ARCHER2 User Forum

ARCHER2 Celebration of Science

15 May 2025

EPSRC
and NERC

THE UNIVERSITY
of EDINBURGH

Hewlett Packard
Enterprise

- 0900 Introductions : Josephine Beech-Brandt (EPCC)
- 0905 Environmental Sustainability : Andy Turner (EPCC)
- 0910 Centre of Excellence Container activity : Holly Judge (HPE)
- 0915 Software Upgrade Project : Kieran Leach (EPCC)
- 0920 Training : Juan Herrera (EPCC)
- 0925 Management Update : Alan Simpson (EPCC)
- 0930 User Forum Discussion

Environmental Sustainability

Andy Turner, ARCHER2 CSE

Environmental Sustainability *(Andy Turner, CSE)*

- Described a methodology for estimating carbon emissions from ARCHER2 system based on Greenhouse Gas (GHG) Protocol.
  - Includes embodied and operational emissions estimates
  - https://www.archer2.ac.uk/news/2024/11/28/emissions.html
- Developed tools to allow users to estimate emissions from their use of ARCHER2.
  - Can be used to look at historical use or predict future emissions
  - https://docs.archer2.ac.uk/user-guide/energy/#estimating-your-emissions
- Developed open-source training to help all HPC stakeholders become more carbon literate and take action to reduce emissions from HPC.
  - Two courses run so far, and another planned for London in July 2025
  - Part of Carpentries Incubator and HPC Carpentry
  - https://carpentries-incubator.github.io/green-software-hpc/

Centre of Excellence container activities

15/05/2025

Holly Judge - CoE

ARCHER2 Centre of Excellence

- Part of ARCHER2 service, 3 staff based in Edinburgh, 2 remote
- Core activities:
  - Deep CSE and Application Support
    (includes issue resolution via helpdesk)
  - Training and Education
  - Future Systems Evaluation
    (GPU platform)
  - Research Software Development
    (System monitoring, energy optimization)
  - Recent focus on directly assisting HEC community

Container strategy

- Some of the installed software on ARCHER2 is not the latest available
- Containerised versions of the Cray programming environment (CPE) are available on ARCHER2 including the very latest v25.03
  - These give developers the opportunity to try out the latest compilers.
- Newer ROCm can be installed and used within a container.
  - For GPU applications which are unsupported with v5.2.3
  - Performance improvements
  - Ease of use for setting up machine learning environments which can include many python packages.
- Even when ARCHER2 is upgraded newer versions of software will be released
  - CPE 25.03 now the latest
  - New ROCm release almost monthly

Currently installed on ARCHER2

Cray programming environment (CPE):

22.12

23.09

GPUs: ROCm 5.2.3

Container options

Cray Programming environment (CPE)

23.12
24.03
24.07
24.11
25.03

- Test new versions of the CPE than available on ARCHER2
- New CCE compilers, cray-mpich, cray-python etc.
- COE enhancements to the image to use lmod and Slurm and add packages.

Standalone ROCm

v5.2.3 – 5.7.1

- New ROCm needed for some applications
- Allows to easily use custom python environments in container – convenient for python ML frameworks using GPUs.
- Can also install ROCm aware MPI

Cray Programming environment (CPE) + ROCm

23.09 w/ ROCm 5.7
23.12 w/ ROCm 5.7

- Useful for applications which have GPU offloading and need newer ROCm than 5.2.3
- Use of CCE and cray libraries e.g. cray-mpich and ROCm
- CPE versions which are compatible with ROCm 5

Using CPE containers

- Compiler environment:

Launches singularity shell with the image CCPE image and binds host libfabric, xpmem and slurm

```
user@ln03:/work/group/group/user/osu-micro-benchmarks> $CCPE_SHELL
Singularity>
Singularity> module load rocm/5.7.0
Singularity> module load craype-accel-amd-gfx90a
Singularity> module load craype-x86-milan
Singularity> export MPICH_GPU_SUPPORT_ENABLED=1
Singularity> module li

Currently Loaded Modules:
  1) libfabric/1.12.1.2.2.0.0            4) cce/17.0.0        7) cray-mpich/8.1.28    10) rocm/5.7.0
  2) craype-network-ofi                  5) craype/2.7.30     8) cray-libsci/23.12.5  11) craype-accel-amd-gfx90a
  3) xpmem/2.5.2-2.4_3.30__gd0f7936.shasta   6) cray-dsmml/0.2.2   9) PrgEnv-cray/8.5.0    12) craype-x86-milan

Singularity> CC=cc CXX=CC ./configure --enable-rocm --with-rocm=/opt/rocm-5.7.0
Singularity> make
```

- Launching in a job script:

Launches singularity exec with the image CCPE image binds host libraries and slurm

```
srun $CCPE_RUN osu-micro-benchmarks/c/mpi/pt2pt/osu_bw -d rocm D D
```

Recap

- We can provide access to CPE and CPE with GPU support containers for use on ARCHER2
- Can help you to:
  - Investigate if issues are fixed with newer software
  - Provide workaround until fixes are installed on ARCHER2
  - Convenience as a start point to build more complex environments

- Note that in same cases the containers are running software not technically supported in the host environment so there may be issues
- Please come to talk to us if you are interested in this (or submit a query)
- See also (from EPCC): https://docs.archer2.ac.uk/user-guide/containers/

Software Upgrade Project

Kieran Leach, ARCHER2 SP

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Background

- ARCHER2 compute and login node OS is historically tied to the system management software version
  - Upgrades to system management software have historically required multiple weeks of system downtime
  - Newer versions of the system management software also offer no particular benefits to our service
- Regardless of these issues we have a preference for upgrading compute/login node OS to gain access to security updates
- HPE have identified a method to separate the compute and login node OS from the system management software version

Implementation

- HPE have now completed testing and demonstration of a new way of delivering compute and login node OS
- This has been tested on the TDS (Test and Development System)
- ARCHER2 RSE Team are currently testing a proposed new image based on an installation of SUSE Linux Enterprise Server 15 SP4
  - This is the same OS version as current ARCHER2 images are based upon
  - HPE customisations are integrated after installation rather than added before install as at present
- A 140-node reservation is currently being used for testing
- Consortia are nominating select users to test against these nodes

What's next?

- Testing on 140 nodes across the rest of May
- Scale testing on 600-1200 nodes in early June which will both:
  - Validate the new deployment methodology for compute and login node OS and;
  - Support testing of application software at scale
- If testing is successful we will migrate to the new software version
  - This should take on the order of 1-2 days
  - Much of this time will be to allow for system-scale testing
- Future upgrades are anticipated to be deployable via rolling reboot
- SLES 15SP4 will have long term support available throughout the anticipated life of the service

Training

Juan Herrera, ARCHER2 CSE

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Training *(Juan Herrera, CSE)*

- **60+ days of interactive face-to-face and online courses and webinars**
- Course catalogue aimed to cover users' needs
- Self-service courses also available:
  - MPI
  - OpenMP
  - GROMACS+CP2K
  - Intro to HPC
- Past course materials and recordings available on the ARCHER2 website
- Feedback from:
  - Past course attendees
  - ARCHER2 user forum
  - ARCHER2 training panel

Training *(Juan Herrera, CSE)*

Topic	Number of days
Software Carpentry (#1), Data Carpentry (#1), HPC Carpentry (#2)	8
Introduction to LAMMPS	1
Introduction and Advanced MPI	4
Modern C++ (#2)	4
Introduction and Intermediate Fortran	4
Intro to Data Science and ML, Data Analysis and Visualisation in Python	4
GPU training (#5)	13
Containers, Efficient Parallel IO, Green HPC, Intermediate RSE, Single-Node Opt.	12
Training delivered by HPE	3
HPC System Administration basics	2
Webinars (#16)	8
	63

Training *(Juan Herrera, CSE)*

- What topics would you add/remove/keep?
- Is there any course that you (or your consortium) might be particularly interested in?
- Would you prefer to enrol in any of the below courses in a self-service format?

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Management Update

Alan Simpson, ARCHER2 Service Director

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Management *(Alan Simpson, Service Director)*

- ARCHER2 continues to meet all service metrics and utilisation remains very high
  - Celebration of Science demonstrates the excellent range of research delivered by ARCHER2!

- As some of you may know, I significantly reduced my hours about 6 months ago
  - My exclusive focus is now on my role as ARCHER2 Service Director
  - …with primary responsibility for ensuring ARCHER2 delivers a high quality service to users
- ARCHER2 management team remains in situ
  - Paul Clark, Lorna Smith, George Beckett, Andy Turner, Jo Beech-Brandt,…
- Jo Beech-Brandt has now taken over my previous role as Director of HPC Services
  - Congratulations and best wishes to Jo!

Feedback from Users

- EPCC are very keen to ensure ARCHER2 service is tailored to user requirements
- We get valuable feedback from:
  - Queries
  - Annual User Survey
  - User Forum
  - Training Panel/Forum
  - User Advisory Group
    - https://www.archer2.ac.uk/about/uag/
- We welcome feedback on any aspect of ARCHER2
  - Please do speak to me or any of my colleagues (yellow badges)
- UKRI have recently commissioned London Economics to undertake a socio-economic impact assessment of ARCHER2
  - See printed sheets on tables

Future Plans

- **Software Upgrade:** as discussed previously
- **ACF Power Outage:** there will be a 2-week full outage of ARCHER2 in September to address a significant switchgear Health and Safety risk
  - More details in plenary talk from Prof. Mark Parsons
- **Audits:** our annual external ISO audits are due in June
  - Covering: Quality; Information Security; Business Continuity
- **Extension:** UKRI have indicated that they intend to extend ARCHER2 for another year until November 2026

- **Key Target:** ensure ARCHER2 continues to enable high quality research for the remainder of its lifetime

User Forum: Discussion

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