High Performance Computing

What is it used for and why?

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

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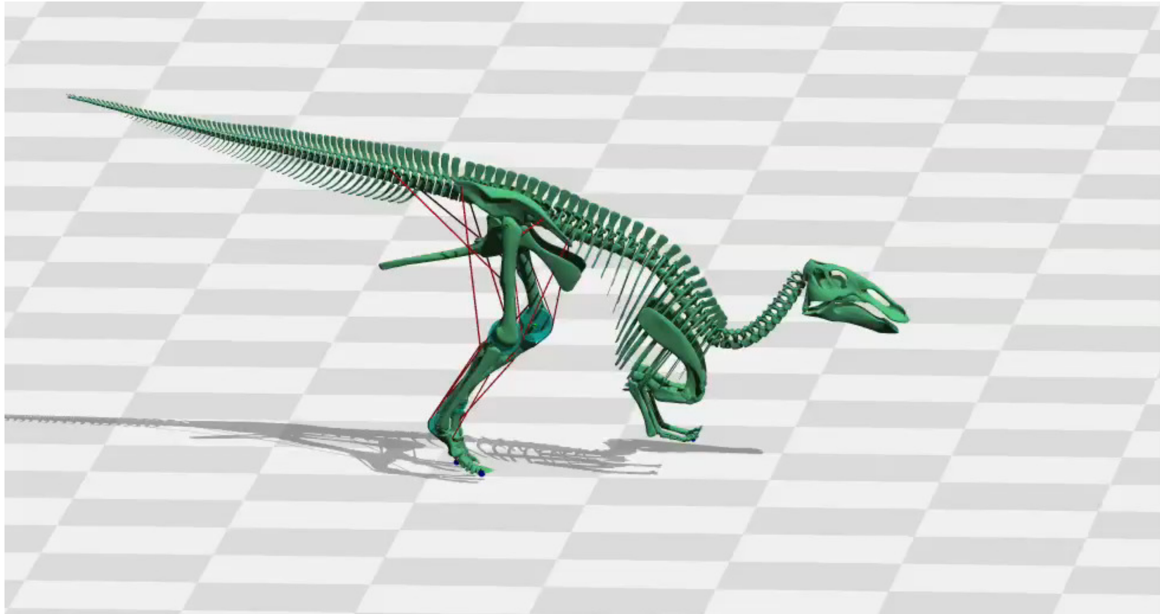
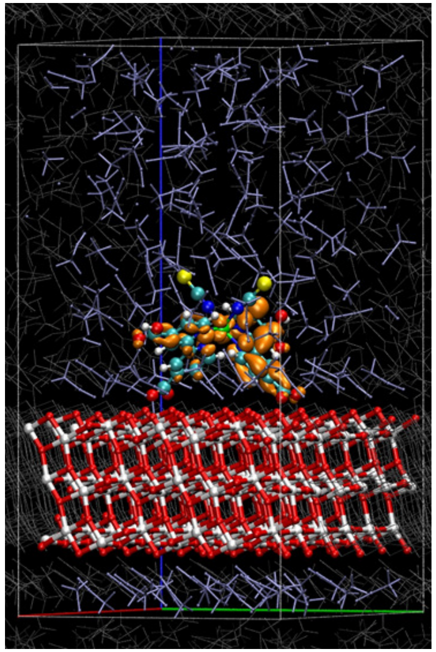
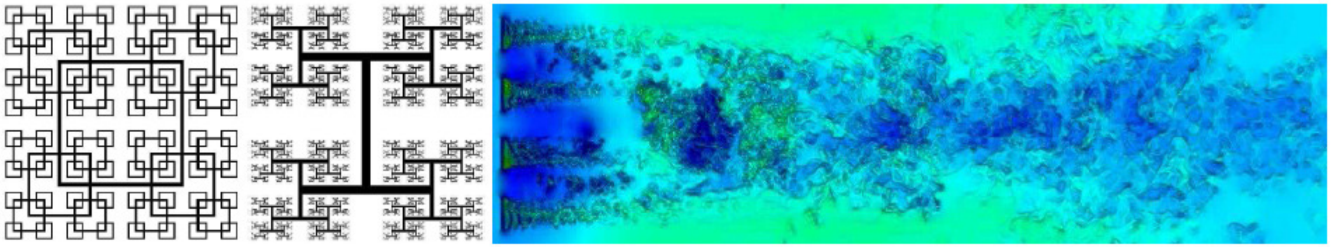


Modelling dinosaur gaits
Dr Bill Sellers, University of Manchester

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



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



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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

Differences from Cloud Computing

- Performance
  - Clouds usually use virtual machines which add an extra layer of software.
  - In cloud you often share hardware resource with other users – HPC access is usually exclusive.
- Tight-coupling
  - HPC parallel programming usually assumes that the separate processes are tightly coupled
  - Requires a low-latency, high-bandwidth communication system between tasks
  - Cloud usually does not usually have this
- Programming models
  - HPC use high-level compiled languages with extensive optimisation.
  - Cloud often based on interpreted/JIT.

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, …

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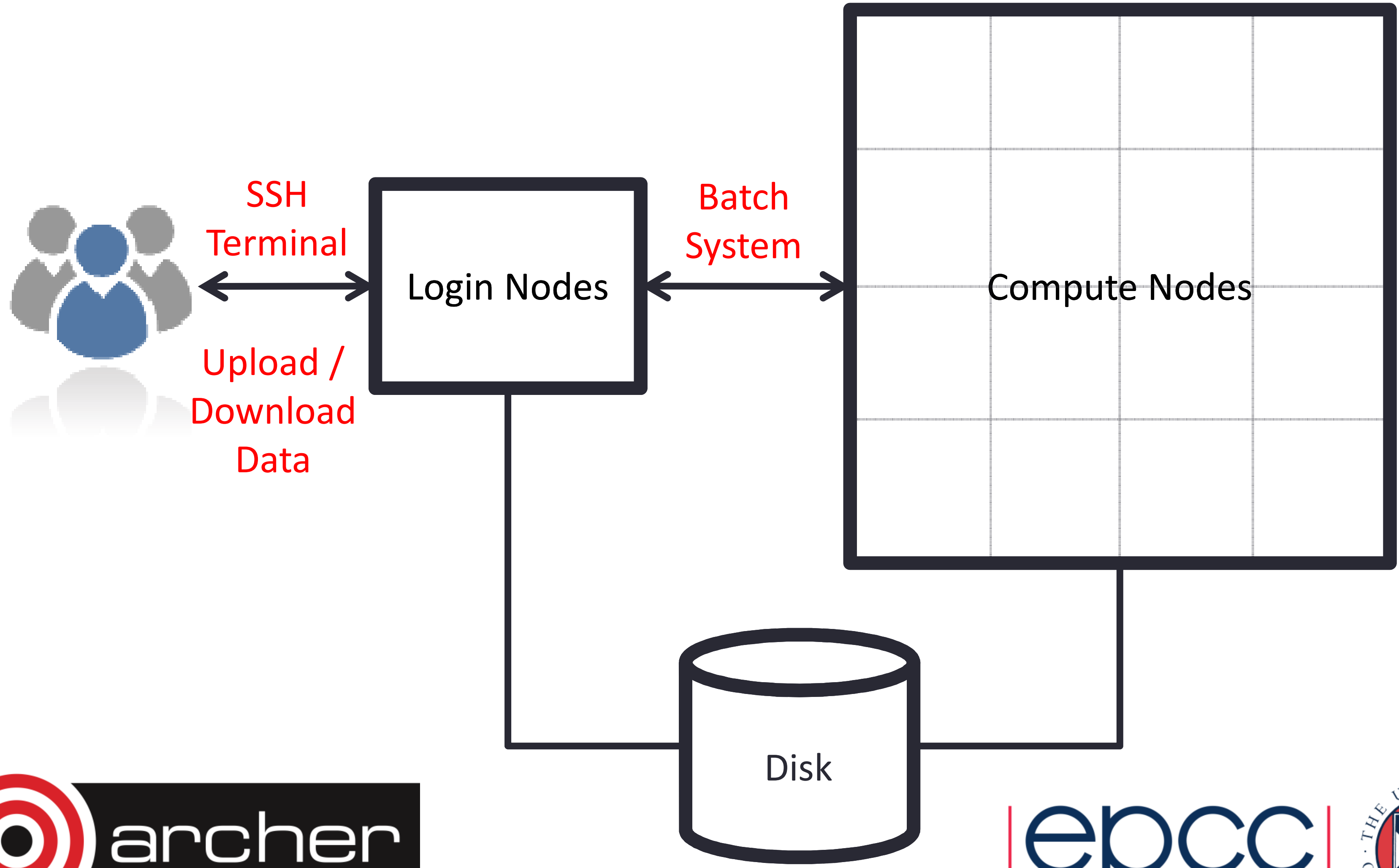
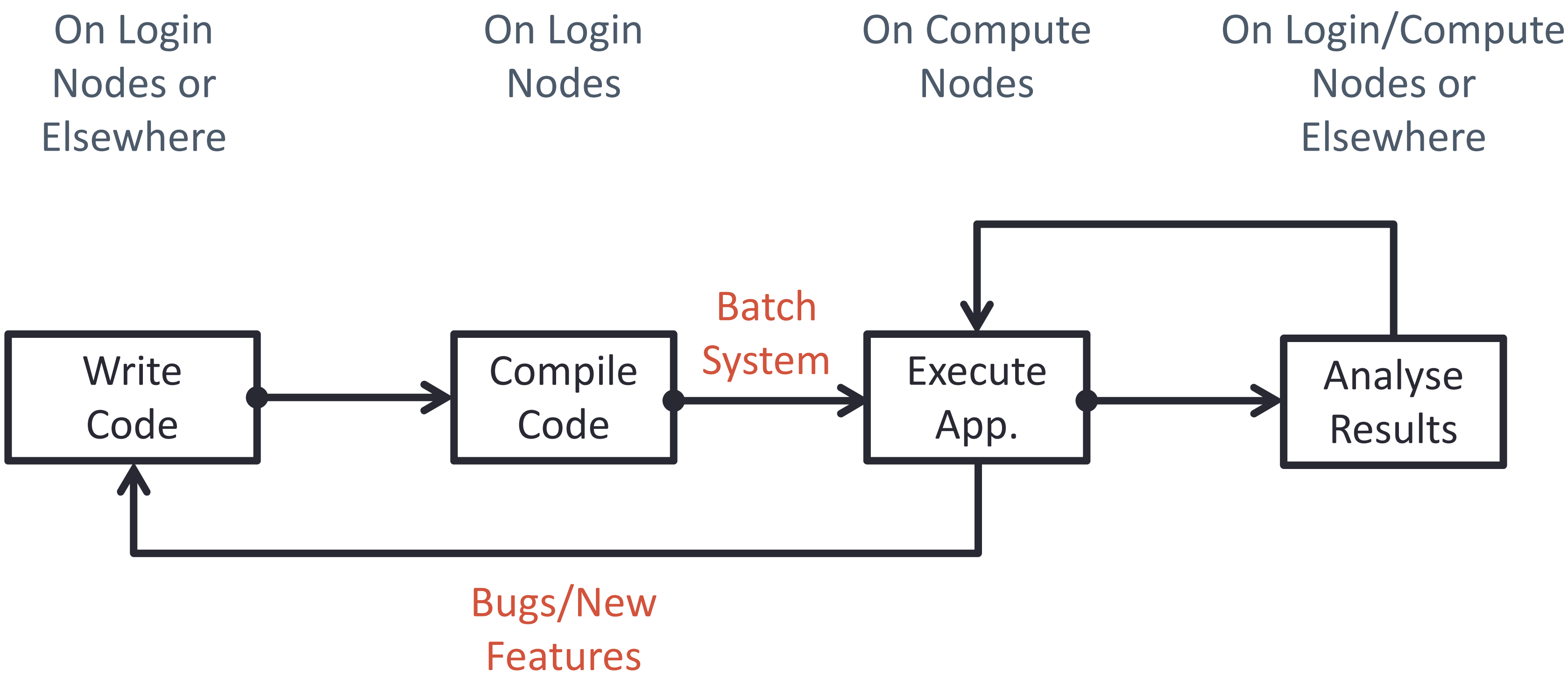
HPC Layout and Use

Starting concepts

Typical HPC system layout



Typical Software Usage Flow



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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