Experiences with Emerging HPC Architectures

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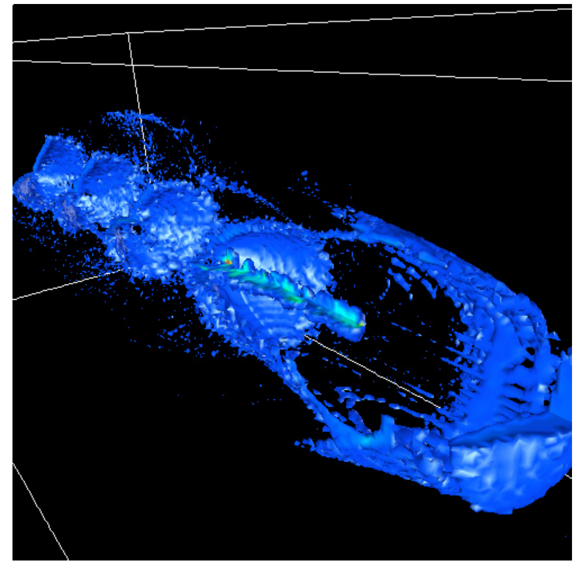
This work was supported by
NASA SBIR Phase II Award No. NNG06CA13C
DOE Office of Science, SciDAC Program, COMPASS Project, Grant #DE-FC02-07ER41499
DOD Navy SBIR Phase I, Award #N68335-09-C-0247
NVIDIA Corp. and Tech-X Corp.

TECH-X CORPORATION

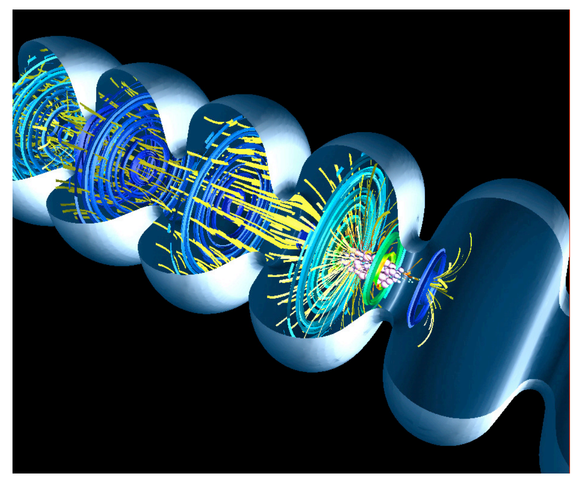
Motivation/Outline

- Need fast turnaround time for EM/Plasma Simulations
  - Particle in Cell (PIC)
  - Finite-Difference Time-Domain (FDTD)



- Coarse grain parallelization has its limits
  - Local problems getting too small
  - “time does not parallelize”
  - Access to large systems can be painful

- Many algorithms memory bandwidth limited
  - Almost no data reuse -> caches useless
  - Multi-core CPU makes it even worse

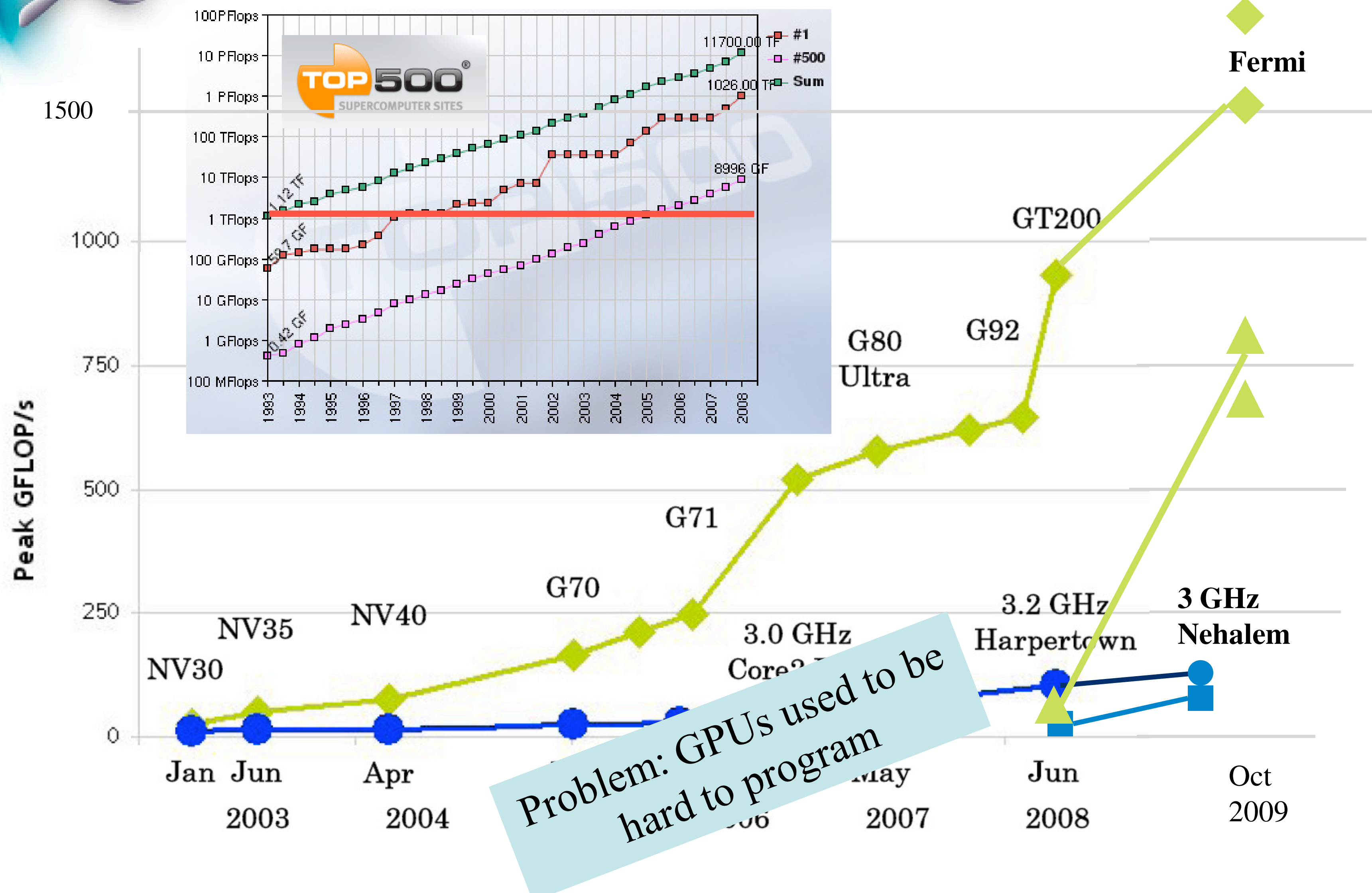


⇒ Need high memory bandwidth accelerator

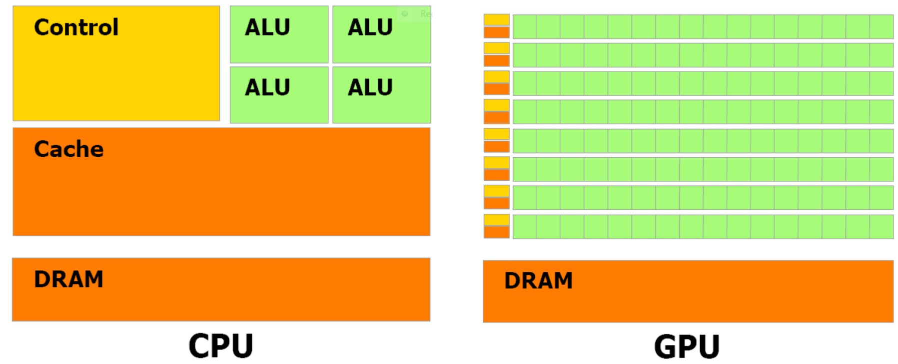
Outline

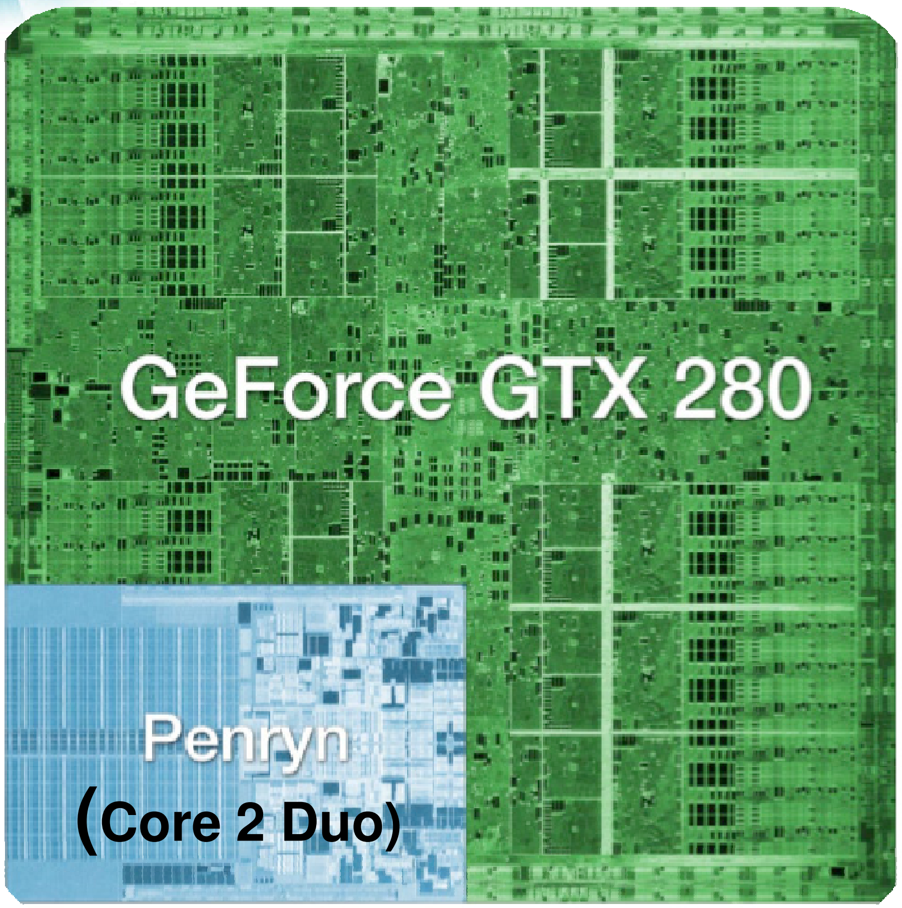
- GPU architecture, programming
- GPULib: A rapid GPU code development environment
- Implementation of EM algorithms on GPU
- Conclusion

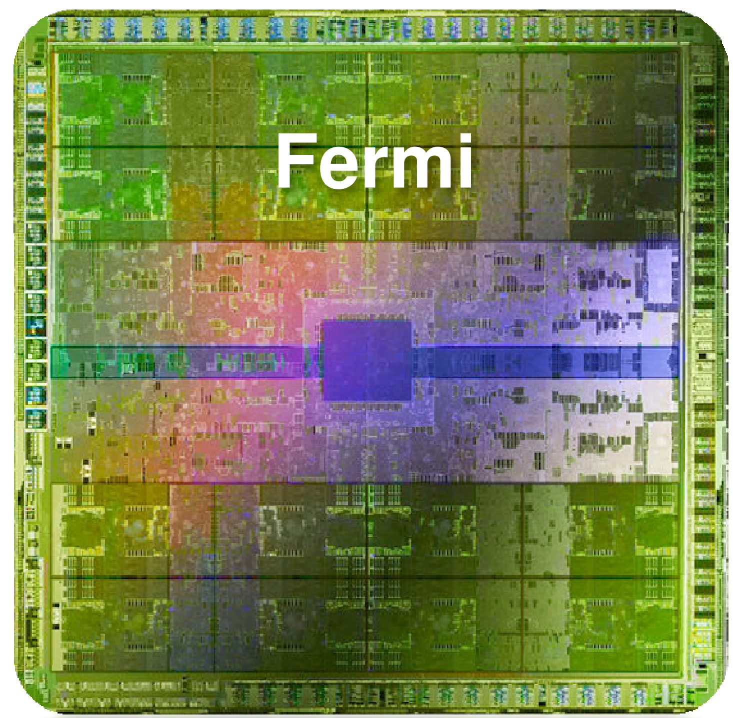
Why scientific computing on GPUs?



Sources: Nvidia, Techreport.com, cse.scitech.ac.uk


Control
ALU
ALU
ALU
ALU
Cache
DRAM
CPU
DRAM
GPU

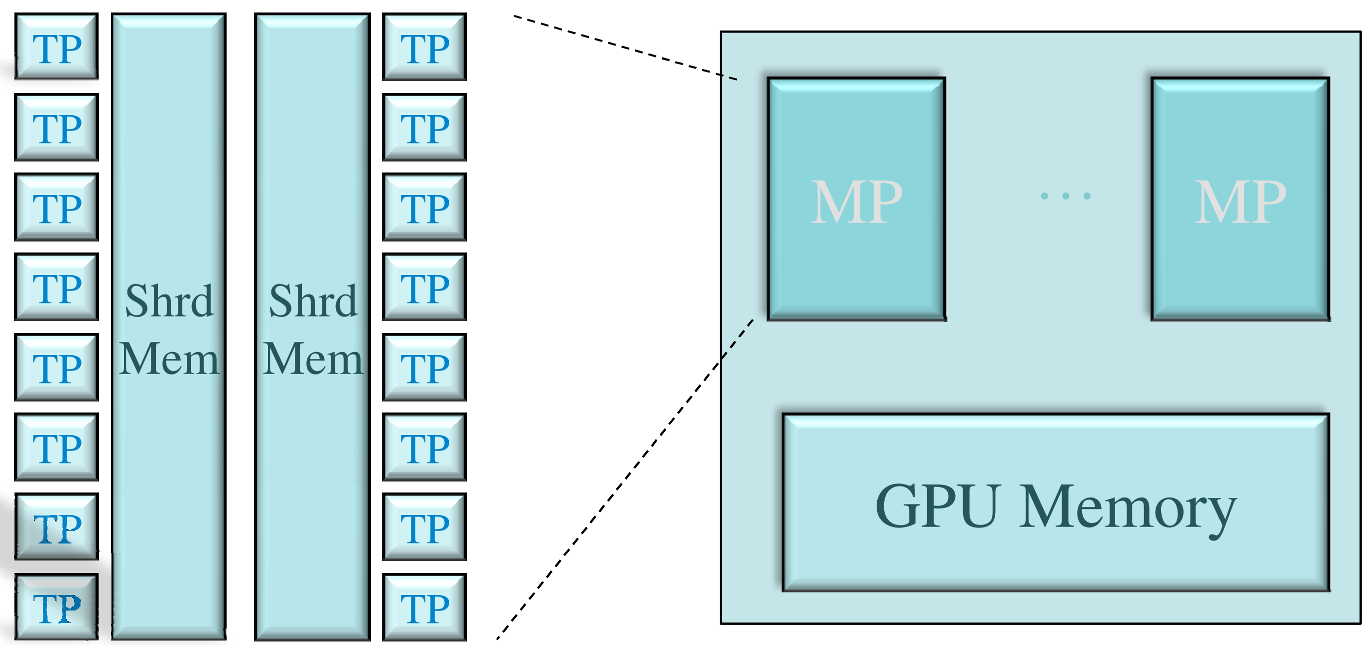

GeForce GTX 280
Penryn
(Core 2 Duo)


Fermi

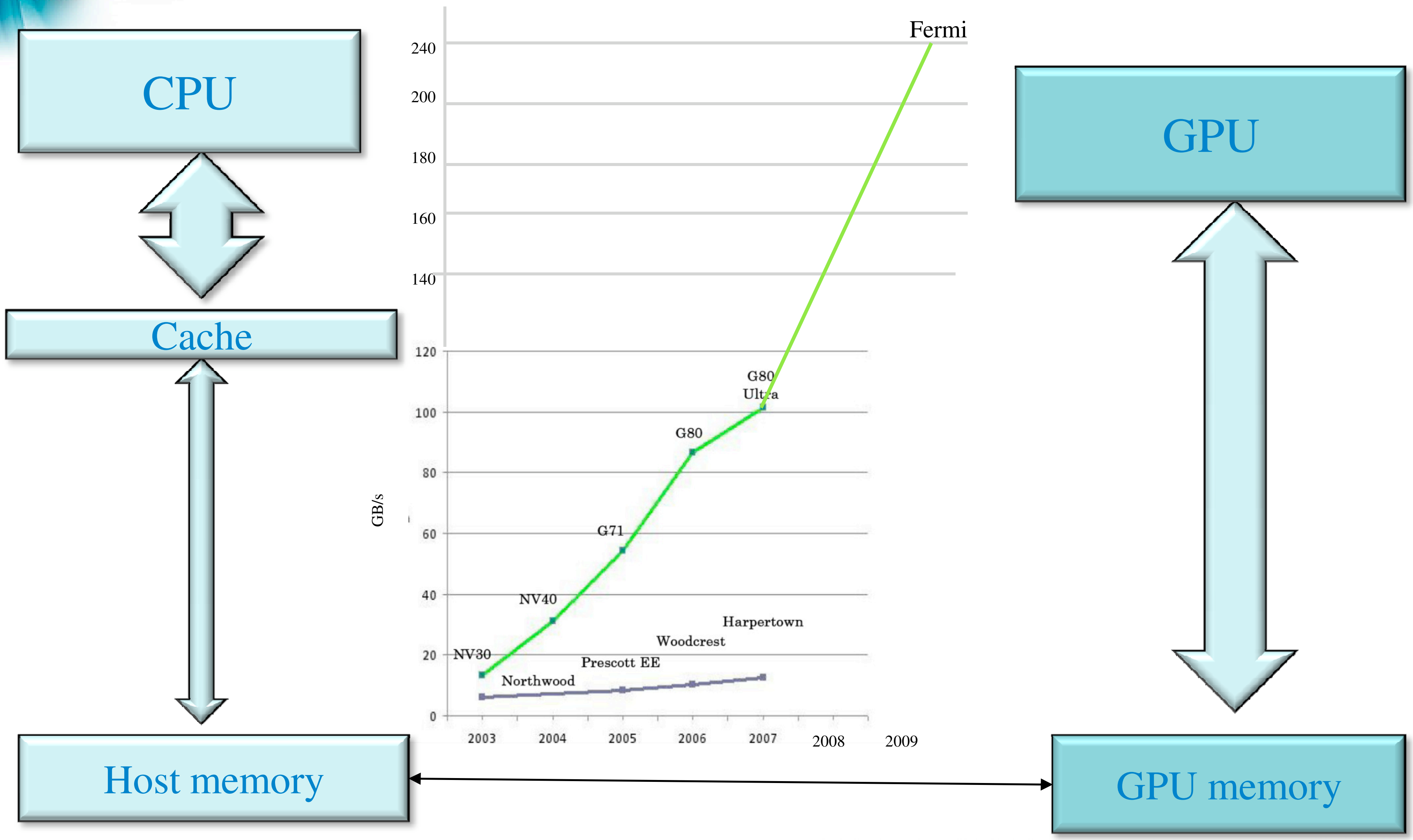
NVIDIA GPUs
A Collection of Specialized SIMD ...essors

- Silicon used for ALUs, rather than large caches
  - Up to 240 processing elements ("thread pro...
  - running at 1.3 GHz, statically sched...
  - Small software managed c...
- Organized as 'Multi...
  - Software ma... ...ti-processor
  - Synchronizat... ...ut global synchronization
- Active thread ma...
  - Work on next th... ...et while waiting for a memory request

Fermi: 512 "thread processors ("GPU cores")
64kB/MP Shared Memory or L1 cache
768k L2 cache

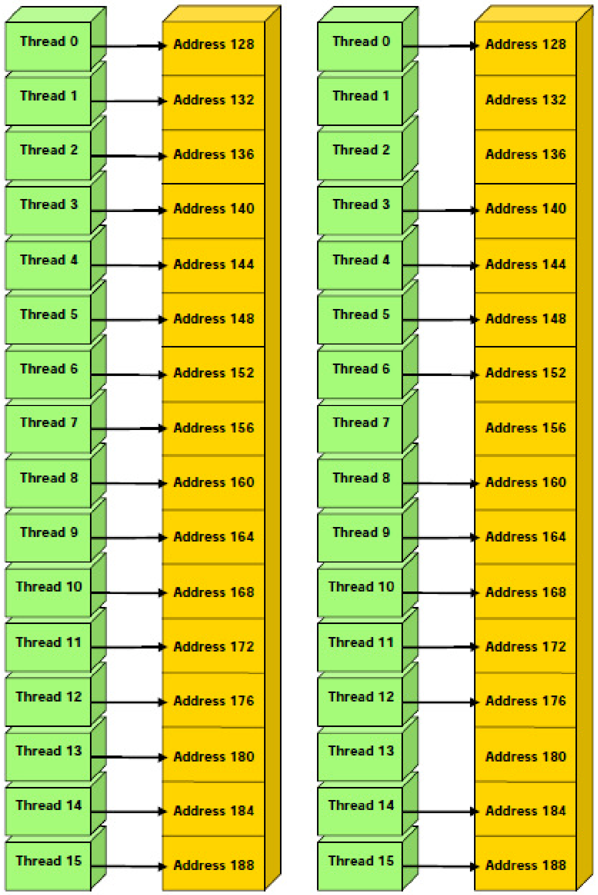


The large memory bandwidth on GPUs can benefit many scientific computing applications



The Flipside: GPUs need regular memory access

(but newer generation GPUs are getting less picky)

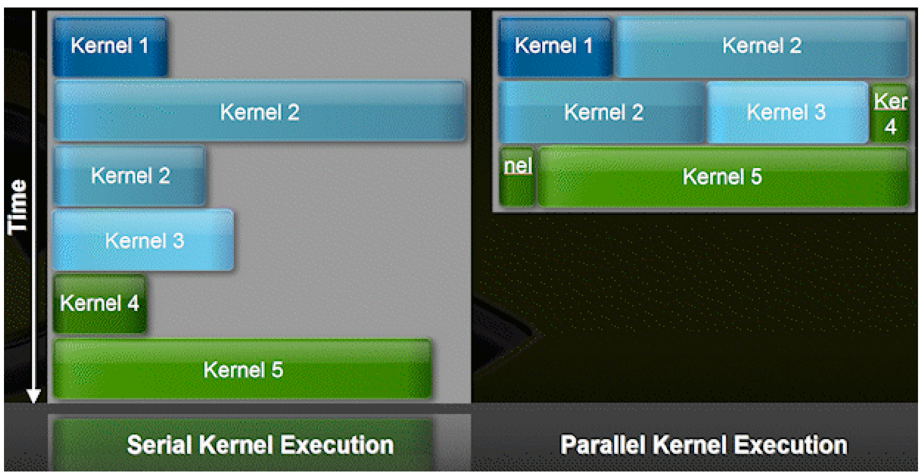


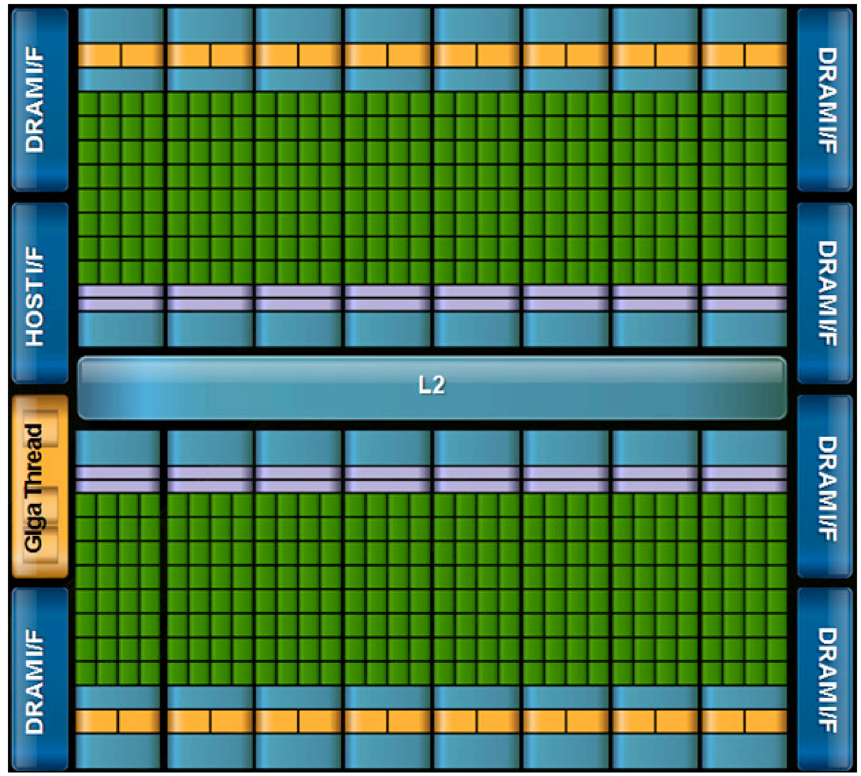
Ideal access pattern

No problem on C1060 and newer

The future: Fermi introduces new level of flexibility

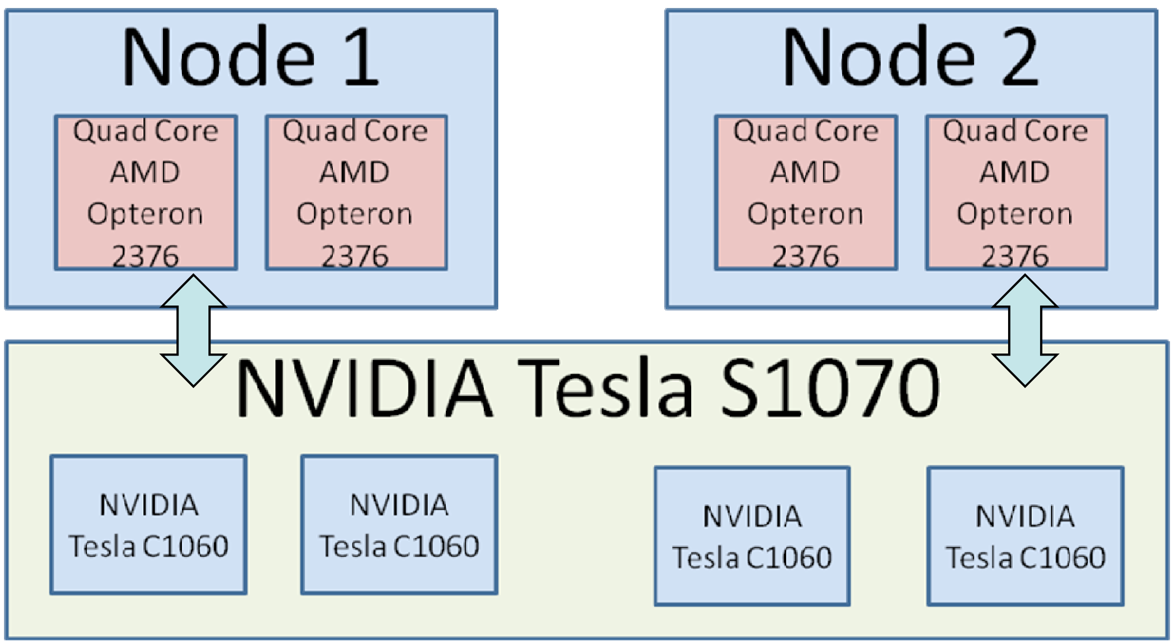
- Multiple kernels executed concurrently
  - Better performance on kernels with low degree of parallelism
- Hardware managed L1, L2 caches
  - Relaxes coalescing requirements
- C++ support on device
- Enhanced atomic performance
- ECC for reliable scaling





Oxygen: Tech-X' Production cluster with GPU accelerated nodes

- 32 nodes, each with dual quad core Opteron
- 8GB RAM per node
- Infiniband interconnect
- Lustre file system
- 4 nodes accelerated with 2 Tesla GPU blades

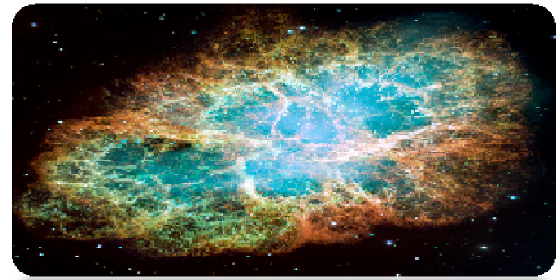


CUDA: Development Environment for NVIDIA GPUs

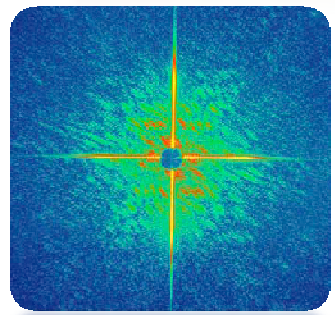
- Early GPGPU efforts heroic
  - Graphics API (OpenGL, DirectX) no natural fit for scientific computing
- Compute Unified Device Architecture (http://www.nvidia.com/cuda)
  - Supported on all modern NVIDIA GPUs (notebook GPUs, high-end GPUs, mobile devices)
  - Co-Existence with OpenCL (OpenCL basically *IS* CUDA)
- Single Source for CPU and GPU
  - Host code C or C++
  - GPU code C(++) with extensions
    - "Kernel" describes one thread
    - Host invokes a collection of threads
  - nvcc: NVIDIA cuda compiler
- Runtime libraries
  - Data transfer, kernel launch, ..
  - BLAS, FFT libraries
- Simplified GPU development, but still "close to the metal"!
- NEXUS: Visual Studio plug-in for GPU development

GPULib:

High-Productivity GPU Computing



- IDL (ITT Vis), MATLAB (Mathworks)
  C, Fortran
- Rich set of data parallel kernels
- Extensible with proprietary kernels
- Seamless integration into host language
- Explicit or implicit management of address spaces
- Interface to Tech-X' FastDL for multi-GPU/DMPP computing



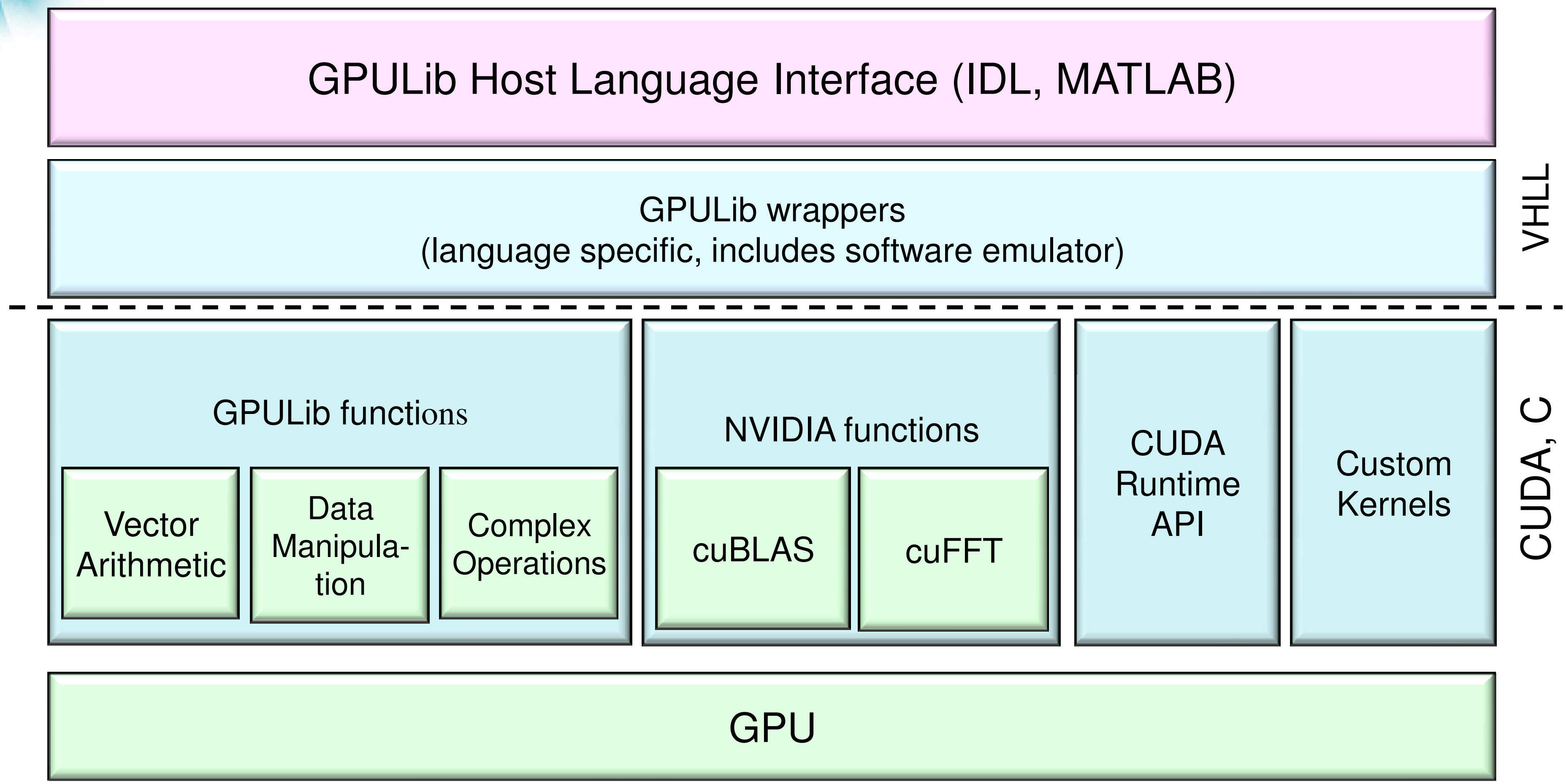
FastDL

http://gpulib.txcorp.com

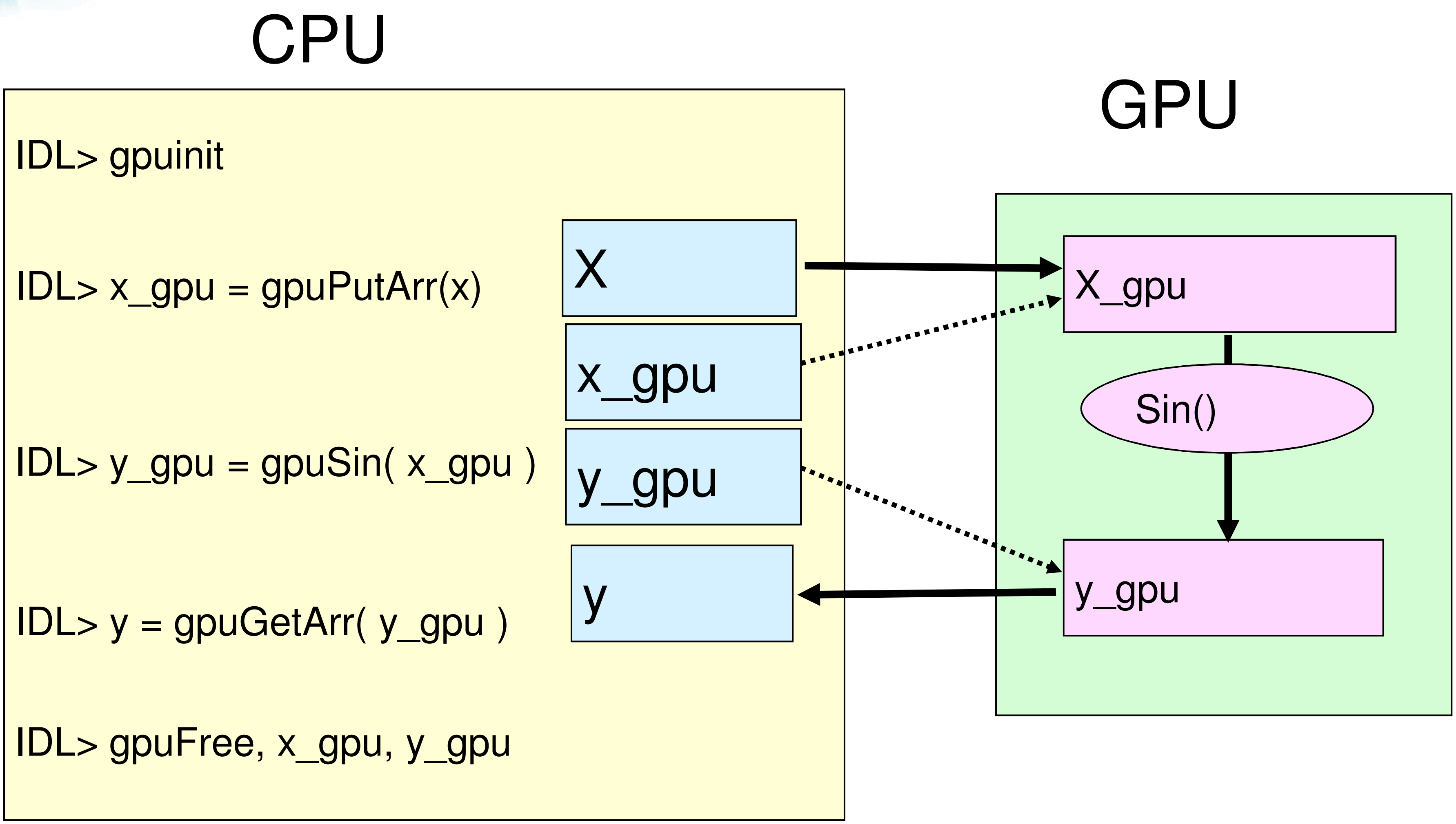
(free for non-commercial use)

Messmer, Mullowney, Granger, *"GPULib: GPU computing in High-Level Languages",* Computers in Science and Engineering, 10(5), 80, 2008.

GPULib's Extensible Architecture

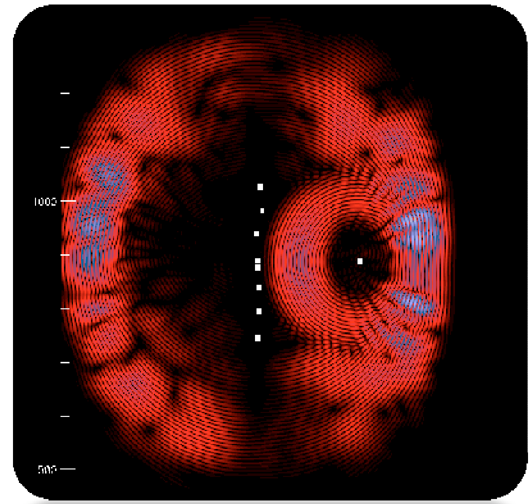


An example of using GPULib in IDL

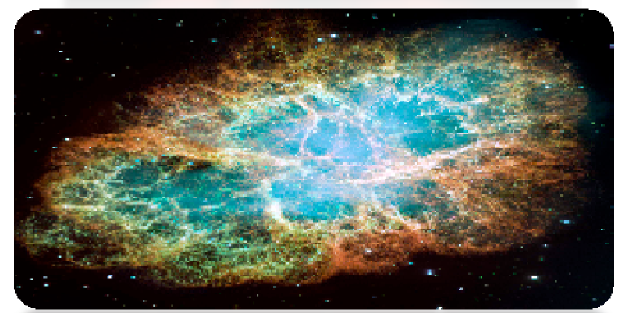


GPULib is currently used in a broad range of applications

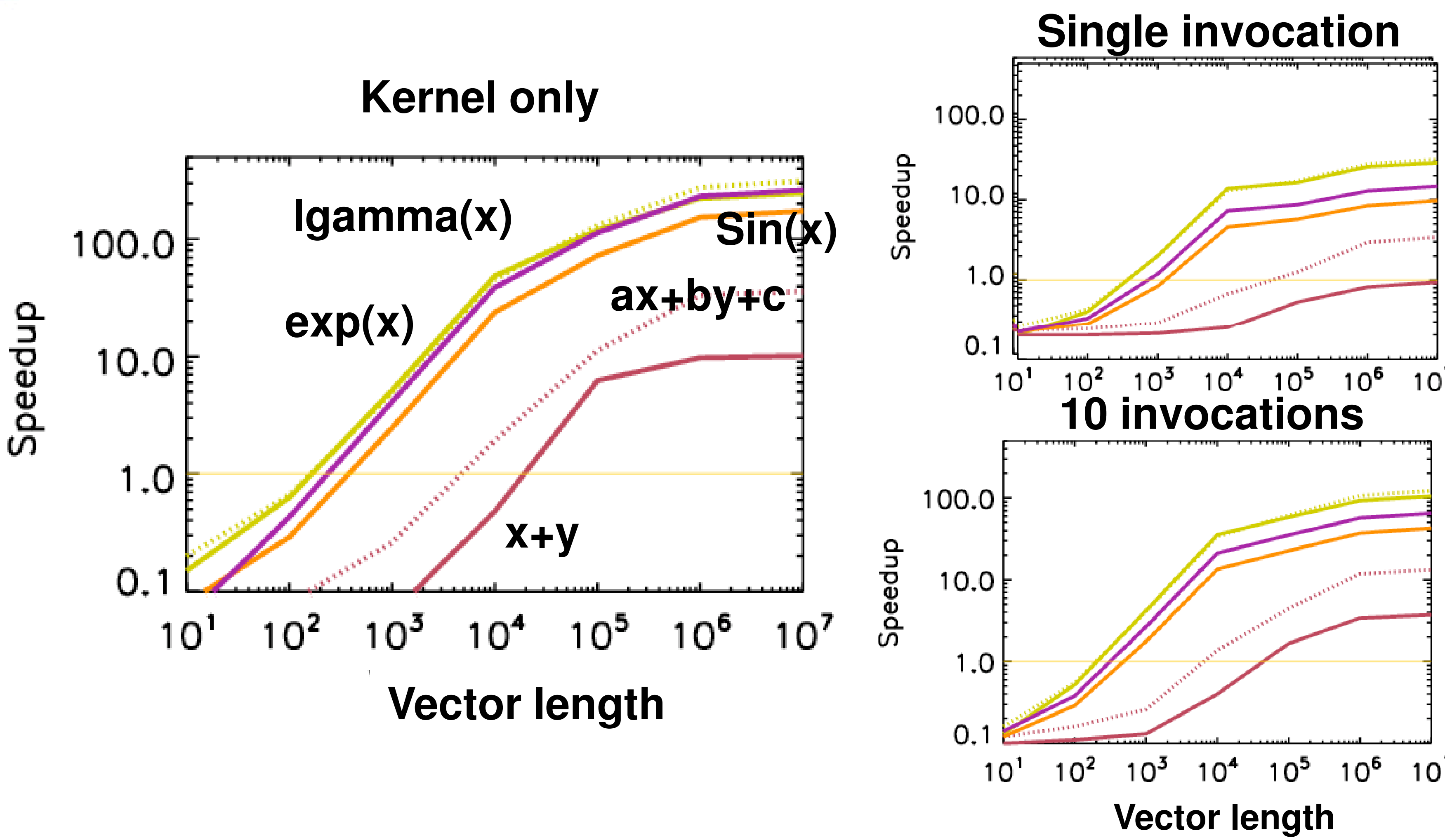
- Simulation / Modeling
  - Neutron scattering experiments
  - Computational Fluid Dynamics (CFD)
  - Linear optimization
  - Tsunami modeling
  - Option pricing
  - Convection zone in stars
  - Galaxy formation
  - Neural tissue simulations



- Data analysis
  - Image enhancement, deblurring
  - Real-time image processing
  - Synthetic Aperture Radar (SAR)
  - Hyperspectral imaging
  - Astronomical imaging
  - Medical imaging
  - Seismic data processing



Key to performance: Multiple kernel invocations per CPU-GPU transfer



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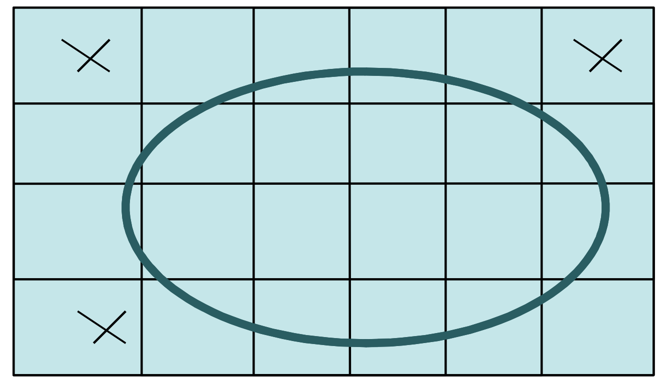
GPU accelerated FDTD Implementation with GPULib

- FDTD usually implemented as stencil operation
  - Traverse e.g. E mesh
  - Grab B values necessary for updating E
  - Special treatment for domain boundaries
  - Interior boundaries: do not update 'outside'

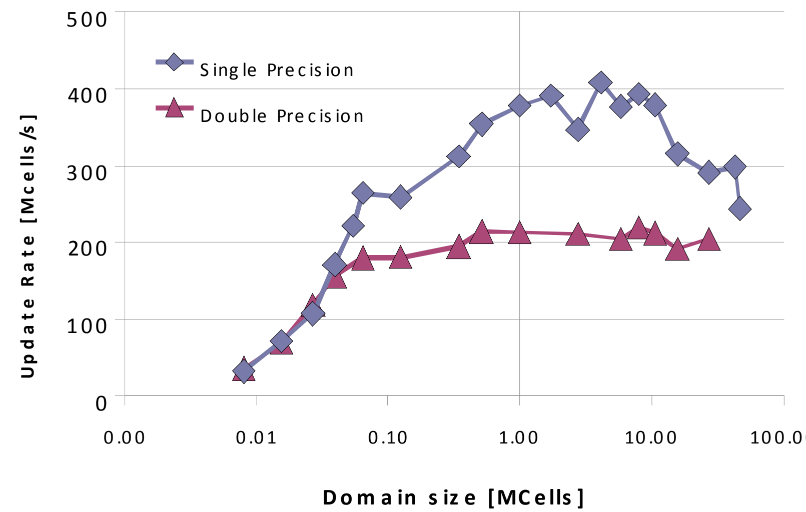


- Problem 1: Short vector operations
- Problem 2: Poorly aligned boundaries
- Problem 3: Skipping cells

- Solution: Treat 3D domain as large 1D vectors
  - Shifted vector operations 'cheap'
    - Pointer arithmetic possible on GPUs
  - 'Dirt' at domain boundaries due to wrap-around
    - Removed by applying boundary conditions
  - Accept 'unnecessary' work

3D FDTD in GPULib

- 3D FDTD
  - Cut-Cell or stair-stepped boundaries
  - Uses VORPAL geometry output
- Performance
  - Up to 400 Mcells/s on
    - ~70% theoretical memory bandwidth
  - ~10 Mcells/s on CPU



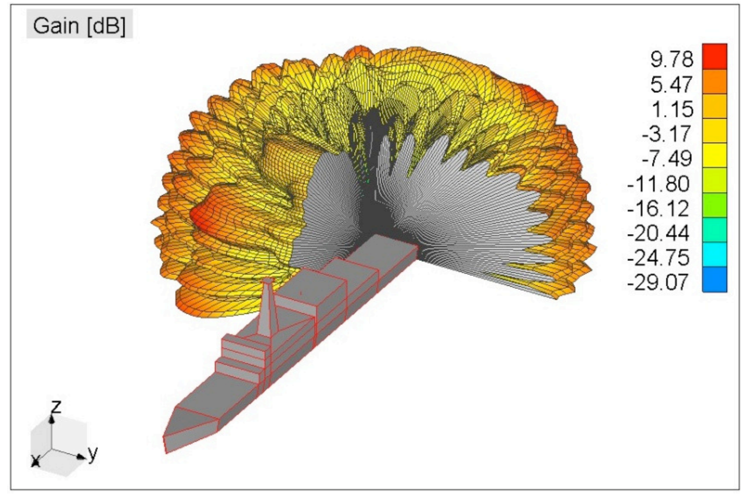
⇒ ~ 40-50x speedup compared to CPU based implementation
  - Comparable to ~48 Franklin cores

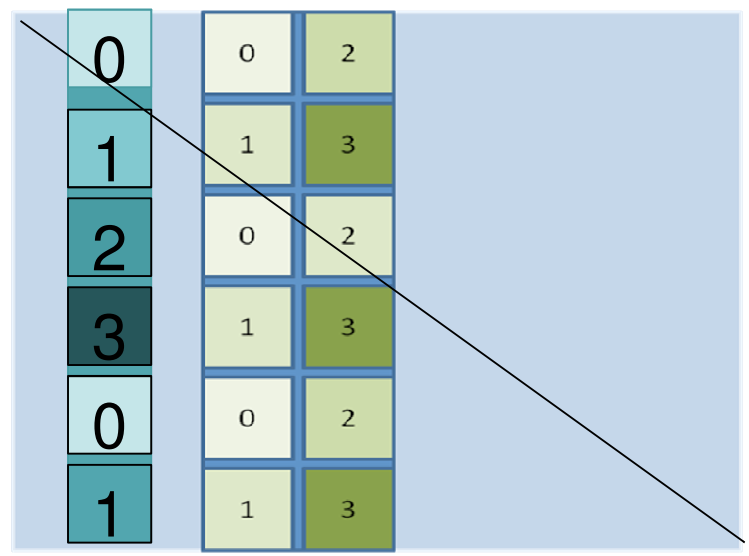
- Double precision hit only due to memory bandwidth
  - Think about your units!
- Multi-GPU via message passing among GPU accelerated nodes
  - Eg. 2.6x speedup on a 3 GPU ‘cluster’ (PSC)
- Now part of VORPAL (ongoing)

Benefit of GPUs not limited to FDTD: Boundary Element Methods

- Large systems of linear equations
  - O(100k)-O(1M) unknowns or larger
- Large matrices
  - 100k unknowns: 80 GB
  - 1M unknowns: 8 TB
- Direct or iterative method
  - LU for dense systems, reuse for different RHS
  - Iterative possibly faster for single solution
- Too large to fit into memory of small cluster
- Solution time scales with $O(N^3)$
  - Interesting problems take days to weeks

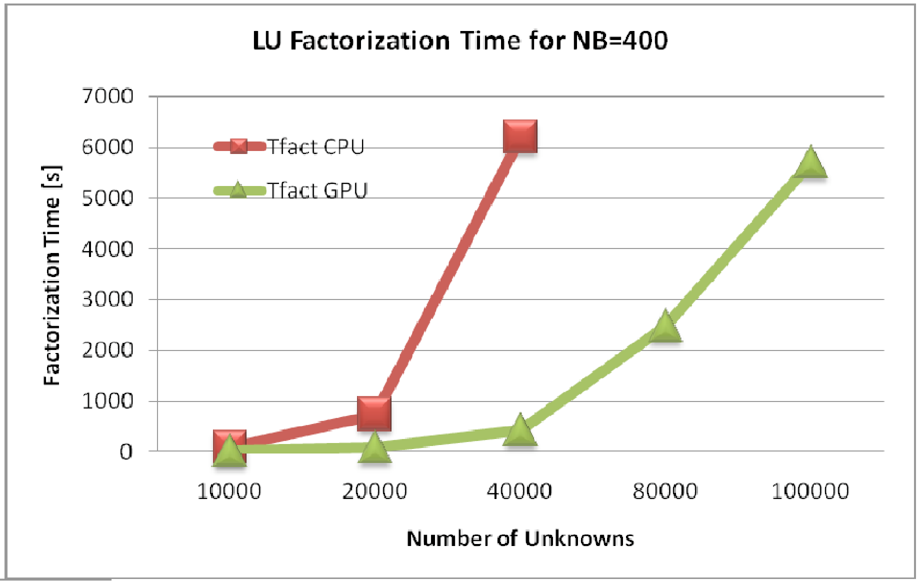
⇒ need fast parallel out-of-core solvers
⇒ Use GPUs as low-cost accelerators



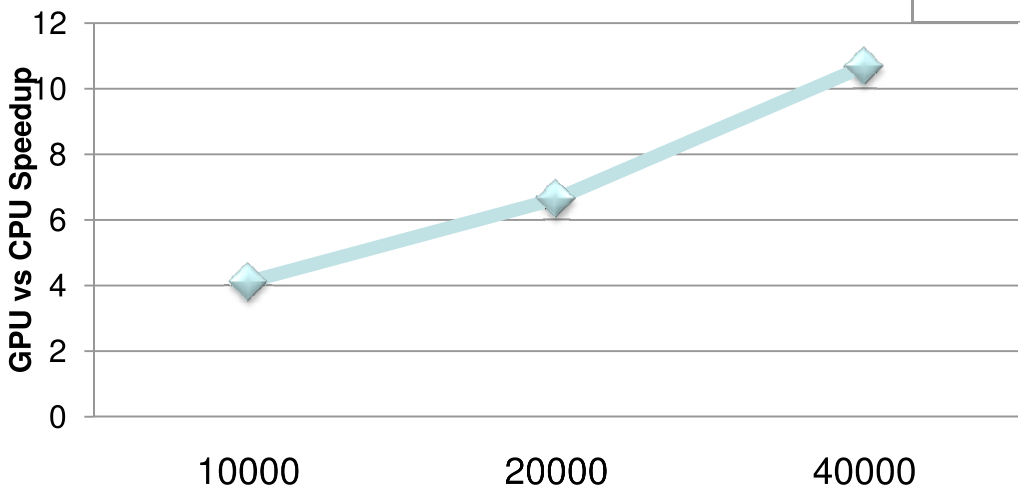


GPUs can significantly accelerate out-of-core LU decompositions

- Based on Azevedo/Dongarra OOC solver



GPU vs CPU Speedup for 8 way parallel OOC LU decomposition



Single precision, real

Summary/Conclusions

- GPUs offer large potential for accelerating scientific applications
- GPULib enables GPU development from within VHLLs
- FDTD solver benefits well from GPU
- Parallel GPU accelerated OOC solver for MOM codes
- GPUs yields ~10x-40x speedup compared to CPU
- Fermi a big leap forward, both in performance and usability