Pipelines and Workflows

Adapting to HPC

Partners

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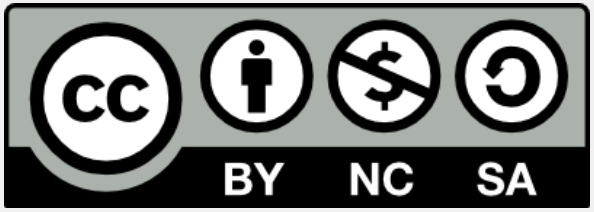

Outline

- Bioinformatics pipelines and HPC
  - What's the problem?
- MapReduce - another parallel pattern
- Hadoop – a MapReduce engine
- Halvade: distributing pipelines
- Common Workflow Languages and Pipeline Frameworks

Bioinformatics pipelines and HPC
what's the problem?

- Many bioinformatics tools parallelised using threading only
  - Best suited to shared-memory machines with a large amount of memory and modest numbers of cores (compared to HPC)
- On distributed-memory systems, restricted to single node
  - Indications are many multithreaded tools used in pipelines don't scale well to typical full number of single-node cores (low parallel efficiency)
- Few tools use MPI
  - Not the only way to scale, but an important / powerful one that would give instant ability to run on HPC machines

Bioinformatics pipelines and HPC
what's the problem?

Example:

```
user@machine:~> bwa mem -t $NSLOTS -M $BWA_INDEX_REF -R
"@RG\tID:$PU\tPL:illumina\tPU:$PU\tSM:$SAMPLE" $READS1
$READS2 | samblaster --splitterFile >(samtools view -hSu /dev/stdin |
samtools sort -@ $NSLOTS /dev/stdin > $SAMPLE.sr.bam) --
discordantFile >(samtools view -hSu /dev/stdin | samtools sort -@
$NSLOTS /dev/stdin > $SAMPLE.disc.bam) | samtools view -hSu
/dev/stdin | samtools sort -@ $NSLOTS /dev/stdin >
$SAMPLE.raw.bam
```

Bioinformatics pipelines and HPC
what's the problem?

Example simplified:

A | B --arg1 >(C | D > file1) --arg2 >(E | F > file2) | G | H > file3

- 8 executables (A – H)
  - 4 multithreaded
  - potentially using different threading standards (pthreads, OpenMP, …)
- Efficiency of parallel executables unknown
  - No idea of optimal number of threads to assign to each (assuming we can)
- Linux pipes don't allow straightforward control over parallel execution
  - Mostly relying on operating system to do the right thing
  - Data flow through pipes and pipe buffers adds addtional complications

Bioinformatics pipelines and HPC
what's the problem?

- Can take days to run
  - Difficult to determine which stages are taking the most time
  - Can't use many standard performance profiling tools
  - Difficult to understand, let alone improve runtime
  - Need to carefully tease apart performance of each step
    - Still leaves questions regarding dataflow between piped commands
- Linux piping *may* be very efficient in some circumstances
  - but don't have a good handle on this
- Risk is this approach became common because it was available, convenient (interactive), and sufficiently fast for smaller data sets
  - Possibly running into problems with more and more data
  - Issues surrounding robustness, checkpointing (can't run > 48 hours on ARCHER)
  - Need a solution engineered for purpose to tackle larger scale in a controlled manner

MapReduce – another parallel pattern

- Like Task Farm, but three categories of worker:
  - Mapper (user supplies this code)
    - Takes a (local) list of key-value pairs, and for each pair, returns another (intermediate) key-value pair
    - Writes these out locally
  - Grouper (part of the run-time), can be done by the master
    - Groups by (intermediate) key on local disk
  - Reducer (user suppliers this code)
    - One reducer for each (intermediate) key
    - Takes the (intermediate) key-value pairs from all relevant disks, performs a reduction operation and returns another (usually) shorter list of (final) key-value pairs

Hadoop

- Hadoop is an implementation of the MapReduce pattern
- Engine to manage execution of many data processing tasks
- Includes a distributed filesystem
- Used as an engine to distribute data to where it's needed, including to perform compute and gather results

Halvade

- Example framework to run sequencing pipelines in parallel
  - based on Hadoop
  - multicore **AND multi-node**
  - alignment (BWA) → data preparation (Picard) → variant calling (GATK)
- Developers analysed
  - single-node threaded efficiency of each tool
    - used to allocate optimum number of threads for each tool in Halvade
  - Optimal task size (experimentally) - found granularity sweet spot

- Good parallel efficiency (~90%) running whole human genome on distributed-memory cluster (up to 16 nodes - 512 cores, 60GB memory per node)

Barriers

- Parallel pipeline performance of Halvade and similar that rely on Hadoop (or Spark) seem promising
- Barrier to deployment on especially the largest HPC systems is conflict with existing file systems, resource management, etc.
  - Potential disruption of environment finely tuned for performance of tightly-coupled traditional HPC codes?
  - Not enough demand or incentive?
  - Gap between (potential) users and service providers?
  - HPC hardware and service mainly funded by non-bioinformaticians?
  - … ?
- Smaller HPC machines more flexible
  - EPCC HPC service Cirrus used for genomics analyses, has Hadoop, Spark

Common Workflow Languages and Pipeline Frameworks

- Currently observe a diversity of CWLs and pipeline frameworks
  - Varying approaches to parallelism
  - Future prospects of any given framework uncertain
    - Hampers adoption / traction, decreases incentive for continued development

- Similarities with earlier decades of parallel computing:
  - Early diversity of message-passing libraries
  - Later adoption of a common standard
  - Allowed applications to be written in parallel once and run everywhere
  - Single standard for parallelism enabled targeting of efforts to improve performance from software and hardware sides
    - Great success - led to portable applications that can run on many different and constantly newer HPC machines

Common Workflow Languages and Pipeline Frameworks

- CWL and pipeline frameworks and their users might benefit from similar
  - Single common framework could potentially improve uptake, deployment and usage on HPC machines, similar to historical emergence of MPI

- Software development efforts could focus on parallelisation of CWL execution layer(s)
  - Would allow separation of concerns, with relevant expertise directed at each level of software and hardware

Summary

- Some bioinformatics pipelines / workflows are problematic from the point of view of HPC
  - Understanding and improving performance is challenging
- Frameworks for massively parallel data-centric computing appear promising
- There are some barriers to uptake / deployment on HPC systems
  - Situation is made more complicated by diversity of approaches without one unambiguous favourite