Tools to Execute an Ensemble of Serial Jobs on a Cray

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Outline

- The Biology Application
- What are ensemble serial jobs?
- Why use Cray machines?
- A survey of solutions
    - BigJob
    - PCP
    - aprun
- Experiments and Analysis
- Conclusion

mlRho – A Biology Application

- mlRho software: a serial program that estimates mutation, recombination and sequencing error rates
- SciAPT assisting Biologists at IU
- Data-parallel, hundreds to thousands of iterations can be performed independently
- I/O is the limiting factor
- Open source, available here: https://github.com/CIPaGES/mlrho
- Biologists came up with a plan to do the analyses on tens of genomes
- A total need of ~6 millions compute hours

XSEDE

- XSEDE is the place to go if you are looking for millions of compute hours
- Need a proposal, with performance and scalability numbers
- Did not have an easy way to do this on Kraken
- Did our experiments on Ranger and Stampede
    - Using BigJob, and
    - An MPI wrapper
- But found a couple of solutions on how to do this on a Cray
- Put some more effort into this given that IU has its own Cray

What is an ensemble of serial jobs?

- A set of serial jobs that are ready to go
  - The ensemble of serial jobs are not sequential
  - They are all ready to go at the same time
- Usually independent, data-parallel, parameter-sweep type applications
- When do we need specific tools?
  - Total workload: 100 serial jobs? 1000? 10,000?
  - 100,000 compute hours? 1 Million?
  - Concurrency
  - A few serial jobs at a time is a separate discussion

Traditional v. Non-traditional

- Traditional fields: physics, math, astronomy, chemistry, etc.
    - Highly parallel, MPI applications
- Non-traditional fields: biology, bioinformatics, finance, geology, psychology, etc.
    - Serial, non-scalable, analytical, text-processing
- The diversity of users and applications is increasing as computing becomes cheaper

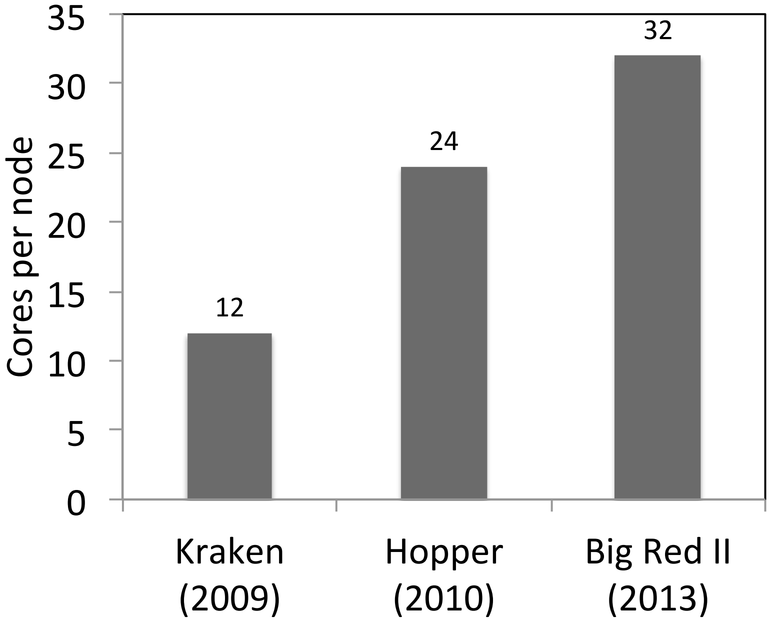
Why do we want to run these jobs on a Cray?

- General Purpose machines
    - Hopper
    - Kraken
    - Big Red II
- Users will have to use compute hours where they can find them
- Cray machines are becoming more and more common

Image Sources: http://www.nics.tennessee.edu/computing-resources/kraken, http://www.nersc.gov/users/computational-systems/hopper/, http://newsinfo.iu.edu/pub/libs/images/usr/15356_h.jpg

Why not let the users figure this out?

- Running serial jobs on a Cray is not a difficult task
- There is a good chance that users will just submit serial jobs
- Without shared node scheduling, 90% of a compute node is unutilized
- Processor parallelism has been growing
    - So has cores per compute node
- Need tools and queue policies to avoid this



A survey of solutions

- Shared node computing using Cluster Compatibility mode (CCM)
    - Service needs to be provided by the admins
- Using regular batch job submission
    - with or without packing all the cores on a node
    - aprun and back grounding the jobs
- PCP – parallel command processor
- BigJob – SAGA based pilot-job tool
- Swift – a parallel scripting language

Adapt to Queue Policies

- Why don’t we stick to aprun?
    - The users can be told to pack enough jobs per node
    - Or the users will waste 90% of their allocation
- But, even with this solution, the user is required to submit many single node requests to the scheduler
- Many centers with large Cray machines prioritize or prefer large jobs
    - Scheduler policies, discounts, etc.
- Need a tool that allows one to bundle as many serial jobs as needed in to one large job of a size that makes it appropriate for a particular machine
- Should make it possible to use multiple compute nodes and all the cores on an individual node
- **Allows users to adapt to the available machines and their policies**

BigJob, PCP and aprun

- Out of all the tools we found, we chose these three
- Reason for that:
  - Previous experience with BigJob, can be used as a container job
  - PCP is easy to use, can be used to bundle jobs
  - aprun is the default choice, used as a baseline
- PCP is a really simple tool, thank NICS user support group for referring PCP
- BigJob is more sophisticated
  - Gives the users more options and control over workflow
  - But adds complexity

BigJob

- Developed and supported by the RADICAL Lab at Rutgers University
- Not necessary to understand the architecture
  - There's an API.
  - A python script defines the workload
  - Asks the scheduler for nodes
  - Runs the jobs
  - Need to understand more if you are running jobs across multiple machines
- Can be used:
  - as a container job,
  - to distribute jobs to multiple resources
  - to coordinate the launch and interaction of jobs within the container
  - And to design lot of other exotic workflows
- We use it as a simple container job

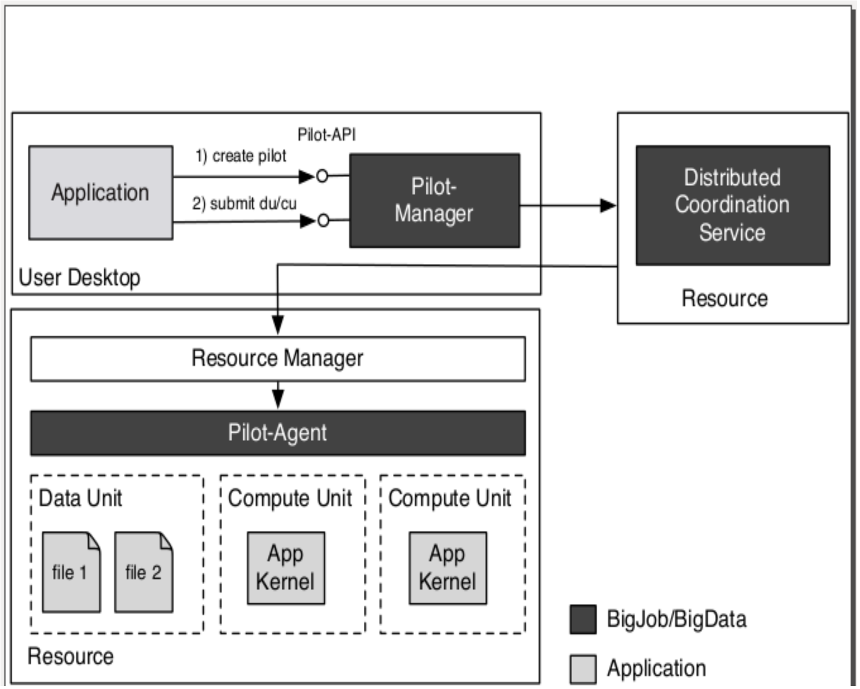


Image source: https://github.com/saga-project/BigJob/wiki/BigJob-Architecture

More about BigJob

- Available for download from the Python Package Index
- API preview:
    - Job request submitted to the scheduler

```
"service_url": "xt5torque+gsissh://kraken.nics.xsede.org",
"number_of_processes": 960,
"allocation": "TG-123456",
"queue": "debug",
"working_directory": "/work/user/",
"walltime":120, #minutes
```

Individual mlRho job descriptions:

```
for i in range(0, NUMBER_JOBS):
 compute_unit_description =
    "executable": "/work/user/mlRho",
    "arguments": [" -m "+ str(start) +" -M "+ str(end)+  "
-n profileDb"],
    "number_of_processes": 1,
    "spmd_variation":"single”, #MPI or serial
    "working_directory":"/work/user/",
    "output": "output"+str(i)+".out",
    "error": "error"+str(i)+".err”,
```

Need to know basis…

- The user only needs to know what the software can do for them and how to get the software to do it
- The only interaction the user has with the BigJob software is via the python job submission script
    - which takes in the same details as a batch job submission script.
    - A quick-start guide is available on the BigJob website https://github.com/saga-project/BigJob/wiki/BigJob-Tutorial-Part-3:--Simple-Ensemble-Example
    - Good to be familiar with python

Parallel Command Processor (PCP)

- Original implementation of the tool was produced by the Ohio Supercomputer Center (OSC)
- Ported by the NICS team to work on a Cray specific architecture
- The source code of PCP is available from NICS
- Tested this code on multiple Cray machines, works as expected.
- PCP expects a text file containing a list of commands to be run
- We have used PCP to run hundreds of mlRho jobs concurrently.
- Basic scripting knowledge useful in creating text files with the jobs that need to be executed
- The barrier to entry for using PCP is very low compared to other similar tools

More about PCP

- Build as simple as: “cc pcp.c”
- `“aprun -n 512 ./pcp list.txt”`
- Where list.txt contains the 512 commands to run:

```
mlRho -m 1000 -M 1005 diatom.pro > out_1
mlRho -m 1006 -M 1010 diatom.pro > out_2
.
.
.
mlRho -m 2551 -M 2555 diatom.pro > out_511
mlRho -m 2556 -M 2560 diatom.pro > out_512
```

All the advantages of a container job… but

- No control over job management
- Job/load balancing not available
- For very similar jobs that are independent and have the same running time, both BigJob and PCP work.

	BigJob	PCP
Container Job	X	X
Job Management	X	
Load Balancing	X	
Data Management	X	
API	X	

aprun

- The default choice
- Scripts that each contain as many binary commands as there are cores on a single node
- Cannot runs jobs across multiple nodes
- Without CCM, whether we can run more than one unique job on a single node is questionable
- If there are 1000,000 jobs to run, need to submit ~10,000 separate jobs
- Lot of scripting

The usual batch script

- On Kraken: `aprun -n 1 -d 12 -cc none -a xt run.sh`
    - -n 1 # run on a single node
    - -d 12 # allows the script to access all the cores on a node
    - -cc none # allows each serial process to run on its own core
    - -a xt # required by aprun to run a script instead of a program

- Where run.sh contains:

```
mlrho -m 1 -M 2500 input.pro > data1.out &
mlrho -m 2501 -M 5000 input.pro > data2.out &
.
.
.
mlrho -m 27501 -M 30000 input.pro > data12.out &
wait
```

Experiments on Kraken

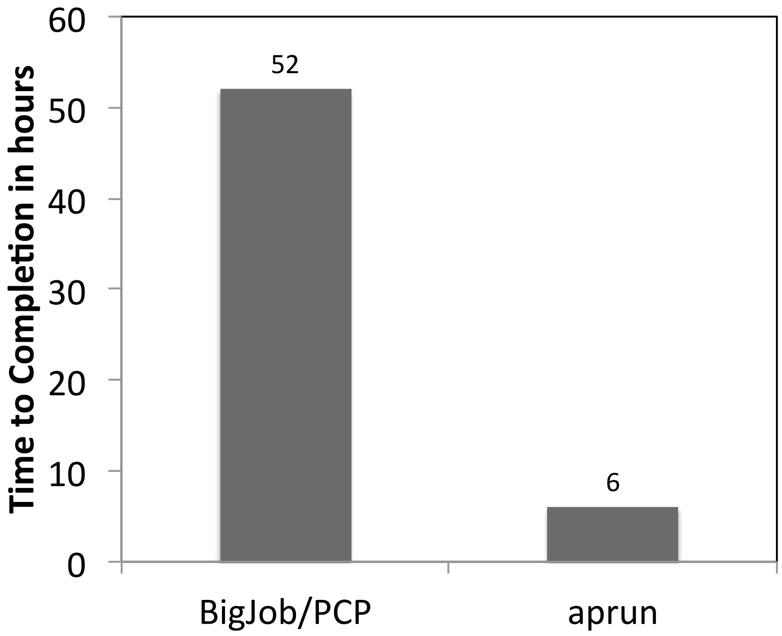
- A trial run to see if:
  - The tools work
  - check whether it is beneficial to bundle serial jobs in general into larger jobs to get better throughput.
- Metric of interest is total time to solution
- Disclaimer: not useful to make broad generalizations, either with respect to Kraken or other large machines, further studies are planned to support more general claims

Workload

- Kraken is a 112,896 core Cray XT5 machine operated by NICS
- A variety of queues are supported
- Same workload with all three tools on Kraken
- We selected a job size of 960 cores, which is 80 compute nodes on Kraken
- One instance of mlRho was run on each core and, in the runs where actual computations were done, ran 250 iterations on a zebra genome.
- Yes, we just collected the queue wait time in all but one experiment
    - Can't waste those SUs!

Experiments

- BigJob and PCP:
  - Single set of experiments will work for both
  - A single job is submitted to the queue in both cases, requesting 80 nodes
- aprun:
  - 80 separate single node job requests submitted to the queue
- Experiments repeated 5 times
- Surprising result:
  - BigJob/PCP type took 52 hours
  - aprun type took 6 hours
  - mlRho runtime is ~4 hours



Analysis

- It appears that aprun was faster than PCP/BigJob
- But need to consider many factors
- While this may be true at 80 nodes, it may not be true at 120 or 200 nodes
- Many machines have queued and run limits:
  - the number of jobs from one user that can be queued at a time
  - The number of jobs from one user that can be running at a time

	Kraken	**Hopper**
Queued Limit	100	16
Run Limit	25	16

- Hopper has a separate throughput queue, where the queued limit is 500 and run limit is 250, but a maximum of only 2 nodes can be requested per job
- The run limit on Kraken is probably not being enforced

Other factors

- Backfilling:
    - the backfilling algorithm attempts find any unused nodes or “holes” in the schedule and fill them with appropriately sized jobs
- While BigJob/PCP jobs were submitted with a gap of multiple days, all 80 of the aprun jobs were submitted simultaneously.
- It is possible that all 80 jobs re-used a single, since these jobs were only collecting waiting time
- We recorded all the node numbers of the compute nodes that our jobs ran on
    - With the exception of one set of runs the number of unique nodes used for the 80 jobs was in the 65-80 range.
    - One set ran on the same five nodes, however this set of runs did not have the smallest overall wait time
    - it had the third longest wait time in the set of five aprun submissions

Conclusion

- Non-traditional applications on the Cray are one the rise
    - Both Cray and non-traditional users are moving towards each other
- Parametric sweeps are not new to the supercomputing field, they are new to Cray supercomputers.
- Previous obstacles to running multiple binaries on the same compute node have now been overcome
- Submitting separate single node job requests to the scheduler is straightforward and easy to implement
- BigJob and PCP are more elegant, offer the ability to submit much larger job requests
    - can be advantageous depending on site specific policies
- **Factors specific to the application, machine, scheduler policies and ease of use determine best tool for the task**

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