

Single Node Optimisation Overview



Reusing this material



This work is licensed under a Creative Commons Attribution-NonCommercial-ShareAlike 4.0 International License.

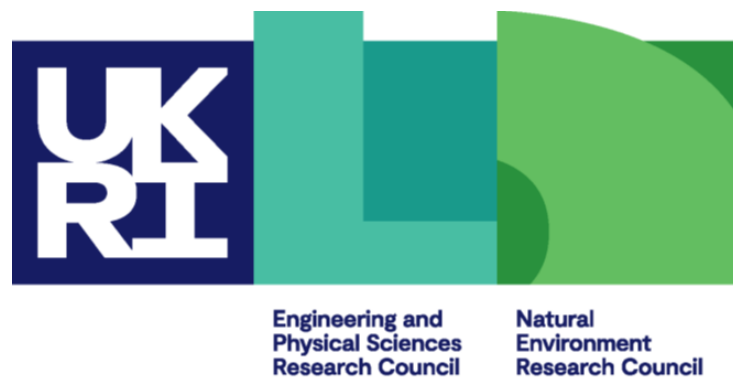
<https://creativecommons.org/licenses/by-nc-sa/4.0/>

This means you are free to copy and redistribute the material and adapt and build on the material under the following terms: You must give appropriate credit, provide a link to the license and indicate if changes were made. If you adapt or build on the material you must distribute your work under the same license as the original.

Note that this presentation contains images owned by others. Please seek their permission before reusing these images.



Partners



THE UNIVERSITY
of EDINBURGH

CRAY[®]
a Hewlett Packard Enterprise company





- UK National Supercomputer Service
 - managed by UKRI/EP SRC
 - 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 are we?



Mark Bull markb@epcc.ed.ac.uk

- Senior research fellow at EPCC
- Lecture on EPCC's MSc in HPC
- EPCC's representative on the OpenMP ARB

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

- Research Fellow at EPCC
- 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 `ta039` project accounts
 - Small amount of budget
 - `ta039` 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!
- 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

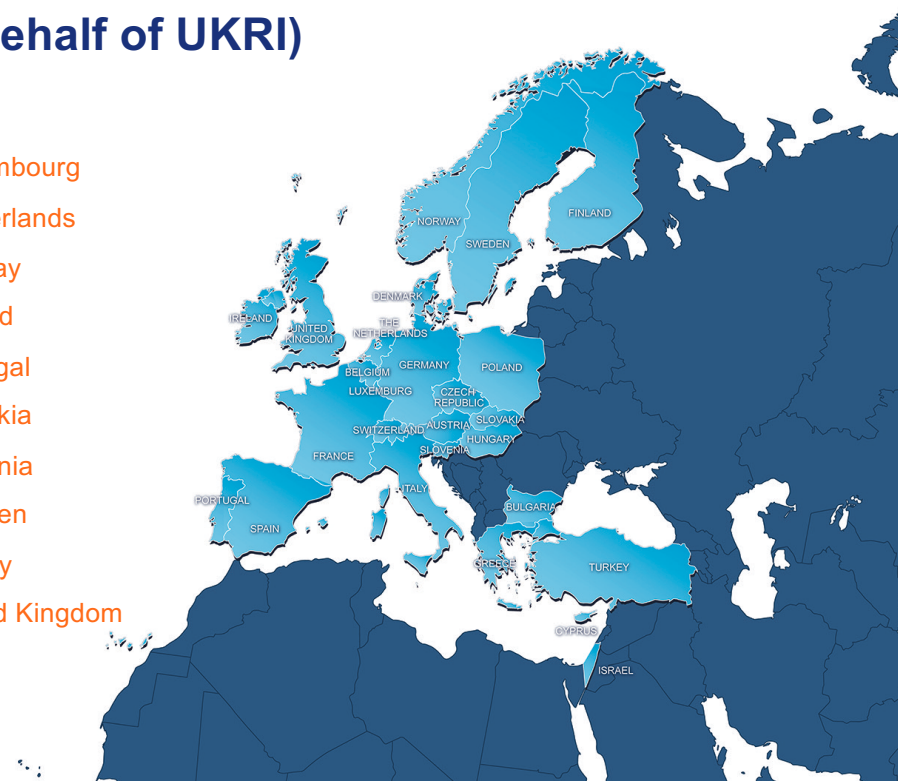
- ▶ France
- ▶ Germany
- ▶ Italy
- ▶ Spain
- ▶ Switzerland

Observers

- ▶ Croatia
- ▶ Romania

General Partners (PRACE 2)

- | | |
|------------------|------------------|
| ▶ Austria | ▶ Luxembourg |
| ▶ Belgium | ▶ Netherlands |
| ▶ Bulgaria | ▶ Norway |
| ▶ Cyprus | ▶ Poland |
| ▶ Czech Republic | ▶ Portugal |
| ▶ Denmark | ▶ Slovakia |
| ▶ 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/2021-09-07>



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!*

