Overview and Introduction
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Nodes: The building blocks

The Cray XC30 is a Massively Parallel Processor (MPP) supercomputer design. It a distributed memory system built from thousands of individual shared-memory nodes. There are two basic types of nodes in any Cray XC30:

• **Compute nodes**
  - These only do user computation, also referred to as the “back-end”

• **Service/Login nodes**
  - e.g. the ARCHER “front-end”: login.archer.ac.uk
  - These provide all the additional services required for the system to function, and are given additional names depending on their individual task:
    - Login nodes – allow users to log in and perform interactive tasks
    - PBS Mom nodes – run and managing PBS batch scripts
    - Service Database node (SDB) – holds system configuration information
    - LNET Routers - connect to the external filesystem.

• There are usually many more compute than service nodes
Differences between Nodes

Service/Login Nodes

- The node you access when you first log in to the system.
- Run a full version of the CLE Linux OS (all libraries and tools available)
- Used for editing files, compiling code, submitting jobs to the batch queue and other interactive tasks.
- Shared resources that may be used concurrently by multiple users.
- There may be many service nodes in any Cray XC30 and can be used for various system services (login nodes, IO routers, daemon servers).

Compute nodes

- These are the nodes on which production jobs are executed
- They run Compute Node Linux, a version of the Linux OS optimised for running batch workloads
- Can only be accessed by submitting jobs to a batch management system (PBS Pro on ARCHER)
- Exclusive resources, allocated (by PBS) to a single user at a time.
- Many more compute nodes in any Cray XC30 than login / service nodes.
ARCHER Layout

Compute node architecture and topology
Cray XC30 Intel® Xeon® Compute Node

The XC30 Compute node features:

- **2 x Intel® Xeon® Sockets/die**
  - 12 core Ivy Bridge
  - QPI interconnect
  - Forms 2 NUMA regions

- **8 x 1833MHz DDR3**
  - 8 GB per Channel
  - 64/128 GB total

- **1 x Aries NIC**
  - Connects to shared Aries router and wider network
  - PCI-e 3.0
Terminology

- A **node** corresponds to a single Linux OS
  - on ARCHER, two sockets each with a 12-core CPU
  - all cores on a node see the same shared memory space
  - ARCHER comprises many 24-core shared-memory systems
  - i.e. maximum extent of an OpenMP shared-memory program

- Packaging into compute nodes is visible to the user
  - minimum quantum of resources allocation is a node
  - user given exclusive access to all cores on a node
  - ARCHER resources requested in multiples of nodes

- Higher levels (blade/chassis/group) not explicitly visible
  - but may have performance impacts in practice
XC30 Compute Blade

- Intra Group/Rank-3 (Optic Cable x 10 links) 12.5 Gbps
- Chassis/Rank-1 (Backplane x 15 links) 14 Gbps
- Dual QPI SMP Links
- 4 Channels DDR3
- PCIe-3 16 bits at 8.0 GT/s per direction
- Aries 48-port Router 4 NICs, 2 router tiles each 40 router tiles for interconnect
- 6-Chassis Group/Rank-2 (Copper Cable x 15 links) 14 Gbps
ARCHER System Building Blocks

- Compute Blade
  - 4 Compute Nodes
- Chassis
  - Rank 1
  - Network
  - 16 Compute Blades
  - No Cables
  - 64 Compute Nodes
- Group
  - Rank 2
  - Network
  - Passive Electrical Network
  - 2 Cabinets
  - 6 Chassis
  - 384 Compute Nodes
- System
  - Rank 3
  - Network
  - Active Optical Network
  - 12 Groups
  - 4920 Compute Nodes

ARCHER System

EPCC
Cray XC30 Dragonfly Topology + Aries
Cray Aries Features

• Scalability to > 500,000 X86 Cores
  • Cray users run large jobs – 20-50% of system size is common
  • Many examples of 50K-250K MPI tasks per job
  • Optimized collectives MPI_Allreduce in particular

• Optimized short transfer mechanism (FMA)
  • Provides global access to memory, used by MPI and PGAS (OpenSHMEM, UPC, Fortran coarrays, ...)
  • High issue rate for small transfers: 8-64 byte put/get and atomic memory operations in particular

• HPC optimized network
  • Small packet size 64-bytes
  • Router bandwidth >> injection bandwidth
  • Adaptive Routing & Dragonfly topology

• Connectionless design
  • Doesn’t depend on a connection cache for performance
  • Limits the memory required per node

• Fault tolerant design
  • Link level retry on error
  • Adaptive routing around failed links
  • Network reconfigures automatically (and quickly) if a component fails
  • End to end CRC check with automatic software retry in MPI
Cray XC30 Rank1 Network

- Chassis with 16 compute blades
- 128 Sockets
- Inter-Aries communication over backplane
- Per-Packet adaptive Routing
Cray XC30 Rank-2 Copper Network

- 16 Aries connected by backplane
- 6 backplanes connected with copper cables in a 2-cabinet group:
- Active optical cables interconnect groups
- 4 nodes connect to a single Aries
- 2 Cabinet Group 768 Sockets
Cray XC30 Network Overview – Rank-3 Network

• An all-to-all pattern is wired between the groups using optical cables (blue network)
• Up to 240 ports are available per 2-cabinet group
• The global bandwidth can be tuned by varying the number of optical cables in the group-to-group connections

Example: A 4-group system is interconnected with 6 optical “bundles”. The “bundles” can be configured between 20 and 80 cables wide
Adaptive Routing over optical network

- An all-to-all pattern is wired between the groups.

Assume Minimal path from Group 0 to Group 3 becomes congested.

Traffic can “bounce off” any other intermediate group.

Doubles load on network but more effectively utilizes full system bandwidth.
Filesystems

- /home – NFS, not accessible on compute nodes
  - For source code and critical files
  - Backed up
  - > 200 TB total
- /work – Lustre, accessible on all nodes
  - High-performance parallel filesystem
  - Not backed-up
  - > 4PB total
- RDF – GPFS, not accessible on compute nodes
  - Research Data Facility
  - Long term data storage
Filesystems

- No /tmp on backend nodes
- Users assigned to projects: filesystems based around projects:
  - /home/projectcode/projectcode/username
  - /work/projectcode/projectcode/username
- Group permissions also done per project
- Sharing data
  - Within projects
    - /work/projectcode/projectcode/shared
    - /home/projectcode/projectcode/shared
  - Between projects
    - /work/projectcode/shared
    - /home/projectcode/shared
Summary of ARCHER

- Each node contains 24 Intel IvyBridge cores
- 4920 Compute Nodes connected by Aries network
  - 64 GB per node; 1/12\textsuperscript{th} of the nodes (one group) have 128 GB
- Total of 118,080 cores
  - over 300 TB memory
- Peak performance of 2.55 PF
ARCHER Software

Brief Overview
Cray’s Supported Programming Environment

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Cray developed
Licensed ISV SW
3rd party packaging
Cray added value to 3rd party
Cray MPI

- Cray MPI
  - Implementation based on MPICH2 from ANL
  - Includes many improved algorithms and tweaks for Cray hardware
    - Improved algorithms for many collectives
    - Asynchronous progress engine allows overlap of computation and comms
    - Customizable collective buffering when using MPI-IO
    - Optimized Remote Memory Access (one-sided) fully supported including passive RMA
  - Full MPI-2 support with the exception of
    - Dynamic process management (MPI_Comm_spawn)
  - MPI-3 support coming soon
Cray Performance Analysis Tools (PAT)

- From performance measurement to performance analysis

- Assist the user with application performance analysis and optimization
  - Help user identify important and meaningful information from potentially massive data sets
  - Help user identify problem areas instead of just reporting data
  - Bring optimization knowledge to a wider set of users

- Focus on ease of use and intuitive user interfaces
  - Automatic program instrumentation
  - Automatic analysis

- Target scalability issues in all areas of tool development
Debuggers on Cray Systems

• Systems with hundreds of thousands of threads of execution need a new debugging paradigm
  • Innovative techniques for productivity and scalability
    • Scalable Solutions based on MRNet from University of Wisconsin
    • STAT - Stack Trace Analysis Tool
      • Scalable generation of a single, merged, stack backtrace tree
      • running at 216K back-end processes
    • ATP - Abnormal Termination Processing
      • Scalable analysis of a sick application, delivering a STAT tree and a minimal, comprehensive, core file set.

• Support for traditional debugging mechanism
  • Allinea DDT 4.0.1
  • gdb
User administration

- SAFE website used for user administration
  - https://www.archer.ac.uk/safe
- Apply for accounts
- Manage project resources
- Report on usage
- View queries
- Etc....