Enabling High–Throughput Research on HPC Systems

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Introduction

Two types of fundamental workflow for HPC

- Large distributed memory (MPI) jobs
- High-throughput jobs

High-throughput jobs covers

- Monte-Carlo simulations
- Parameter space sweeps
- Processing of large data sets

It is characterised by doing a task over and over again with a different input.

The problem

MPI machines

Machine like the Power7 cluster at BlueFern and Fitzroy at NIWA are geared towards distributed memory jobs (MPI).

High-throughput job

Running high-throughput jobs efficiently on these systems requires a little bit of thinking ahead and care. We will "steal" the MPI workflow to achieve this. Machines like Pan in Auckland are geared more towards high-throughput and medium size MPI jobs but applying the techniques presented here could be beneficial on it as well.

Ehsan's Simulations

Ehsan Yasdi is a PhD student in computer science. His problem is simulating wireless networks to improve the efficiency of the communication in mobile devices.

- first submission to the cluster was 40,000 simulations
- done 4 at a time
- first reaction: increase the number of simulations he can run (after all they are not big MPI jobs)
- Bad idea: the simulations were spread all over the cluster blocking big MPI jobs
- developed a custom solution to contain him to a set of nodes
- Since then, his time to run simulations has gone from 3 weeks to 3 days. He presented 5 talks at international conferences
- we later found out that it was equivalent to using MPMD

We now identify high-throughput projects quickly and offer them better solutions as soon as possible.

Solutions

Presentation

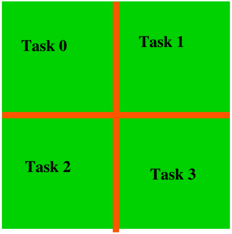
There are two main ways of packaging serial jobs to pass them as MPI distributed memory job, we'll look at them through the work of two researchers.

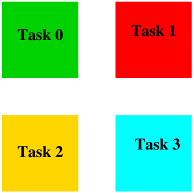
1. MPMD (Multiple Program Multiple Data): Nick's network
2. Batcher: Jing Wang DNA matching work

Nick's Networks

- Nick Baker is a PhD student in biological sciences with a background in mathematics. He studies ecological networks (complex food chains).
- His work focuses on analysing networks to find "keystone" species that are essential to the network. The work is what we call embarrassingly parallel, he has to go through a high number of networks and perform his analyses on each and every one of them.
- I spotted him on the cluster running four jobs at a time out of close to a hundred. There was definitely room for improvement. He became a test subject for MPMD
- The throughput increase will enable him to study how networks react to other variations such as climate change and loss of habitat amongst other parameters.

MPMD: Multiple Program Multiple Data





SPMD: Instances of a program process the data distributed amongst them.

MPMD: Programs, not necessarily identical, process distinct data.

Jing Wang, DNA matching with batcher

- Jing Wang is a researcher at ESR and came to us for several NeSI research projects
- The problem is to compare strands of DNA against a database to match sequences of genes
- The task can be further broken down by splitting the strands in sections and searching for match in these.
- Searching for sequences in one long DNA strand can take a long time. Doing it on a section is much quicker but now you have to do it on potentially thousands of sections. This has become a high-throughput task
- The main focus of the project was to identify new virus and develop a process that can be used in the event of emerging infectious disease outbreaks

Batcher: Master and Worker

A batcher program uses a different MPI mode: the ability for one program to be a master that spawns workers to do various jobs on demand.

Like MPMD, the batcher program will take a list of tasks. Unlike MPMD, however, batcher does not start all tasks at once. If you give batcher more tasks than you have cores, it will fill the cores given. When one task finishes, it will start the next one in the list until all tasks are completed.

Instead of building packets to match the number of cores requested (MPMD) you can package in units that make sense.

Pros and Cons

Batcher

Pros:

- Can group any number of tasks
- tasks that complete quickly will be replaced by new tasks while the longer ones finish

Cons:

- one core is used by batcher and not available to do tasks

MPMD

Pros:

- all cores are used

Cons:

- if some tasks are much longer than others some cores will be idle
- number of tasks must be equal to number of cores

Conclusions

- Lots of serial jobs are not a good thing on a machine tuned for MPI jobs
- We solve this by packing the serial jobs in a way that make look like MPI jobs
- It increases your throughput at BlueFern and Fitzroy
- It makes the life of your cluster administrator easier
- MPMD is best suited for tasks of equal length (lattice QCD, Monte-Carlo)
- batcher is best suited for the rest
- Jobs can also be packaged on the Pan cluster in Auckland but the MPMD submission would be different.

Questions & Answers

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