CENTER FOR HIGH THROUGHPUT COMPUTING

Advance Your Research: Scale Out Your Computing

OSG User School 2023
August 7, 2023

Why Scale Out Your Computing?

Richard Ayoade in the IT Crowd, Series 1, Episode 2
https://giphy.com/gifs/richard-ayoade-it-crowd-maurice-moss-dbtDDSvWErdf2

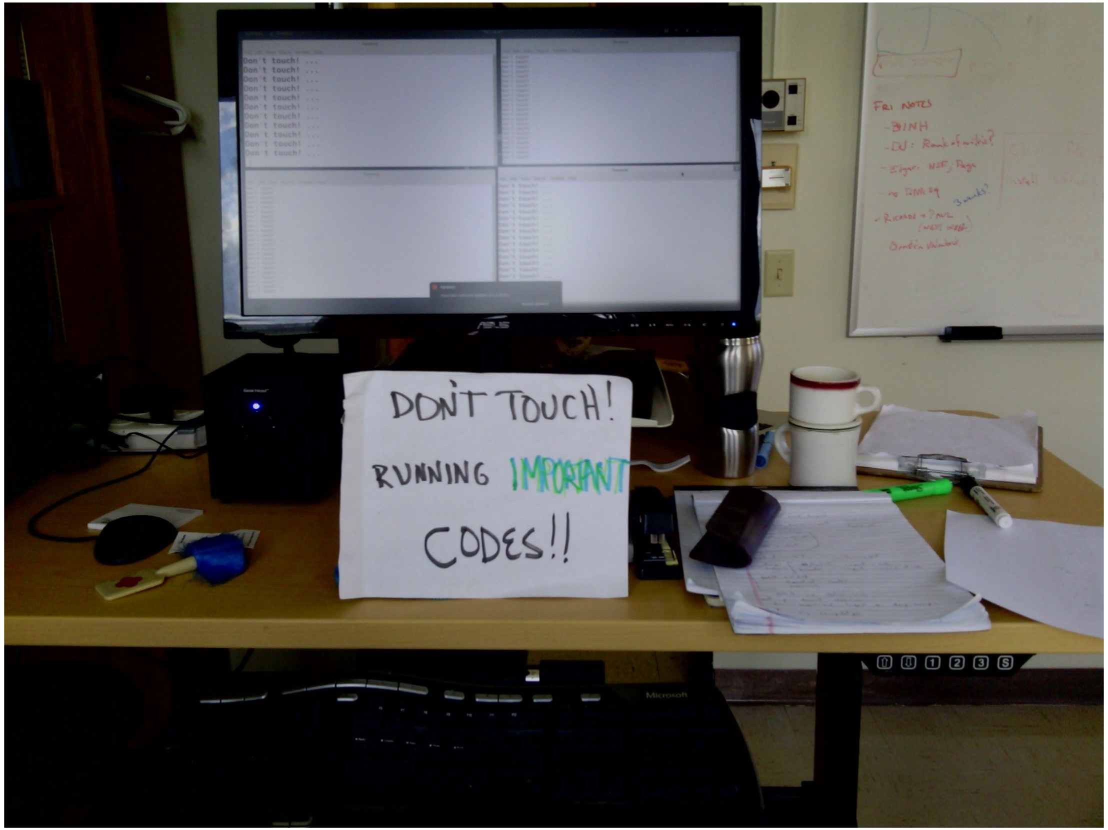


Photo credit Steve Goldstein

Dr. Timothée Poisot
@tpoi

Just use this simple heuristic: if it's slow and the computer goes WOOOOOOOOSH, the bottleneck is the CPU; if it's slow and the mouse stop moving, the bottleneck is the memory.

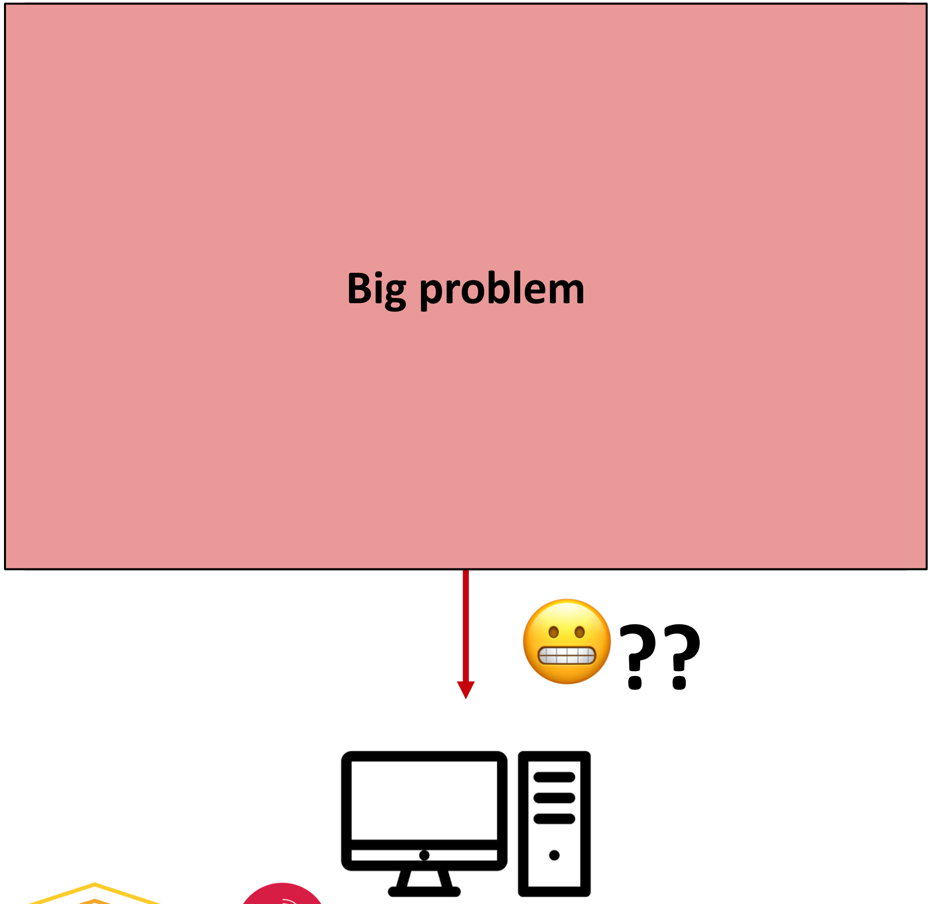
https://twitter.com/tpoi/status/1169692855201402885

Big Problems

How do you solve a big computational problem?

For example:

- Lots of data
- Thousands of parameters
- Many grid points

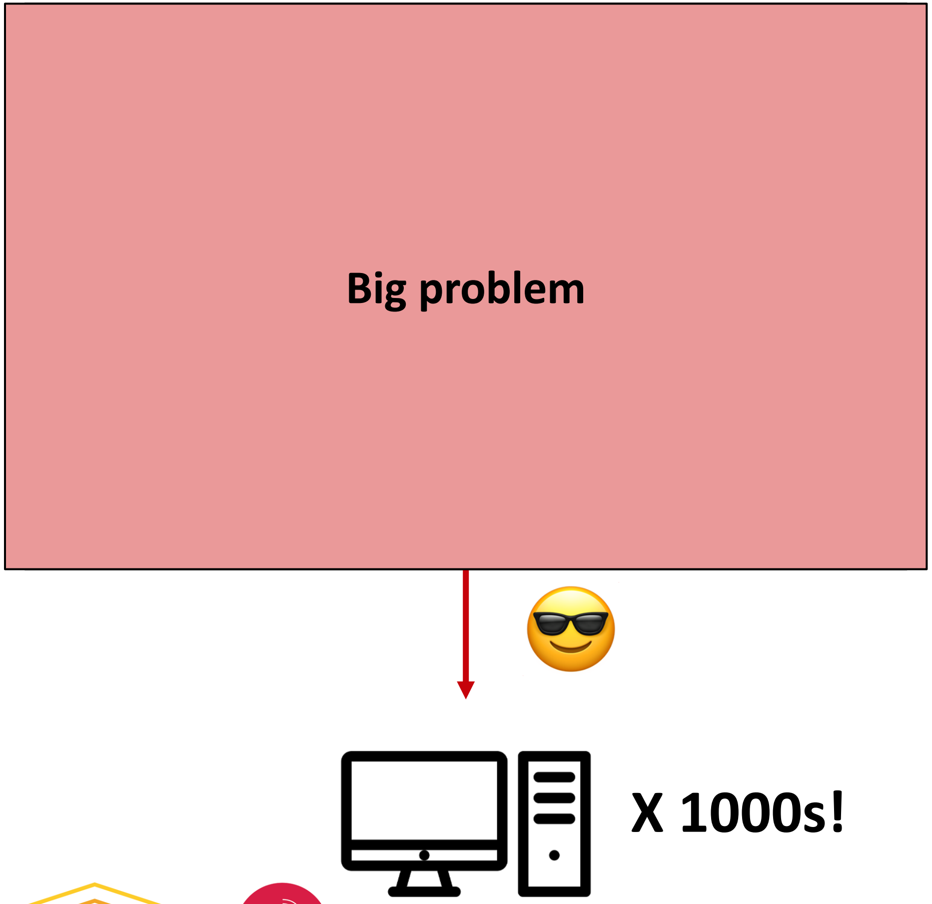


Our Goal: Scaling Out

We want to be able to tackle big problems.

We want to go from using a small number of resources to a LOT of resources.

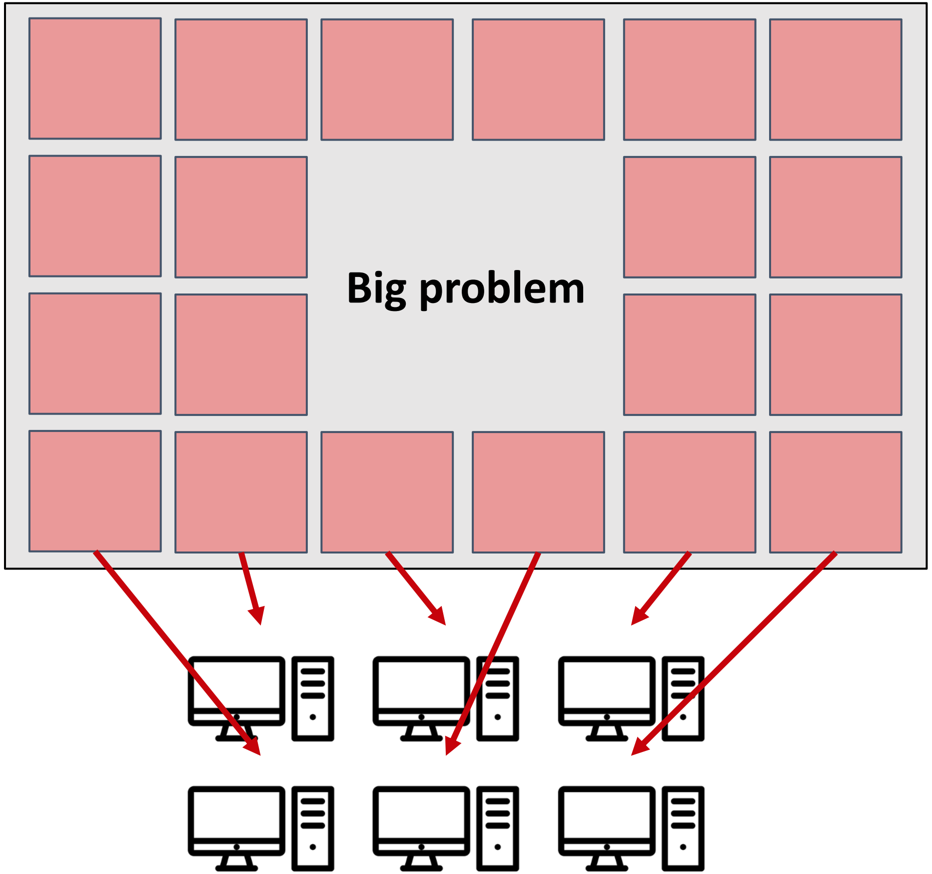
There is one strategy to do this with computers: divide and conquer



Big Solutions

To solve a big problem, break it into many sub-problems and use more/specialized computers.

There are different ways to do this.



Large Scale Computing Approaches

A bigger computer

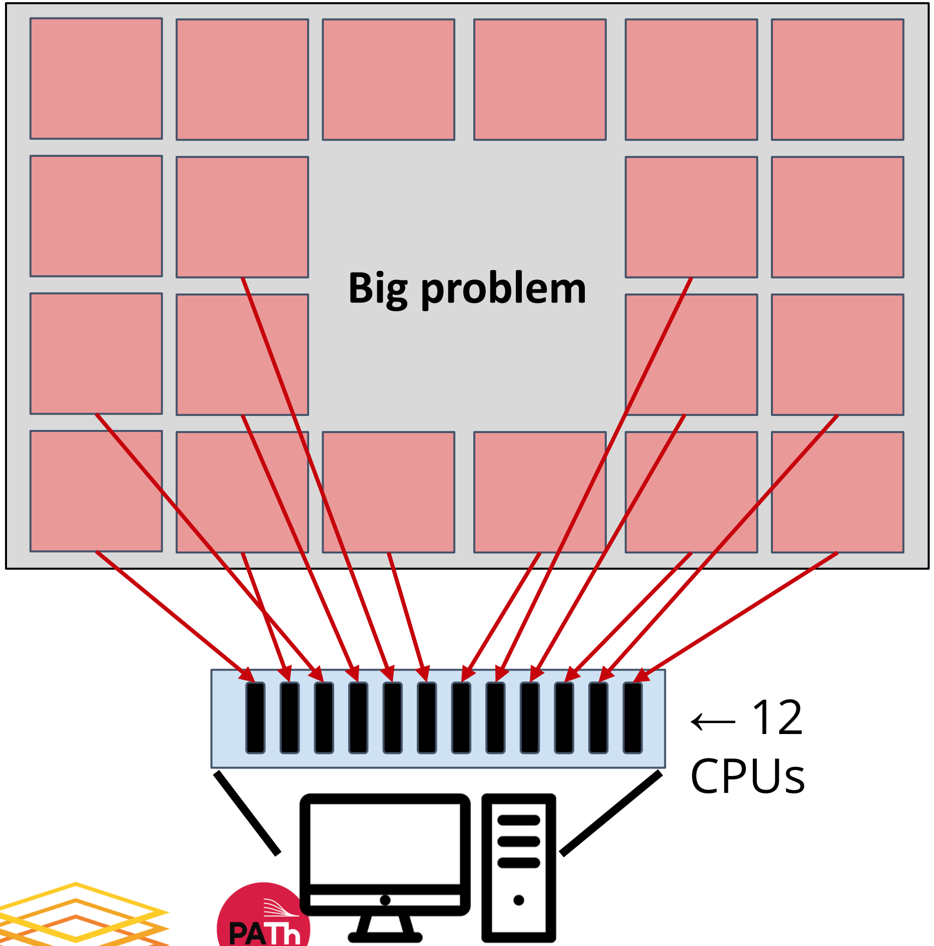
Sometimes, getting a larger computer can solve your problem - more CPUs, more memory, more disk space.

- Workstation
- Server that requires remote log in

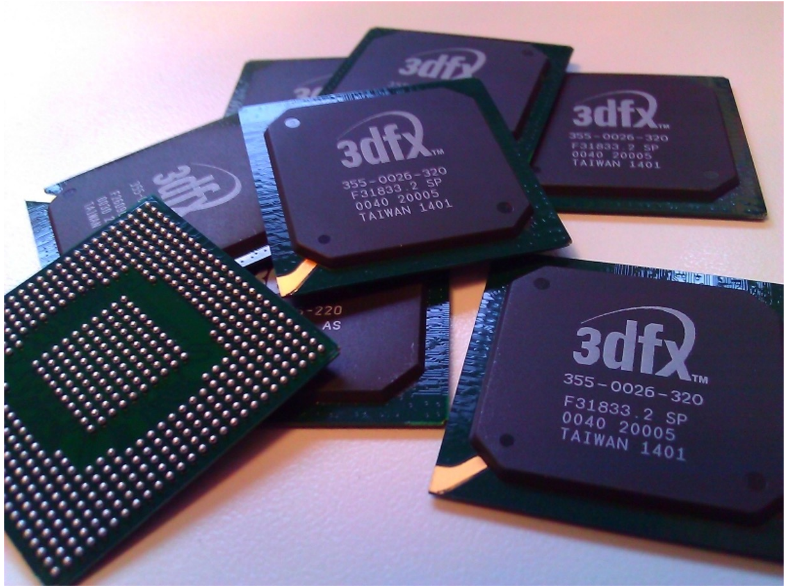
Option 1: More CPUs

Run sub-problems on individual CPUs.

Requires programming this capability into the code.



Specialized computer components (like GPUs)



GPUs are a common way to accelerate certain kinds of computing.

Like before, can be used from a:

- Workstation
- Server

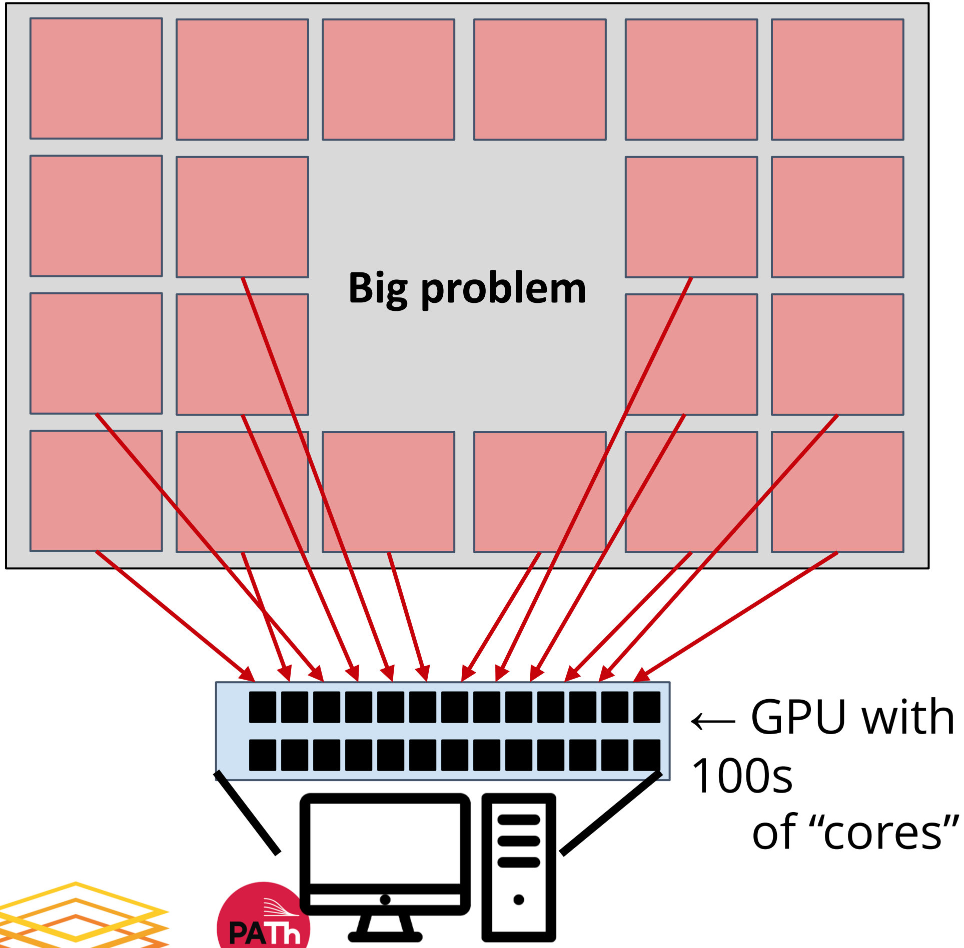
Option 2: Use a GPU

Run sub-problems on "cores" inside a GPU card.

Like before, requires programming this capability into the code.

Examples:

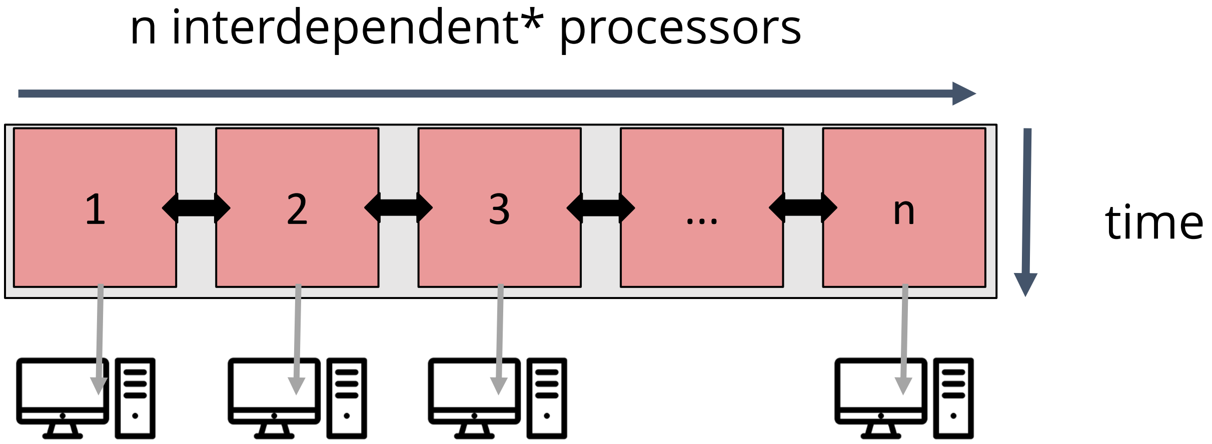
- Neural networks and other deep learning algorithms
- Certain molecular dynamic codes



Use more computers at once.

This is the idea behind the large-scale computing systems like the Open Science Pool.

Option 3: High Performance Computing (HPC)



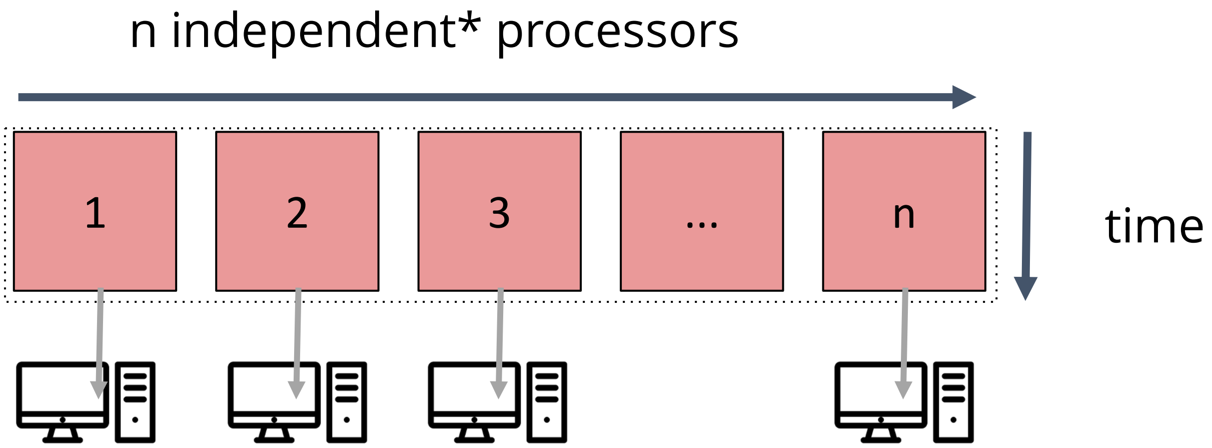
Solve sub-problems by distributing across multiple CPUs on multiple computers.

Also requires special coding (MPI) to coordinate calculations across multiple computers.

HPC Examples:

- Complex physical simulations with many inter-connected components.
- Optimization problems that use many local calculations to drive the global optimization.

Option 4: High Throughput Computing (HTC)



Sub-problems are independent and self-contained, can be run on many computers.

Most scalable.

No special programming needed.

HTC Examples:

- Test many parameter combinations
- Analyze multiple images or datasets
- Do a replicate/randomized analysis
- Align genome/RNA sequence data

One of our favorite HTC examples: baking the world's largest/longest cake

In computational terms: solving a big problem (the world's longest cake) by executing many small, self-contained tasks (individual cakes) and joining them.

Photos: Arun Sankar via https://www.theguardian.com/world/2020/jan/16/indian-bakers-rise-to-task-of-making-worlds-longest-cake

Use Case 1: Random Simulations

- **Typical task**: running a simulation
- **One computation needs**:
  - 1 core, 512Mb of memory
  - almost no data
  - 10 seconds
- **How many times?** Millions
- **Are there multiple steps involved?** No.
- **Bottleneck**: total number of simulations

Mei Monte Carlo

Needs to run many random simulations to estimate a statistical value.

Use Case 2: Analyzing Multiple Files

- **Typical task**: analyzing a data sample
- **One computation needs**:
  - 1-16 cores, 8 – 32GB of memory
  - Input of 5GB, output of 10GB
  - 8-10 hours for whole pipeline
- **How many times?** Dozens (number of samples)
- **Are there multiple steps involved?** Yes.
- **Bottleneck**: Size of data, number of samples, certain steps

Ben Bioinformatics

Needs to process 100s of genomic data files.

Discussion

See handout.

OSG School = HTC School

- This week is all about learning more about the practice of high throughput computing:
  - Job submission + troubleshooting (Mon/Tues)
  - Software portability (Tues)
  - Data handling (Wed)
- On two different high throughput computing resources
  - The PATh Facility (Mon)
  - the Open Science Pool (Tues onward)

Acknowledgements

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