

HPC Architectures

Types of resource currently in use



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Outline

- Shared memory architectures
- Distributed memory architectures
- Distributed memory with shared-memory nodes
- Accelerators
- Filesystems

- What is the difference between different tiers of machine?
 - Interconnect
 - Software
 - Job-size bias (capability)

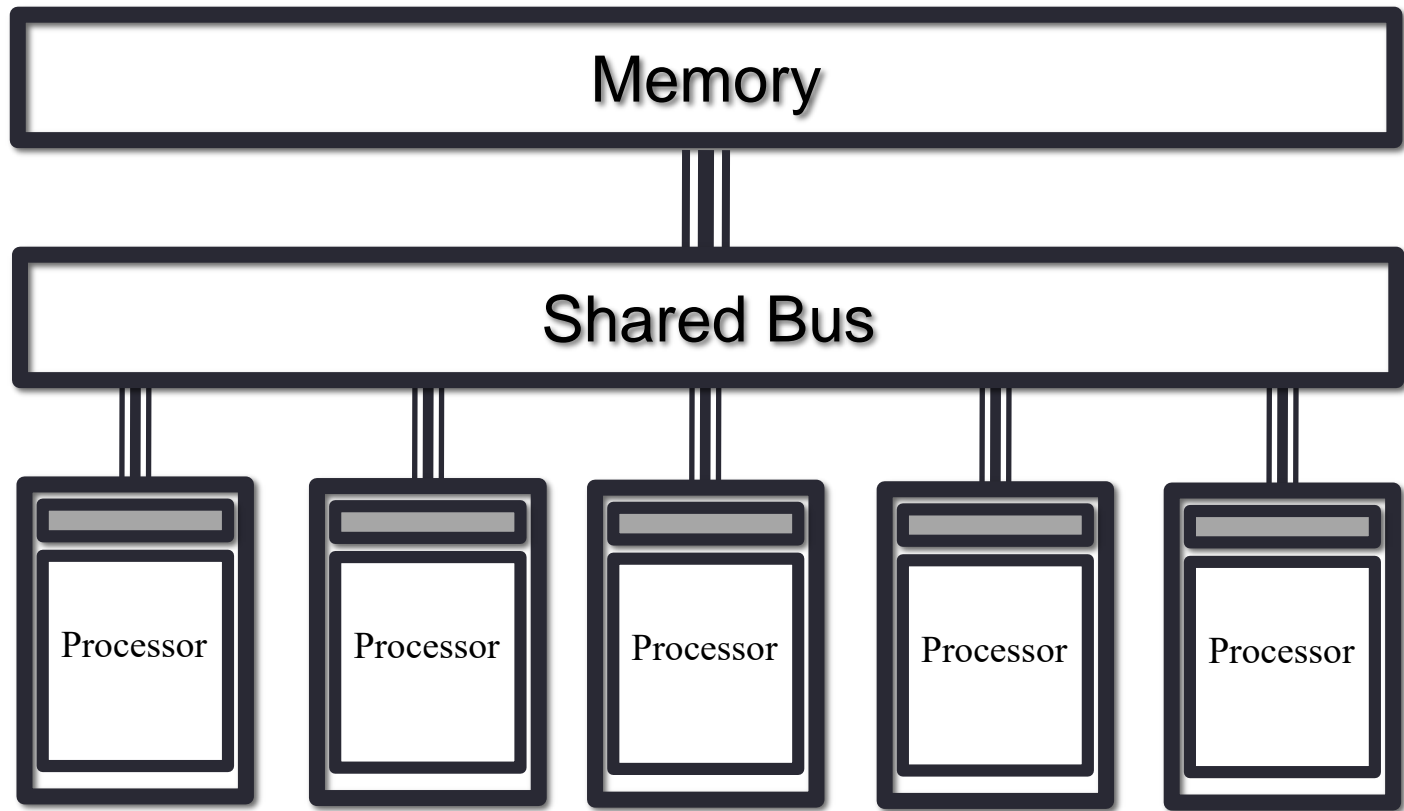
Shared memory architectures

Simplest to use, hardest to build

Shared-Memory Architectures

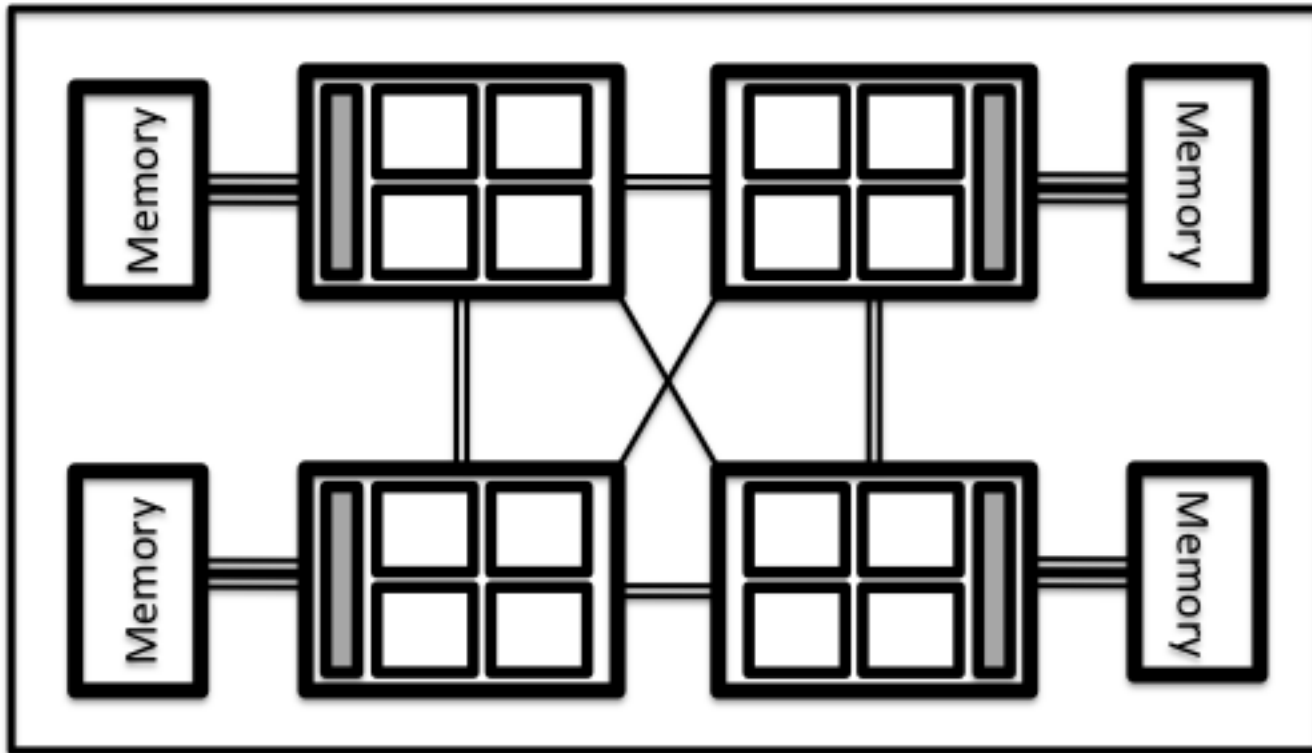
- Multi-processor shared-memory systems have been common since the early 90's
 - originally built from many single-core processors
 - multiple sockets sharing a common memory system
- A single OS controls the entire shared-memory system
- Modern multicore processors are just shared-memory systems on a single chip
 - can't buy a single core processor even if you wanted one!

Symmetric Multi-Processing Architectures



- All cores have the same access to memory, e.g. a multicore laptop

Non-Uniform Memory Access Architectures



- Cores have faster access to their own local memory

Shared-memory architectures

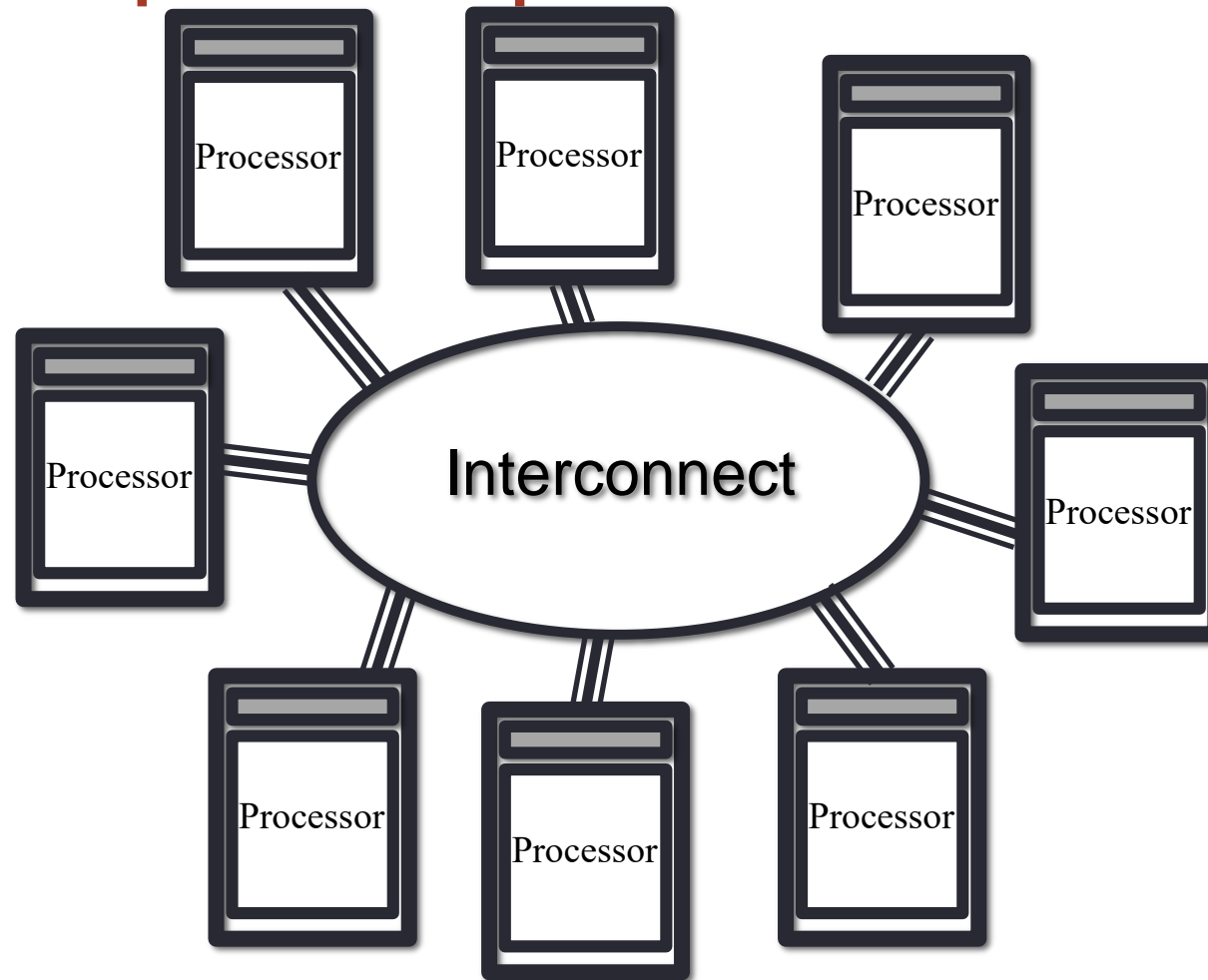
- Most computers are now shared memory machines due to multicore
- Some true SMP architectures...
 - e.g. BlueGene/Q nodes
- ...but most are NUMA
 - Program NUMA as if they are SMP – details hidden from the user
 - all cores controlled by a single OS
- Difficult to build shared-memory systems with large core numbers (> 1024 cores)
 - Expensive and power hungry
 - Difficult to scale the OS to this level

Distributed memory architectures

Clusters and interconnects



Multiple Computers



- Each self-contained part is called a *node*.
- each node runs its own copy of the OS

Distributed-memory architectures

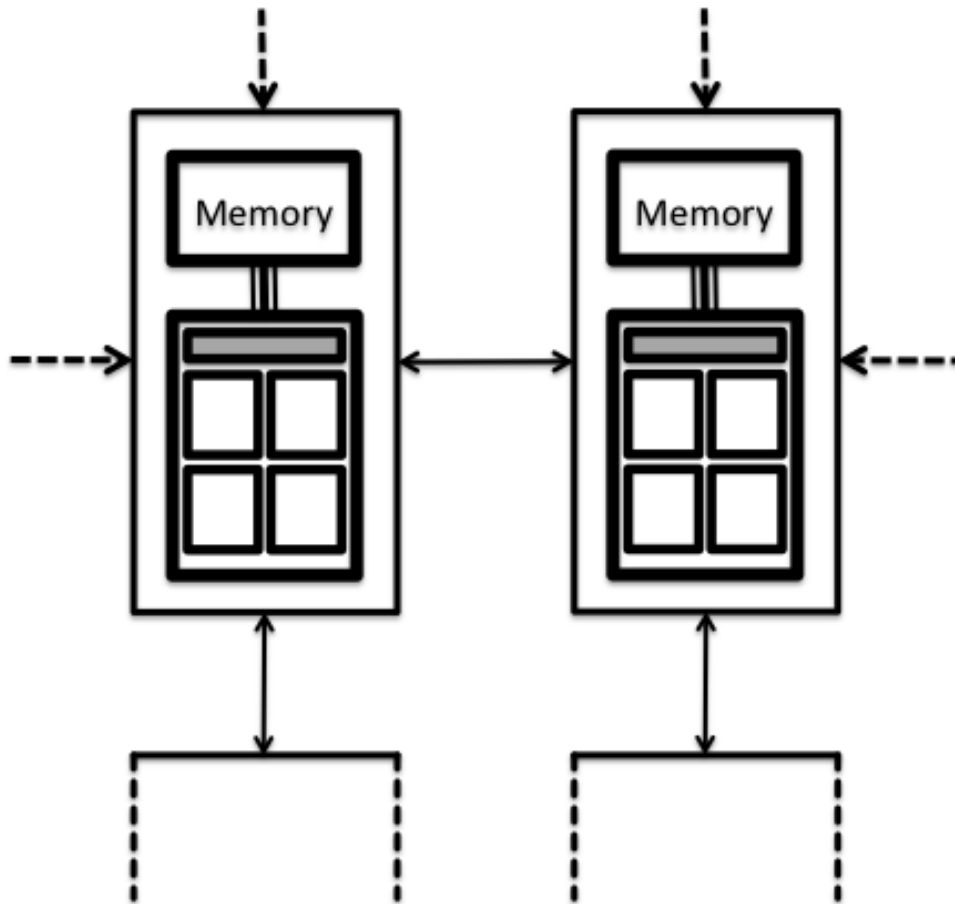
- Almost all HPC machines are distributed memory
- The performance of parallel programs often depends on the *interconnect* performance
 - Although once it is of a certain (high) quality, applications usually reveal themselves to be CPU, memory or IO bound
 - Low quality interconnects (e.g. 10Mb/s – 1Gb/s Ethernet) do not usually provide the performance required
 - Specialist interconnects are required to produce the largest supercomputers. e.g. Cray Aries, IBM BlueGene/Q
 - Infiniband is dominant on smaller systems.
- High bandwidth relatively easy to achieve
 - low latency is usually more important and harder to achieve

Distributed/shared memory hybrids

Almost everything now falls into this class

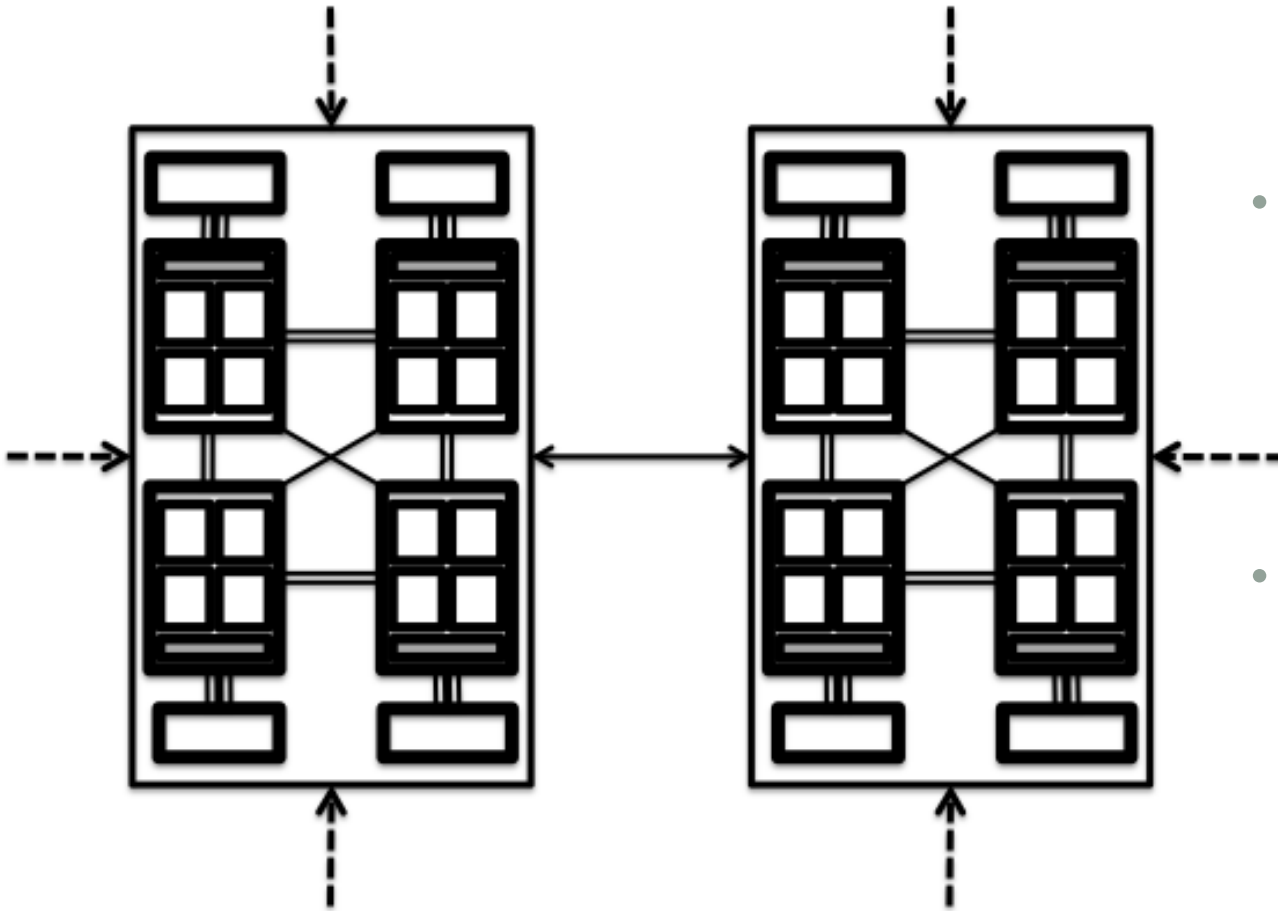


Multicore nodes



- In a real system:
 - each node will be a shared-memory system
 - e.g. a multicore processor
 - the network will have some specific topology
 - e.g. a regular grid

Hybrid architectures



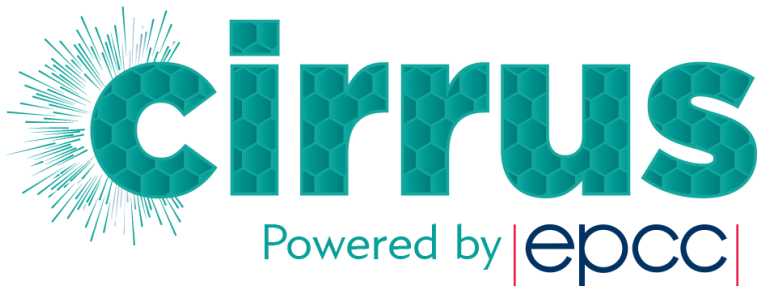
- Now normal to have NUMA nodes
 - e.g. multi-socket systems with multicore processors
- Each node still runs a single copy of the OS

Hybrid architectures

- Almost all HPC machines fall in this class
- Most applications use a message-passing (MPI) model for programming
 - Usually use a single process per core
- Increased use of hybrid message-passing + shared memory (MPI+OpenMP) programming
 - Usually use 1 or more processes per NUMA region and then the appropriate number of shared-memory threads to occupy all the cores
- Placement of processes and threads can become complicated on these machines

Examples

- ARCHER has two 12-way multicore processors per node
 - 2 x 2.7 GHz Intel E5-2697 v2 (Ivy Bridge) processors
 - each node is a 24-core, shared-memory, NUMA machine
 - each node controlled by a single copy of Linux
 - 4920 nodes connected by the high-speed ARIES Cray network
- Cirrus has two 18-way multicore processors per node
 - 2 x 2.1 GHz Intel E5-2695 v4 (Broadwell) processors
 - each node is a 36-core, shared-memory, NUMA machine
 - each node controlled by a single copy of Linux
 - 280 nodes connected by the high-speed Infiniband (IB) fabric



Accelerators

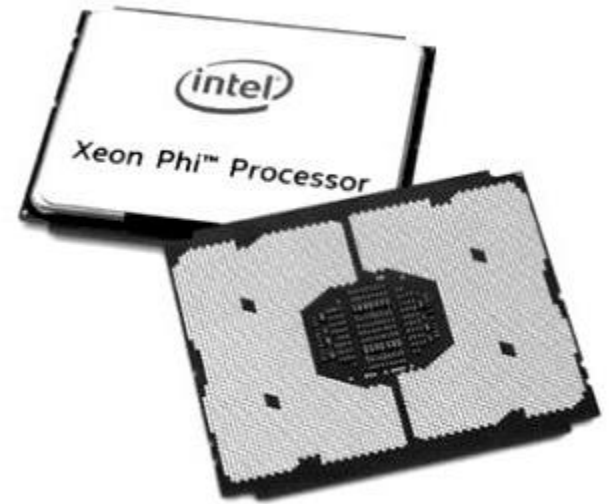
How are they incorporated?

Including accelerators

- Accelerators are usually incorporated into HPC machines using the hybrid architecture model
 - A number of accelerators per node
 - Nodes connected using interconnects
- Communication from accelerator to accelerator depends on the hardware:
 - NVIDIA GPU support direct communication
 - AMD GPU have to communicate via CPU memory
 - Intel Xeon Phi communication via CPU memory
 - Communicating via CPU memory involves lots of extra copy operations and is usually very slow

Example: ARCHER KNL

- 12 nodes with Knights Landing (Xeon Phi) recently added
- Each node has a 64-core KNL
 - 4 concurrent hyper-threads per core
 - Each node has 96GB RAM and each KNL has 16GB on chip memory
- The KNL is self hosted, i.e. in place of the CPU
 - Parallelism via shared memory (OpenMP) or message passing (MPI)
 - Can do internode parallelism via message passing
- Specific considerations needed for good performance



Filesystems

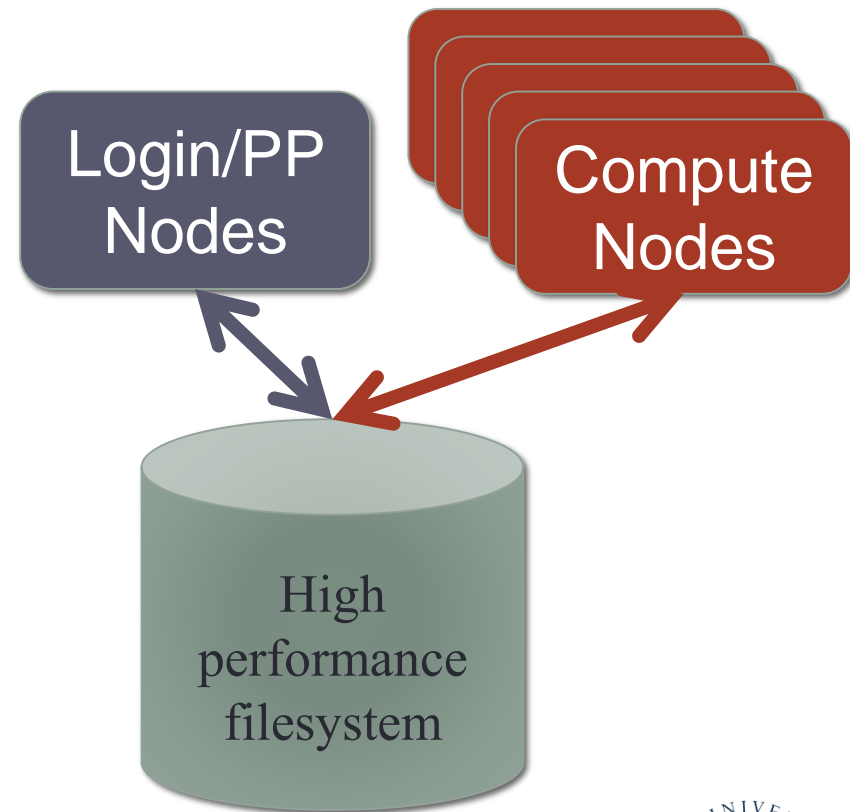
How is data stored?

High performance IO

- We have focused on the significant computation power of HPC machines so far
 - It is important that writing to and reading from the filesystem does not negate this
- High performance filesystems
 - Such as Lustre
 - Computational nodes are typically diskless and connect via the network to the filesystem
 - Due to its size this high performance filesystem is often NOT backed up
 - Connected to the nodes in two common ways
 - Not a silver bullet! There are lots of configuration and IO techniques which need to be leveraged for good performance and these are beyond the scope of this course.

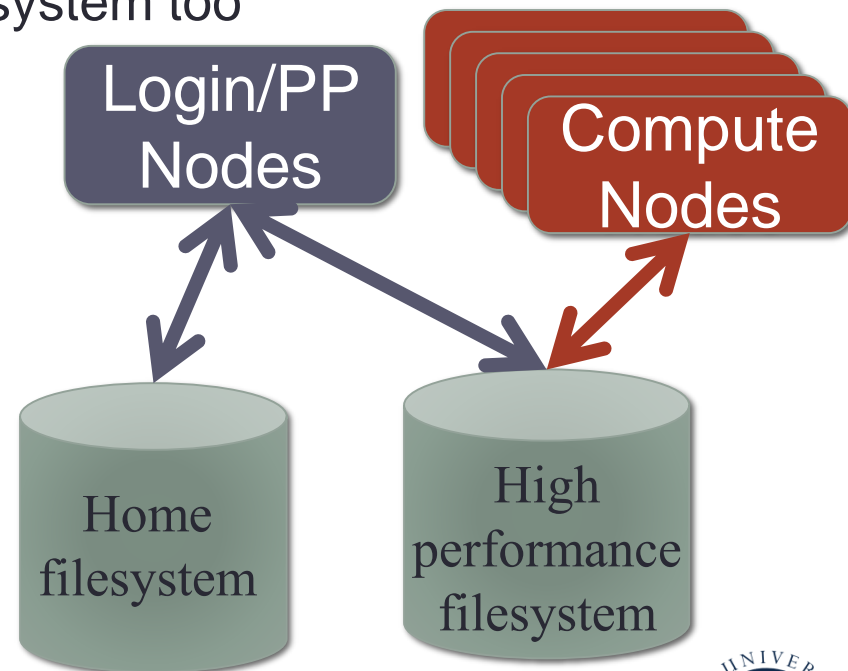
Single unified filesystem

- One filesystem for the entire machine,
 - All parts of the machine can see this and all files are stored in this system
 - E.g. Cirrus (406 TiB Lustre FS)
- Advantages
 - Conceptually simple as all files are stored on the same filesystem
 - Preparing runs (e.g. compiling code) exhibits good IO performance
- Disadvantages
 - Lack of backup on the machine
 - This high performance filesystem can get clogged with significant unnecessary data (such as results from post processing/source code.)



Multiple disparate filesystems

- High performance filesystem focused on execution
 - Other filesystems for preparing & compiling code, as well as long term data storage
 - E.g. ARCHER which has an additional (low performance, huge capacity) long term data storage filesystem too
- Advantages
 - Home filesystem is typically backed up
- Disadvantages
 - More complex as high performance FS is only one visible from compute nodes
- High performance FS sometimes called work or scratch

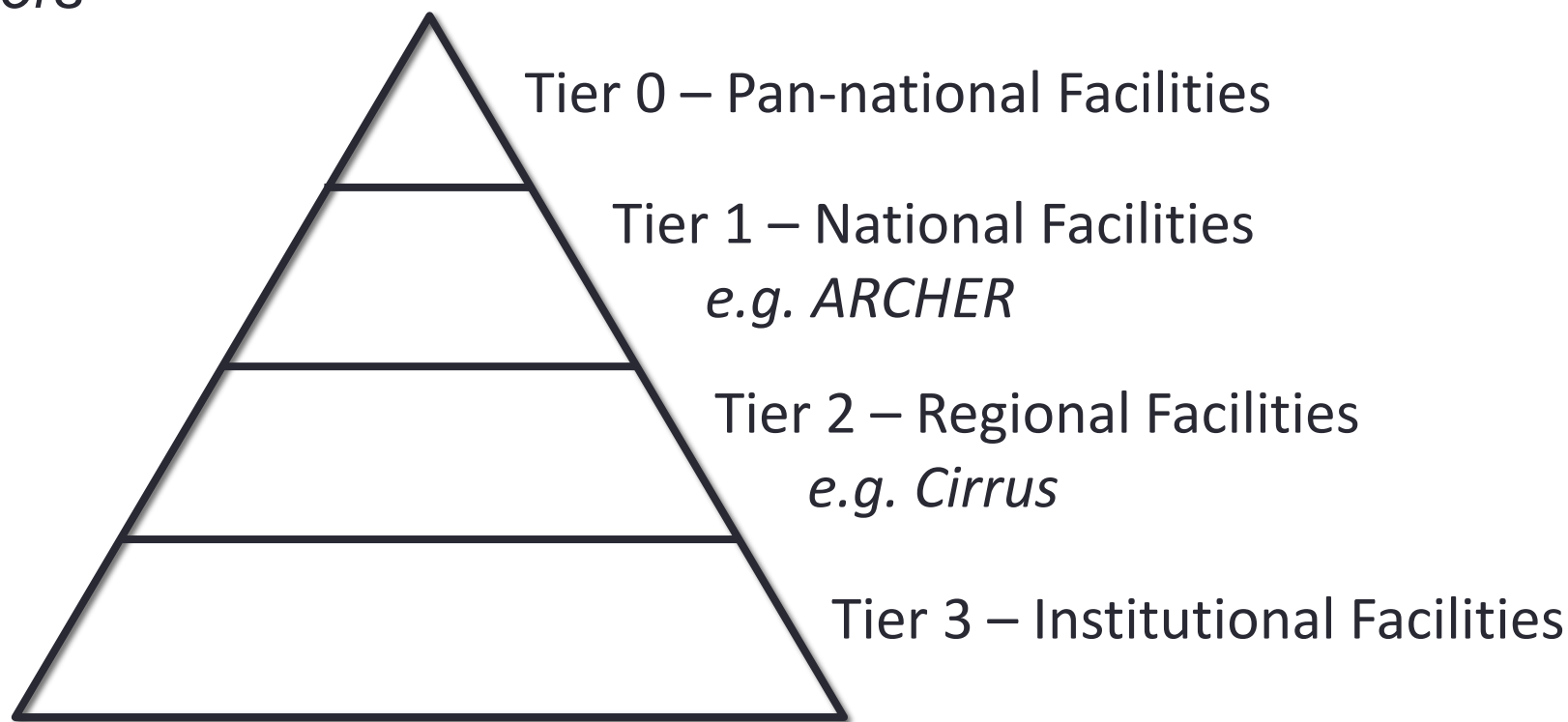


Comparison of machine types

What is the difference between different tiers of machine?

HPC Facility Tiers

- HPC facilities are often spoken about as belonging to *Tiers*



List of tier 2 facilities at

<https://www.epsrc.ac.uk/research/facilities/hpc/tier2/>



Summary

Summary

- Vast majority of HPC machines are shared-memory nodes linked by an interconnect.
 - Hybrid HPC architectures – combination of shared and distributed memory
 - Most are programmed using a pure MPI model (more later on MPI)
 - does not really reflect the hardware layout
- Accelerators are incorporated at the node level
 - Very few applications can use multiple accelerators in a distributed memory model
- Shared HPC machines span a wide range of sizes:
 - From Tier 0 – Multi-petaflops (1 million cores)
 - To workstations with multiple CPUs (+ Accelerators)