

Scientific Simulation on Emerging Technologies

Alan O'Cais
Scientific Coordinator
CaSToR^C

Outline:

- Capacity or capability?
- Capability architecture
 - Accelerators
- Project tools and management

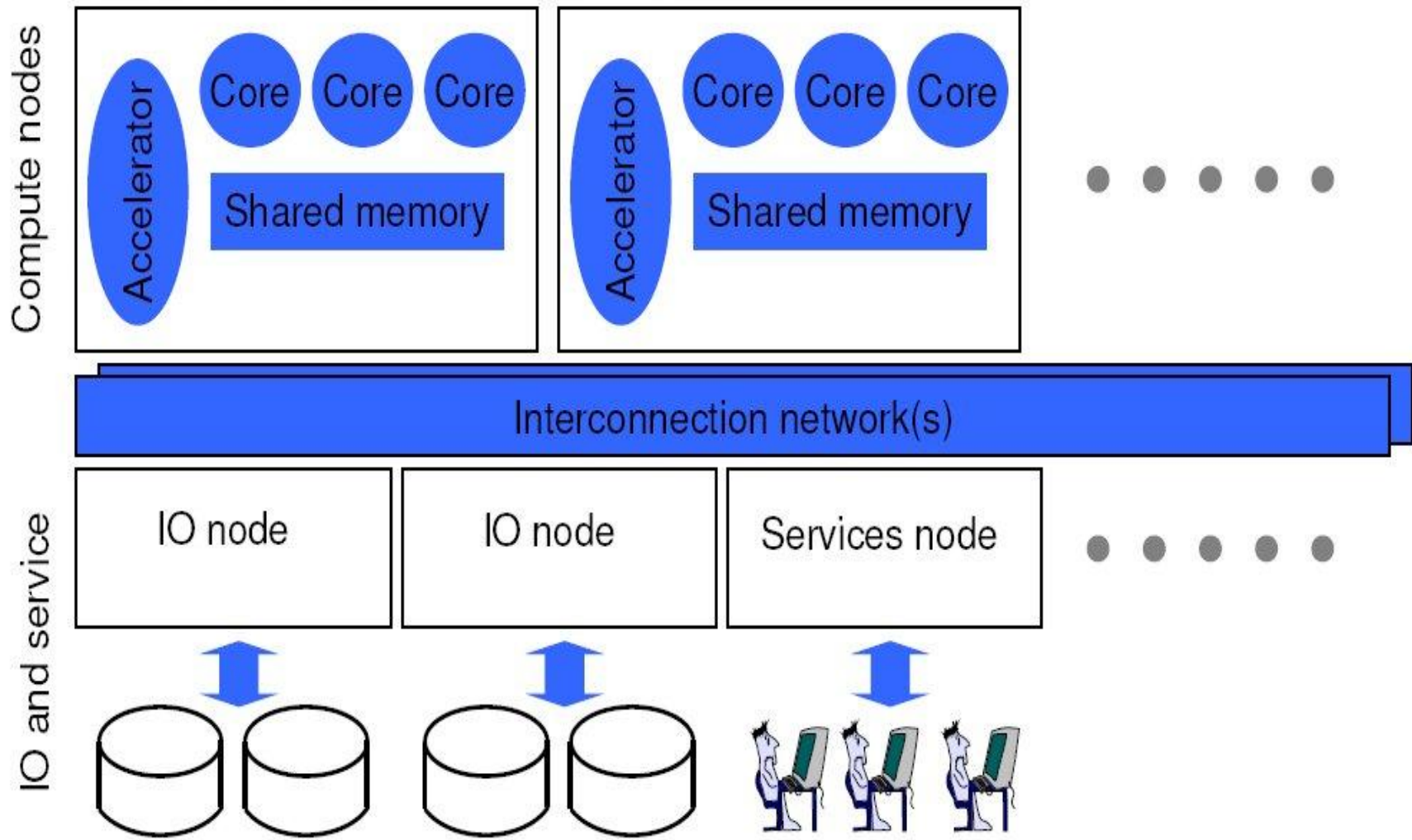
Strong/Weak Scalability and HPC Systems

- Strong scaling
 - Same problem size in shorter time
- Weak scaling
 - Larger problem size in same time
- Capacity computing
 - Cycle-scavenging
 - GRID systems
- Capability computing
 - Larger problems, more expensive systems

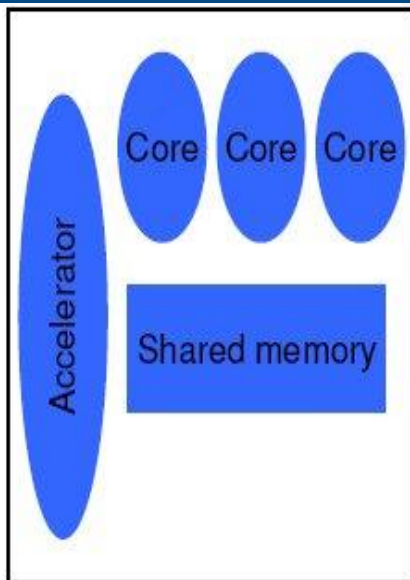
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Architecture: A generic view



Compute nodes



Low power μ p
Ex: IBM/BG/P,
 $\approx 3,5$ Gflops/core

Commodity μ p
Ex: Intel/Xeon,
 ≈ 10 Gflops/core

High performance μ p
Ex: IBM/Power6,
 ≈ 20 Gflops/core

Accelerators (GPU, Cell, FPGA, ...)
Ex: AMD FS 9250, ≈ 200 Gflops DP ≈ 150 W
Ex: IBM PowerXcell 8i, ≈ 100 Gflops DP ≈ 90 W
Ex: ClearSpeed CSX700 ≈ 100 Gflops DP ≈ 25 W

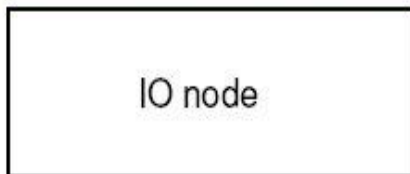
Vector processors
Ex: NEC SX9, ≈ 100 Gflops/core

Commodity thin-nodes
 $\approx 2-4$ sockets / node

High performance fat-nodes
 $> 2-4$ sockets / node

Integration and system software
(ex: BULL/BAS - based on OpenSource)

IO and service



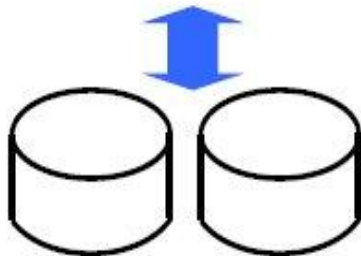
Software RAID

Intelligent storage

SATA disks
 $> \approx 2$ TB

SSD storage
 ≈ 10 s GB

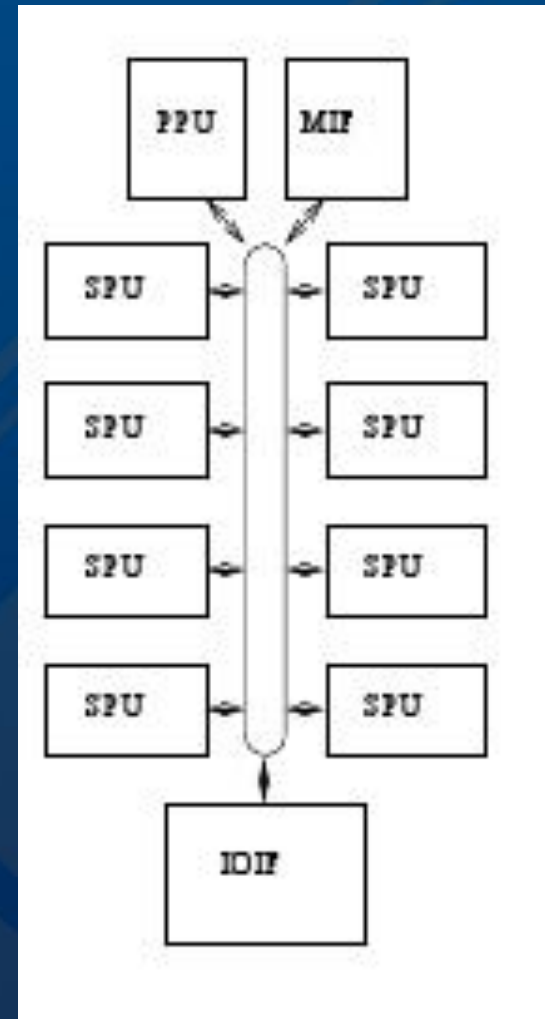
SAS disks
 ≈ 1 TB



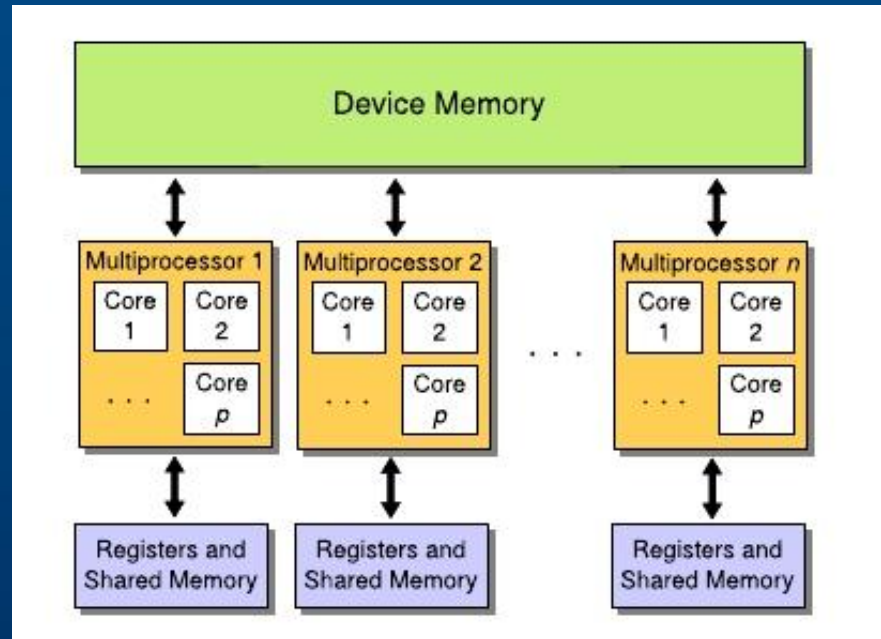
Ingredients for a Petaflop/s system in 2009/2010

Cell

- One PowerPC Processor Element (PPE)
- 8 Synergistic Processor Elements (SPE)
- 204.8 (102.4) GFlops SP (DP)
- ~ 90W



GPU



- 30 multiprocessors consisting of a total of 240 cores
- Compute Unified Device Architecture (CUDA)
- ~ 150W

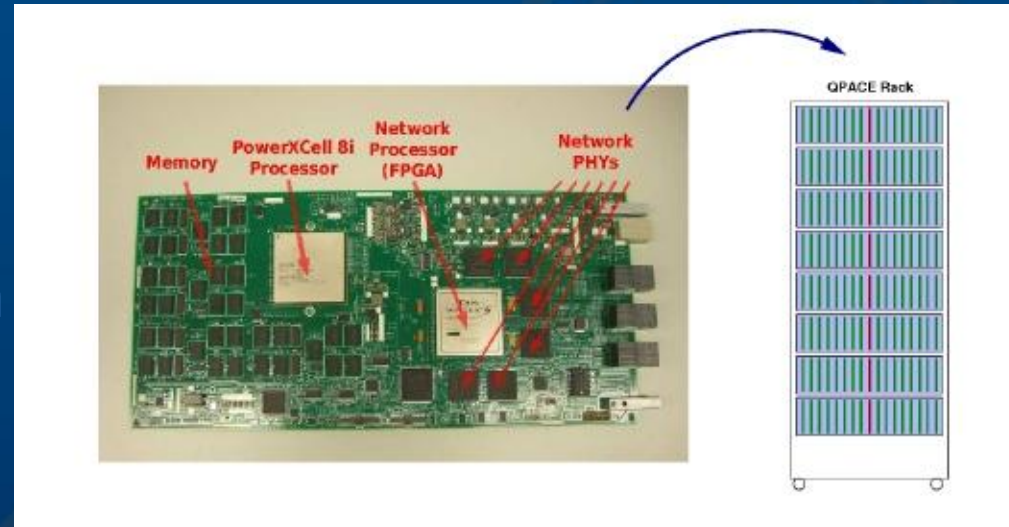
FPGA

- Field Programmable Gate Array
- Circuit design can be loaded
- Adapt architecture to program
- Require hardware design skills (?)
- Still following Moore's Law
- ~ 25W

Success stories in Lattice QCD

- QPACE

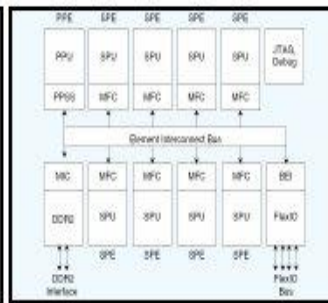
- FPGA for network
- Cell for computation
- 25% of peak



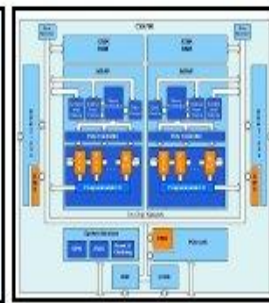
- Boston University (one of many)

- Data layouts, local storage
- 80 GFlops sustained (compared to 5GFlops for CPU)
- \$450 per board

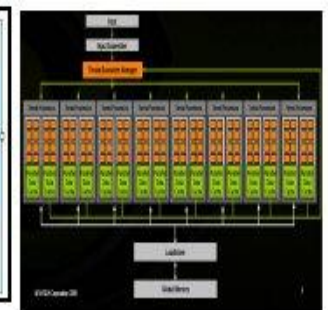
Evolution of Accelerators



IBM PowerXCell 8i
>0.1 Tflops DP



ClearSpeed CSX700
0,1 Tflops DP



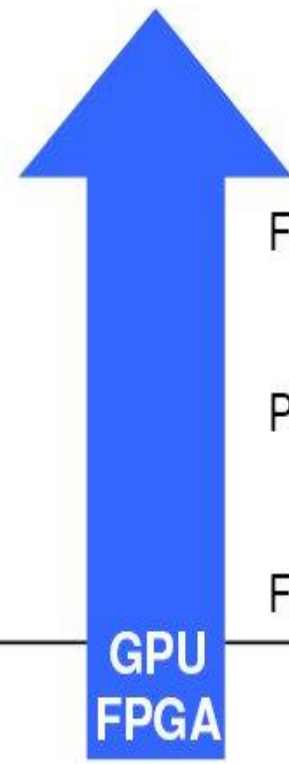
Nvidia Tesla T10
1 Tflops SP >0.1 Tflops DP
AMD FireStream 9250
1 Tflops SP, 0.2 Tflops DP

Outstanding performance/price and performance/electricity ratio for well suited and programmed applications

- GPU**
 - Evolving toward general-purpose computing
 - Addressing the HPC market (data-parallel programming)
- FPGA**
 - Less flexible but best performance/watt

Programmability

Performance



**GPU
FPGA**

- Fully programmable
- Partially programmable
- Fixed function

Beginning the Project

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- Understand the system
 - Heterogeneity
 - Memory (at all levels)
 - Network

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- Understand the system
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- Use all the available tools
 - Ease of development
 - Ease of management

Creating the Project

- Language
 - Programming (PGAS languages, hybrid programming)
 - Accelerator (CUDA, RapidMind, OpenCL, ...)
- Algorithm
 - Software technology doubles speed every 6 years
- Libraries
 - BLAS, LAPACK, FFTW...

Controlling the project

- Version control
 - CVS, SVN
- Debugging
 - Alinea DDT, TotalView
- Compiling
 - PGI, Pathscale, GCC, Intel, IBM,...
- Profiling
 - Gprof, Vtune, Intel Trace Analyzer,...
- Documentation

Implementing the Project

- GNU/Linux
- Scripting
 - Perl, Python, RUBY,...
- Job submission and queue management
- Fault tolerance and checkpointing
- Visualization
 - Parallel I/O
 - Paraview, OpenDX, AVS,...

Conclusions

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- Must attempt to use available tools
- Must exhibit **capacity** to exploit **capability**

The End