ARCHER2 for Data Scientists

Introduction

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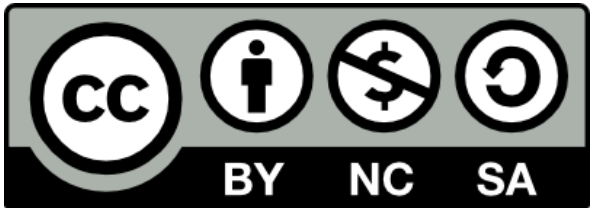

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- New UK National Supercomputer Service
  - managed by UKRI/EPSRC
  - Housed, operated and supported by EPCC
  - hardware supplied by Cray
- Training provided by the ARCHER2 Computational Science and Engineering (CSE) support team
  - 60 days per year at various locations
  - free to all academics

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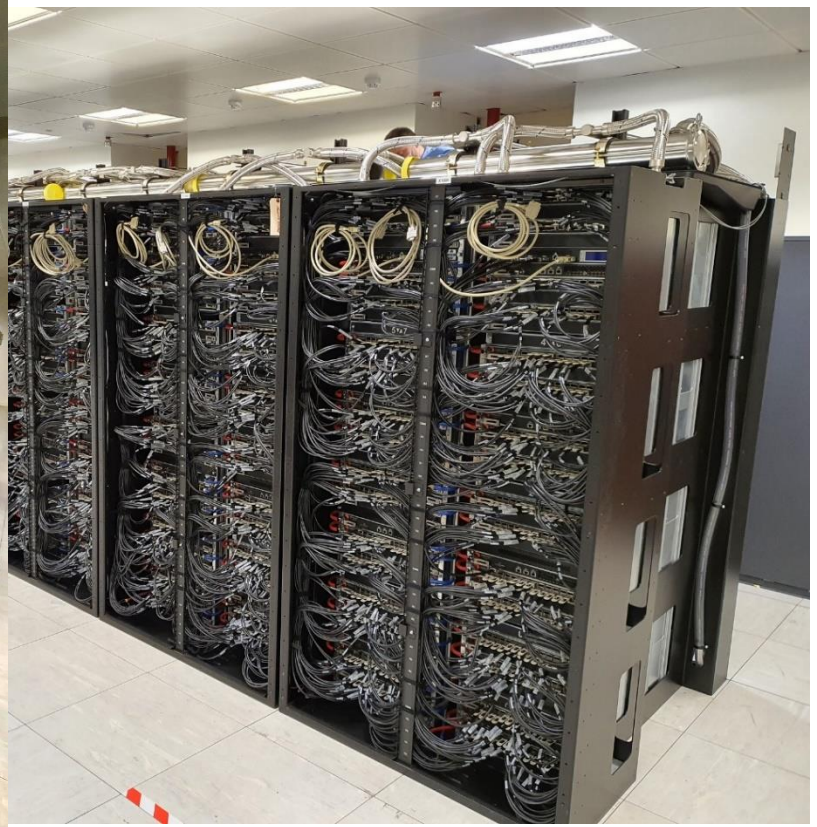
Located at EPCC's Advanced Computing Facility (ACF)



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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)
  - http://www.archer2.ac.uk/training/
- Documentation
  - http://www.archer2.ac.uk/documentation/

Who am I?

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

- Teach at EPCC on HPC and program optimisation:
  - MSc, PhDs
  - PRACE Advanced Training Centre
  - ARCHER training programme
  - commercial training
  - ...
- Also do HPC research
  - Porting and optimizing community codes
  - new parallel programming models, accelerators, performance, memory hardware, ..

Other Resources

- Please fill in the feedback form!
  - you will be sent a link at the end of the course
- General enquiries about ARCHER2 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 during course

- Personal accounts for duration of course
  - will allow machine access for up to a month afterwards
- 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) will continue to be available from ARCHER2 website
  - archived on ARCHER2 training pages for future reference

Code of Conduct

https://www.archer2.ac.uk/about/policies/code-of-conduct.html

- 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.

- See https://www.archer2.ac.uk/ecse/ for details

ARCHER2 hardware / software setup

- 5,860 nodes each with 128 AMD CPU-cores
  - made up of 2x64-Core AMD multicore processors
  - more than 750,000 CPU-cores!
- Batch access via SLURM: sbatch, squeue, ...
- Two file systems – you have two directories:
  - /home/project/project/username
  - /work/project/project/username
- You must run all parallel jobs from /work/
  - I recommend you “cd” straight there every time you log in
- If required, reserved queues each day for fast turnaround

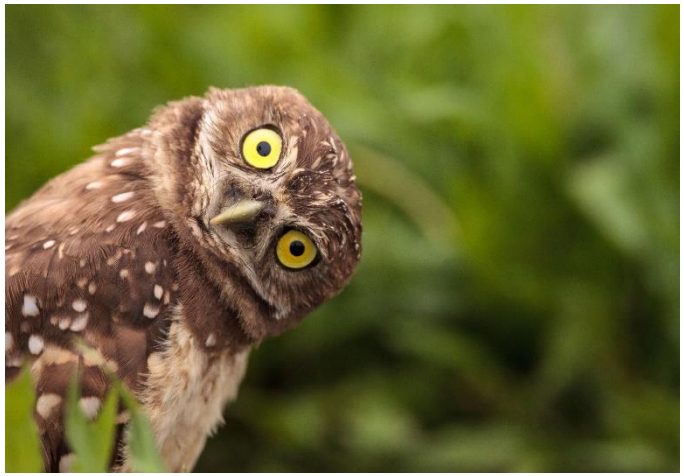
Timetable

- 10:00 - Registration and check connections
- 10:10 - L01: Introduction to ARCHER2
- 10:30 - L02: Containers and installing software
- 11:15 - Break
- 11:30 - Exercise: Containers
- 12:30 - L03: Parallel Python on ARCHER2
- 13:00 - Lunch
- 14:00 - Exercise: Parallel Python
- 14:30 - L04: Dask
- 15:30 - Break
- 16:00 - L05: Parallel R on ARCHER2
- 17:00 - Exercise: Parallel R
- 17:30

Course aims

- ARCHER2 for Data Scientists
  - Teach you want you need to know to:
    - Understand what ARCHER2 is suitable for
    - Run your workflows on ARCHER2
    - Install new software on ARCHER2
    - Use the hardware as efficiently as possible
  - Not aiming to teach you:
    - How to undertake data science
    - The one tool you need use
- Focussing on:
  - Containers
  - Python
  - R

I hope you enjoy the course



- ... and *please ask questions*!