ARCHER2 Training

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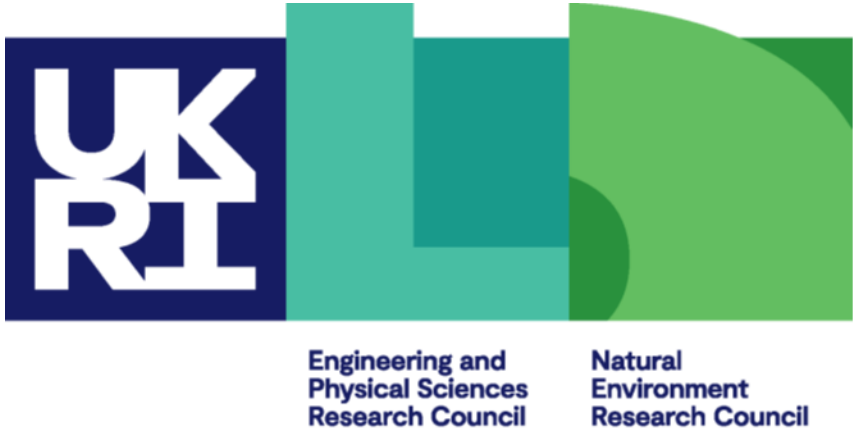
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EPCC and Training

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Past experience

- 50% staff involved (in some capacity) in Training.
- 25 years of experience running training for national HPC services.
  ARCHER (72 days of training per year since 2013, 446.5 days, around 200 courses).
- PRACE Training Centre (since 2012).
- ACM SIGHPC Education Chapter.
  Co-chairs of Content and Outreach sub-committees.
- Regular tutorials and workshops at SC and ISC conferences.
- Free online Supercomputing MOOC on FutureLearn, completed by almost 1,000 people.
- Hands-on courses at 9 International HPC Summer Schools since 2010 at locations around Europe, the USA and Canada.
- Training at EPSRC-funded HPC Autumn Academies in Cambridge from 2011.

Academia involvement

- Post-graduate programmes at The University of Edinburgh:
  - MSc in HPC (since 2001). Available fully online from Sep 2020.
  - MSc in HPC with Data Science (since 2014). Available fully online from Sep 2020.
  - Data Science, Technology and Innovation (University-wide online).

  Resulting in over 300 post-graduates trained in RSE skills to support researchers using HPC and data science.
- Past publications:
  - **C. Barrass**, and **D. Henty** (2017). *Novel Approaches to HPC User Engagement.* Cray User Group 2017 in Washington, US.
  - J. Kunkel, K. Himstedt, N. Hübbe, H. Stüben, S. Schröer, M. Kuhn, M. Riebisch, S. Olbrich, T. Ludwig, **W. Filinger**, J.-T. Acquaviva, A. Gerbes, and L. Lafayette. *Towards an HPC certification program*. Journal of Computational Science Education, 10 (1), pp. 88-89, 2019. ISSN 2153-4136, DOI 10.22369/issn.2153-4136/10/1/14.

Collaborations

- The DiRAC national HPC service.
- Centres of excellence: Hartree Centre, Alan Turing Institute, PRACE Training Centres, Software Sustainability Institute, The Carpentries…
- The VI-HPS Institute (help deliver collaborative HPC performance tools courses).
- Vendors: Cray, Intel, AMD, ARM, NVIDIA and HPE.
- Code developers: VASP, CASTEP, CP2K, Code Saturne, Unified Model…
- Leading HPC projects: BioExcel, INTERTWinE, EUDAT, Women in HPC…


ARCHER2 Training: Highlights
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Scope and Mission

- Training is a function inside the Computational Science and Engineering (CSE) service.
- ARCHER2 will provide a rich, diverse programme of training that is responsive to users' evolving needs.
- 60 days of training per year around the UK.
- EPCC's training activity is underpinned by our ISO9001-accredited Quality Management System.

Challenges

1) COVID-19 outbreak
   - Courses will be delivered online for the foreseeable future.
2) ARCHER2 Hardware
   - Delayed until later in 2020.
   - Use of ARCHER in the meantime.
   - Thanks to Cray/HPE, EPCC will get remote access to some of the new equipment in the factory, enabling EPCC to learn about the new Shasta system and prepare the course materials.
   - ARCHER2 specific courses will be delivered later in the year.

Delivery mechanisms and tools

- Use of Blackboard Collaborate.
  - Collaborate has coped with more than 100 attendees
- Course materials available via Github.
- Use of Etherpad (collaborative editing in real-time).
- We record all online sessions and put videos on the web afterwards.

Innovations

- We will offer ARCHER2 access before courses.
- Ongoing machine access after the course ends for users to practise putting skills into action.
- **Follow-up virtual consultancy session** around one month after a course ends to allow attendees to ask questions after they have started to put the course material into practice in their research.

Accessibility and diversity

- Course materials are available on the webpage with at least 24 hours in advance.
- Building and room are accessible to those who can not use stairs. This includes teaching rooms, catering and toilet facilities.
- There is a microphone for instructors. We also prefer rooms to be equipped with a hearing induction loop, though if required we can provide a portable loop.
- ARCHER2 website follows the WCAG guidelines (level AA).
- We have a *Diversity and Inclusion Policy*:
  https://www.archer2.ac.uk/about/policies/diversity-inclusion.html
  - Promote a welcoming and positive learning environment on all our courses.
  - ARCHER2 Code of Conduct (based on The Carpentries CoC).

Feedback

- Comments on post-course questionnaires.
- Feedback from training staff at internal post-course reviews (mandatory for every course).
- Input from annual ARCHER2 user survey and training impact survey.

Programme tailored to users' needs

A training programme that is flexible and responsive to user's need, with an independent

- ARCHER2 User Training Forum to provide ongoing input into the design and delivery of the training programme.
- ARCHER2 Training Panel to approve this programme.

ARCHER2 Training User Forum

- Mission: provide ongoing input into the design and delivery of the training programme.
- Members:
  - One nominated member per all core consortia.
  - User community members with significant interest/experience in/of HPC training.
- The forum will be consulted for input on the training plan from year 2 onwards before it is sent to the ARCHER2 Training Panel for approval.
- This forum will help ensure our ARCHER2 training programme is a strategic fit to on-going community training needs.
- It will be set up soon.

ARCHER2 Training panel

- Programme approved by an independent Panel, whose functions are:
  - Approve each annual programme
  - Address the balance of delivery routes
  - Ensures scientific and technical diversity
  - Considers courses topics, course levels and geographic distribution.
- Panel members:
  - External chair: Jo Lampard (UCL, UK).
  - Six members from the UK and overseas such as Sweden, US, and Australia.

ARCHER2 Training: Course plan

Course levels

We have classified the ARCHER2 courses into 3 levels:

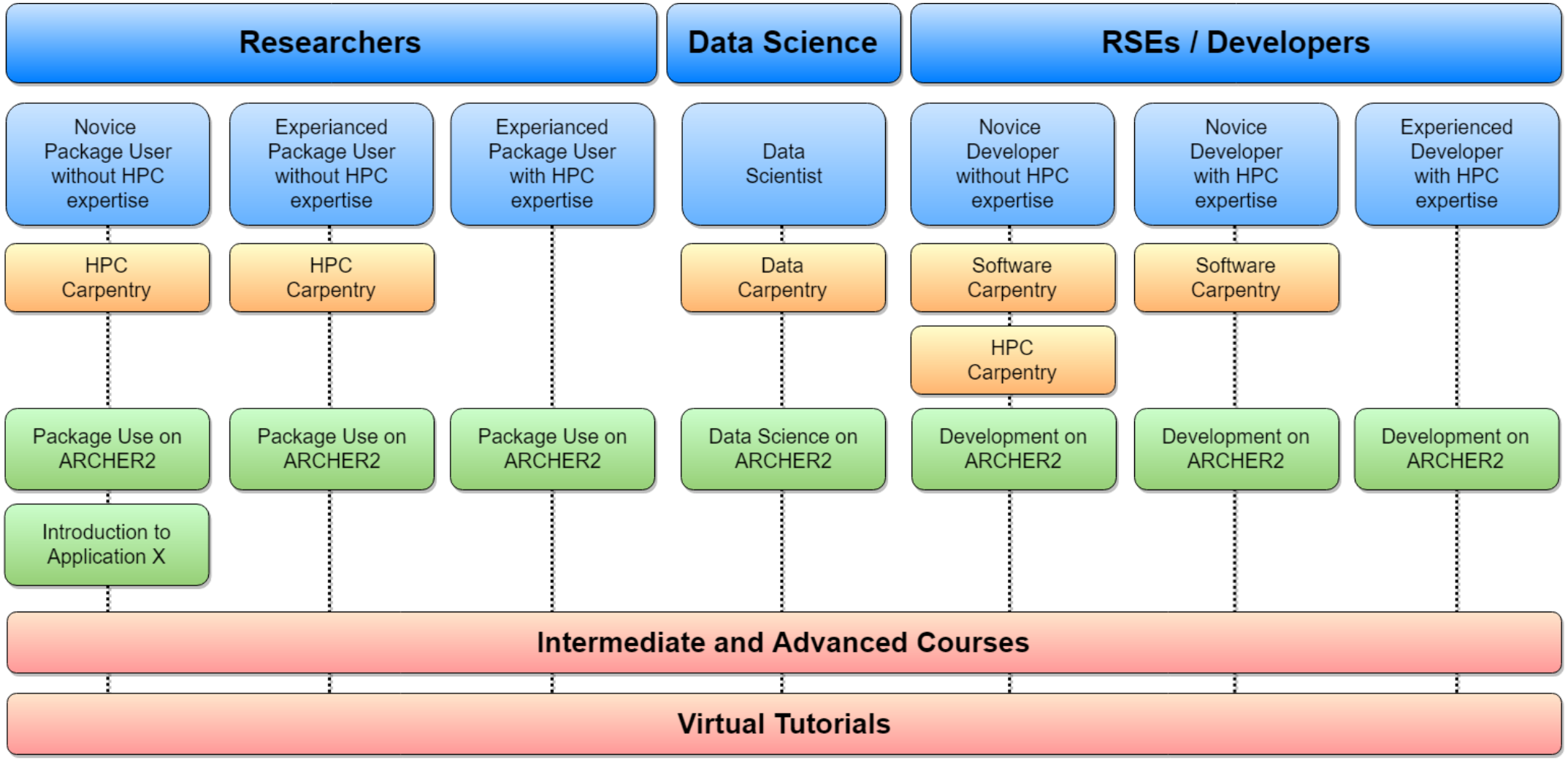
1) **Introductory**: Requiring no substantial programming skills or knowledge of HPC; these courses only assume basic computer literacy.
2) **Intermediate**: These require some existing knowledge, for example the ability to program in C or Fortran, or experience of running parallel applications on HPC systems.
3) **Advanced**: These require an existing knowledge of parallel programming.

Courses for different types of user

Training tracks aimed specifically at:

- **Package users,** who primarily use existing research software packages for their research).
- **Developers,** who develop research software packages for their own research or for use by the wider research community.
- **Data Scientists,** who apply data science tools and techniques using data processing frameworks such as Spark as well as packages for data analysis, machine learning, and deep learning.

User journeys



The Carpentries

- Teach foundational computational and data science skills.
- Lessons delivered using evidence-based teaching practices.
- We offer:
  - Software Carpentry
  - Data Carpentry
- Carpentries-based courses
  - HPC Carpentry
  - ARCHER2 specific courses.

ARCHER2 specific courses

Different introductory courses for different user categories:

- **Package Use on ARCHER2 (1 day):**
  - Essentials of the ARCHER2 service.
  - How pre-installed software packages can be used.
  - Efficient use of pre-installed research software packages on ARCHER2.
- **Development on ARCHER2 (2 days):**
  - ARCHER2 application development environment.
  - Core parallel and scientific software libraries
  - Available debugging and profiling tools.

Both online and face-to-face.

ARCHER2 for Data Scientists

- **Data Science on ARCHER2 (1 day):**
  - The essentials of ARCHER2.
  - The basic use of core data science packages on ARCHER2 (e.g. R, Pandas),
  - Data handling best practice on ARCHER2.
- Intermediate courses:
  - Data Analytics with HPC.
  - Data Analysis using Python.

  Overview of data science and the analytical techniques that form its basis as well as exploring how HPC provides the power that has driven their adoption.

Package specific courses

The chosen packages will be directed by requests from the user community and the various feedback mechanisms described before.

Initial plans:

- Introduction to LAMMPS
- Introduction to Code Saturne
- Introduction to Unified Model
- QM/MM simulations with CP2K and GROMACS
  - Introduction to CP2K and Gromacs
  - Advanced use of CP2K and Gromacs

Intermediate and Advanced courses

Intermediate courses

- Understanding Package Performance
- Containers for HPC
- Message Passing Programming with MPI
- Shared Memory Programming with OpenMP

Advanced courses

- Performance Optimisation on AMD EPYC
- Efficient use of the Cray Shasta System ARCHER2
- Performance Analysis Workshop

Scheduled online courses for May, June, July

Title	Date	Level
Introduction to LAMMPS	May	Introductory (level 1)
Message-passing programing with MPI	May	Intermediate (level 2)
HPC Carpentry	June	Introductory (level 1)
Containers for HPC (full)	July	Intermediate (level 2)

Further online courses can be found here:
https://www.archer2.ac.uk/training/#upcoming-training

Virtual tutorials

- Interactive live webinars where experts can share their knowledge on a range of intermediate and advanced topics.
- Regular slot: Wednesdays at 3pm BST (sometimes at 11am BST).
- Recordings available on the ARCHER2 Youtube channel:
  https://www.youtube.com/channel/UCZi-oBdxoDV5CPEQnhmrCAg

Scheduled Virtual Tutorials

Title	Speaker	Date
ARCHER2 Spectrum of Support	George Beckett, EPCC	13th May 2020
The determination of clusters structures combining infrared spectroscopy and density functional theory calculations	Piero Ferrari, KU Leuven	20th May 2020
ARCHER2 eCSE	Chris Johnson, EPCC	27th May 2020
ARCHER2 Outreach	Jane Kennedy, EPCC	3rd June 2020

Further Virtual Tutorials can be found here:
https://www.archer2.ac.uk/training/#upcoming-training

Self-service courses

- Use of **online self-service courses** to allow people to access training when it suits them.
- Specifically tailored to be followed at a user's own pace.
- During the first year, two self-taught courses will be available:
  - Shared-memory programming with OpenMP, available from 1st Sep. 2020.
  - Message-passing programming with MPI, available from 1st Feb. 2021.
- Full recordings of several previous ARCHER courses available online.
- All online self-service courses will be available in addition to the 60 days of scheduled training.

ARCHER2 Driving Test

- Test based on online training material with a multiple-choice test.
- Anyone who passes this test can apply for an ARCHER2 account with a small amount of compute time.
- Modelled on previous ARCHER driving test, developed when hardware is available.
- Different versions:
  - Researchers using pre-installed research software.
  - Data scientists.
  - Developers.
- The ARCHER2 Driving Test lowers barriers to access and ensures that anyone with key basic knowledge can get access to try out ARCHER2 for their research.

Summary

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Key points

- **Training tracks** aimed at **package users, developers,** and **data scientists.**
- Improved **accessibility** and **inclusivity** of HPC training.
- A training programme that is **flexible** and **responsive** to users' needs.
- User Training Forum and Training Panel.
- **Collaboration** with the community.
- Providing **internationally recognised leadership** in the HPC and data science training community.
- An approach to training that offers **diversity** in **subject areas, pedagogical approaches** and **delivery mechanisms.**
- A training programme that is **open to all** UK researchers.

Summary

The ARCHER2 training plan has the aims of:

1) Addressing the needs of all users.
2) Enabling them to make efficient use of ARCHER2 as soon as it is available.

Next Virtual Tutorial:

ARCHER2 Spectrum of Support (Wed 12th May at 3pm BST)

Follow us on:

- Website: https://www.archer2.ac.uk/training/
- ARCHER2 mailing list (further info on the above URL)
- Twitter: @ARCHER2_HPC