

High Performance Computing

What is it used for and why?

EPSRC

NERC SCIENCE OF THE ENVIRONMENT



CRAY
THE SUPERCOMPUTER COMPANY

epcc



Overview

- What is it used for?
 - Drivers for HPC
 - Examples of usage
- Why do you need to learn the basics?
 - Hardware layout and structure matters
 - Serial computing is required for parallel computing
 - Appreciation of fundamentals will help you get more from HPC and scientific computing



What is HPC used for?

Drivers and examples



Why HPC?

- Scientific simulation and modelling drive the need for greater computing power.
- Single-core processors can not be made that have enough resource for the simulations needed.
 - Making processors with faster clock speeds is difficult due to cost and power/heat limitations
 - Expensive to put huge memory on a single processor
- Solution: parallel computing – divide up the work among numerous linked systems.

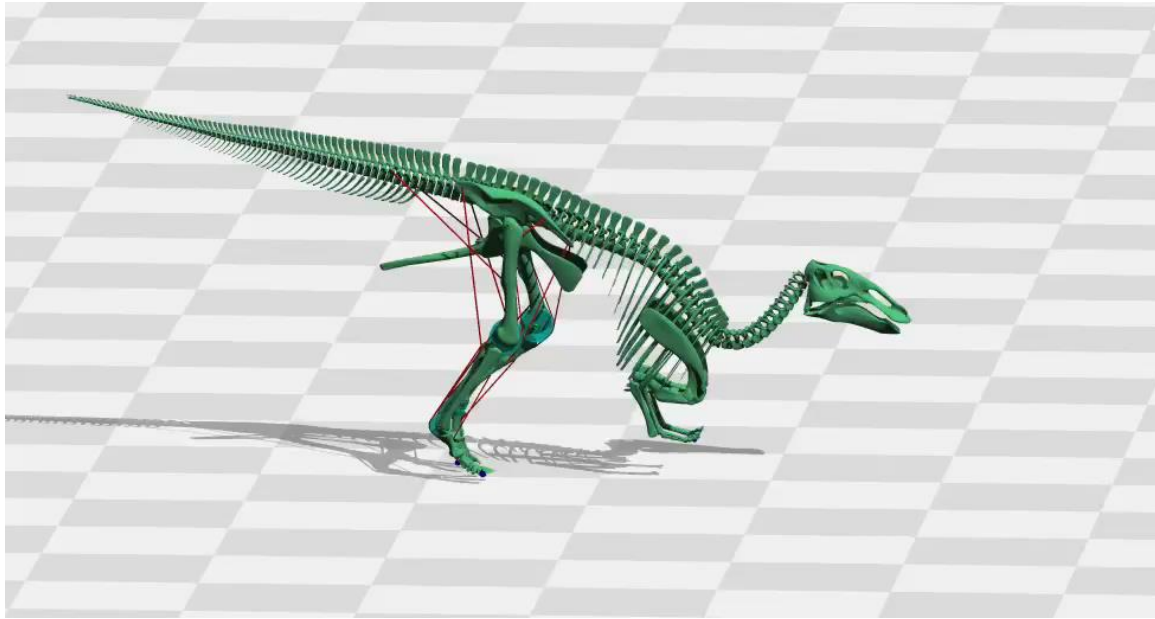


Generic Parallel Machine

- Good conceptual model is collection of multicore laptops
 - come back to what “multicore” actually means later on ...
- Connected together by a network

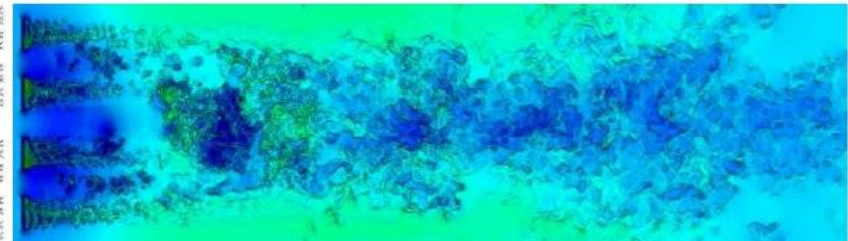
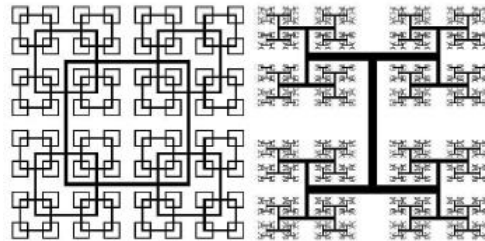
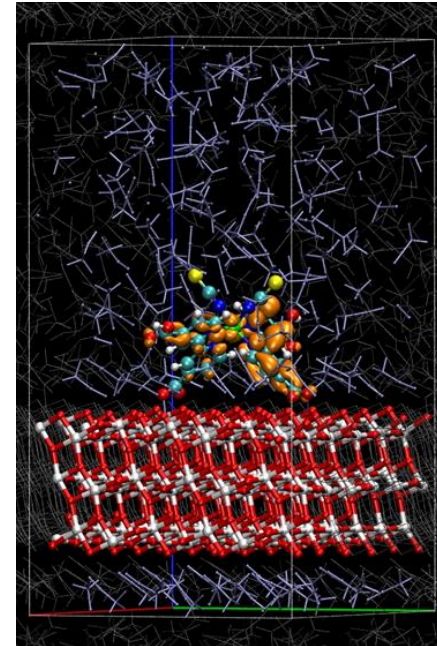


- Each laptop is called a *compute node*
 - each has its own operating system and network connection
- Suppose each node is a quadcore laptop
 - total system has 20 processor-cores



Modelling dinosaur gaits
 Dr Bill Sellers, University of Manchester

Dye-sensitised solar cells
 F. Schiffmann and J. VandeVondele
 University of Zurich



Fractal-based models of turbulent flows
 Christos Vassilicos & Sylvain Laizet,
 Imperial College



The Fundamentals

Why do I need to know this?



Parallel Computing

- Parallel computing and HPC are intimately related
 - higher performance requires more processor-cores
- Understanding the different parallel programming models allows you to understand how to use HPC resources effectively



Hardware Layout

- Understanding the different types of HPC hardware allows you to understand why some things are better on one resource than another
- Allows you to choose the appropriate resource for your application
- Allows you to understand the ways to parallelise your serial application
- Gives you an appreciation of the parts that are important for performance



Serial Computing

- Without an understanding of how serial computing operates it is difficult to understand parallel computing
 - What are the factors that matter for serial computation
 - How does the compiler produce executable code?
 - Which bits are automatic and which parts do I have to worry about
 - What can or can't the operating system do for me?



Differences from Desktop Computing

- Do not log on to compute nodes directly
 - submit jobs via a batch scheduling system
- Not a GUI-based environment
- Share the system with many users
- Resources more tightly monitored and controlled
 - disk quotas
 - CPU usage



What do we mean by “performance”?

- For scientific and technical programming use FLOPS
 - Floating Point OPerations per Second
 - $1.324398404 + 3.6287414 = ?$
 - $2.365873534 * 2443.3147 = ?$
- Modern supercomputers measured in PFLOPS (PetaFLOPS)
 - Kilo, Mega, Giga, Tera, Peta, Exa = 10^3 , 10^6 , 10^9 , 10^{12} , 10^{15}
- Other disciplines have their own performance measures
 - frames per second, database accesses per second, ...

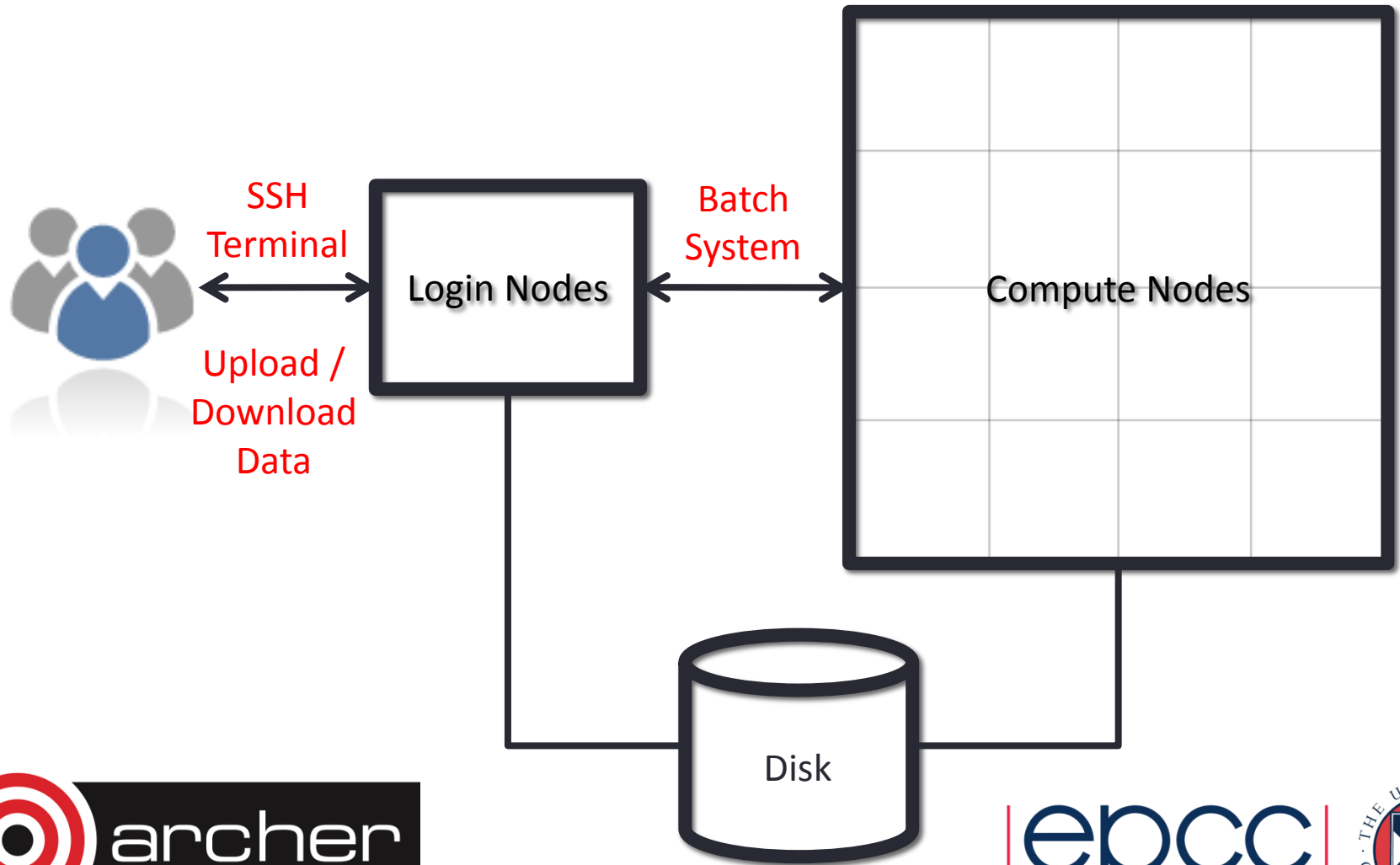


HPC Layout and Use

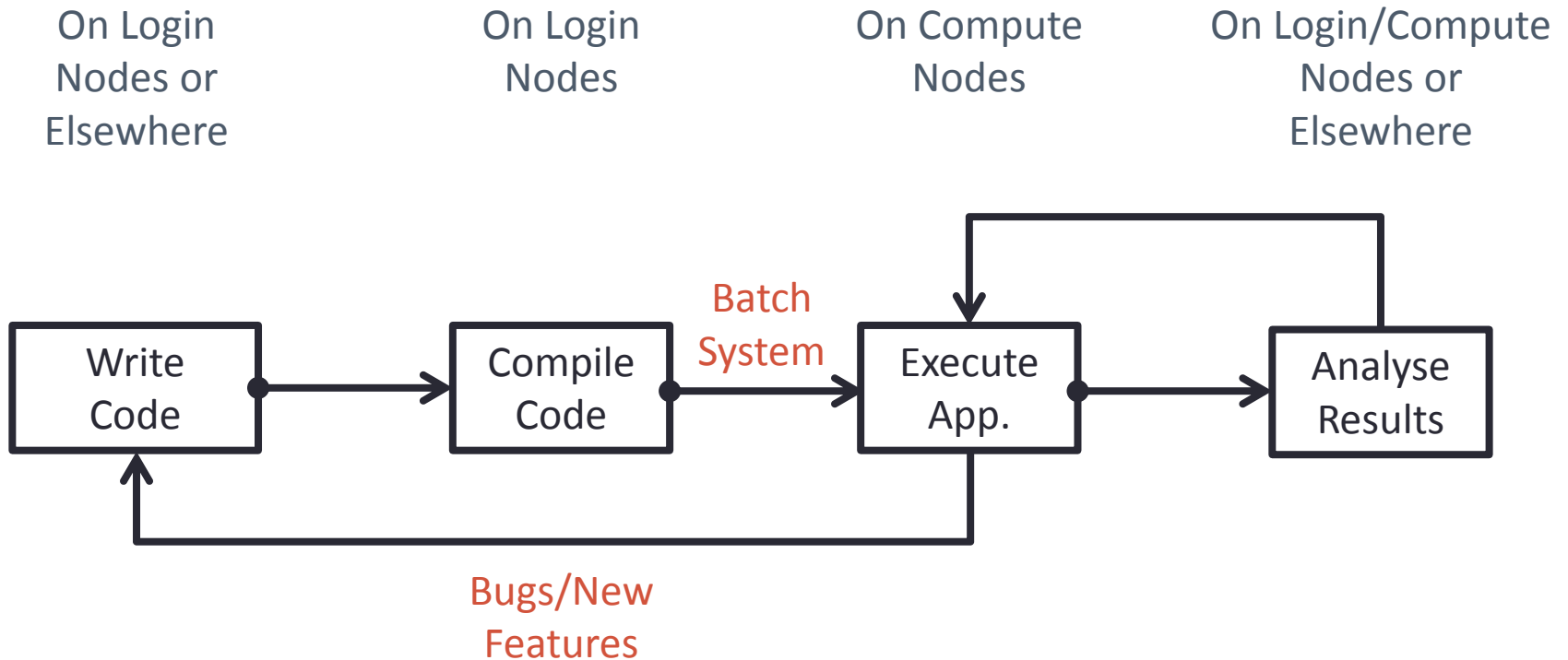
Starting concepts



Typical HPC system layout



Typical Software Usage Flow



ARCHER



ARCHER

- UK National Supercomputing Service
 - funded by EPSRC and NERC
 - operated by EPCC



ARCHER in a nutshell

- Peak performance of 2.55 PFLOPS
- Cray XC30 Hardware
 - Intel Ivy Bridge processors: 64 (or 128) GB memory; 24 cores per node
 - 4920 nodes (118,080 cores) each running CNL (Compute Node Linux)
 - Linked by Cray Aries interconnect (dragonfly topology)
- Cray Application Development Environment
 - PBS batch system
 - Cray, Intel, GNU Compilers
 - Cray Parallel Libraries
 - DDT Debugger, Cray Performance Analysis Tools



Summary

- High Performance Computing = parallel computing
- Run on multiple processor-cores at the same time
- Typically use fairly standard processors
 - but many thousands of them
- Fast network for inter-processor communications

