Improving NeSI researchers' productivity with a consultancy service

Chris Scott Alex Pletzer Wolfgang Hayek Georgina Rae

New Zealand eScience Infrastructure (NeSI)

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Outline

What is NeSI Consultancy?

Introduction

- Goals of NeSI's Consultancy service
  - Enable increased scale and complexity of research
  - Help researchers use NeSI's computing capabilities to increase research outputs and impacts

- How we achieve this
  - Working on projects with researchers; typically 1 day per week for 3-4 months
  - The scope of projects we work on is very broad and covers topics such as:
    - Code optimisation and/or parallelisation
    - Workflows
    - Improving software sustainability
    - Porting code to NeSI's platforms
    - Custom code development
    - Visualisation

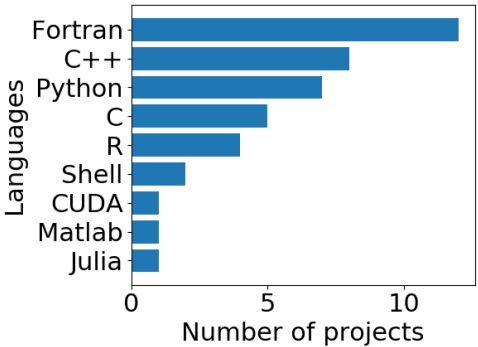
Consultancy projects

Applying for a project

- Usually researchers who meet the following criteria can access consultancy at no cost to themselves, based on their institution's or MBIE's investment into NeSI:
  - Researchers with Merit or postgrad projects
  - Researchers based at collaborator institutions
    - University of Auckland
    - NIWA
    - University of Otago
    - Manaaki Whenua - Landcare Research
- Others may be able to pay to access the service
- Application form
  - Usually filled out after an initial meeting
  - Defines the current state of the problem
  - Defines the scope of the work

Consultancy projects

Languages



- The programming languages that we have worked with
- Some projects had more than one language
- Fortran, C++/C still dominate
- Python and R are popular too
- We started work on our first project with Julia recently

Getting closer to more accurate climate predictions for New Zealand

Researchers:

Erik Behrens & Jonny Williams
National Institute of Water & Atmospheric Research (NIWA)

"The NZESM is a community project. With this upgrade we have an exciting tool with which to study the climate."

NeSI delivered:

- High performance computing resources
- Computational science expertise

Code development

NZESM project

- Multiple models that need to be coupled together (atmosphere, ocean, . . .)
- Using a tool called OASIS for coupling these models together
- We added a new feature to OASIS to enable an ocean coupling scheme for coupling a high resolution regional ocean component
- Important step to setting up customised earth, ocean and weather system modelling for New Zealand

Cascade trajectories project

- Infrastructure
  - Added a CMake build system
    - Easy to port to di erent systems
    - Easy to try di erent compilers Cray compiler 40% faster
  - Adding tests
- Optimisation
  - Optimised performance of serial Fortran code
    - 22 % boost
- Work ows
  - Instead of running one long calculation they can run many shorter calculations
  - Created Python/Slurm scripts to enable this parallel work ow and give a big boost in performance

Fractal analysis project

Code optimisation

- Matlab code
- Identi ed two functions with big loops that were performance bottlenecks
- Converted these functions to C++ and call from Matlab mex'ing
- Total speedup of 8x from converting these functions
- Other outcomes
  - Taught the researcher how to use git version control
  - Importance of testing adding a checksum to easily check result

Trinity project overview

Work ows and runtime tuning

- Genomics code - de novo assembly
- Complex work ow consisting of two distinct computational phases
  - Initial phase is multithreaded with high memory requirements (100s GB)
  - Second phase has many millions of short, serial embarrassingly parallel jobs with low memory requirements (5 GB)
- By default Trinity runs everything at once within a single high memory node not optimal

Trinity project solution

Work ows and runtime tuning

- HPCGridRunner launch embarrassingly parallel jobs on a compute grid (cluster)
  - Accumulated I/O bandwidth of many nodes gives much better performance

Type	Num cores	Elapsed time (hh:mm:ss)	Core hours
Single node	16	24:09:36	387
Grid	20	07:59:58	168
Grid	40	04:10:45	171
Grid	60	02:36:58	160

The NeSI consultancy service has drastically improved my work ow by reducing RNA de novo assembly time from 7 days to 24 hours!

Alexis Marshall, University of Waikato