High Performance Computing in High Energy Physics

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FOR PRECISION TESTS OF FUNDAMENTAL SYMMETRIES



Agenda HPC

HPC

Motivation

HPC

Motivation

What is HPC?

HPC

Motivation

What is HPC?

Design

High Energy Physics: LHCb

High Energy Physics: LHCb

Evolution of Experiment

High Energy Physics: LHCb

Evolution of Experiment Implications for Physics

Software Challenges

Software Challenges

Race Conditions

Software Challenges

Race Conditions

Deadlocks

Why HPC?

Motivation: HEP

Pattern Recognition and Parallel Processing for Triggering



Basic Classification



Basic Classification



Design Principles

Goal: Maximize the maximum computing power given a fixed budget and specific application field

Past

Present



Design Principles

Goal: Maximize the maximum computing power given a fixed budget and specific application field



Designs for HPC

Massive Parallel Architectures

Designs for HPC

Massive Parallel Architectures

Local/Dispersed



Grid Computing

- heterogeneous hardware & OS
- connected via Internet or low speed communication system (bus)
- nodes are autonomous and can opt out
- every node manages its own resources

Designs for HPC

Massive Parallel Architectures

- homogenous, local
- perform same task
- connected via high-speed bus or LAN
- Scheduling done by central server
- Whole system behaves as if it were one system

Cluster Computing



What is HPC? CPU & GPU

Core L1 Cache	Con trol	Core L1 Cache	Con trol	
Core	Con trol	Core	Con trol	
L1 Cache		L1 Cache		
L2 Cache		L2 Cache		
L3 Cache				
DRAM				
CPU				

[1]

CPU & GPU

Core	Con trol	Core	Con trol	
L1 Cache		L1 Cache		
Core	Con trol	Core	Con trol	
L1 Cache		L1 Cache		
L2 Cache		L2 Cache		
L3 Cache				
DRAM				
CPU				



What is HPC? CPU & GPU

CPU

- Serial Processing
- ≻ Few Cores

➢ Focuses on Low Latency

GPU

Parallel Processing

≻ Lot of Cores

Focuses on High Throughput What is HPC? CPU & GPU

CPU

- Serial Processing
- ≻Few Cores

➢ Focuses on Low Latency

GPU

Parallel Processing

≻ Lot of Cores

Focuses on High Throughput

Multithreading





[2]

What is HPC? Multithreading



Multithreading

Sequential Programming

Deterministic Process

Easy - Medium

Casual Software Bugs

Highly Reproducible

Multithreading Programming

Multithreading

Sequential Programming

- Deterministic Process
- Easy Medium
- Casual Software Bugs
- > Highly Reproducible

Multithreading Programming

- Non-Deterministic Process
- Difficult very Difficult
- Bugs ~ number of interactions
- > Highly Non-Reproducible

Why does HEP needs HPC?

Evolution of LHCb Experiment



Why does HEP needs HPC?

Implications for Physics



Higher amount of Data enables to push analysis forward reducing uncertainties - just better statistics

Example for Multithreading





Software-Challenges

Race Conditions





Software-Challenges

Race Conditions

Dead Locks

Counter: U		
Thread 1	Thread 2	
Read C (0)		
	Read C (0)	
Increment C (0)	Increment C	
Write C (1)	(0)	
	Write C (1)	

Software-Challenges

Race Conditions

Dead Locks

16/18



Software-Challenges

Race Conditions

Dead Locks

Mutual Exclusion

Signaling and Waiting

No Preemption

Circular Dependency

Conclusion

Future of HPC

- HPC is needed in order to enable research institutes and companies to process huge amount of data or to build complex simulations
- HEP cannot evolve without HPC, HEP will heavily rely in the future on the state of HPC
- > My Predictions for the 2020s: Cloud HPC, AI HPC (MLOps)



- [1] CUDA Toolkit Dokumentation, Nvidia, Developer Zone, https://docs.nvidia.com/cuda/cuda-cprogramming-guide/index.html
- [2] R. Arpaci-Dusseau, A. Arpaci-Dusseau, Operating Systems: Three Easy Pieces, https://pages.cs.wisc.edu/~remzi/OSTEP/

Supercomputers



Supercomputers

Deep Blue

Riken MDGRAPE-3

> Folding @home

Riken Fugaku

IBM Supercomputer

1997: After upgrade, it won against Garry Kasparov in 6-game match: 3 - 1 - 2

~ 11.38 GFLOPs

Supercomputers



Institute of Physical and Chemical Research (RIKEN) 2006: announced to be completed, molecular dynamics (esp. protein structure predictions) ~ 1 petaFLOPs

7/x

Supercomputers



Washington University, led by Greg Bowman 2000 (initial release): protein dynamics 2021: COVID-19 Research Acceleration

~ 1.22 exaFLOPs

Supercomputers

Deep Blue

Riken MDGRAPE-3

> Folding @home

Riken Fugaku

Riken & Fujitsu

2014: development started 2020: debut, in June became the fastest supercomputer in the world (TOP500)

> ~ 442 petaFLOPs (HPL) ~ 1.42 exaFLOPs (HPL-AI)

Challenges of HPC: Multithreading

Advantages

Disadvantages

Thread A waits, Thread B goes

Software needs to be optimized for multithreading

Higher Performance if correctly used

Lower Performance if incorrectly used

Resource Sharing

Thread Scheduler!

Cost-Effective on Hardware Side

Cost-intensive on Software Side

Challenges of HPC: Multithreading

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