An Introduction to CUDA

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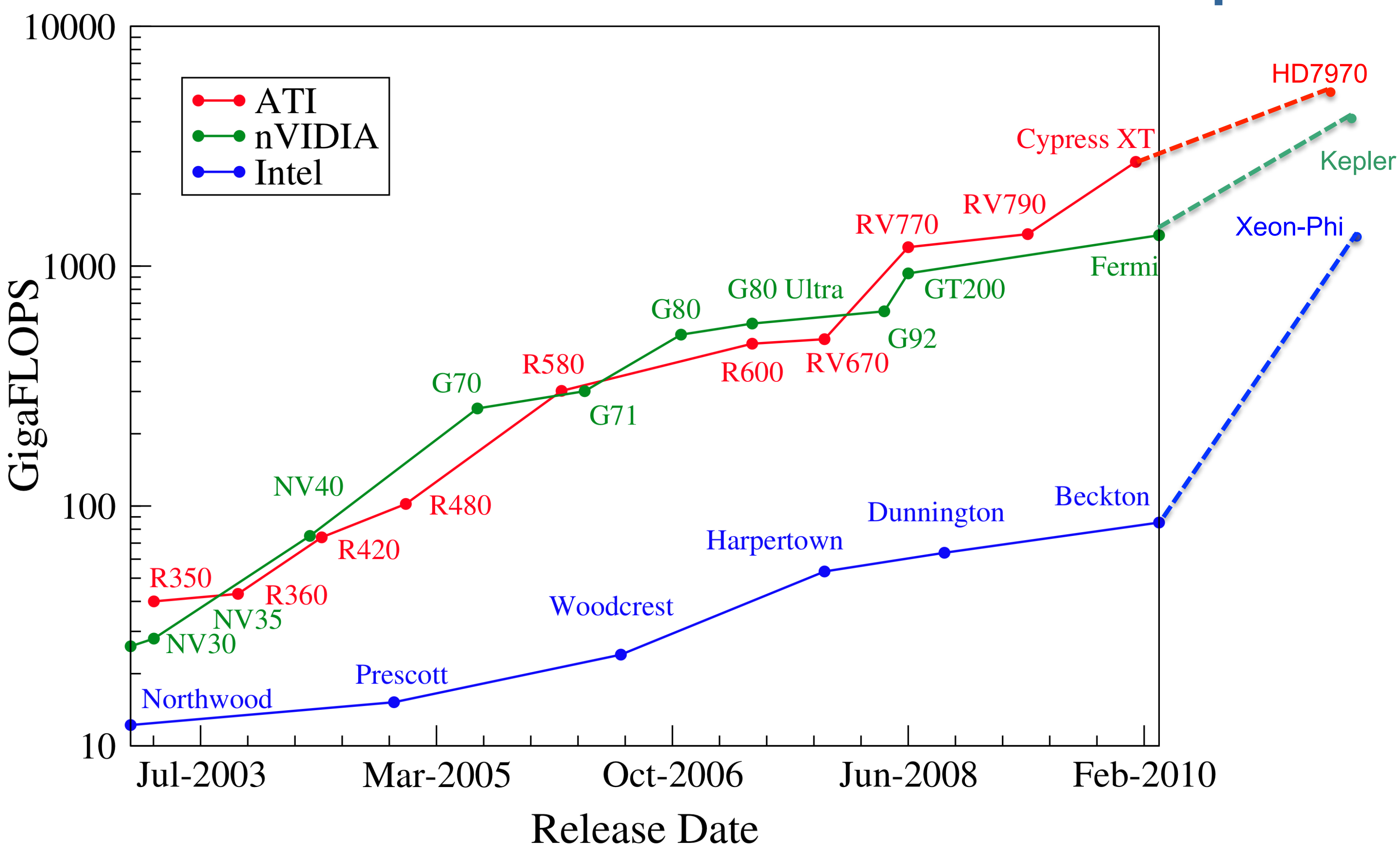
Motivation: Why GPU?

- Kepler Series GPUs vs. Quad-core Sandy Bridge CPUs
  - Kepler delivers equivalent performance at:
    - 1/18th the power consumption
    - 1/9th the cost

- So
  - Awesome performance per Watt
  - Awesome performance per $
- Price/Performance/Power:
  - NVIDIA GeForce GTX 680 3,090 GFLOPS at 195 W for $460
  - 3,090 GFLOPS / 195 W ≈ 15.8 GFLOPS/W
  - 3,090 GFLOPS / $460 ≈ 6.7 GFLOPS/$
- "The Soul of a Supercomputer in the Body of a GPU"

Which costs more: buying a Playstation or running it continuously for a year?

Performance Graph



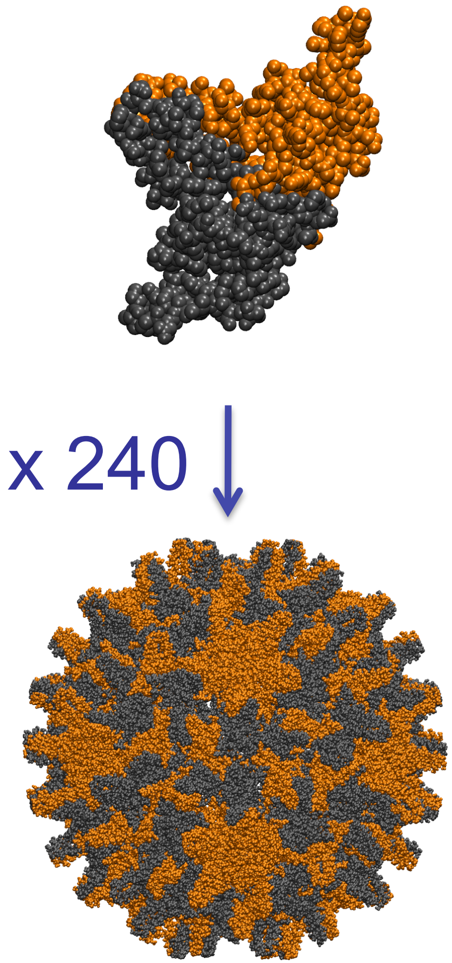
Is a speedup of 1400x for a GPU implementation plausible?

The Effect of Memory Bandwidth

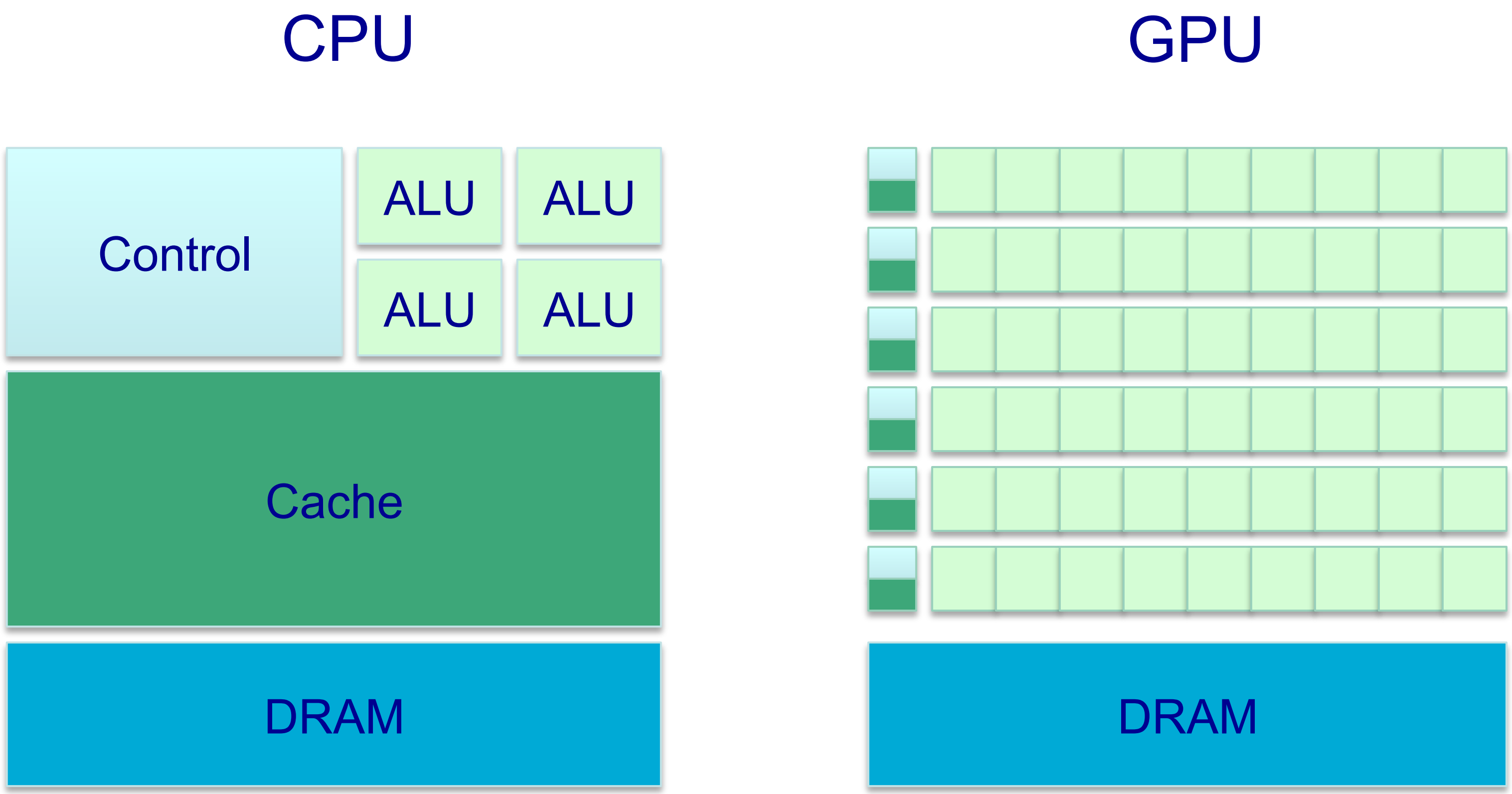
- Theoretical Peak FLOPS
  - An unrealistic measure obtained by multiplying the ALU throughput by number of cores
  - A good measure would also account for I/O performance, cache coherence, memory hierarchy, integer ops
- GPUs win again on memory transfer
  - On average 7X higher internal memory bandwidth
  - 177.4 GB/s (GTX4xx,5xx) vs 25.6 GB/s (Intel Core i7)
  - However CPU - GPU transfer much slower (~8 GB/s)

Case Study: Molecular Docking

- 1400-fold speed-ups are possible for the right problem and with sufficient development effort
- Coarse-grained replica exchange Monte Carlo protein docking
  - A statistical sampling approach to aligning molecules
- Viral capsid construction:
  - 680,000 residues, 100 million iterations
  - 3000 years on a single CPU
  - < 1 year on a cluster of GPUs



A Difference in Design Philosophies



Design Implications

- CPU:
  - Optimized for sequential code performance
  - Lower memory bandwidths (< 50 GB/s)
  - Large cache and control
- GPU:
  - Optimized for parallel numeric computing
  - Higher memory bandwidths (> 150 GB/s)
  - Small cache and control
- Ideal is a combination of CPU and GPU, as provided by CUDA

Motivation: Why CUDA?

- What is it?
  - Compute Unified Data Architecture (CUDA)
  - Offers control over both CPU and GPU from within a single program
  - Written in C with a small set of NVIDIA extensions
- Better than the GLSL/HLSL/Cg alternative:
  - Forcing a square peg into a round hole (forcing a Computer Graphics program to be general purpose)
- More features:
  - Shared memory, scattered reads, fully supported integer and bitwise ops, double precision if needed

Motivation: Why *not* GPU?

- GPU's are not a cure-all
- Not suited to all algorithms
  - Work needs to be divisible into small largely-independent fragments
  - Does not cope well with recursive highly-branching tightly-dependent algorithms
- Difficult to program
  - Relatively easy to get moderate speedups (2-5X)
  - Better performance requires understanding of the architecture and careful tuning

Feeding the Beast

- Need thousands of threads to:
  - Saturate processors
  - Hide data transfer latency
  - Handle other forms of synchronisation
- Supported by low thread scheduling overhead
- But not all problems are amenable to such a decomposition

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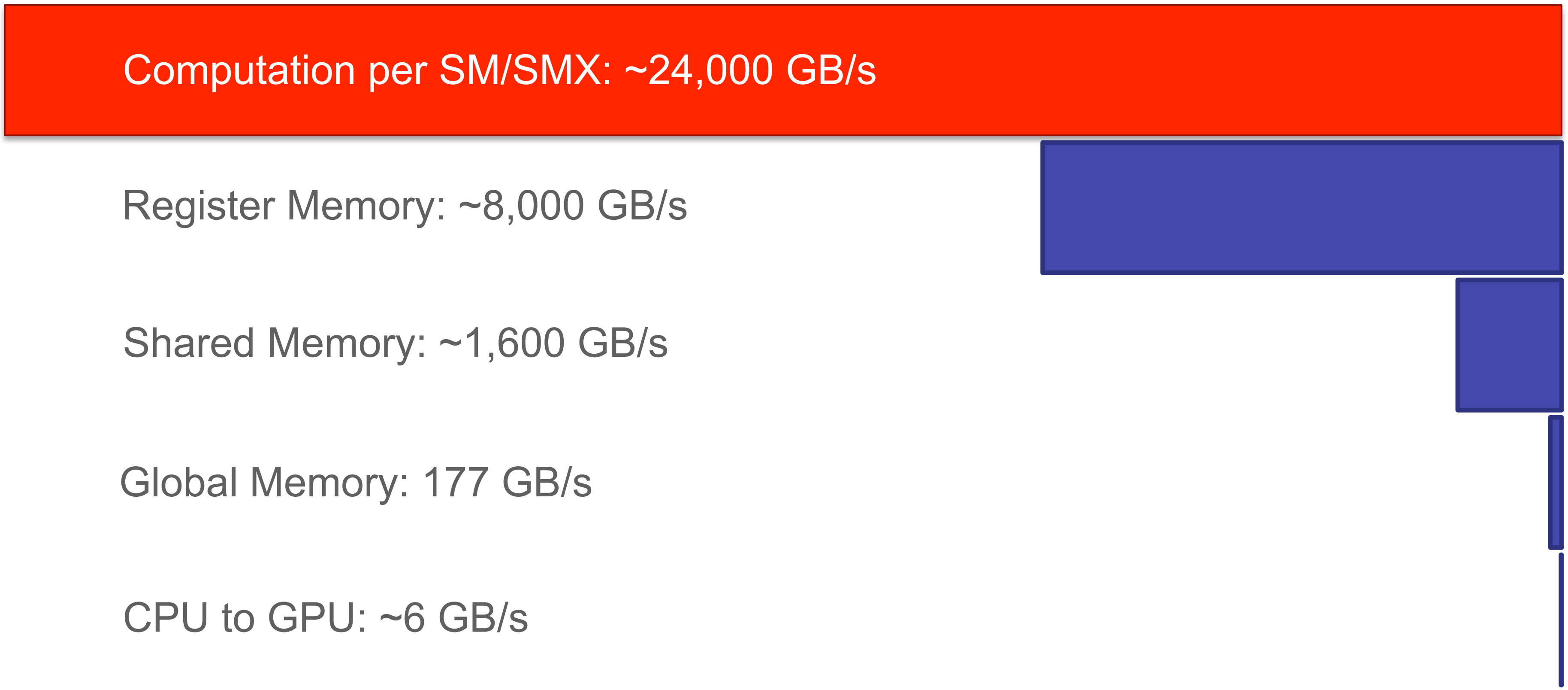
Memory Bandwidth



Effective memory use is absolutely crucial to GPU acceleration

Motivation: Why *not* CUDA?

- Proprietary product
  - Only supported on NVIDIA GPUs
- Stripped down version of C:
  - No recursion (< cc2.0), no function pointers
- Branching may damage performance
- Double precision deviates in small ways from IEEE 754 standard

CUDA Compared

Platform	✗	✔
Shader Languages (GLSL, Compute)	• Contorted code (for a non-graphics fit) • More passes required • Restricted access to features • Harder to learn	• Supported on more GPUs
OpenCL	• Still underdeveloped • Somewhat verbose	• Cross-platform standard • Similar in design to CUDA
ATI Stream	• Late to the party • Also proprietary • DEAD?	

Implications of Computer Graphics Legacy

- Games Industry:
  - Constant drive for performance improvement
  - Commoditisation – high demand leads to high volumes, lower prices
- Massively multi-threaded:
  - Millions of incoming polygons and outgoing pixels, each largely independent
  - Best supported by millions of lightweight threads

Computation Implications

- Coherence:
  - Nearby pixels / vertices have similar access patterns and computation
  - Consequently, GPU's expect memory access and branch coherence
- Single-precision floating point:
  - Geometric operations in CG require floating point but don't need the accuracy of double precision
  - Consequently, integers and doubles weren't well supported until recently

Memory Implications

- Memory Bandwidth:
  - Must transfer millions of elements from vertex buffers and to the framebuffer or the frame rate stalls
  - Consequently, memory transfers have high bandwidth
- Textures:
  - Images that are wrapped onto geometry to cheaply provide additional realism
  - Consequently, GPU's support large on-chip memories with high bandwidth coherent access

CUDA Programming Model

- Data parallel, compute intensive functions should be off-loaded to the device
- Functions that are executed many times, but independently on different data, are prime candidates
  - i.e. body of for-loops
- CUDA API:
  - Minimal C extensions
  - A host (CPU) component to control and access GPU(s)
  - A device component
  - CUDA source files must be compiled with the nvcc compiler

Summary

- With current barriers to higher clock speeds, Parallel Computing is recognised as the only viable way to significantly accelerate applications
- Many-core GPU architectures are a strong alternative to multi-core (dual-core, quad-core, etc) CPU architectures
- Programming in CUDA can provide considerable speedup for numerically intensive applications
  - But more significant speedups often require extensive tuning and algorithm restructuring

Take-home Messages

[1] Not all problems are suited to a GPU solution

[2] Refactoring and careful tuning required for best performance

Slide References

- J. Seland. Cuda Programming, Jan 2008. http://heim.ifi.uio.no/˜knutm/geilo2008/seland.pdf
- David Kirk and Wen-mei Hwu, 2007-2009. ECE 498AL Spring 2010, University of Illinois, Urbana-Champaign.
- David Kirk and Wen-mei Hwu, Programming Massively Parallel Processors: a Hands-on Approach, Morgan Kaufmann, 2010.