ARCHER: UK National HPC Service

Nottingham HPC User Conference 2017

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Reusing this material

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Outline

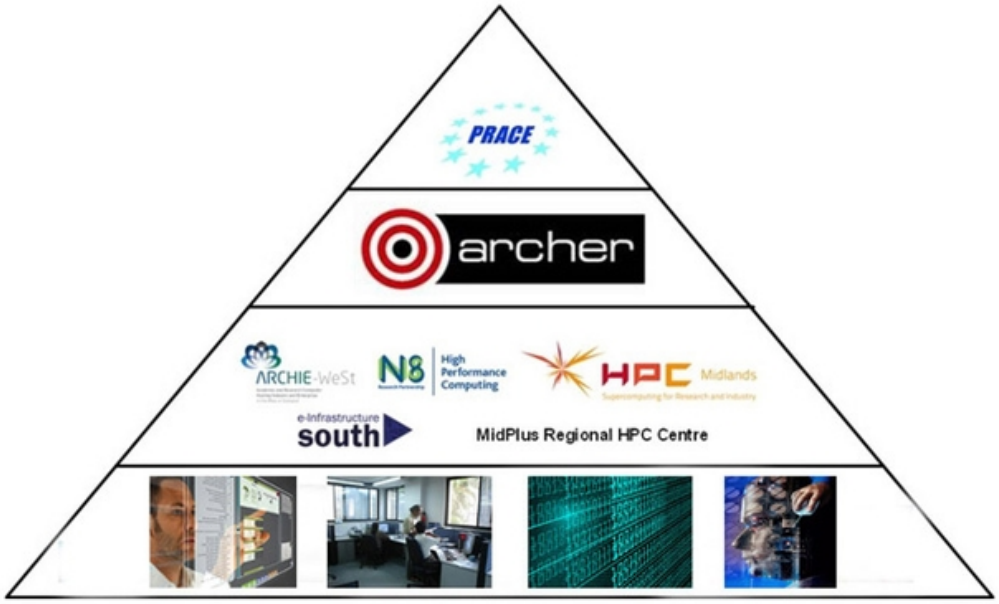
- Service Overview
- ARCHER Hardware & Software
  - Routes to access
- CSE Support
  - Scientific Software Packages
- Training
- Embedded Computational Science and Engineering (eCSE) Funding
- Cirrus Tier-2

Service Overview

National HPC Service(s)?

- Tier-0: International
- Tier-1: National
- Tier-2: Regional
- Tier-3: Institutional/

  Departmental / Group



Service Overview

- UK National Supercomputing Service
  - 2013-2018
  - Follow-on from HECToR, HPCx, CSAR …
- Funded by EPSRC and NERC
  - Managed by EPSRC
- Service provision, accommodation and Computational Science and Engineering (CSE) support service by EPCC
- Hardware provided by Cray

www.archer.ac.uk

Service Overview

- Advanced Computing Facility (ACF)
  - Purpose built, secure, world-class facility
- Houses wide variety of leading-edge systems and infrastructures
  - National services
    - ARCHER
    - Cirrus (EPCC Tier-2)
    - IBM BlueGene/Q (DiRAC)
    - UK Research Data Facility (RDF)
  - Local services
    - ECDF, EDIM1 – DIR machine
- Major expansion for ARCHER
  - 6MW, 850m^2 plant room, 550m^2 machine
  - HECToR PUE = 1.25, ARCHER PUE < 1.1

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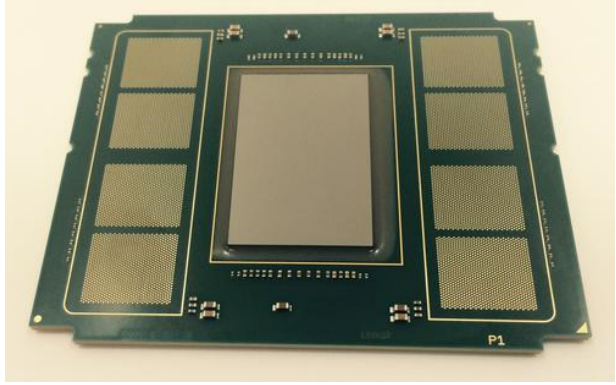
ARCHER Hardware

- Cray XC30 architecture
  - 4920 nodes:
    - 24 Intel Ivy Bridge cores per node ➔ 118,080 cores
    - Most nodes have 64 GB memory (~2.3 GB/core)
    - 1 group (376 nodes) have 128 GB memory (~5.6 GB/core)
  - Cray Aries interconnect with Dragonfly all-to-all topology
    - ~1.4us latency, 11 TB/s bisectional bandwidth
  - 4.4 PB high performance parallel filesystem (Lustre)
  - Direct access to Research Data Facility (20PB disk + backup tape)

ARCHER Hardware

- ARCHER Knights Landing (KNL) platform
  - 12 nodes:
    - 64 core Intel Xeon Phi 7210 processor
    - 96 GB main memory and 16GB high-bandwidth MCDRAM
    - Cray Aries interconnect
  - Similar programming environment to ARCHER
  - Home filesystem shared with ARCHER
  - Intended for trialling applications on KNL
  - Opportunity to experiment with a manycore CPU



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ARCHER Hardware

- Pre/post-processing (PP) nodes
  - 2 nodes
  - 40 Intel Westmere cores per node
  - 1 TB memory per node
  - Access to Lustre file system and RDF

- Data Analytic Cluster (DAC)
  - 12 compute nodes (20 Ivy Bridge cores, 128 GB memory)
  - 2 high-memory nodes (40 Westmere cores, 2 TB memory)
  - High-bandwidth connectivity to RDF storage

Image: Gordon Fraser, www.scotsman.com

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ARCHER Software

- Fully-featured Cray Programming Environment
  - Cray, Intel and GNU compiler suites
  - Cray MPI & Libsci libraries
  - Many popular scientific libraries:
    - PETSc, HDF5 & NetCDF, FFTW…
  - Python
    - 'Native' distribution (MPI4Py, NumPy, SciPy available…)
    - Anaconda distributions
    - Customisable with Virtual Environments
  - Debuggers and performance analysis tools
    - Allinea DDT
    - Cray Performance Analysis Toolkit

Find out more at:
https://www.archer.ac.uk/documentation/

Routes to access

- Access via Scientific consortia
  - Significant resources pre-allocated to EPSRC & NERC consortia:
    - Materials Chemistry Consortium
    - UK Turbulence Consortium
    - HEC Biomolecular Simulation Consortium
    - Oceanography
    - …

See https://www.archer.ac.uk/community/consortia/

- Access via ARCHER Driving Test
  - Small amount of compute time (1200 kAUs) for 12 months
  - Suitable for new users to ARCHER
  - Online training material and multiple-choice assessment

See https://www.archer.ac.uk/training/online/driving_test.php

Routes to access

- Access via EPSRC & NERC Grants
  - ARCHER time may be included in research grant applications / fellowships etc.
  - Need to complete an ARCHER Technical Assessment (TA), which is submitted along with your application
    - 10 days turnaround

See https://www.archer.ac.uk/access/

- Access via ARCHER Calls (EPSRC only)
  - ARCHER Resource allocation panel (RAP)
  - Significant amounts of compute resource (>1 MAUs, 1 year)

Current call closes 25th May 2017:
https://www.epsrc.ac.uk/funding/calls/rapaccessarcherspring2017/

  - 'Instant Access' for small projects (< 1.2 MAUs, 6 months)

CSE Support

safe https://www.archer.ac.uk/safe

Email: support@archer.ac.uk

Phone: +44 (0)131 650 5000

Support 0830-1800 Mon-Fri excluding UK Bank Holidays

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CSE Support

- ‘In-depth’ support
  - Porting & debugging codes
  - Software development support
  - Performance optimisation advice
  - Support for centrally installed software packages
  - ARCHER / HPC ‘Gurus’

Image: Jorge Cham, www.phdcomics.com

- Consortium contacts
  - Liaison between ARCHER service and scientific consortia
  - Understanding of key codes, methods & workflows
  - Provide tips, training, one-to-one support

See https://www.archer.ac.uk/community/consortia/

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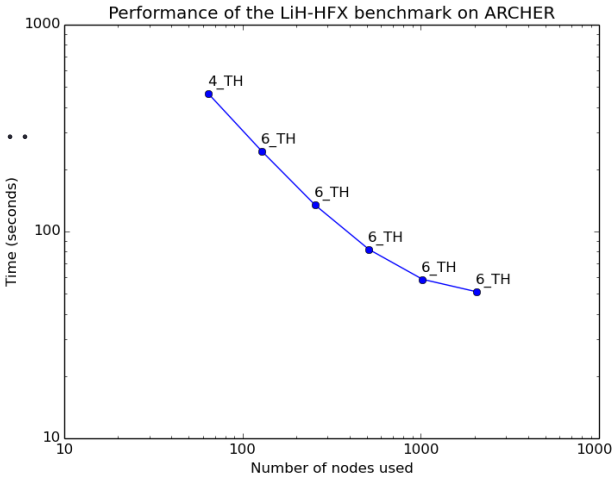
CSE Support

- Scientific Software Packages
  - Relatively few users bring their own code to ARCHER
  - 40+ popular packages are pre-installed
    - Optimised & tested
  - E.g. VASP, GROMACS, CP2K, OpenFOAM, Code_Saturne, FEniCS, Paraview…
    - License restrictions apply to some packages
  - Documentation, benchmark performance, scripts…
  - Often as easy as: `module load cp2k`

See https://www.archer.ac.uk/documentation/software/

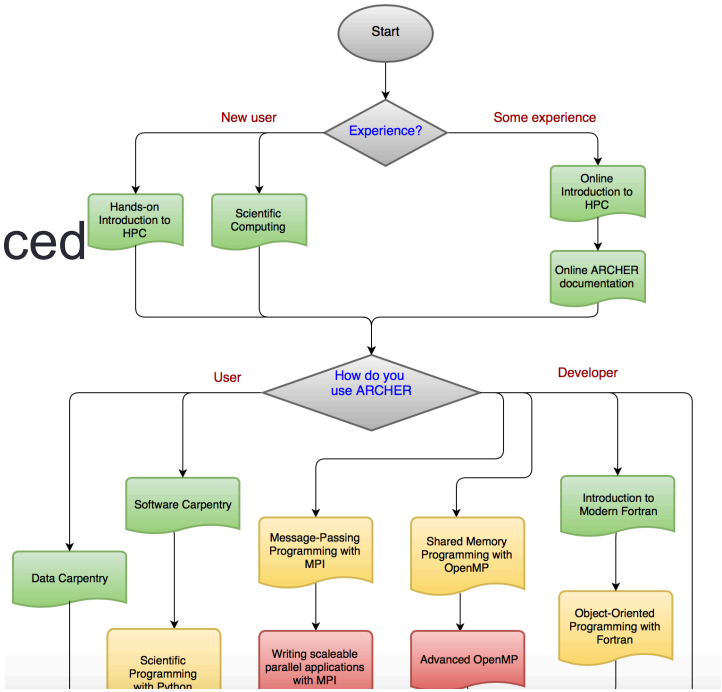


Training

- Extensive training programme
  - Mix of online and classroom courses
  - Not just for existing ARCHER users (free to all academics)

See https://www.archer.ac.uk/training/

- Courses
  - Range of venues around the UK
  - Mixture of introductory / intermediate / advanced
  - Courses for ‘users’ and ‘developers’
  - All material archived on the web!



- Virtual Tutorials / Webinars
  - 3pm, Wednesdays
  - Presentation / live demos and Q&A

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Embedded CSE Funding

- Regular calls for software development projects:
  - To sustain development of key applications on ARCHER
  - To facilitate efficient use of ARCHER resources through enhanced code performance/functionality
  - Code porting/scale-up from Tier-2/3, bringing new communities onto ARCHER

See https://www.archer.ac.uk/community/eCSE

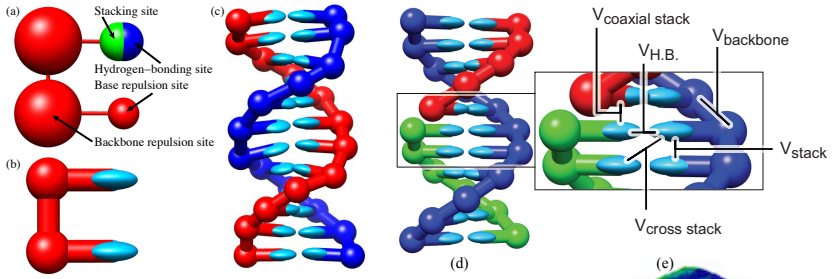
- 3-12 person-months
  - Effort provided by EPCC, Institutional RSEs, group members…
  - Expect close interaction with ARCHER CSE team

- Calls 3 or 4 times per year

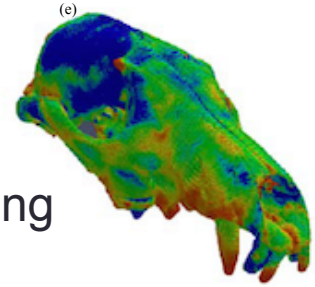
Current call closes on 9th May
Next (final) call closes 12th Sept

Embedded CSE Funding

- Some recent projects:
  - "Adding Multiscale Models of DNA to the LAMMPS Molecular Dynamics code"
    - 12 PMs EPCC staff effort
    - New functionality



  - "VOX-FE: New functionality for new communities"
    - 6 PMs Postdoc at Hull, 3 PMs EPCC
    - New GUI for model setup and analysis, improved load balancing



  - "Enabling HPC for tools for the analysis of single molecule ion channel currents"
    - 12 PMs UCL RSE team, re-architected and parallelised for ARCHER

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Cirrus Tier-2

- One of the new EPSRC Tier-2 Services
- 280 nodes
  - 36 Intel Broadwell cores per node ➔ 10,080 cores
  - 128 GB memory per node (~3.5 GB per core)
- 30% EPCC
  - Industry & research projects
- 70% EPSRC access
  - Instant Access – 7,000 CPUh for 6 months
  - National Open Access – TBC
  - EPSRC Grant Access

Callum Bennetts/Maverick Photography

www.cirrus.ac.uk

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Summary

- ARCHER is the largest academic HPC resource in the UK
- Supports ‘capability’ jobs of up to 100,000s CPU cores
- Free access for EPSRC and NERC-remit research
- Extensive training, support and documentation available
- Funding for software development in support of research

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Any questions?

support@archer.ac.uk

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