

Single Node Optimisation

Overview

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Partners



Engineering and
Physical Sciences
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Environment
Research Council



THE UNIVERSITY
of EDINBURGH



a Hewlett Packard Enterprise company





- 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



ARCHER2



- Full system will be 5848 nodes
 - 128 cores per node, 748,544 cores
 - 256 GB per node (512 for some large memory nodes)
 - Cray Slingshot interconnect
 - 4 Lustre filesystems (14PB)
 - 1 Burst buffer filesystem (1PB)
- Current system, 4 cabinets, 1024 nodes
 - One filesystem
 - No large memory nodes
 - No burst buffer filesystem

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 65 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 Fellow 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 `ta013` project accounts
 - Should be active for a month after the course has finished
 - Small amount of budget
 - `ta013` 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



The Partnership for Advanced Computing in Europe | PRACE

EPCC's PRACE Training Centre

PRACE | 26 members

(UK represented by EPCC on behalf of UKRI)

Hosting Members

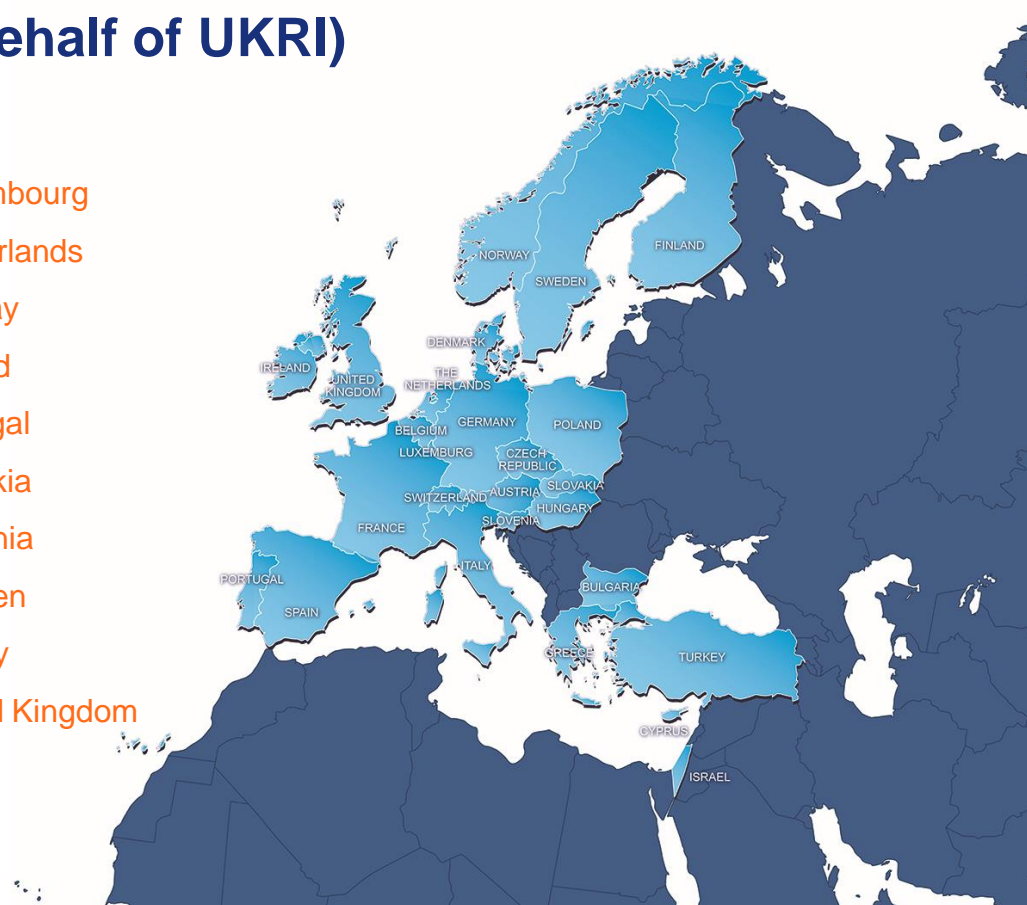
- ▶ France
- ▶ Germany
- ▶ Italy
- ▶ Spain
- ▶ Switzerland

Observers

- ▶ Croatia
- ▶ Romania

General Partners (PRACE 2)

- | | |
|------------------|------------------|
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| ▶ Finland | ▶ Slovenia |
| ▶ Greece | ▶ Sweden |
| ▶ Hungary | ▶ Turkey |
| ▶ Ireland | ▶ United Kingdom |
| ▶ Israel | |



PRACE | 10 Training Centres (PTCs)

- ▶ Hubs for world-class HPC training for researchers in Europe: www.training.prace-ri.eu
 - ▶ Barcelona Supercomputing Center (Spain)
 - ▶ CINECA - Consorzio Interuniversitario (Italy)
 - ▶ CSC - IT Center for Science Ltd (Finland)
 - ▶ EPCC at the University of Edinburgh (UK)
 - ▶ Gauss Centre for Supercomputing (Germany)
 - ▶ GRNET (Greece)
 - ▶ ICHEC (Ireland)
 - ▶ IT4I (Czech Republic)
 - ▶ Maison de la Simulation (France)
 - ▶ SURFsara (Netherlands)

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/2021-01-29>

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!*