Single Node Optimisation

Overview

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Reusing this material

Partners

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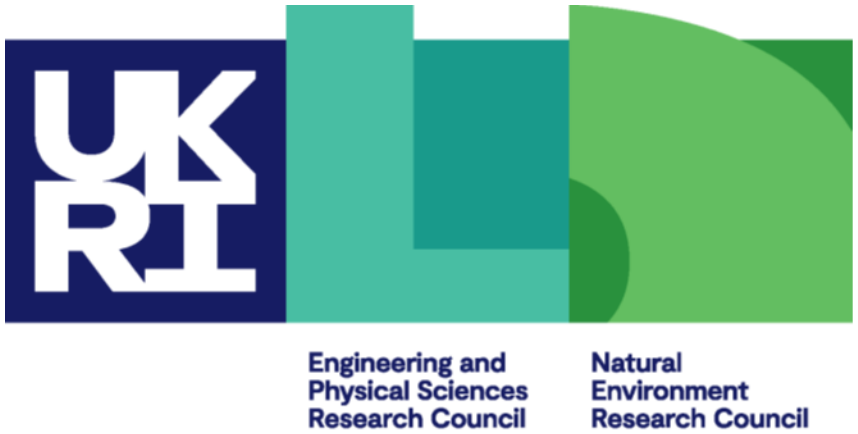

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THE UNIVERSITY of EDINBURGH

CRAY®

a Hewlett Packard Enterprise company

archer2

- UK National Supercomputer Service
  - managed by UKRI/EPSRC
  - to be housed, operated and supported by EPCC
  - hardware Supplied by Cray

- Training provided by the ARCHER2 Computational Science and Engineering (CSE) support team
  - 60 days per year at various locations
  - free to all academics

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ARCHER2

- System is 5860 nodes
  - 128 cores per node, 750,080 cores
  - 256 GB per node (512 for some large memory nodes)
  - Cray Slingshot interconnect
  - 4 Lustre filesystems (14PB)
  - 1 Burst buffer filesystem (1PB)

What is EPCC?

- UK national supercomputer centre
  - founded in 1990 (originally Edinburgh Parallel Computing Centre)
  - a self-funding Institute at The University of Edinburgh
  - running national parallel systems since Cray T3D in 1994
  - around 120 full-time staff
  - a range of academic research and commercial projects
  - one-year postgraduate masters in HPC www.epcc.ed.ac.uk/msc/
- Get in contact if you want to collaborate
  - many staff are named RAs on research grants
  - joint research proposals
  - European project consortia
  - ...

Key ARCHER2 Resources

- Upcoming courses
  - http://www.archer2.ac.uk/training/
- Material from past courses
  - https://www.archer2.ac.uk/training/materials/
- Virtual tutorials (online)
  - https://www.archer2.ac.uk/training/online/
- Documentation
  - https://www.archer2.ac.uk/documentation/

Who am I?

Adrian Jackson a.jackson@epcc.ed.ac.uk

- Research at EPCC
  - Interests in parallel algorithms, parallel programming models, benchmarking, novel uses of HPC, computing hardware
- Lecture on EPCC's MSc in HPC

Other Resources

- Please fill in the feedback form!
  - https://www.archer2.ac.uk/training/feedback/
- General enquiries about ARCHER go to the helpdesk
  - support@archer2.ac.uk
- EPCC runs one-year taught postgraduate masters courses
  - ***MSc in HPC*** and ***MSc in HPC with Data Science***
  - awarded by the University of Edinburgh since 2001
  - scholarships available
  - http://www.epcc.ed.ac.uk/msc/

Access to ARCHER2

- Your ARCHER2 `ta129` project accounts
  - Should be active for a month after the course has finished
  - Small amount of budget
  - `ta129` project accounts allow us to use a reservation to access dedicated compute nodes and get our jobs to run more quickly
  - Other ARCHER2 accounts can be used

- Accounts will be closed two weeks after access ends
  - all files etc. will be deleted
  - take copies of all your work beforehand!

- Take copies of all your work before that time if you want to keep it!

- Course materials (slides, exercises etc) available from ARCHER2 website
  - archived on ARCHER2 web pages for future reference

Code of Conduct

https://www.archer2.ac.uk/training/code-of-conduct/

- We expect all course trainers and attendees to:
  - Use welcoming and inclusive language
  - Be respectful of different viewpoints and experiences
  - Gracefully accept constructive criticism
  - Focus on what is best for the community
  - Show courtesy and respect towards other community members
- See web page for full details and incident reporting form

Funding calls

- Embedded CSE support
  - Through a series of regular calls, Embedded CSE (eCSE) support provides funding to the ARCHER2 user community to develop software in a sustainable manner to improve research on the ARCHER2 service.
  - The funding allows the employment of a Research Software Engineer (RSE) to carry out software development of ARCHER2 software.
- Scope of funding
  - Implementation of algorithmic improvements within an existing code in a portable manner
  - Improving the scalability of software on higher core counts in a portable manner
  - Improving a code to enhance sustainability and maintainability
  - Improvements to code that allow new science to be carried out on ARCHER2
  - Migrating, porting and optimising a code in significant use by an EPSRC or NERC community to run efficiently on ARCHER2 and next generation architectures. (This will be used to prioritise the NERC projects).
  - Adding new functionalities to existing codes
  - Code development to take a code from a Tier-2 (Regional) or local university cluster to ARCHER2
- See https://www.archer2.ac.uk/ecse/ for details

Timetable – Day 1

- 09.30 – 09.45 Introduction
- 09.45 – 10.30 Node Architecture
- 10.30 – 11.00 Practical – memory performance
- 11.00 – 11.30 Break
- 11.30 – 12.30 Profiling
- 12.30 – 13.00 Practical – profiling
- 13.00 – 14.00 Break
- 14.00 – 15.00 Optimising with the compiler
- 15.00 – 15.30 Break
- 15.30 – 17.00 Practical – profiling and optimization
- 17.00 – 17.10 Summary
- 17.10 – 17.30 Practical – profiling and optimization

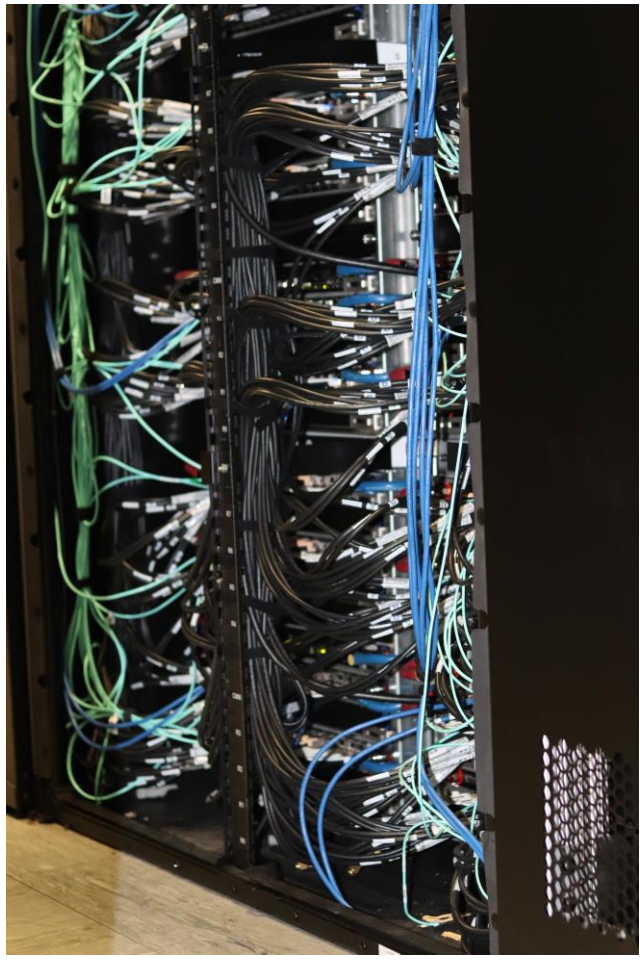
Timetable – Day 2

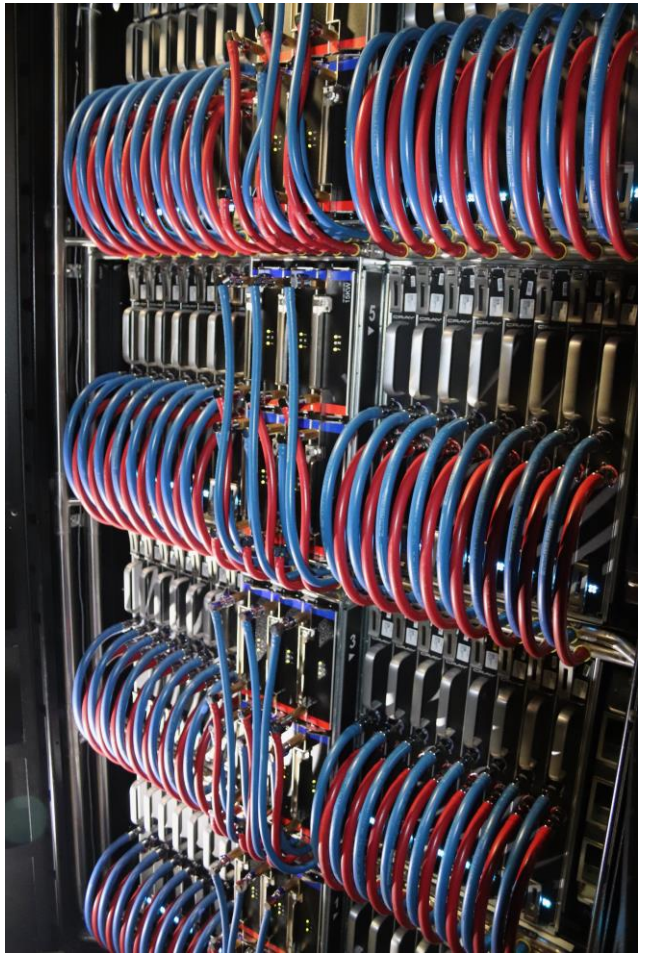
- 09.30 – 11.00 OpenMP optimisation
- 11.00 – 11.30 Break
- 11.30 – 12.30 Practical – OpenMP optimisation
- 12.30 – 13.30 Break
- 13.30 – 15.00 Vectorisation, Memory Hierarchy Optimisation
- 15.00 – 15.30 Break
- 15.30 – 16.30 Practical – memory and cache blocking

Lecture notes etc.

Go to

https://github.com/EPCCed/single-node-optimisation-course/tree/2023-11-23





Practical exercises source code

To download the source code for the practical exercises, make sure you are in your **work** directory on ARCHER, then use the following command :

```
cp /work/z19/shared/SNO.tar .
tar xvf SNO.tar
```

I hope you enjoy the course

- ... and *please ask questions*!