Introduction to High Performance Computing

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Outline

- What is High Performance Computing?
- Characteristics of HPC
- Building Blocks of an HPC System
- Evolution of Supercomputers
- A Modern Supercomputer
- Architecture of a Supercomputer
- Vector Processing
- Accelerators
- Why Use HPC
- HPC is not just…
- Paradigms Influenced by HPC
- HPC Domains

What is High Performance Computing?

- As the name suggests: computing on high performance computers
- Combination of hardware & software
- Originally implemented in supercomputers for scientific research
- Main purpose is development of parallel processing software which can be executed simultaneously on multiple processors
- Modern day HPC does not require a supercomputer

Characteristics of HPC

- Massively Parallel Processing
- Vector Processing
- Floating Point Arithmetic
- Multi Threading
- Low Latency
- High Bandwidth
- Efficiency measured in FLOPS

Building Blocks of an HPC System

- Compute Hardware
  - Cluster of computers
  - Accelerators (GPU or MIC)
  - Specialized Accelerators (FPGA or ASIC)
- Network Fabric
  - Infiniband
  - Gigabit Ethernet
  - Others (MyriNet, Quadrics etc.)
- Software (Programming Models)
  - MPI (Message Passing Interface)
  - SHMEM (Shared Memory)
  - PGAS (Partitioned Global Address Space)

Evolution of Supercomputers

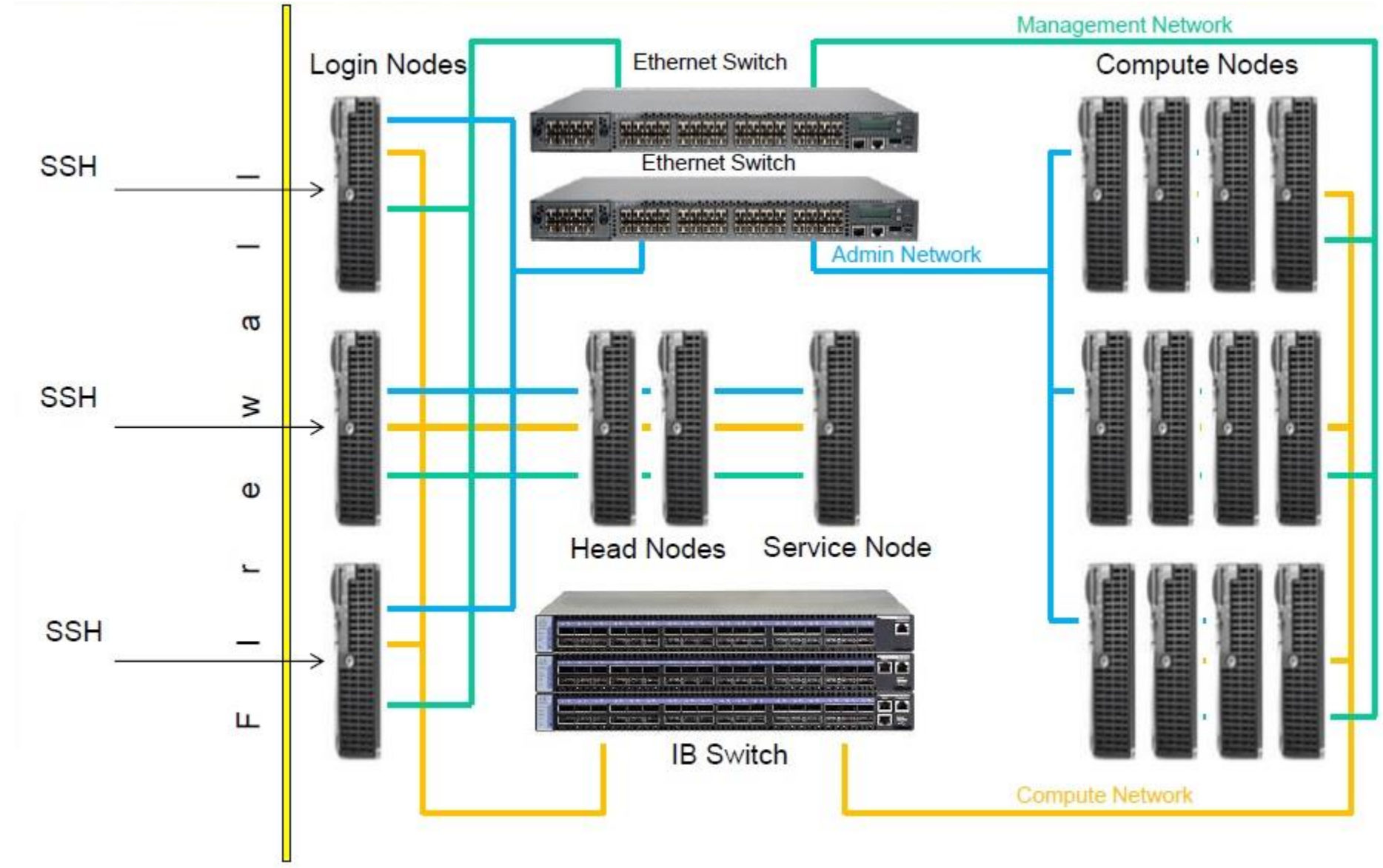
- Vector Computers (VC)
  - Designed keeping in mind the numerical problems at hand
  - Too specific
- Massively Parallel Processors (MPP)
- Symmetric Multiprocessors (SMP)
- Distributed Systems
- Clusters
  - Easier to integrate
  - Cost effective
  - Serves a wide variety of purpose

A Modern Supercomputer

- Modern Supercomputer: cluster of commercially available off the shelf (COTS) computers
- Compute units: multi socket, multi core CPUs or Accelerators
- Interconnected via high throughput network fabric
- Parallel File System
- Message Passing Interface

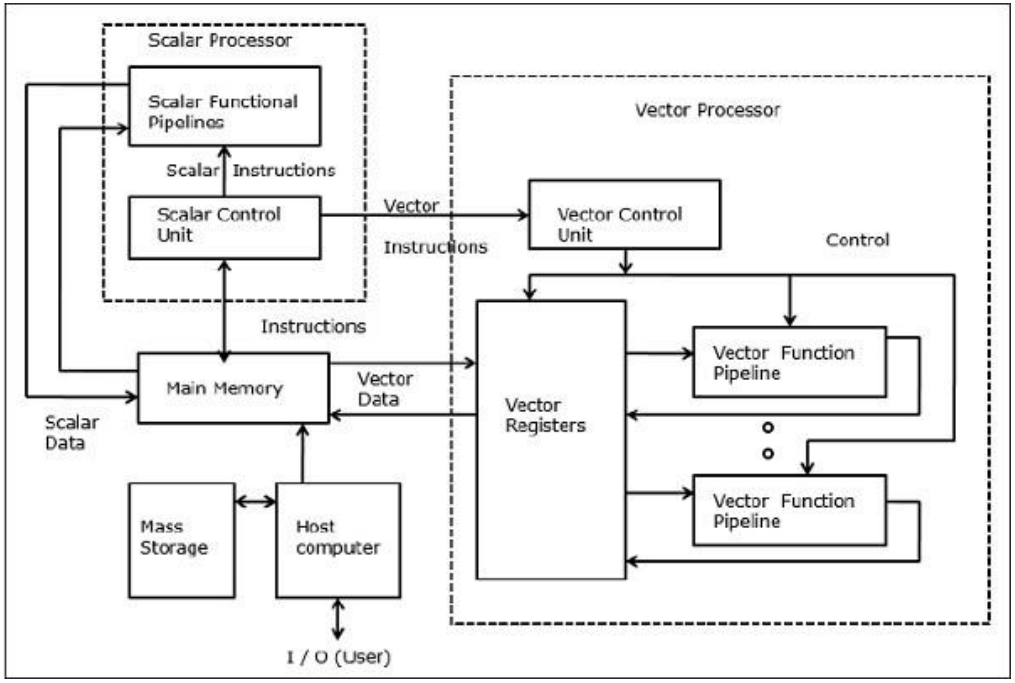
Supercomputer (A Visual Example)

Architecture of a Supercomputer



Vector Processing

- The diagram below shows the architecture of a vector supercomputer during the early ages of HPC



- In modern times similar processing and much more is achieved within a normal CPU

Accelerators

Nvidia GPU

Intel MIC

Altera FPGA

Bitmain Bitcoin ASIC Unit

Why Use HPC?

- Simulation & modelling
  - Cost of real experiment is too high
    - E.g. CFD analysis of an aircraft
  - Real experiment may be too dangerous
    - E.g. simulation of nuclear fission reaction
- Time bound completion
  - Application must finish within set time limits
    - E.g. weather forecasting
  - Application needs to perform in real time
    - E.g. high performance trading
- Experimental data is too large
- Allows more permutations & combinations to be tried

HPC is not just…

- Supercomputing
- Grid Computing
- Distributed Computing

Paradigms influenced by HPC

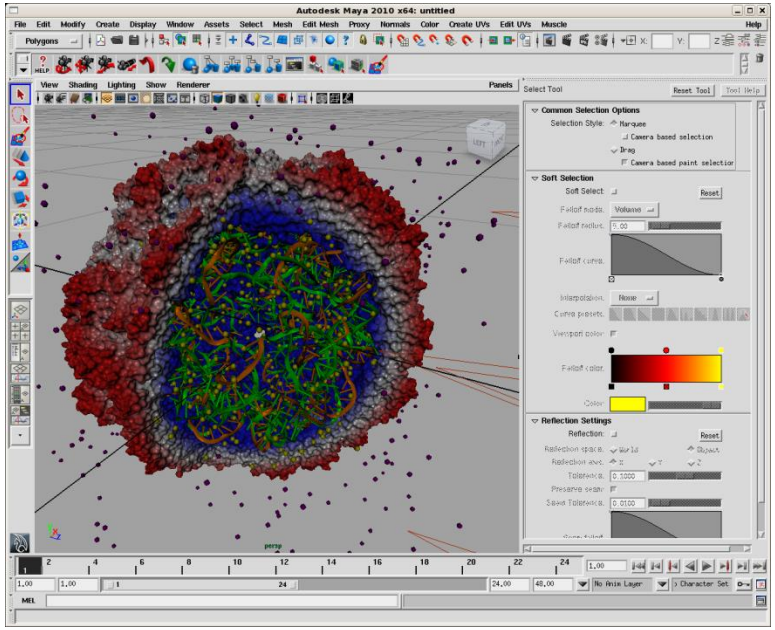
- Many computing paradigms have been influenced by HPC, often to be confused as being part of HPC
  - Big Data
  - Cloud Computing
  - Machine Learning

HPC Domains

- HPC has moved beyond the domains of scientific research and has gone mainstream
- HPC touches our day to day life in form of medicines, weather forecasts, automobiles, banking, animated movies etc.

Life Sciences & Molecular Research

- Utilities
  - Formulation of new molecules
  - Drug discovery
  - Genome sequencing
- Softwares
  - AMBER
  - NAMD
  - LAMMPS
  - GROMACS

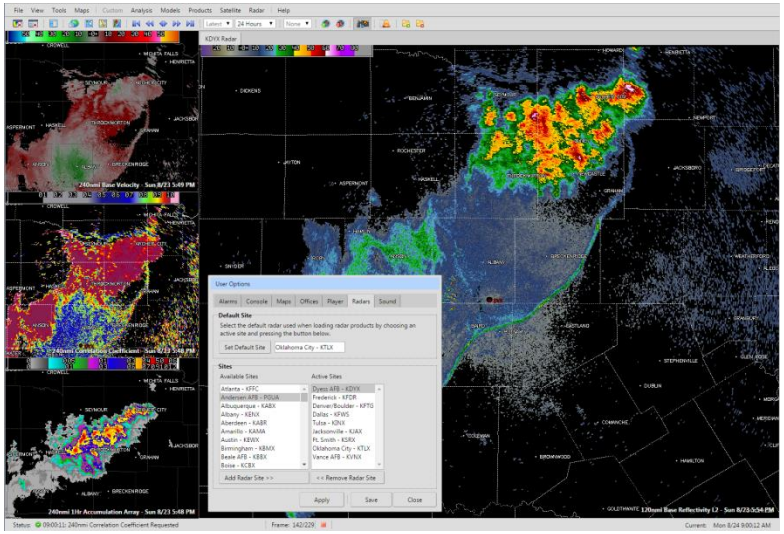


Screenshot of VMD-1.9

Weather Modelling & Forecasting

- Utilities
  - Weather forecasting
  - Atmospheric Research
  - Oceanography
  - Ice cap & glacial modelling

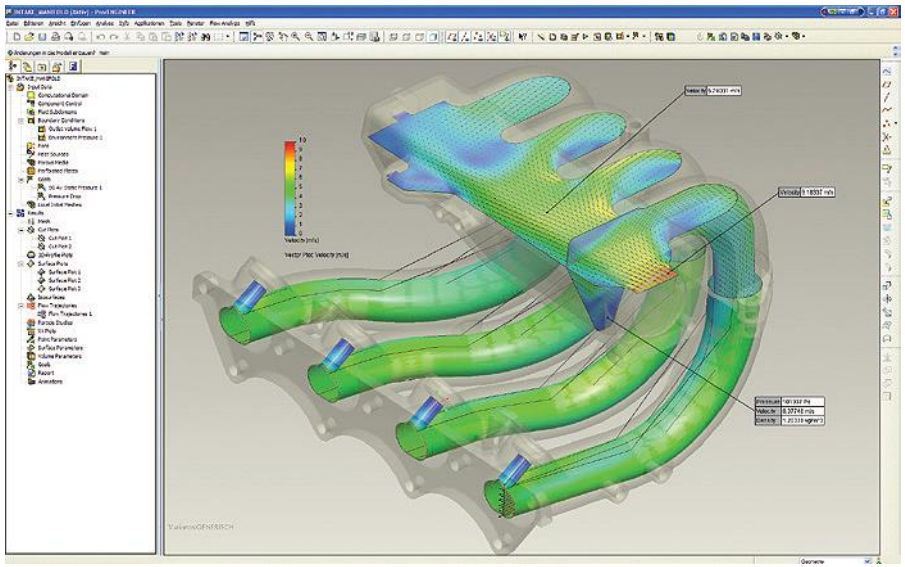
- Softwares
  - WRF
  - ROMS
  - GEOS



Computational Fluid Dynamics

- Utilities
  - Design of aircrafts, automobiles
  - Design of cooling units
  - Design of jet & rocket engines

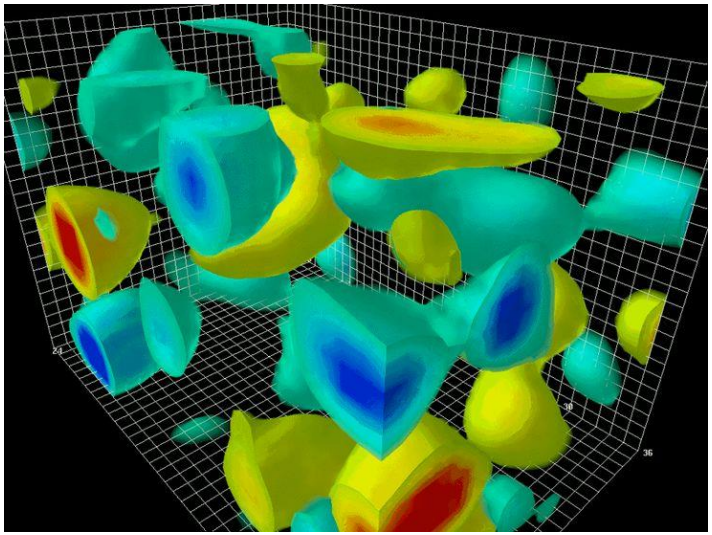
- Softwares
  - OpenFOAM
  - Ansys Fluent
  - Abaqus



Nuclear & Quantum Physics

- Utilities
  - Simulation of nuclear experiments
  - Behaviour analysis of quarks
  - Quantum Chromodynamics
  - Research at Large Hadron Collider

- Softwares
  - MILC
  - QPHIX



A QCD simulation showing quark and gluon field fluctuations

Other HPC Domains

- Finance & trading
  - Banking
  - High performance trading
  - Stock market modelling
  - Cryptocurrencies (e.g. Bitcoin)
- Cryptography & Security
  - Code breaking
  - Cyber forensics
  - Cryptocurrency
- Media & entertainment
  - Animation
  - Special Effects (VFX)
- Oil & gas exploration
- Astronomy & astrophysics


THANK
YOU !