ARCHER2 Technology

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Reusing this material

Partners

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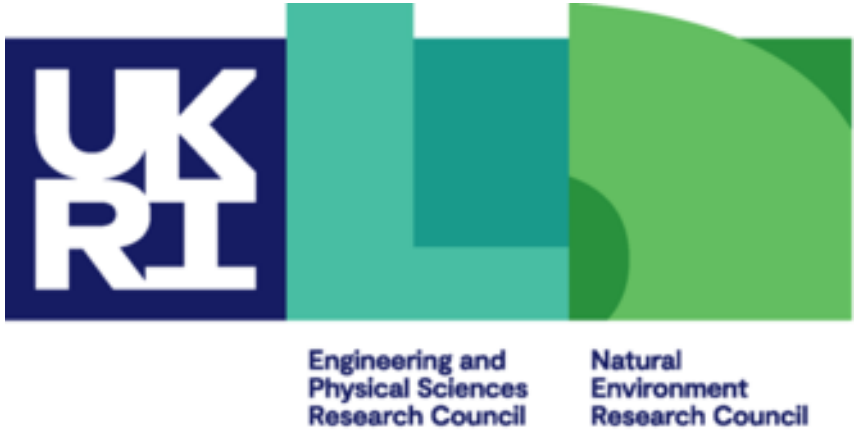

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CRAY®

a Hewlett Packard Enterprise company

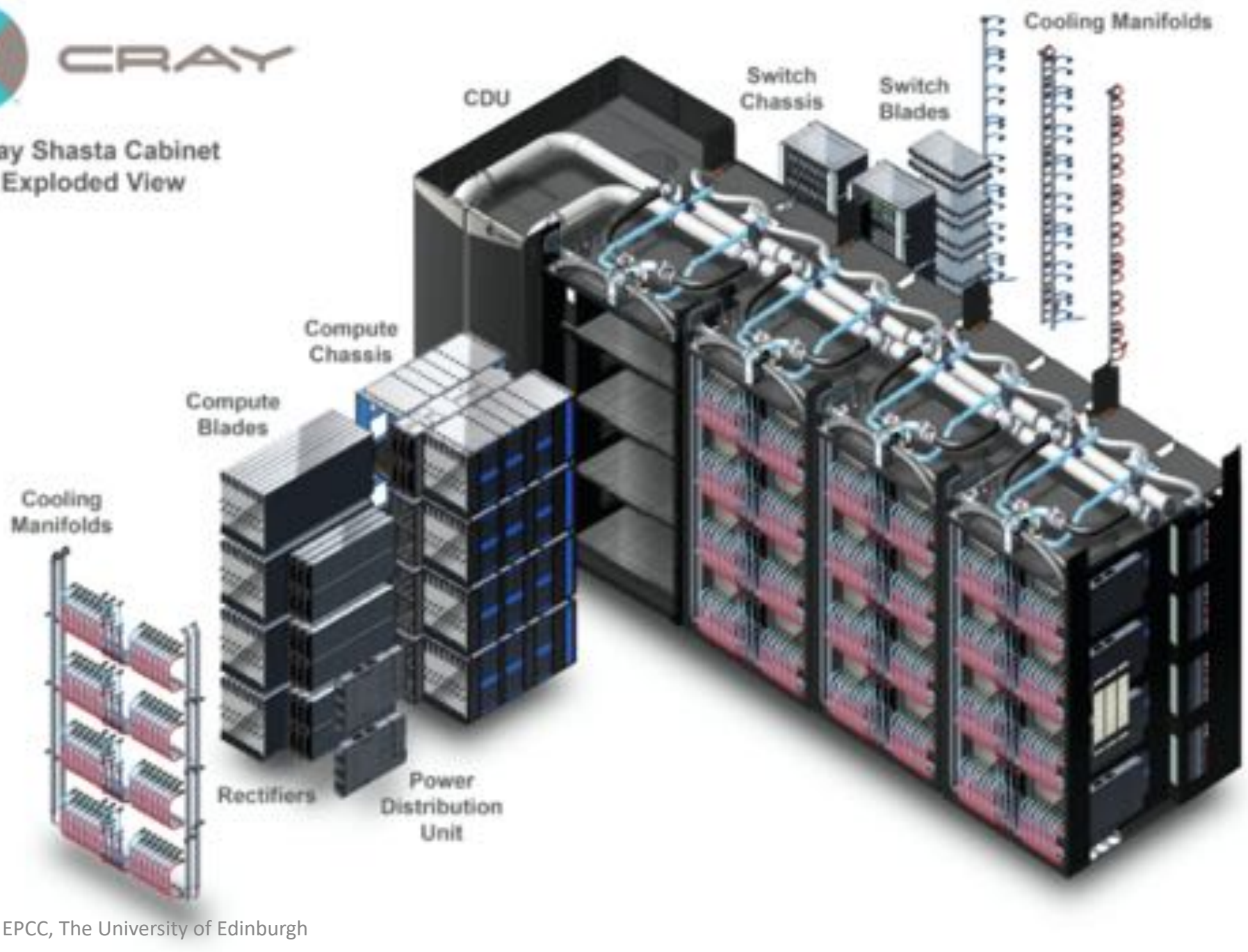
Overview

- Hardware details
  - Node types and architecture
  - Interconnect
  - Storage
  - Comparisons to ARCHER
- Software details
  - Cray-provided software environment
  - EPCC CSE-provided software environment
  - Comparisons to ARCHER
- Details useful for:
  - Users who plan to use pre-installed software on the service
  - Users who plan to develop and compile software on the service

Hardware Overview

System Overview

- Peak performance: ~28 PFlops
  - CASTEP: 11x ARCHER
  - CP2K: 9x ARCHER
  - GROMACS: 13x ARCHER
  - OpenSBLI: 9x ARCHER
  - Met Office UM: 18x ARCHER
- 5,848 compute nodes in 23 Shasta Mountain cabinets
  - 748,544 AMD cores
- 14.5 PB Lustre (4 file systems)
- 1.1 PB solid state burst buffer
- 1 PB home (backed up) storage
- Cray Slingshot interconnect


Cray Shasta Cabinet
Exploded View
CDU
Switch
Chassis
Switch
Blades
Cooling Manifolds
Compute
Chassis
Compute
Blades
Cooling
Manifolds
Rectifiers
Power
Distribution
Unit

Node types visible to users

- Login nodes, each:
  - 2x AMD EPYC Zen2 (Rome) 7742 2.25 GHz, 64-core; 512 GB DDR 3200
  - Same processors as compute nodes so no cross-compile required
- Compute nodes, each:
  - 2x AMD EPYC 7742 2.25 GHz, 64-core; 256 or 512 GB DDR 3200
  - More details coming up…
- Data analysis nodes (e.g. pre- and post-processing), each:
  - 2x AMD EPYC 7742 2.25 GHz, 64-core; 512 GB DDR 3200
- Collaboration system
  - 2 nodes each with 8 AMD GPUs
  - Very little known about this at the moment…
- (c.f. ARCHER: Unlike ARCHER, all nodes have the same architecture and instruction set)

Compute Nodes: AMD EPYC 7742

- Dual socket AMD EPYC (Rome) 7742, 2.25GHz, 64 core
  - 128 cores per node (256 SMT)
  - 8 memory channels per socket
  - DDR 3200MHz
  - Maximum memory bandwidth 381.4 GB/s per node
- 5556 Standard Nodes: 256 GiB
- 292 High Memory Nodes: 512 GiB

Comparison with ARCHER

	ARCHER2	ARCHER	Ratio
Processors	2x AMD EPYC 7742	2x Intel Xeon E5-2697 v2	
Cores per socket (node)	64 (128)	12 (24)	5.3:1
Cores per NUMA region	8-64	12	
Max. SP GFLOP/s per socket (node)	4608 (9216)	518 (1037)	384.0:1
Max. SP GFLOP/s per core	72	43	1.7:1
Memory per node	256/512 GB	64/128 GB	4.0:1
Memory per core	2.0/4.0 GB	2.7/5.3 GB	0.7:1
Memory channels per socket	8	4	2:1
Memory	DDR 3200	DDR 1866	
Max. memory BW per socket (node)	190.7 (381.4) GB/s	59.7 (119.4) GiB/s	3.2:1
Max. memory BW per core	3.0 GiB/s	5.0 GiB/s	0.6:1

Comparison with ARCHER (cache and NUMA)

	ARCHER2	ARCHER	Ratio
L1 data cache (per core)	32 KiB	32 KiB	1.0:1
L2 cache (per core)	512 KiB	256 KiB	2.0:1
L3 cache (shared)	32 MiB (shared by 8 cores) 256 MiB per socket	30 MiB (shared by 12 cores) 30 MiB per socket	8.5:1

- NUMA (and hence cache structure) is more complex on EPYC Zen2
  - Each socket made up of 8-core *chiplets* with a shared L3 cache
  - 8 chiplets connected together using I/O and memory hub chip
  - The I/O and memory hub allows the socket to be configured to present as different numbers of NUMA domains:
    - 8 NUMA domains per socket: matches the underlying hardware
    - …other combinations…
    - 1 NUMA domain per socket: I/O and memory hub manages cache
    - Not sure yet what the configuration will be on ARCHER2

Compute nodes vs ARCHER: Summary

- Much more compute power and memory per node…
- …but the balance is different
  - Many more cores per node
  - Less memory and memory bandwidth on a per-core basis
  - Different cache structure
- Need to stop thinking about cores as the key resource indicator
  - Think about the whole node and how you can best exploit it
  - Potentially under-populate the node (i.e. not use all cores)
  - Explore use of multithreading per process
- Different interconnect may also change characteristics…

Interconnect: Cray Slingshot

- Ethernet-compatible, high-performance interconnect
- 2x 100 Gbps bi-directional interfaces per node: 200 Gbps bi-directional BW per node
  - c.f. current ARCHER Aries network supports over 120 Gbps bi-directional BW per node with one network interface per node
- Diameter 3 dragonfly topology
- Supports dynamic routing and quality of service features (e.g. to manage congestion control)

Storage and I/O

- 4x Cray ClusterStor L300 Lustre file systems, each with 3.6 PB usable storage (/work file systems)
  - No backup
- 1x Cray ClusterStor E1000F solid state storage, 1.1 PB usable
  - No backup
- NetApp FAS8200 providing 1 PB /home file systems
  - Backed-up for disaster recovery

	ARCHER2	ARCHER
/work (Lustre)	14.5 PB	4.4 PB
/home	1 PB	218 TB
Solid state	1.1 PB	N/A

Software Overview

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Cray Software Environment

- OS: Cray Linux Environment
- Cray Developer Environment (CDE)
  - Software modules (similar to current ARCHER setup)
  - SLURM scheduler and job launcher
  - Compilers
  - MPI and SHMEM
  - Optimised scientific and numeric libraries
  - Optimised parallel Python and R
  - Parallel profiler and debugger
- Singularity containers

CDE: SLURM job scheduler and launcher

- Standard SLURM environment
  - `srun` parallel launcher (c.f. ARCHER: `srun` instead of `aprun` on ARCHER2)
  - Script runs on compute node (c.f. ARCHER: no job launcher nodes on ARCHER2)

```
#!/bin/bash
#SBATCH -J my_job
#SBATCH --ntasks=512
#SBATCH --ntasks-per-node=128
#SBATCH --cores-per-task=1
#SBATCH --time=2:0:0

# Load modules, etc.

# srun to launch the executable using parallel options from sbatch
srun my_parallel_app
```

CDE: Compilers

- Three environments provided by CDE
  - Cray Compiler Environment (CCE)
    - Cray Fortran compiler (not Flang-based)
    - Cray C/C++ compiler based on Clang
  - AMD Optimizing Compiler Collection (AOCC)
    - Flang Fortran compiler
    - Clang C/C++ compiler
  - GNU Compiler Collection (GCC)
    - Gfortran Fortran compiler
    - gcc/g++ C/C++ compilers
  - (c.f. ARCHER: no Intel compilers on ARCHER2)
- All Cray-provided libraries and tools work with these environments
- Dynamic linking by default
  - (c.f. ARCHER: static linking by default on ARCHER)

CDE: Parallel, scientific and numeric libraries

- Cray Message Passing Toolkit
  - MPI and OpenSHMEM
- Cray LibSci:
  - BLAS and LAPACK
  - CBLAS and LAPACKE
  - BLACS and ScaLAPACK
- FFTW 3
- HDF5
- NetCDF
- (c.f. ARCHER: no PETSc, no Trilinos, no TPSL provided by Cray on ARCHER2)

CDE: Python and R

- Cray high-performance Python (2 and 3) distribution:
  - **numpy, scipy** - built against Cray LibSci
  - **mpi4py** - built against Cray MPT
  - **dask**
  - Can use `pip install --user` to build on top of the distribution
- Cray R distribution:
  - Less details available
  - Includes standard packages and “parallel” package
- (c.f. ARCHER: no Cray-provided Python and R environments on ARCHER)

CDE: Profiling and debugging

- Debugging:
  - **gdb4hpc**: HPC version of command-line GDB debugging tool
  - **valgrind4hpc**: HPC version of memory debugging tool
  - **stat**: merged stack and backtrace analysis tool
  - **atp**: scalable core file generator and analysis tool
  - **Cray Comparative Debugging**: side-by-side debugging of two versions of the same application
  - (c.f. ARCHER: no Arm Forge DDT available on ARCHER2)
- Profiling
  - **Cray Performance Analysis Toolkit** (CrayPAT)
  - **PAPI**: support in CrayPAT
  - **Cray Reveal**: run time performance stats combined with source code visualisation (CCE only)
  - (c.f. ARCHER: no Arm Forge MAP available on ARCHER2)

Singularity Containers

- Singularity will be available
  - See: https://sylabs.io/
- Support containers for single node use and multi-node using MPI
- Potential applications:
  - Custom environments for particular applications/workflows
  - Support for legacy and custom versions of software
  - Capturing environments to enhance reproducibility
  - Ease of install of software with complex dependencies
- (c.f. ARCHER: no containers available on ARCHER)

EPCC CSE Service Software Environment

- Modelling and simulation research software
  - e.g. VASP, CASTEP, OpenFOAM, GROMACS
- Additional scientific and numeric libraries
  - e.g. PETSc, Boost, Eigen
- Data analysis tools and software
  - e.g. NCO, CDO, (VisiData!)
- Other software as required

- Initial set based on analysis of use on ARCHER and consultation with UKRI scientific consortia

Summary

Summary

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- ARCHER2 is based on new technology
  - New cabinets - Cray Shasta
  - New processers - AMD EPYC Zen2 (Rome)
  - New interconnect - Cray Slingshot
- Compute nodes have much more floating-point power and total memory available compared to ARCHER
  - Efficient use will require investigation of what balance of cores used per node and number of processes/threads to use
  - EPCC ARCHER2 CSE service will provide advice and assistance with this
- A solid-state storage component will be available
  - potentially improve I/O performance for some applications
- Broad research software stack will be available
  - Including support for Python, R and containers
  - Environment will work in a similar way to current ARCHER setup