

Scientific Python ARCHER2

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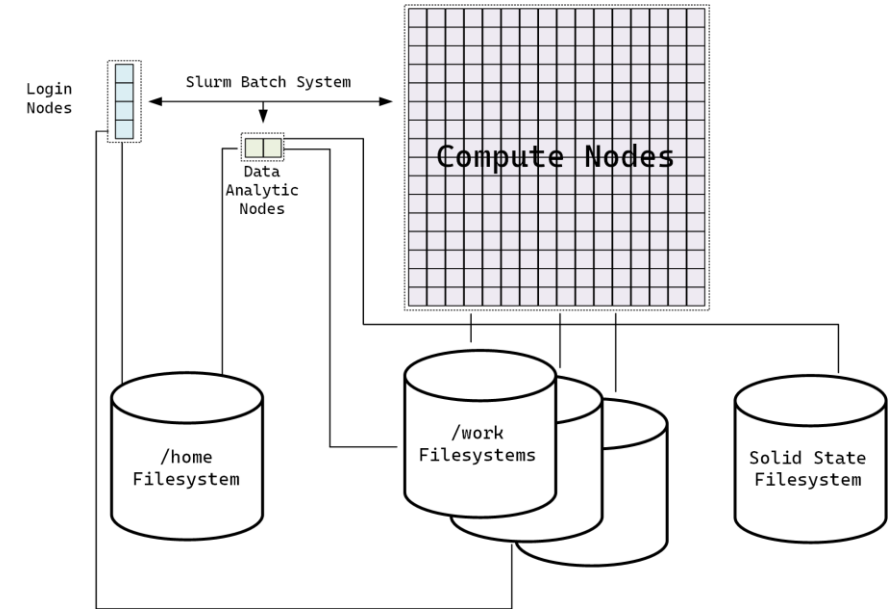
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Hewlett Packard
Enterprise

Hardware

- ARCHER2 is composed of:
 - 5,860 compute nodes
 - High performance network
 - home filesystem
 - work filesystem
 - 4 login nodes
 - 2 data analytics nodes
- Filesystems
 - /home: 1 PB network filesystem
 - Available on login and data analysis nodes
 - /work: 14.5 PB lustre filesystem
 - Available on login, data analysis and compute nodes
 - Solid state storage: 1.1 PB NVMe storage

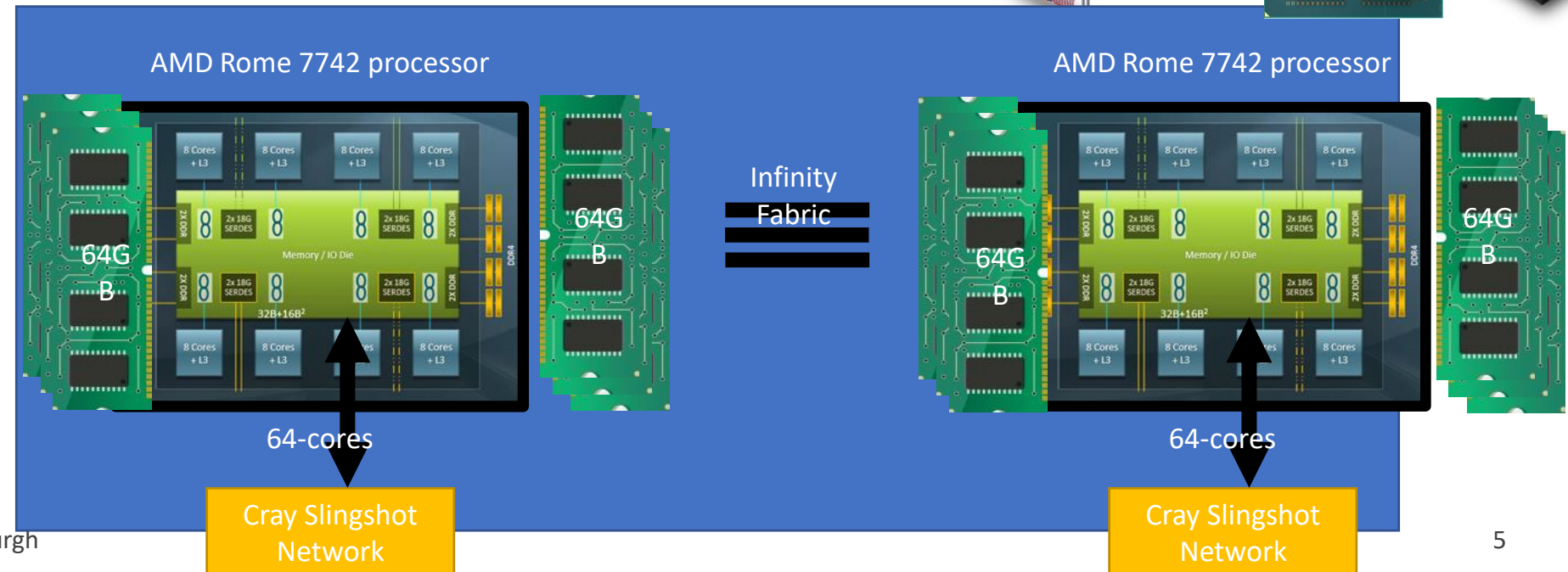
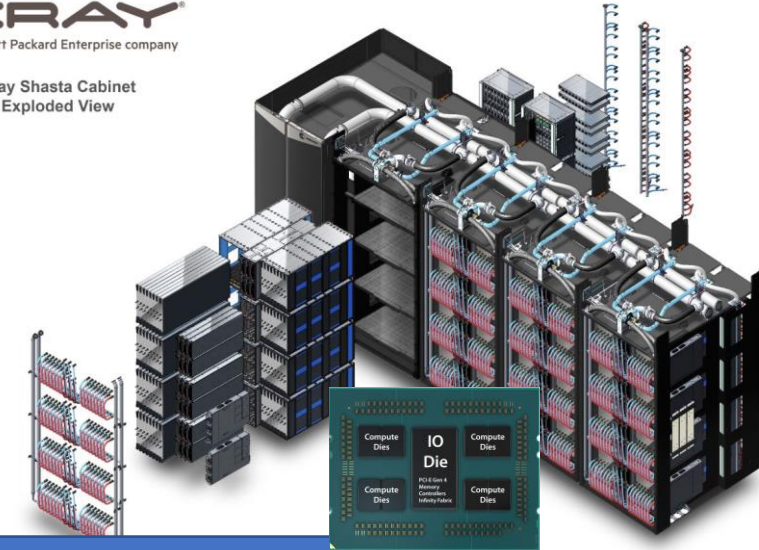


Hardware

- Nodes comprise of:
 - 128 processor cores:
 - 2x AMD EPYC Zen2 (Rome) 7742, 2.25 GHz, 64-core
 - 256/512 GB DDR 3200, 8 memory channels
 - 300 high memory nodes (512 GB)

CRAY
a Hewlett Packard Enterprise company

Cray Shasta Cabinet
Exploded View



Software

- Linux operating system
 - HPE Cray Linux Environment (based on SLES 15)
- Slurm scheduler
 - Access compute and data nodes
- Three compilers
 - Cray: crayftn, craycc, crayCC
 - GNU: gfortran, gcc, g++
 - AMD: clang, clang++, flang
- HPE/Cray MPI and communication libraries
- HPE Cray scientific and numerical libraries:
 - HPE Cray LibSci: BLAS, LAPACK, ScaLAPACK
 - FFTW 3
 - NetCDF
 - HDF5
 - etc...
 - cray-python
- Programming tools:
 - gdb4hpc parallel debugger
 - valgrind4hpc parallel memory debugging
 - STAT stack trace analysis tool
 - ATP abnormal program termination analysis tool
 - HPE Cray Performance Analysis Toolkit (CrayPAT)
- <https://docs.archer2.ac.uk/>

Usage

- Login nodes for compilation and general development
- Data nodes for longer running data movement/processing tasks (limited amounts of resources)
- Compute nodes for everything else
 - Compute nodes require runtime budget
- Usage of cores is restricted
 - Login nodes have fair share
 - Compute nodes having binding/placement enforcement

Batch system

- Full configuration details
 - <https://docs.archer2.ac.uk/user-guide/scheduler/>

```
#!/bin/bash
```

```
#SBATCH --job-name=xthi
```

```
#SBATCH --nodes=2
```

```
#SBATCH --tasks-per-node=128
```

```
#SBATCH --partition=standard
```

```
#SBATCH --qos=short
```

```
#SBATCH --account=z19
```

```
srun -n 256 ./xthi
```