

Canadian Bioinformatics Workshops

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Data Management

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Bioinformatics Workshop
Next Generation Sequencing
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It's a new world

- Next gen sequencers generated Gb of data
- Architecture matters

Why should you care?

- Architecture matters
 - If you are choosing the compute resources for your lab, designing the correct system architecture is important to get the most use out of the systems
 - If you are using the compute resources of your lab, understanding the system architecture will help you get the most out of the system

What you won't learn.

- This lecture will provide you with a basic understanding of computer systems, but....
- Consult your local expert
- If you are the local expert, make friends at a large genome centre 😊

The basics

- CPU
- Disk space
- RAM
- Bandwidth

CPU

- The speed of your CPU determines how quickly it can process instructions
- Many bioinformatics operations fall into the “embarrassingly parallel” category
- Getting a results faster is as simple as adding more CPUs
- => clusters

How many CPUs?

- For current throughputs, you will need ~8 CPU dual quad core nodes per sequencer to handle data rates
- 8 way boxes are relatively easy to come by.

RAM

- RAM is fast storage close to the CPU
- By loading data from disk to RAM, the CPU can execute instructions much more rapidly

How much RAM?

- Typical sizing is 2GB of RAM per CPU
- This works fine for most aligners
- Assemblers typically need much more RAM
- If you don't have enough RAM, the CPU will need to make use of the disk storage –
- When a computer has run out of RAM it is said to be “swapping”
- Some aligners have a minimum memory limit for optimal performance
- Human de novo requires lots of RAM!

Disk space

- Unlike RAM, information is retained after the machine is switched off
- Speed of access is slower than RAM
- Magnetic disks have a seek time and read time
 - Read data from a block is faster than seeking all over the disk to get the data
- Can be RAIDed to improve performance

How much disk space?

- Sequencers generate ~2Gbases a day
- Including quality values and additional files (alignments etc) results in....
- Each machine will generate ~~15~~ 35TB of data per year
- Scaling

Space, or lack thereof, is the problem

- Disk space is probably the biggest problem today
- ~~60~~ 500GB is for sequence data and quality values
- ~~Should you store images?~~
- Should you store intensities

Understanding bandwidth

- Bandwidth of a connection represents the maximum rate of transfer between two points
- Most commonly, we think of network bandwidth, but there is also bandwidth
 - between the disk and CPU
 - between a RAID array and the CPU
 - between the RAM and the CPU

More bandwidth

- Depending on the algorithm, the CPU will process data at a particular rate
- The trick is always max out the CPU's utilization
- Bandwidth to the CPU must be \geq the rate at which the CPU can process data

Even more bandwidth

- E.g. An aligner can process X reads per second on a single CPU at a data rate of Y bytes/sec
 - ~200 million reads in 10 hours
 - Each read 50 bases at 10 bytes per base
 - 2.7 MB/sec
- Design 100TB storage and connect it to a CPU resource
- Design bandwidth to be 10 Mb/sec – plenty of spare bandwidth
- Now we want to complete the job in an hour and get permission to buy 10 more CPUs – great!

Not so great

- For the 10 CPUs to run at maximum speed, they need to be supplied data at 27MB/sec
- Our bandwidth is 10MB/sec
- Therefore, no matter how many CPUs we buy, the job will never run faster than ~ 2.5 hours

Balancing it all

- The best balance of compute resources is application dependant
- Aligners may require a different balance than assembler (or other algorithms)
- Decisions
 - If limited resource, design system to deal with the biggest bottleneck
 - Ideally, have different systems for different parts of the pipeline

Backing it up

- Where to start....
 - Who's backing up their data today?
- Back up to active disk is probably the easiest
- Backup to tape expensive
 - Person time
 - Need to refresh tapes
 - Slow
- Active disk can't be taken offsite
- No great solutions out there... Except perhaps SEP machine...

Clouds

- Clouds, such as Amazon EC2, are emerging as a viable alternative to owning your own resources
 - Remote disk storage
 - Remote CPU
 - Pay as you go
- This could be a good option for a small lab

LIMS

- Generating all that data is no good if you don't know where you've put it
- LIMS provide a mechanism for keeping track of all of the data
- Metadata (i.e. data about data) related to the experiments is stored in a database
- The database stores the location of the data files
- Tracking may be paper based or bar code based
- Essential for a centre running lots of expts

LIMS and other s/w

- Build in-house and off-the-shelf
 - Commercial or free solutions
- Is there a solution that meets your needs?
 - If missing some requirements, will the company/lab modify their s/w for your needs?
- How do you want to spend your time?

Emerging Standards

- Sequence
- Alignment
- Best practises
- Why are standards important?
 - Hint: wouldn't you just like to focus on the science?
- “If you build it, will they come?”