Scientific supercomputing: Teaching practical skills for credit

KO TE TANGATA
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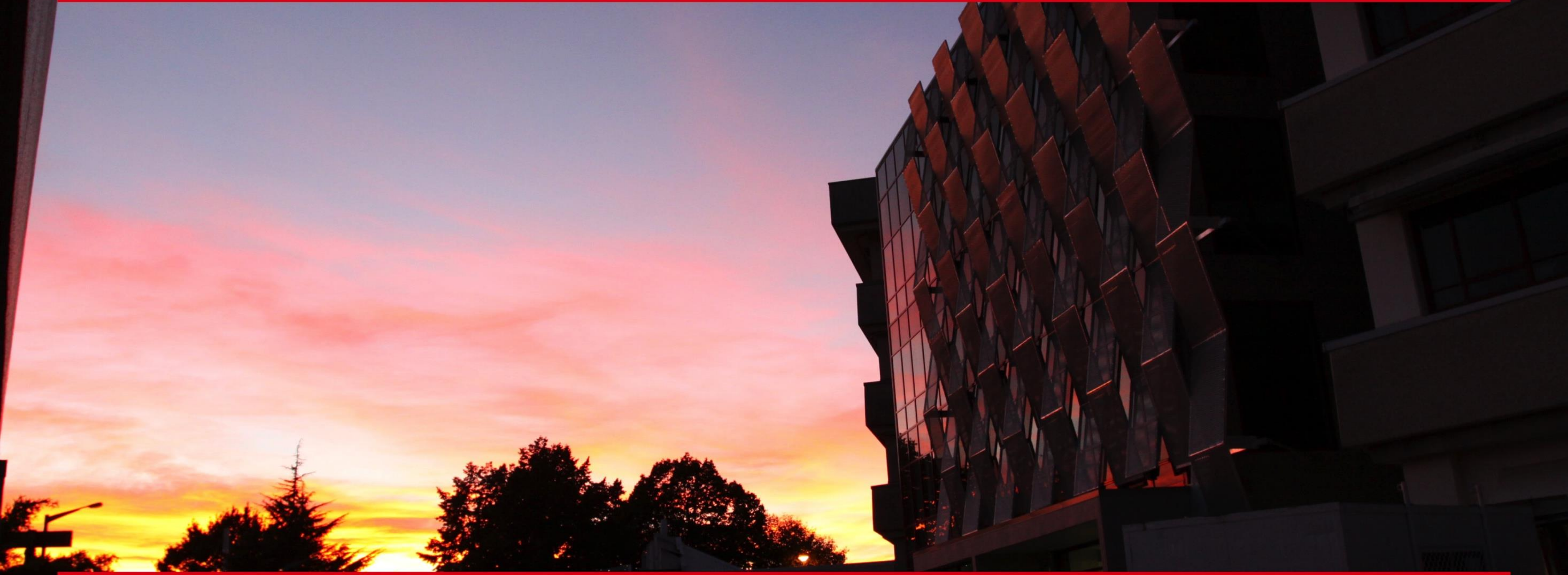

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WHERE THE WORLD IS GOING
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Postgraduate Science review

- Full review of our postgraduate degrees and papers
- Consultation with current/former students, employers, external stakeholders

"I want to learn through doing"

"I don't want to take harder undergraduate papers"

"Graduates need better practical skills"

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"Graduates need better practical skills"

- Led to revised degree structures and redevelopment of all taught papers

SCIEN511 – Scientific Supercomputing

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- 15 point paper (150 learning hours)

- **Overall goal:** To provide students with the skills necessary to run simulations on large-scale shared supercomputing facilities, such as the New Zealand eScience Infrastructure (NeSI).

- Taught via a short block-course, followed by a self-directed mini-research project

SCIEN511 – Scientific Supercomputing

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- ~~Taught via a short block-course, followed by a self-directed mini-research project~~

- Taught via a series of 2-hour workshops for six weeks, followed by a self-directed mini-research project

Learning outcomes

1. Navigate the Linux shell and use scripts to automate common tasks

2. Successfully apply for computer time to undertake research at a high-performance computer facility

3. Undertake a benchmarking exercise to determine the most efficient way to run scientific software on a high-performance computer

4. Undertake a mini-research project using scientific software and write up the results in the style of a journal article

Workshop structure

1. An introduction to the Linux command line (Codecademy)
2. Getting connect to NeSI
3. An introduction to HPC facilities
4. How to efficiently run scientific software on an HPC
5. How to automate simple tasks in Linux
6. How to design a computational research project

Assessment structure

- 100% internally assessed
- Assignment 1: Linux command line tutorial (10%, Pass/Fail)
- Assignment 2: Apply to use the NeSI supercomputers (10%, Pass/Fail)
- Assignment 3: Benchmark your software on NeSI (10%, graded)
- Assignment 4: Automate simple tasks in Linux (10%, graded)
- Mini-research project (60%, graded)

Mini-research project

- Any topic of choice, ideally related to a student's thesis/dissertation

- Written in the style of a relevant journal article for their discipline

- Key focus areas:
  - How to design a computational research project: What question are you ***actually*** trying to answer?
  - How to compare computational and experimental results
  - How to ensure computational results are reproducible
  - How to distill results and create a narrative when writing up

Review of paper

Worked well:

- Attracted students from different natural science disciplines
- Having NeSI onsite for some workshops
- Practical nature of workshops
- Self-directed mini-research projects
- Being open/transparent

Challenges:

- Underestimating assumed knowledge
- Keeping an appropriate pace with students from different backgrounds
- Bespoke preparatory assignments
- Getting some mini-research supervisors motivated

Summary and future outlook

- Overall, student feedback was very positive
- The paper will run again in July 2020 and enrolments look good already
- Students will complete generic rather than bespoke preparatory assignments under a single NeSI project
- Students will apply for their own NeSI project later in the paper, after they've mastered the practical elements and have a better idea of their research project

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