# Accelerating Scientific Applications with GPUs


Presented by

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# The GPU: Ideal candidate for scientific computing

- A massively parallel coprocessor
- Superior memory bandwidth
- Immense raw computing power
- SPMD processing with tens of thousands of threads

# CUDA

- NVIDIA's programming model makes GPUs more accessible than ever
- Decompose parallel sections of applications into kernels
- Execute those kernels on the GPU

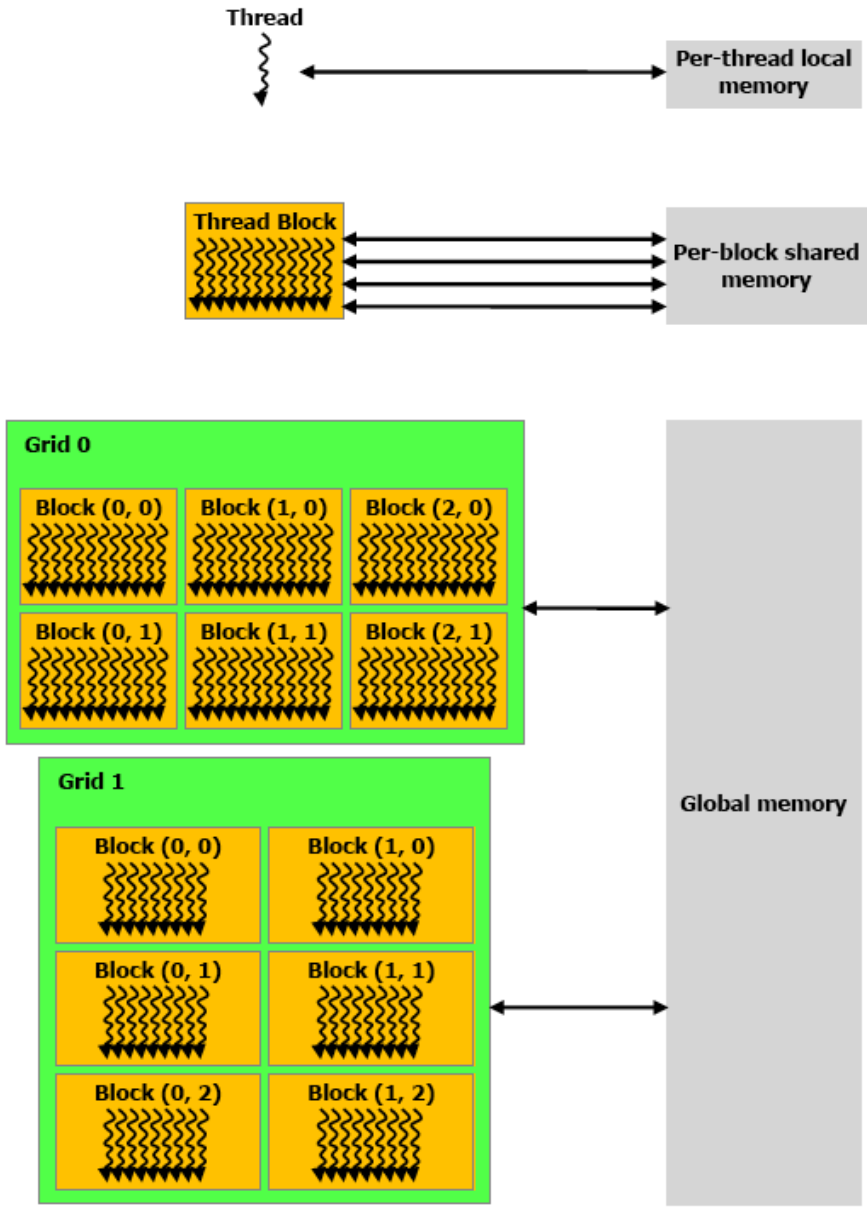



Image from NVIDIA CUDA Programming Guide

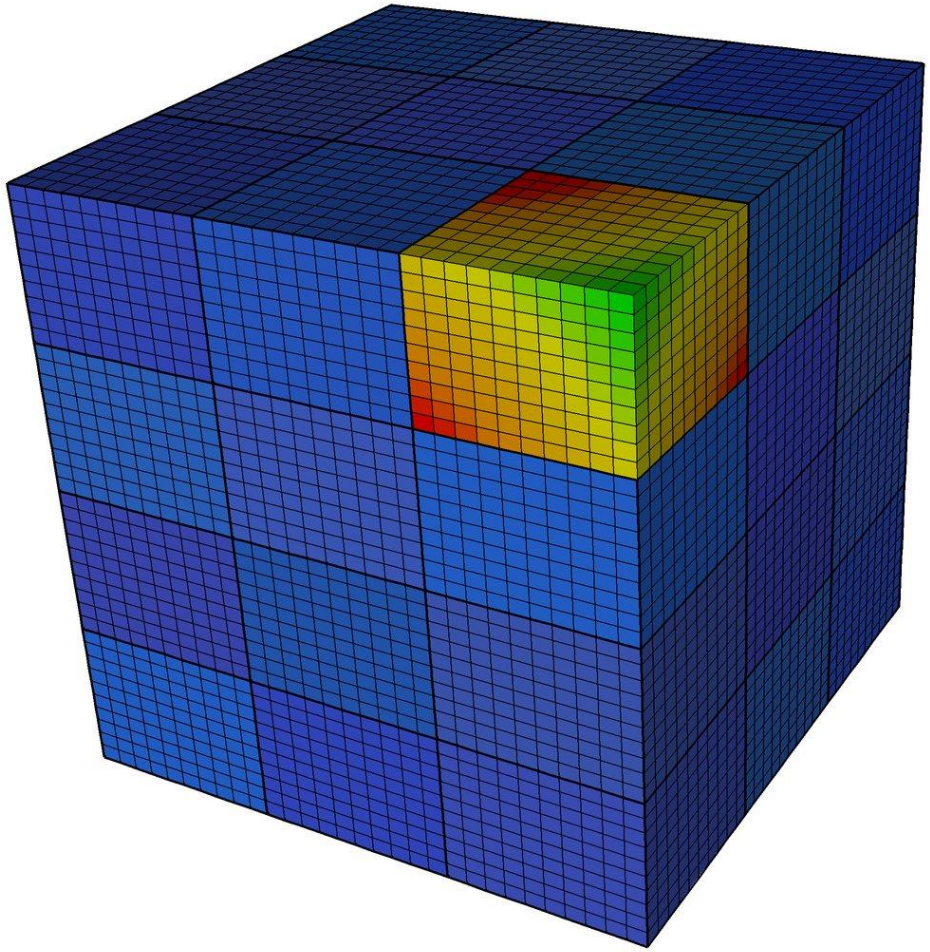
# The S3D simulation code

- S3D is a direct parallel solver for the Navier-Stokes equation, complete with detailed chemistry
- It is used to simulate combustion
- A faster version of S3D would allow scientists to simulate larger chemical domains at higher resolution, for longer periods of time

Image from: "Direct numerical simulation of a lifted ethylene-air flame."
C. S. Yoo, J. H. Chen, et al.

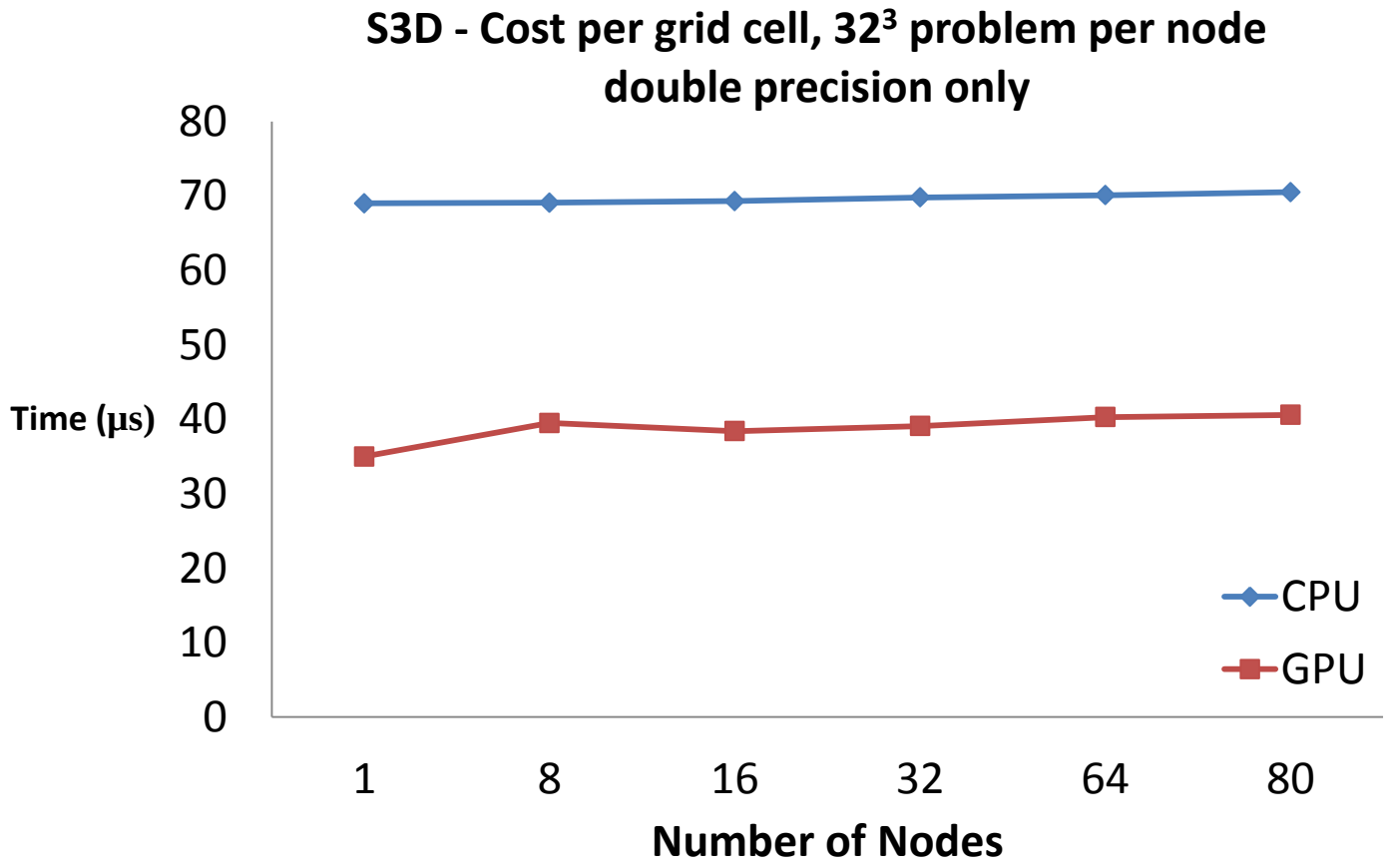
# Mapping S3D to CUDA

- S3D operates on a regular 3-D mesh, which we decomposed spatially into blocks
- Each block is further divided into threads, which solve for an individual point in space



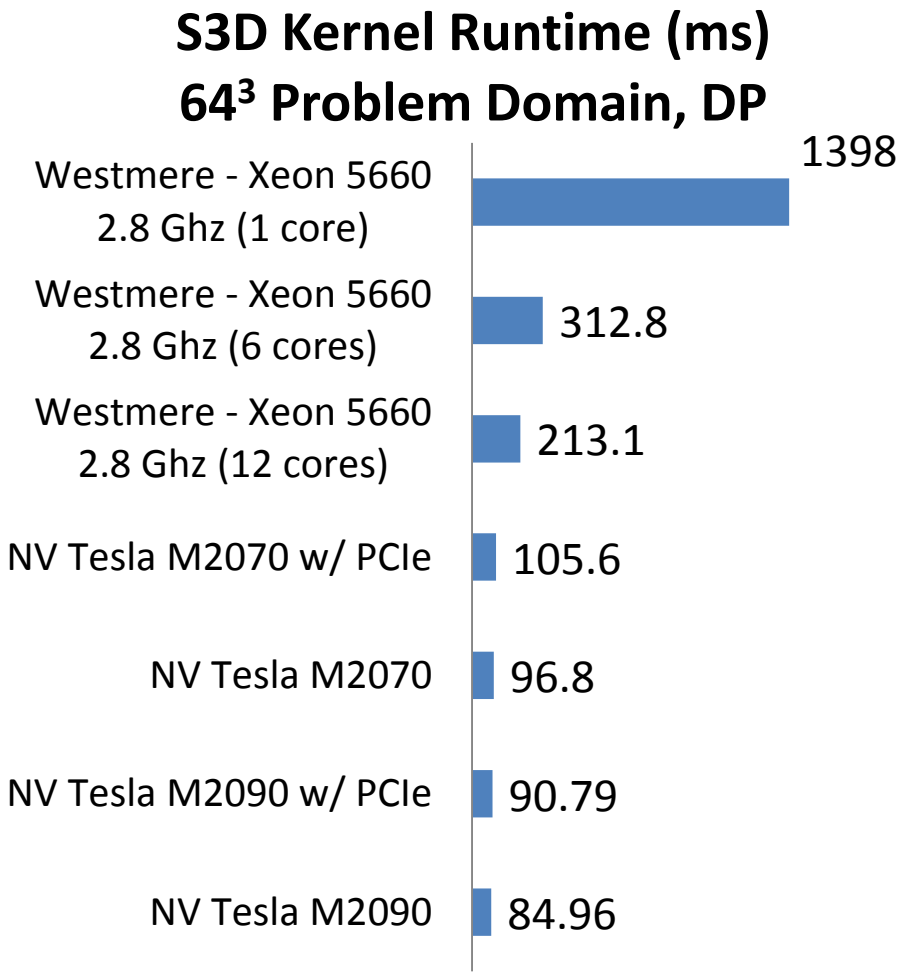
# Accelerating S3D's chemistry

**We implemented an accelerated version of S3D's Getrates kernel. The graph below shows the normalized runtime on Keeneland using one Tesla M2070 GPU or Westmere CPU per node.**

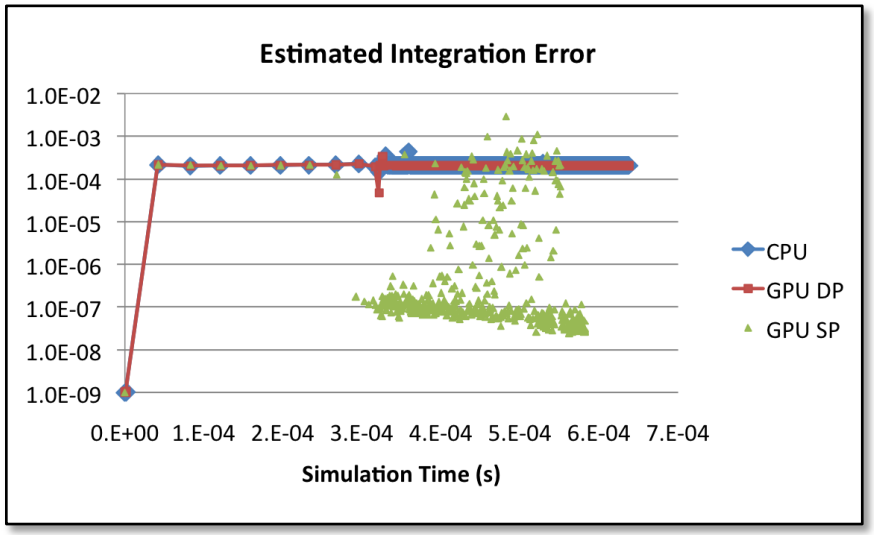


# Detailed Kernel Performance

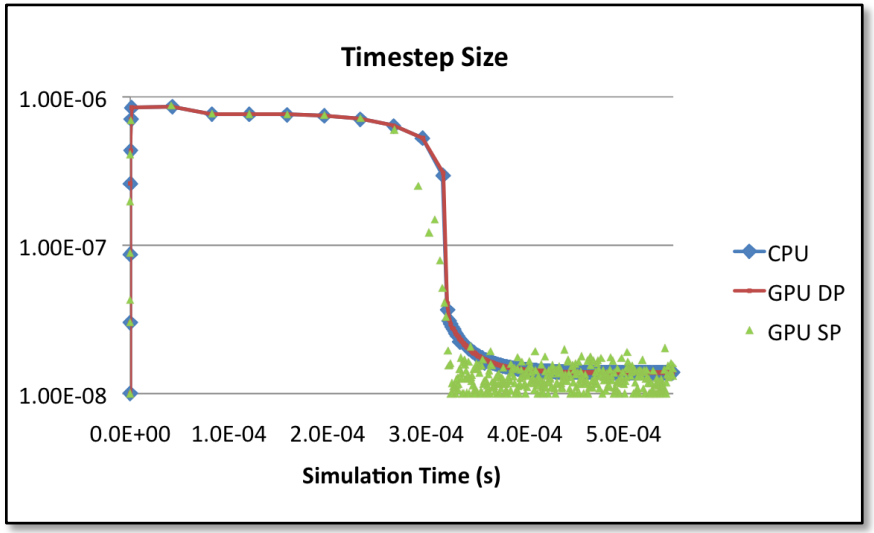
- This chart compares the performance of an optimized CPU version to the GPU version on the NSF Keeneland system.
- Performance measured using CUDA 4.0 and double precision.

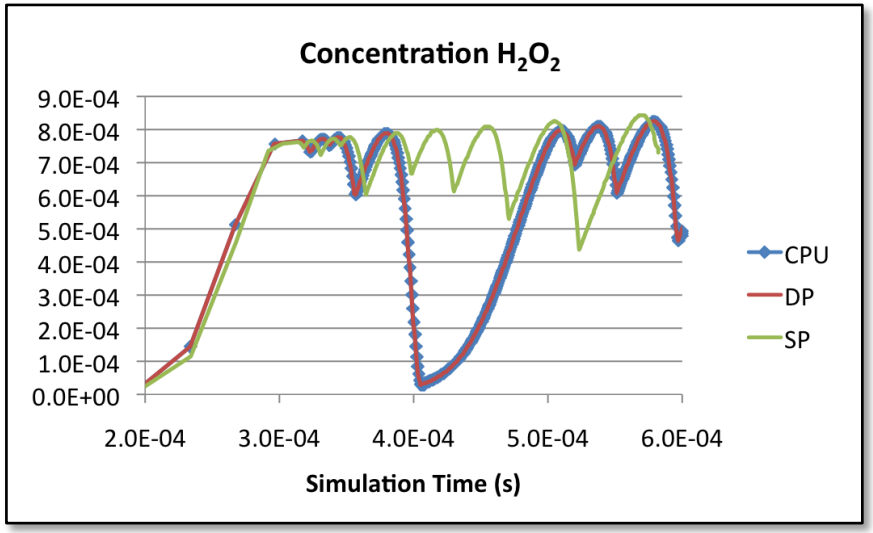


# Accuracy vs performance in S3D

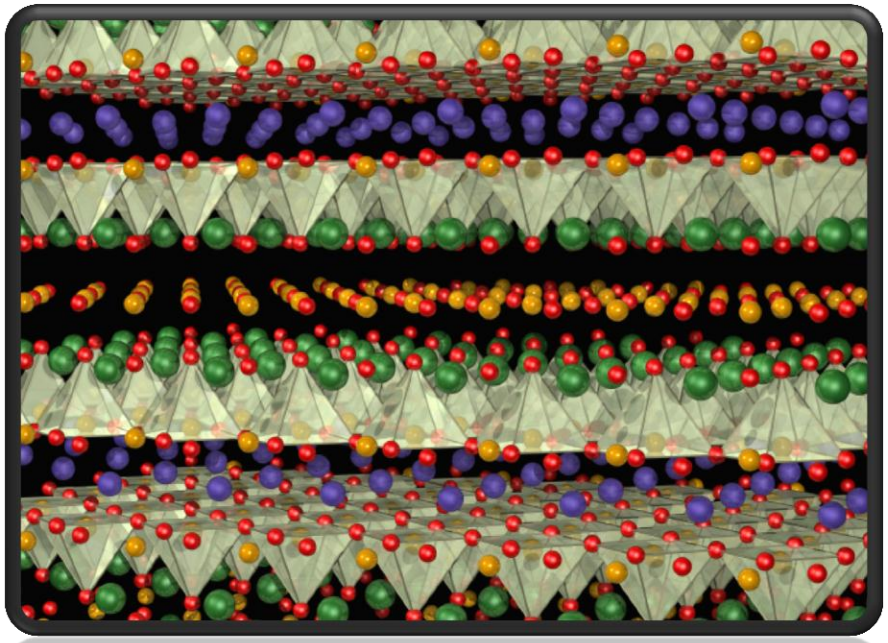


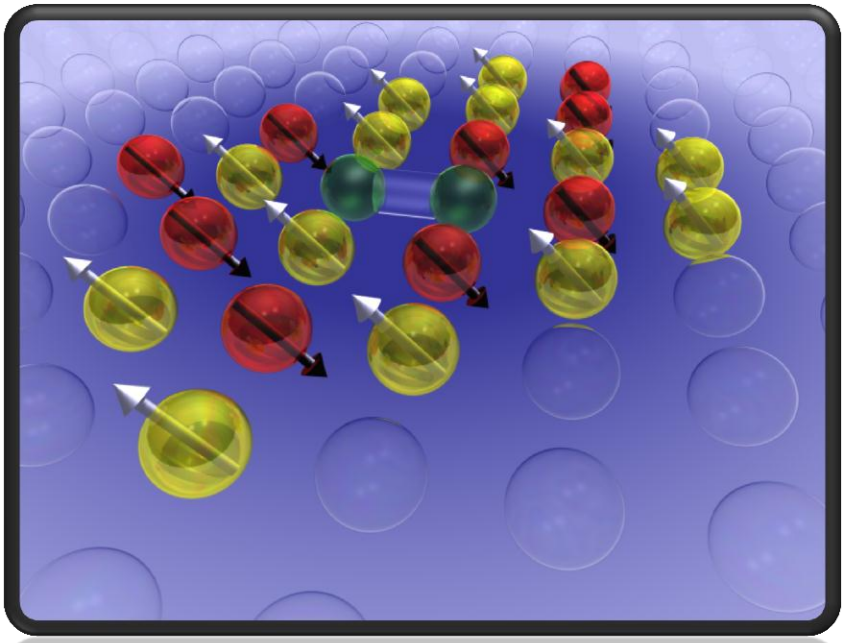

- Single precision is faster, but results in higher integration error
- Time step size shrinks to compensate
- It takes more iterations to simulate the same physical process
- Thus, the trade-off between precision and runtime is complex



# The DCA++ simulation code



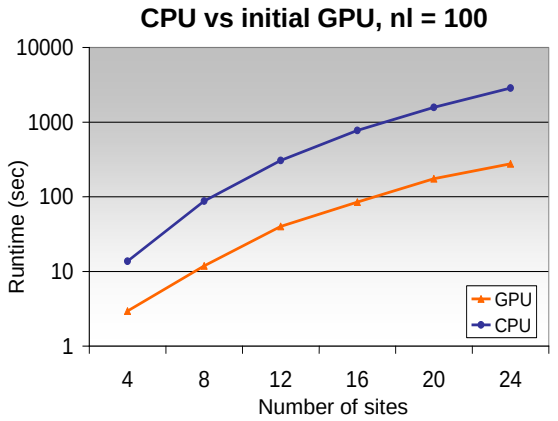


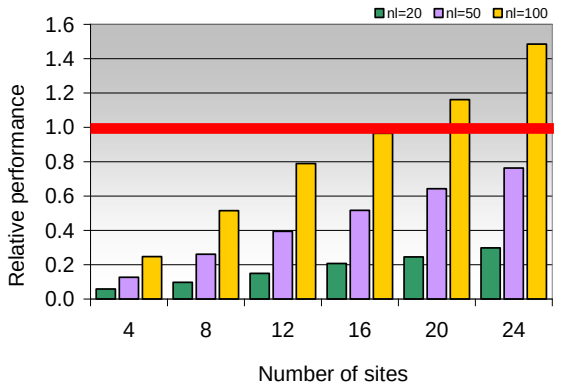
## DCA++ is a Quantum Monte Carlo simulation code

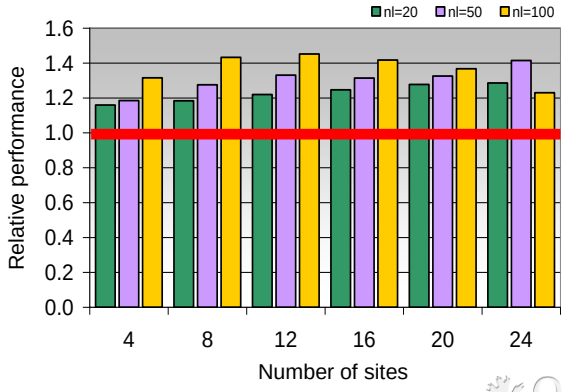
- Studies of high-temperature superconductivity and other materials science
- Implements Dynamic Cluster Approximation

# Mapping DCA++ to CUDA

- GPU BLAS offload alone resulted in significant speedups
- Further improvement by minimizing data transfers was only moderate because some functions remained on the CPU
- Porting remaining functions to GPU helped or hurt performance depending on problem size



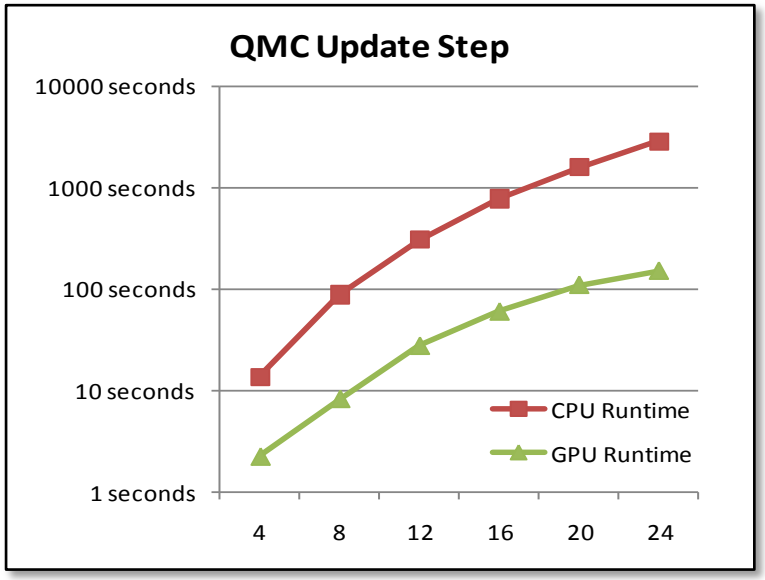



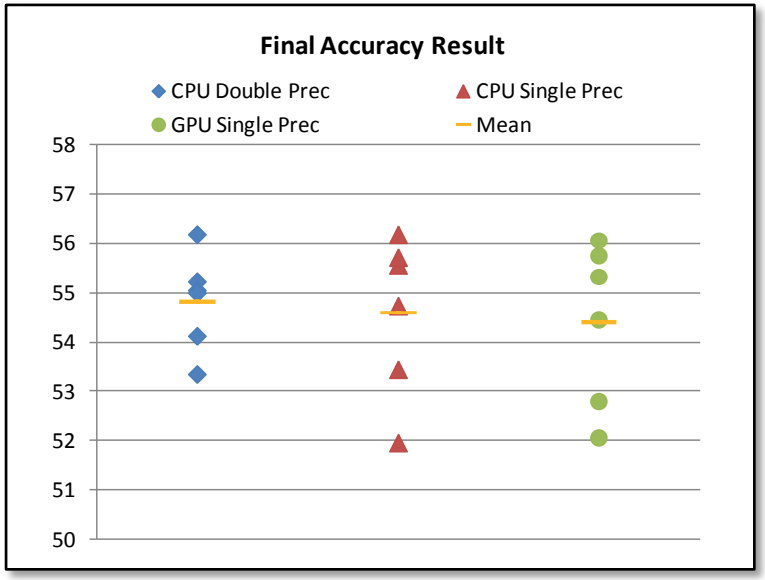



# DCA++ results

- QMC Update step showed almost 20× speedup after acceleration
- Accuracy remained within acceptable levels even when using single precision algorithms
- Full parallel GPU accelerated code showed 5× improvement

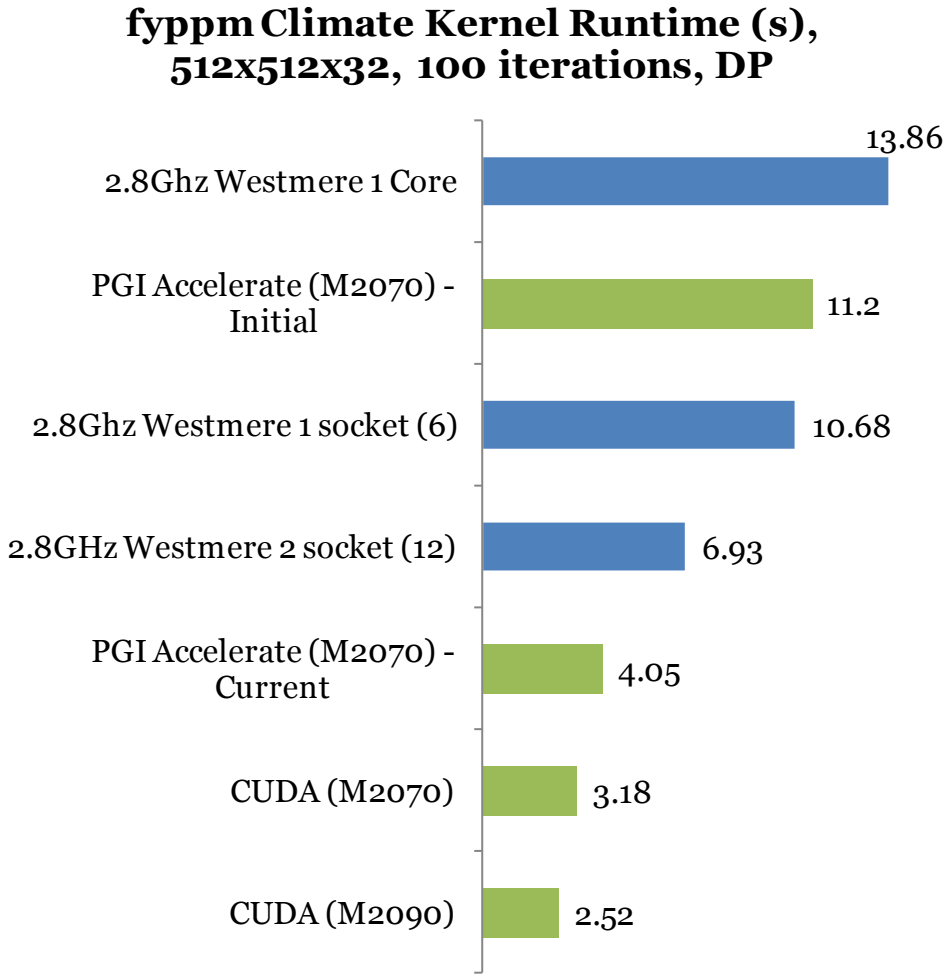
| Parallel Speedup | Median Speedup | Maximum Speedup |
|---|---|---|
| Warm-up phase | 13.46× | 17.28× |
| One QMC step | 13.32× | 17.10× |
| One measurement | 1.00× | 1.00× |
| One iteration | 4.96× | 5.56× |
| Whole code | 5.35× | |



# NOAA GFDL Climate Model Results

- Domain: Climate and weather modeling Cristopher Kerr, NOAA
- Evaluating performance-productivity tradeoff of hand-written CUDA and directive-based acceleration
- Measured kernel performance on Keeneland system and next-gen Sandy Bridge
- Initially legacy FORTRAN
- Currently running on multiple GPUs using OpenMP



# Moving forward

- Productivity and accuracy remain critical goals
  - OpenCL improves code portability
    - Open standard for parallel heterogeneous computing
    - Abstractions are similar to CUDA
    - www.khronos.org/opencl
  - GPU improvements in precision
    - Full double-precision support in latest GPUs
    - Speed is improving relative to single precision performance
- References


K. Spafford, J. Meredith, J.S. Vetter, J. Chen, R. Grout, R. Sankaran. "Accelerating S3D: A GPGPU Case Study," *Proceedings of the Seventh International Workshop on Algorithms, Models, and Tools for Parallel Computing on Heterogeneous Platforms (HeteroPar 2009),* Delft, The Netherlands.

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