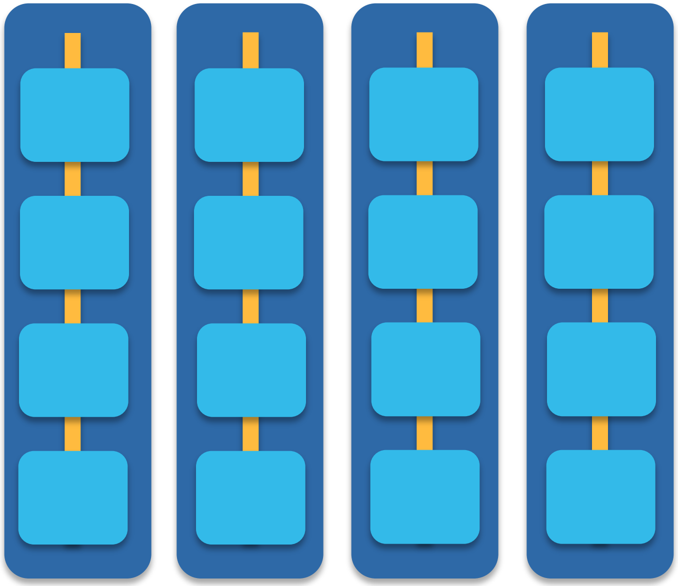
To do SCIENCE!!!

- A lot of science is best-done with computing – sometimes, LOTS of computing
- Science needs to be reproducible
- And, we'd really like science to happen **fast**(er)

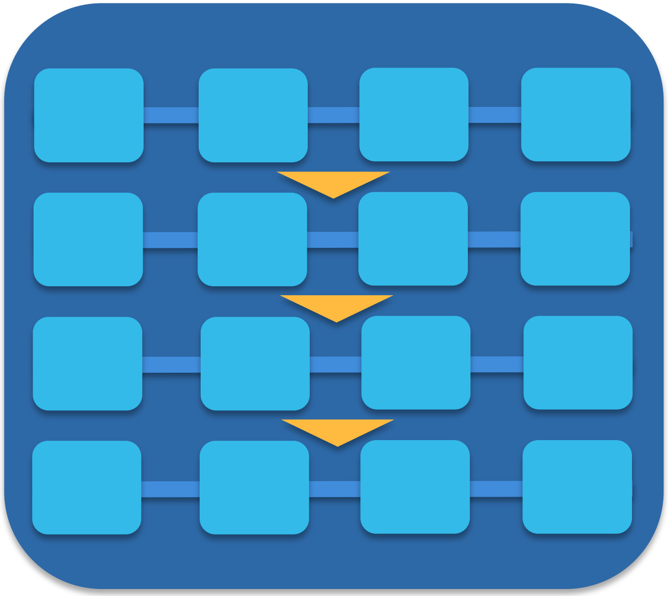
Getting the most out of **computing** (for research)

Computing Types

- At the beginning of the week, we talked about two different approaches for tackling large compute tasks...



high-throughput



high-performance (e.g.MPI)

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Two Strategies

High Throughput

Focus: Workflows with many *small*, *largely independent* compute tasks

Optimize: *throughput*, or time from *submission* to *overall completion*

High Performance

- Focus: Workflows with *large, highly coupled* tasks
- Optimize: *individual tasks*, software, communication between processes

Making Good Choices

How do you choose the best approach?

Is your problem “HTC-able”?

Typical HTC Problems

- batches of similar program runs (>10)
- “loops” over independent tasks
- others you might not think of …
  - programs/functions that
    - process files that are already separate
    - process columns or rows, separately
    - iterate over a parameter space
  - *a lot* of programs/functions that use multiple CPUs on the same server

Ultimately: Can you break it up?

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What is Not HTC?

- fewer numbers of jobs
- jobs individually requiring significant resources
  - RAM, Data/Disk, # CPUs, time

  (though, “significant” depends on the HTC compute system you use)
- restrictive software licensing

The Real World

- However, it's not just about finding the right computing approach to your problem.
- These approaches will be *most* effective if they're running on appropriate compute systems.

The Real World

- Not all compute systems are created equal.

- Two questions to ask:

What resources are available to me?

Which one is the best match for the kind of computing I want to do?

TWO EXAMPLES: LOCAL HTC AND OSG

CHTC Recommendations

	Ideal Jobs	Still very advantageous	Less-so, but maybe
Cpus (Gpus)	1 (1)	<20 (1)	>20 cpus, using multiple nodes
Walltime	<12 hours* *or checkpointable*	<24 hours* *or checkpointable*	up to 2 weeks
RAM	1-2GB	up to TBs	>4TB
Input	<100MB	up to TBs	N/A
Output	<4GB	up to TBs	N/A
Software	'portable'	anything else that's not →	licensed, non-Linux

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OSG Recommendations

	Ideal Jobs! (up to 10,000 cores across jobs, per user!)	**Still Very Advantageous!**	**Less-so, but maybe**
cores (GPUs)	**1** (1; non-specific type)	**<8** (1; specific GPU type)	**>8 (or MPI)** (multiple)
Walltime	**<12 hrs*** *or checkpointable	**<24 hrs*** *or checkpointable	**>24 hrs**
RAM	**<few GB**	**<10s GB**	**>10s GB**
Input	**<500 MB**	**<10 GB**	**>10 GB**
Output	**<1 GB**	**<10 GB**	**>10 GB**
Software	*'portable' (pre-compiled binaries, transferable, containerizable, etc.)*	*most other than →*	*Licensed software; non-Linux*

WHAT ABOUT YOUR LOCAL COMPUTE CENTER?

Campus Resources

- Check out your local campus compute system
- Some considerations:
  - Who has access? Are there allocations?
  - What kind of system? What is it optimized for?
- An HPC cluster may not handle lots of jobs well, in the same way that an HTC system has limited multicore capabilities - be aware of how a system matches/doesn't match your computation strategy.
- Ask questions! Be a good citizen!
- If local resources are limited, explore other options.

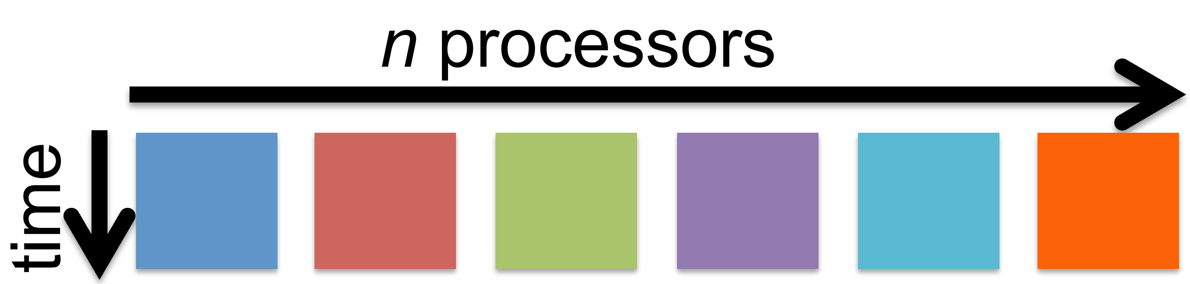
Beyond Your Campus

- Open Science Grid!
  - This afternoon, Tim will talk about ways to access OSG after the school is over

- Other grids
  - European Grid Infrastructure
  - Other national and regional grids
  - Commercial cloud systems

The Payoff

- HTC is, beyond everything, scalable
  - If you can run 10 jobs, you can run 10,000, maybe even 10 million
- Worth pursuing the right kind of resources (if you can) for the right kind of problem.



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Getting the Most out of HTC

The HTC Goal:

RUN AS MANY JOBS AS POSSIBLE ON AS MANY COMPUTERS AS POSSIBLE

Key HTC Tactics

1. **Increase Overall Throughput**
   Optimize for total work, not individual jobs
2. Utilize Resources Efficiently!
3. Bring Dependencies With You
4. Scale Gradually, Testing Generously
5. Automate As Many Steps As Possible

Throughput, revisited

- In HTC, we optimize *throughput*: time from submission to overall completion
- Instead of making individual jobs as fast as possible, optimize how long it takes for all jobs to finish.
- We do this by breaking large processes into smaller pieces (to have more simultaneous processing power)

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Breaking Up

- Break work into parallel (separate) jobs
  - reduced job requirements = more matches
  - not always easy or possible
- Strategies
  - break HTC-able steps out of a single program
  - break up loops
  - break up input
- Use self-checkpointing if jobs are too long
- Consider grouping tasks if jobs are short!

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Self-Checkpointing

Solution for long jobs and “shish-kebabs”

1. Changes to your code
   - Periodically save information about progress to a new file (every hour?)
   - At the beginning of script:
     - If progress file exists, read it and start from where the program (or script) left off
     - Otherwise, start from the beginning
2. Change to submit file:

```
when_to_transfer_output = ON_EXIT_OR_EVICT
```

Solutions for Larger Files

- File manipulations
  - split input files to **send minimal data** with each job
  - **filter** input *and* output files to transfer only essential data
  - use compression/decompression
- Follow file delivery methods from yesterday for files that are still "large"

Key HTC Tactics

1. Increase Overall Throughput
2. **Utilize Resources Efficiently!**

   Jobs will match to more resources

3. Bring Dependencies With You
4. Scale Gradually, Testing Generously
5. Automate As Many Steps As Possible

Know and Optimize Job Use of Resources

- **CPUs** ("1" is best for matching; essential for OSG)
  - restrict, if necessary/possible
  - software that uses all available CPUs is BAD!
- **CPU Time**

  > ~5 min, < ~1 day; **Ideal: 1-10 hours**

- **RAM** (not always easily modified)
- **Disk** per-job (execute) and in-total (submit)
- **Network Bandwidth**
  - minimize transfer: filter/trim/delete, compress

Use the Job Log

```
001 (2576205.000.000) 06/07 11:57:57 Job executing on host:
<128.104.101.248:9618>
005 (2576205.000.000) 06/07 14:12:55 Job terminated.
        (1) Normal termination (return value 0)
                Usr 0 00:00:00, Sys 0 00:00:00  -  Run Remote Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Run Local Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Total Remote Usage
                Usr 0 00:00:00, Sys 0 00:00:00  -  Total Local Usage
        5  -  Run Bytes Sent By Job
        104857640  -  Run Bytes Received By Job
        5  -  Total Bytes Sent By Job
        104857640  -  Total Bytes Received By Job
        Partitionable Resources :    Usage  Request Allocated
           Cpus                 :                 1         1
           Disk (KB)            :   122358   125000  13869733
           Memory (MB)          :       30      100       100
```

Key HTC Tactics

1. Increase Overall Throughput
2. Utilize Resources Efficiently!
3. **Bring Dependencies With You**

   Jobs can run anywhere*
4. Scale Gradually, Testing Generously
5. Automate As Many Steps As Possible

*almost

Bring *What* with You?

- Software (covered Wednesday)
- Data and other input files
  - Parameters and random numbers: generate and record ahead of time (for reproducibility)

- What else?

Wrapper Scripts Recap

- Before task execution
  - transfer/prepare files and directories
  - setup/configure software environment and other dependencies
- Task execution
  - prepare complex commands and arguments
  - batch together many ‘small’ tasks
- After task execution
  - filter/combine/compress files and directories
  - check for and report on errors

Key HTC Tactics

1. Increase Overall Throughput
2. Utilize Resources Efficiently!
3. Bring Dependencies With You
4. **Scale Gradually, Testing Generously**

   Saves you time in the long run!
5. Automate Multiple Steps

Testing, Testing, Testing!

- Will be a major focus of our exercises today.
- Allows you to optimize resource use (see HTC tactic #2), job length (tactic #1)
- Just because it worked for 10 jobs, doesn't mean it will work perfectly for 10,000 jobs (scaling issues)
  - Data transfer (in and out)
  - Discover site-specific problems

Why test? Imagine if:

- You are using a new scientific instrument. Would you run 100 samples without ever running a test (or a few tests)?

- Your job accidentally creates a 3GB core dump file because the code is corrupted. What happens if you submit 1,000 jobs with this issue?

Testing, Testing, One...

- Get one job working
  - Work out software issues, data transfer patterns, etc.
  - Make subsequent memory/disk requests based on results from this job
  - How long does the job run?

...Two...

- Run a medium/small scale test(s) (10-100 jobs)
  - Check memory/disk requests when complete. Are they accurate? If not, change them.
  - Do some percentage of jobs fail? If so, can you figure out why? How will you find/handle failures at a larger scale?
  - Would it make sense to submit **more, smaller** jobs or **fewer, longer** jobs?
  - How much data is being generated? Do you have space on the submit server to store the results of the full-scale run?

...Three!

- If you make significant changes in any of the previous testing steps (or make any other changes to your workflow - new code, new data, new version of your software) -- do another quick test.
- Once you've done a small and medium test, scale up to the full submission.

Introducing the exercises

- Our exercise today will involve developing a workflow (series of sequential pieces)
- What you need to know for the first two exercises:
  - Identify the component pieces (job submissions) of the workflow and the shape of the overall workflow.
  - Test/optimize the pieces, as described in the previous few slides

Questions?

- Now: “Joe’s Workflow”
  - Exercise 1.1 -- Understand and plan (no jobs)
  - Exercise 1.2 -- Testing jobs
  - Work in groups of 2-3
  - Read carefully!
- Later:
  - Lecture: Optimizing Workflows
  - Exercises 2.1, 2.2