Stay Tuned

How NeSI Optimises the Usage of Shared HPC Resources
Computational Science Team @ NeSI

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NeSI

New Zealand eScience
Infrastructure

Outline

About NeSI CS Team

Computational Science Team

Basically, it means that we are the Researchers best friends :-)

About NeSI CS Team

Which is the main goal of a shared HPC facility?

- Run a few jobs really fast, no matter what their efficiency is.
- Run the maximum number of jobs, in favour of short and small jobs.
- NeSI provides a wise combination by optimising the usage of computational resources.

About NeSI CS Team
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Identify the Bottlenecks
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Tuning
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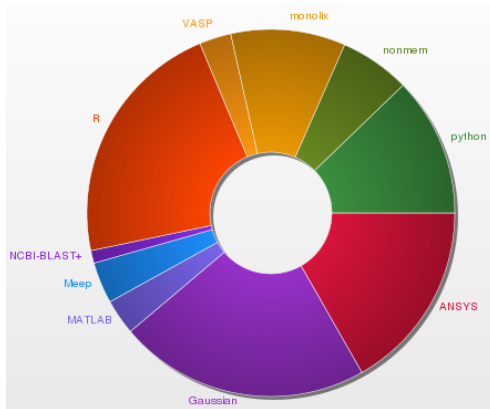Back to the future
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Identify the Most Popular Apps

Figure : Most popular applications in Pan cluster. We are using snoopy to track the applications run in the cluster. This allow us to get a list of the most popular apps.

Tuning

Tuning the most popular applications provides a major impact in

- the walltime of the users of this code.
- the global cluster efficiency.
- the availability of the computational resources.
- the waiting time.
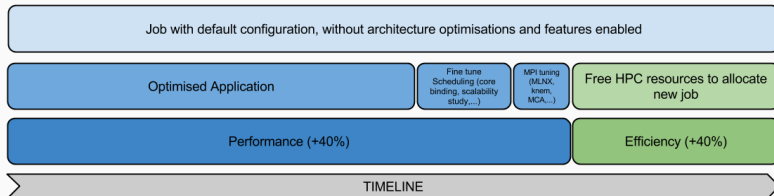
Tuning

There are several ways to tune an HPC Application

- Most obvious : tune the algorithm.
- Choose the right Libraries + Compilers + MPI "Flavour".
- Choose the right Options and Environment.
- Work in the work-flow.
- Explore the scalability (how well it scales).
- Check if benchmark results are good enough.

Profile and Debug

Available software

- Intel Vtune Amplifier & Intel Trace Analyzer
- DDT
- Score-P
- HPC Toolkit
- Scalasca
- Cube
- PAPI
- TAU
- Parallel Profile Visualization (ParaProf)
- Native Slurm profiling tools
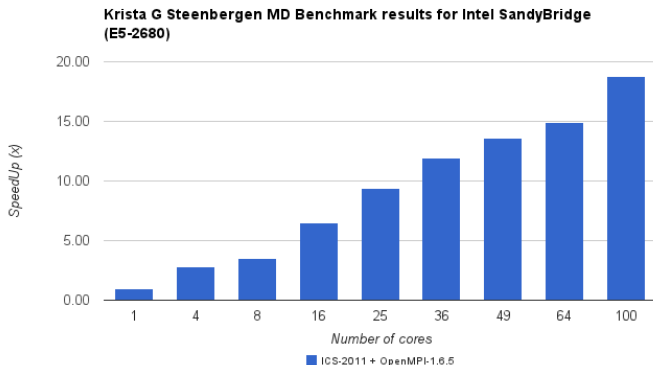
Increase the performance

VASP Case Study

The Vienna Ab initio Simulation Package (VASP) is a computer program for atomic scale materials modelling, e.g. electronic structure calculations and quantum-mechanical molecular dynamics, from first principles.

Benchmark provided by Dr. Krista Grace Steenbergen (Victoria University)

It describes finite temperature molecular dynamics simulation of a 128-atom bulk gallium super-cell (8 atoms to a normal unit cell, 16 unit cells), using 3x3x3 KPOINT mesh at medium precision (higher FFT-gridding) and allowing for spin polarization.
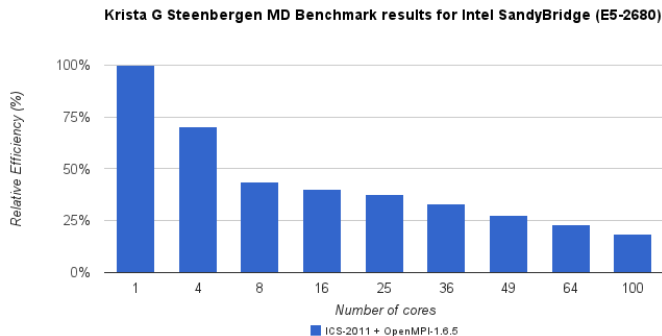
Increase the performance

VASP Case Study : Speed Up

Krista G Steenbergen MD Benchmark results for Intel SandyBridge (E5-2680)

Increase the performance

VASP Case Study : Efficiency

Krista G Steenbergen MD Benchmark results for Intel SandyBridge (E5-2680)
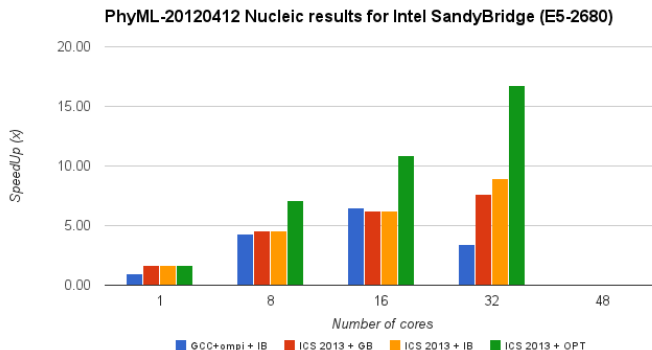
Increase the performance

PhyML Case Study

PhyML is software that estimates maximum likelihood phylogenies from alignments of nucleotide or amino acid sequences. The main strength of PhyML lies in the large number of substitution models coupled to various options to search the space of phylogenetic tree topologies, going from very fast and efficient methods to slower but generally more accurate approaches.

Developed by Dr. Stéphane Guindon (UoA)

PhyML is developed in NZ and is world-famous software in Phylogenetics. In this case, the right compilers and optimization options for an specific architecture increased the performance up to x6.
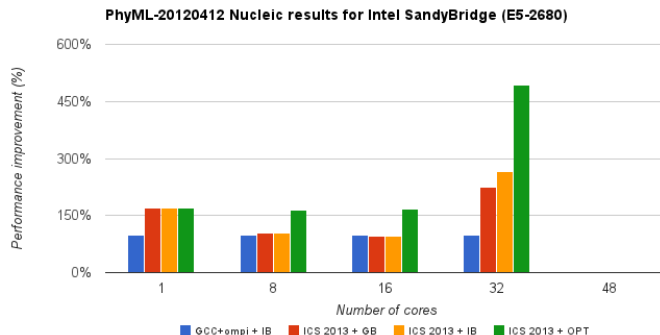
Increase the performance

PhyML Case Study : Speed Up

PhyML-20120412 Nucleic results for Intel SandyBridge (E5-2680)

Increase the performance

PhyML Case Study : Performance

Discover the scalability limits

How well does the code scales?

- There are theoretical limits but the reality can be really surprising!

- The scalability/quality of a code is measured in terms of efficiency (USL).

- The benchmarks can help to discover the real scalability limits.

- With this information you can get even faster results and save computational resources for other jobs.

Discover the scalability limits

Migrate-n Case Study

Migrate estimates effective population sizes and past migration rates between n population assuming a migration matrix model with asymmetric migration rates and different subpopulation sizes.

### Benchmark provided by Dr. Sarah Knight (UoA)

The research group of Dr. Sarah Knight were investigating the population structure and connectivity in the yeast species *Saccharomyces cerevisiae* (which is widely used by industry in the fermentation of beer, wine, bread etc.) in New Zealand. They used MIGRATE to obtain estimates of gene-flow or migration. The data they used was 8 microsatellite markers and they were investigating connectivity between 5 important wine growing regions.

Discover the scalability limits

Migrate-n Case Study
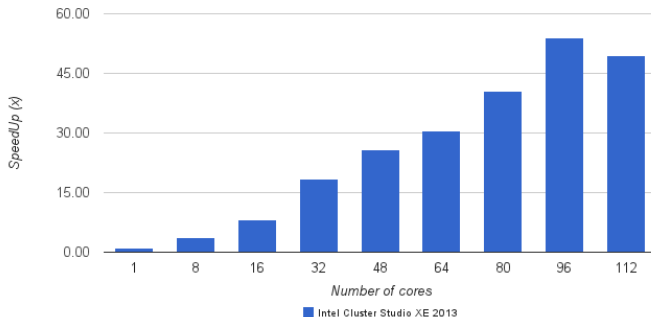
Improve the efficiency

The workflow can save several HPC resources

- Thanks to the nature of some codes, the problem can be transformed into a embarrassing parallel problem.

- In some cases it's possible to split large input file into several small files, allowing to run several copies of the same code using completely independent input files.

- In scenarios like these you can achieve a linear scalability.

- Several problems related with genomics have this approach.

Improve the efficiency
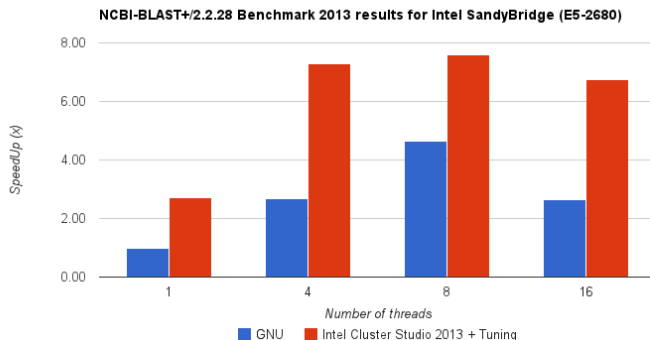
NCBI-BLAST+ Case Study

BLAST (Basic Local Alignment Search Tool) command line
applications developed at the National Center for Biotechnology
Information (NCBI).

Benchmark provided by Dr. Daniel White (Landcare Research)

It describes the dataset as a pathogen discovery dataset using de
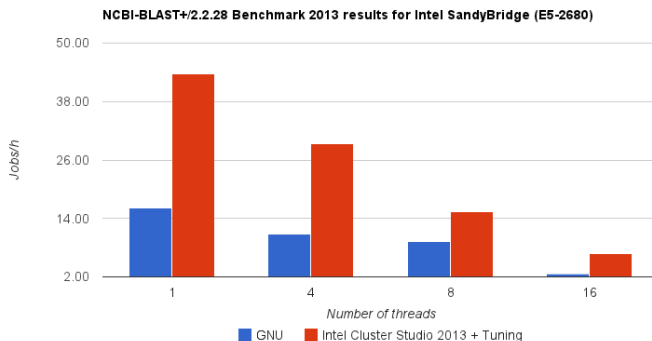novo metagenomics.

Improve the efficiency

NCBI-BLAST+ Case Study : Speed Up

Improve the efficiency
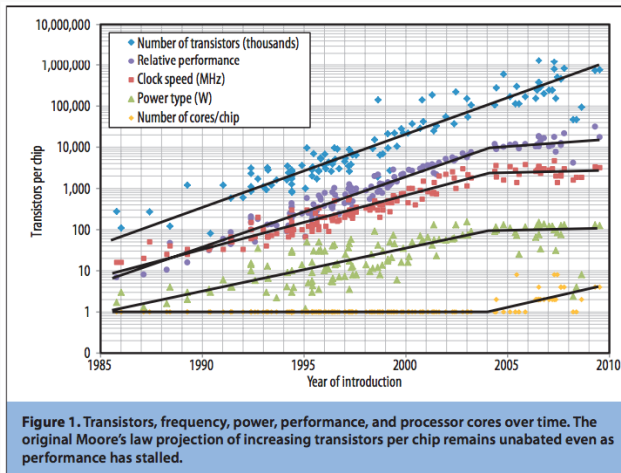
NCBI-BLAST+ Case Study : Efficiency

NCBI-BLAST+/2.2.28 Benchmark 2013 results for Intel SandyBridge (E5-2680)

Improve the efficiency

NCBI-BLAST+ Case Study : Speed Up compared with original code

threads	split	tuned binaries	SHM	Speed Up	Efficiency
1	1000	2.71	●	●	●
4	1000	7.27	●	●	●
8	1000	7.61	●	●	●
16	1000	6.74	●	●	●

Back to the future

Moore's Law

Figure 1. Transistors, frequency, power, performance, and processor cores over time. The original Moore's law projection of increasing transistors per chip remains unabated even as performance has stalled.

Back to the future

Sequencing Cost per Genome

Back to the future

About NeSI CS Team
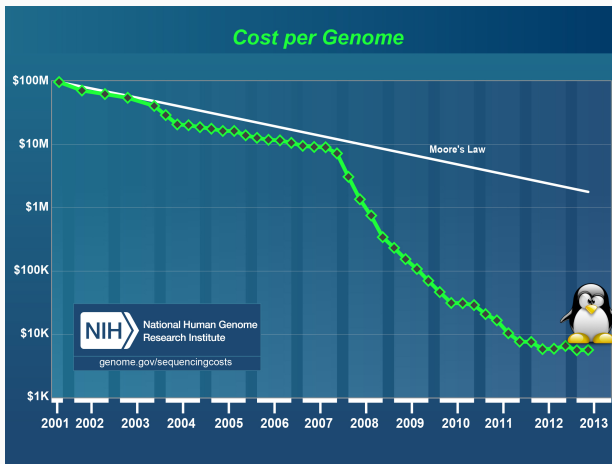oo

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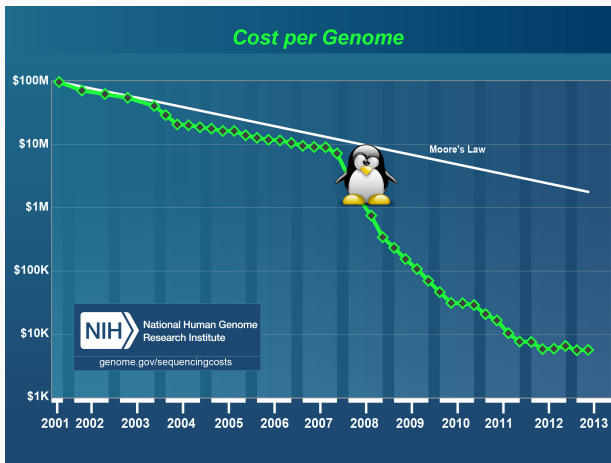
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Back to the future

Sequencing Cost per Genome

Back to the future

Are you still living in the 80's?

Questions & Answers