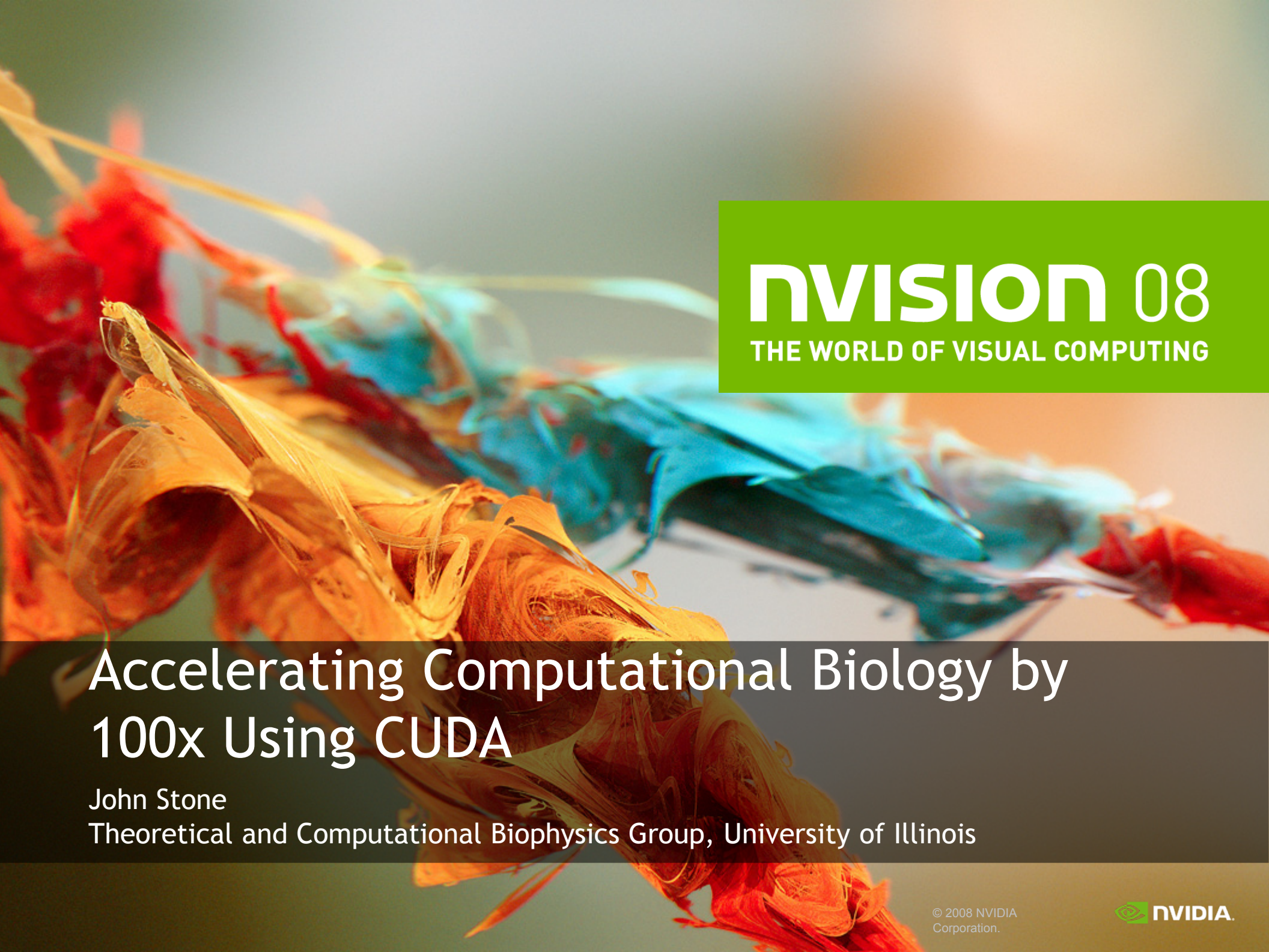


Accelerating Computational Biology by 100x Using CUDA

John Stone
Theoretical and Computational Biophysics Group, University of Illinois

NVIDIA

GPU Computing

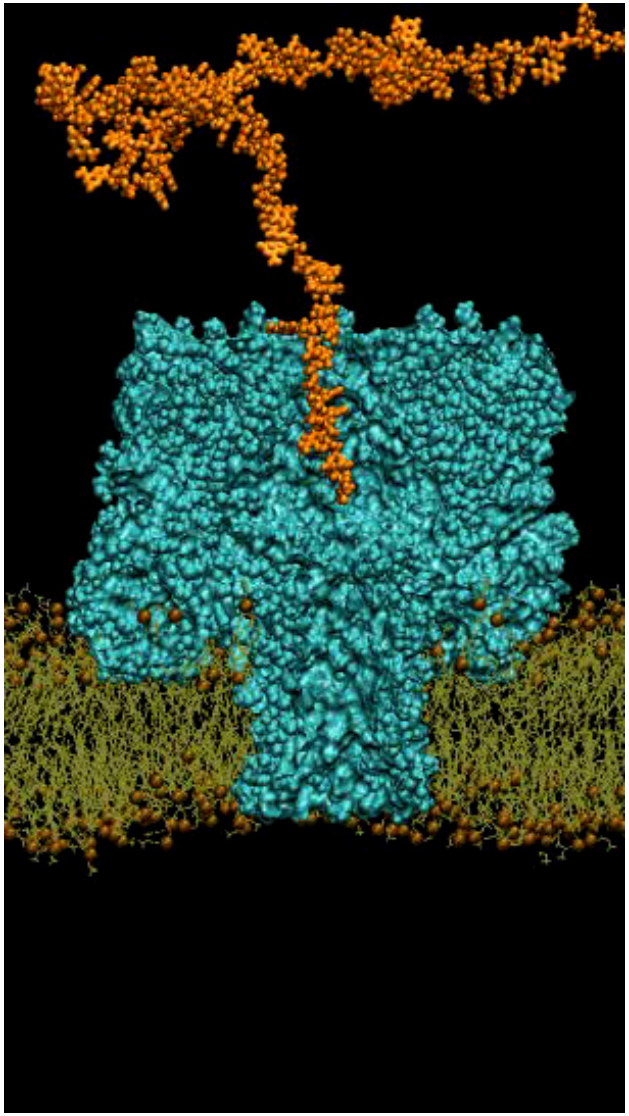
- Commodity devices, omnipresent in modern computers
- Massively parallel hardware, hundreds of processing units, throughput oriented design
- Support all standard integer and floating point types
- Programming tools allow software to be written in dialects of familiar C/C++ and integrated into legacy software
- GPU algorithms are often multicore-friendly due to attention paid to data locality and work decomposition (e.g. MCUDA)

What Speedups Can GPUs Achieve?

- Single-GPU speedups of 8x to 30x vs. CPU core are quite common
- Best speedups (100x!) are attained on codes that are skewed towards floating point arithmetic, esp. CPU-unfriendly operations that prevent effective use of SSE or other vectorization
- Amdahl's Law can prevent legacy codes from achieving peak speedups with only shallow GPU acceleration efforts

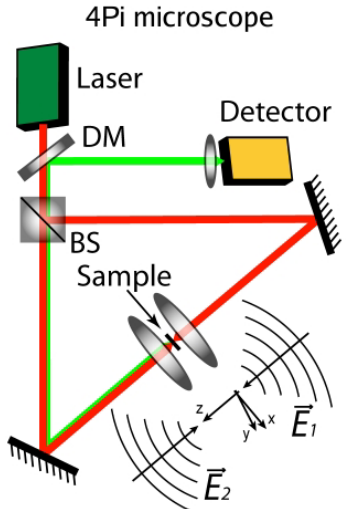
Computational Biology's Insatiable Demand for Processing Power

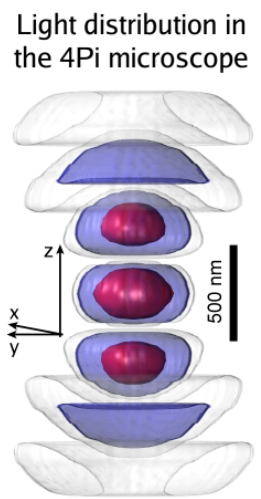
- Simulations still fall short of biological timescales
- Large simulations extremely difficult to prepare, analyze
- Order of magnitude increase in performance would allow use of more sophisticated models



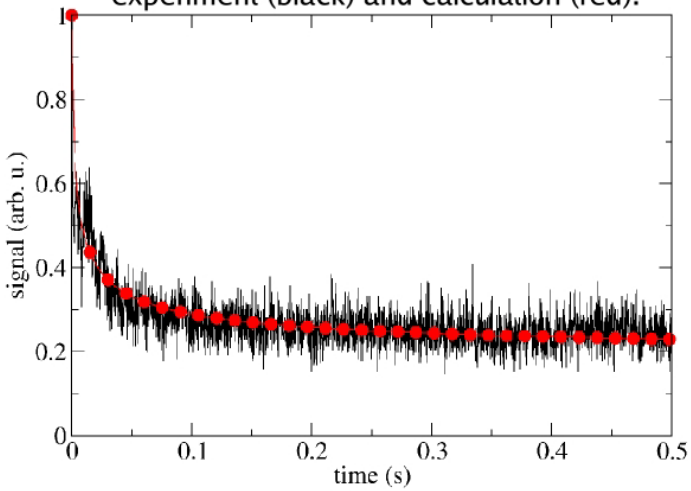
Fluorescence Microscopy

- 2-D reaction-diffusion simulation used to predict results of fluorescence microphotolysis experiments
- Simulate 1-10 second microscopy experiments, 0.1ms integration timesteps
- Goal: <= 1 min per simulation on commodity PC hardware
- Project home page:
  http://www.ks.uiuc.edu/Research/microscope/





Fluorescence from the sample changes due to photobleaching and diffusion: experiment (black) and calculation (red).



Fluorescence Microscopy (2)

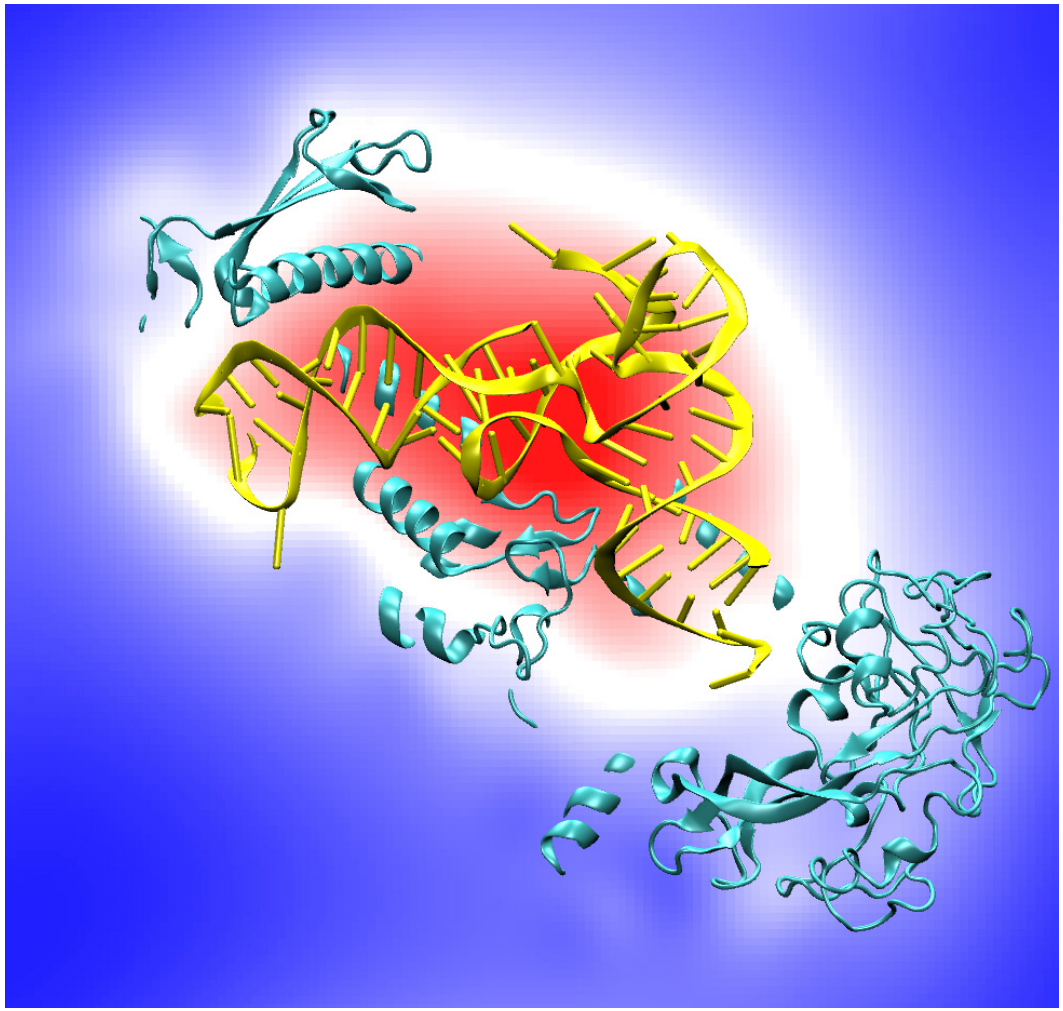
- Challenges for CPU:
  - Efficient handling of boundary conditions
  - Large number of floating point operations per timestep
- Challenges for GPU w/ CUDA:
  - Hiding global memory latency, improving memory access patterns, controlling register use
  - Few arithmetic operations per memory reference (for a GPU…)

Fluorescence Microscopy (3)

- Simulation runtime, software development time:
  - Original research code (CPU): 80 min
  - Optimized algorithm (CPU): 27 min
    - 40 hours of work
  - SSE-vectorized (CPU): 8 min
    - 20 hours of work
  - CUDA w/ 8800GTX: 38 sec, 12 times faster than SSE!
    - 12 hours of work, possible to improve further, but already "fast enough" for real use
    - CUDA code was more similar to the original than to the SSE vectorized version – arithmetic is almost "free" on the GPU

Calculating Electrostatic Potential Maps

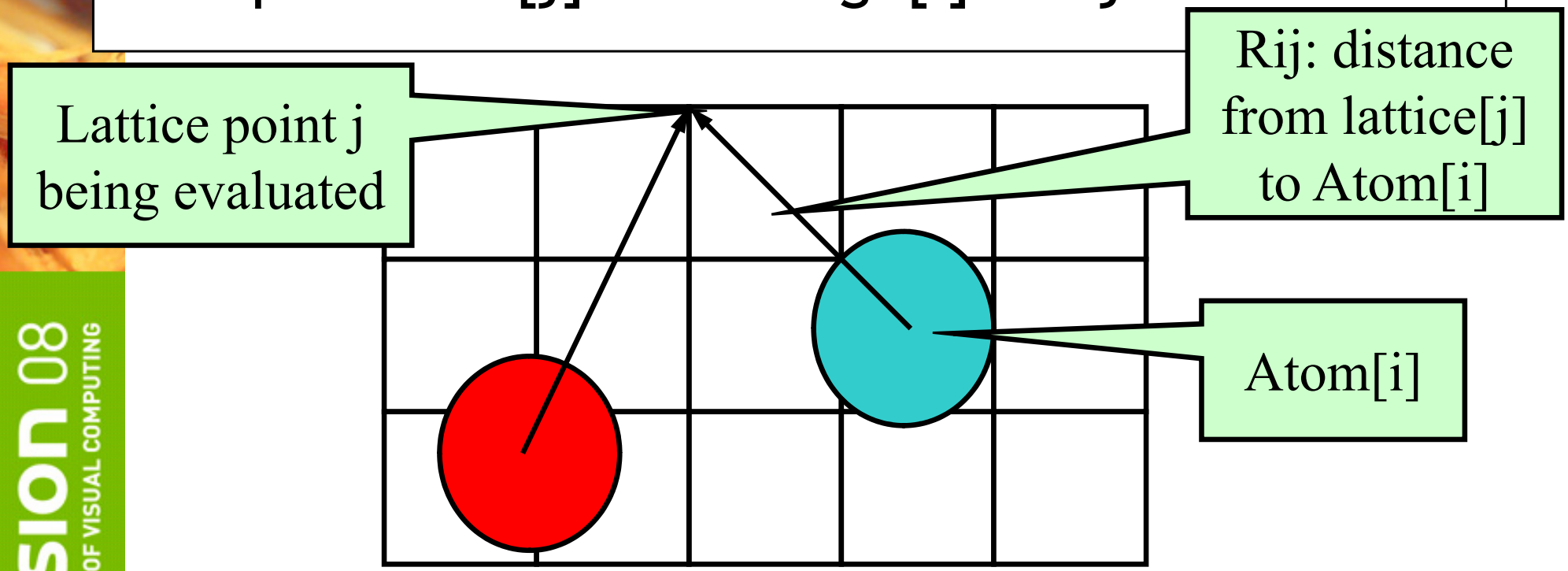
- Used in molecular structure building, analysis, visualization, simulation
- Electrostatic potentials evaluated on a uniformly spaced 3-D lattice
- Each lattice point contains sum of electrostatic contributions of all atoms



Direct Coulomb Summation

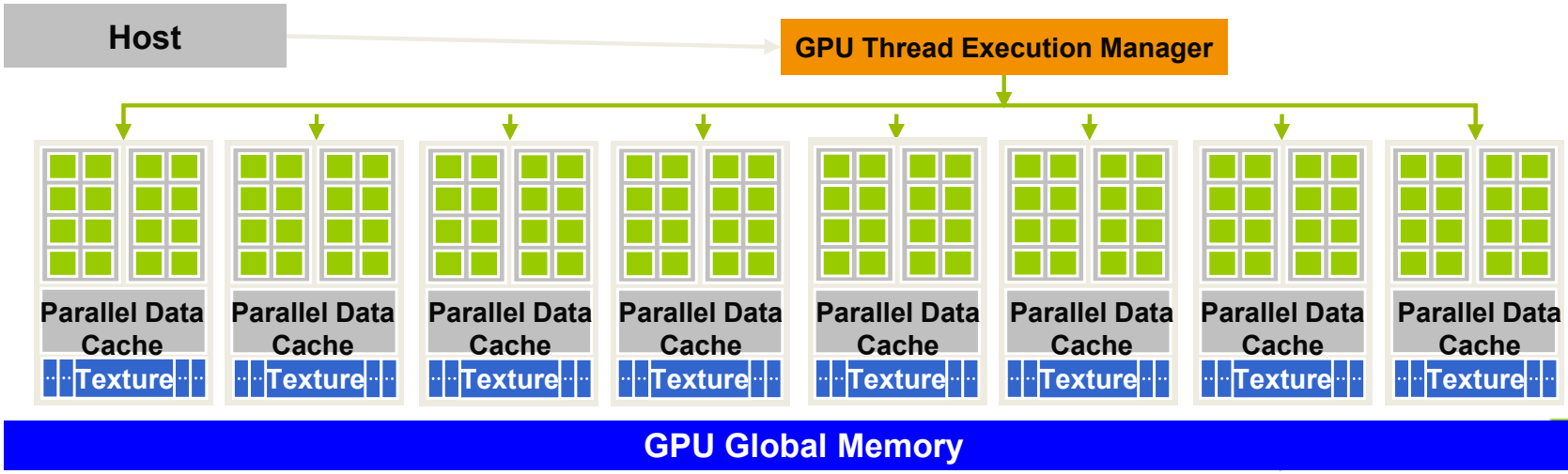
- At each lattice point, sum potential contributions for all atoms in the simulated structure:

  potential[j] += charge[i] / Rij

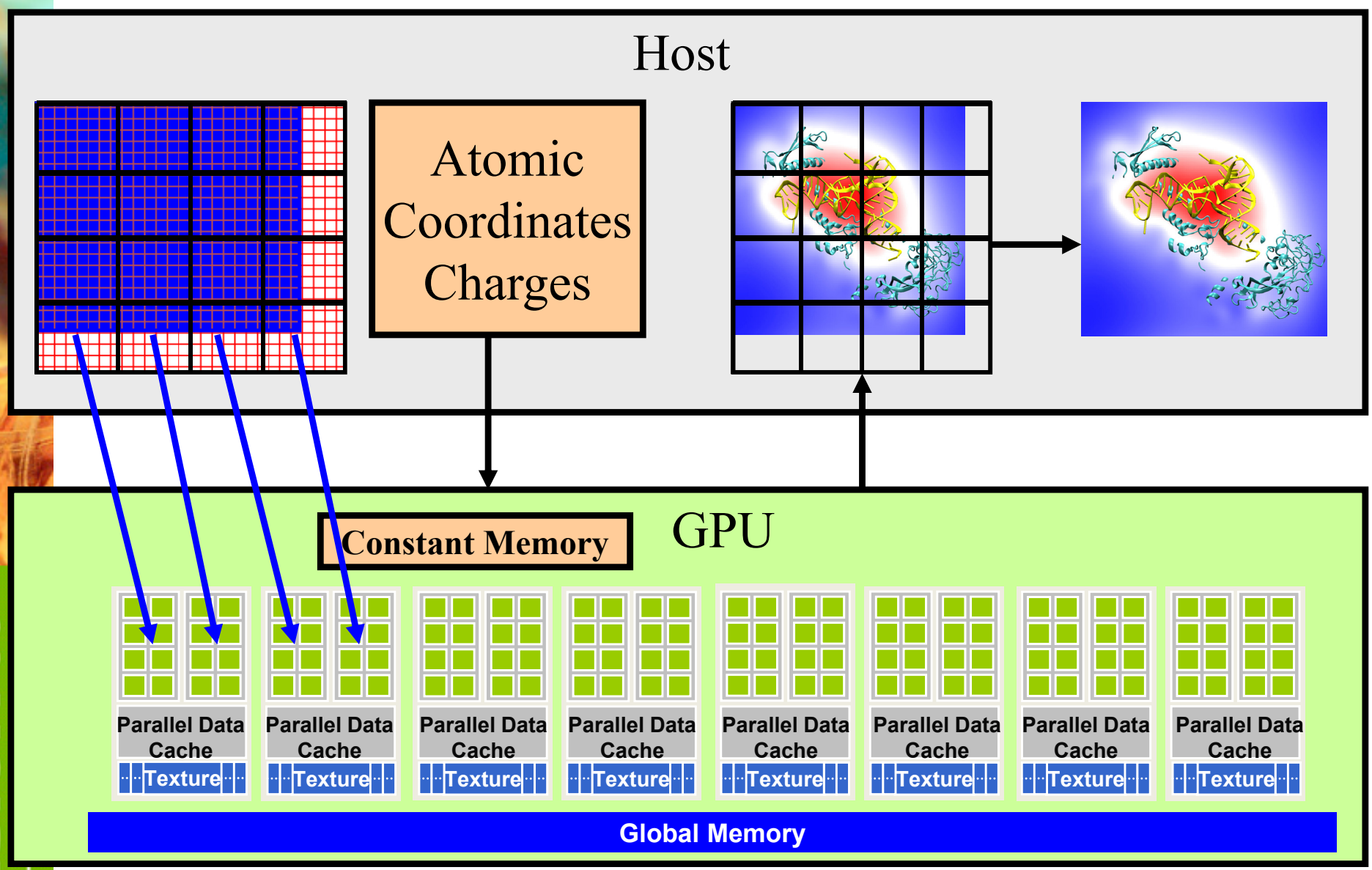


Direct Coulomb Summation on the GPU

- GPU outruns a CPU core by 44x
- Work is decomposed into tens of thousands of independent threads, multiplexed onto hundreds of GPU processor cores
- Single-precision FP arithmetic is adequate for intended application
- Numerical accuracy can be further improved by compensated summation, spatially ordered summation groupings, or accumulation of potential in double-precision
- Starting point for more sophisticated algorithms

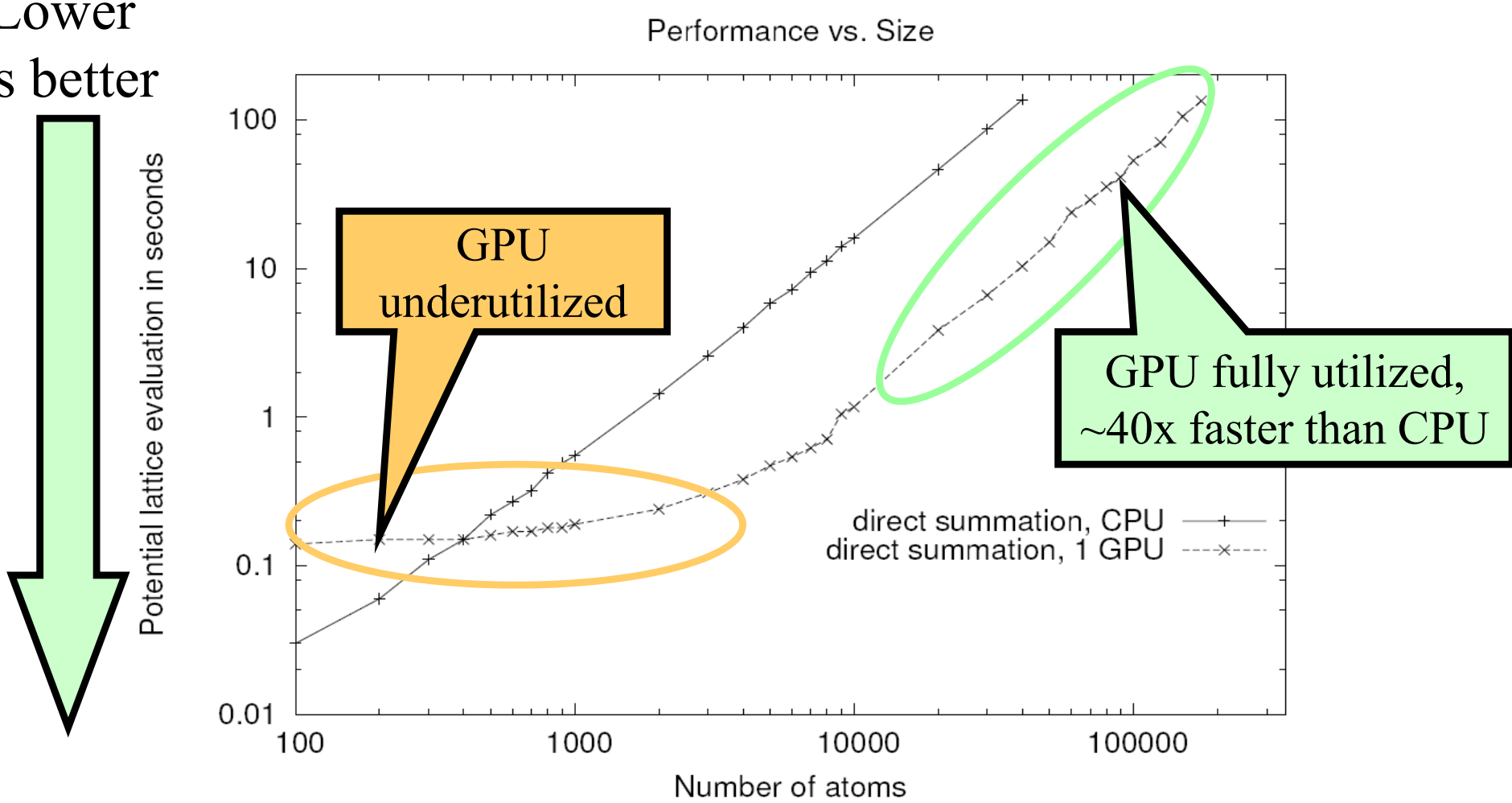


Direct Coulomb Summation on the GPU



Direct Coulomb Summation Runtime

Lower is better



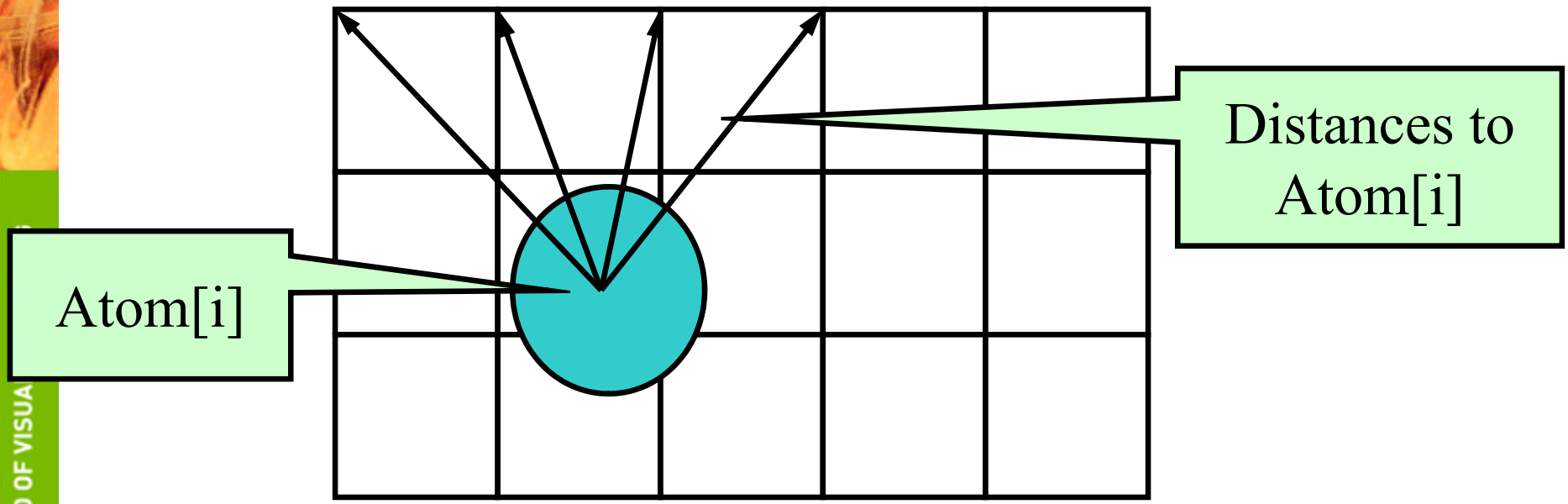
Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.

Optimizing for the GPU

- Increase arithmetic intensity, reuse in-register data by "unrolling" lattice point computation into inner atom loop
- Each atom contributes to several lattice points, distances only differ in the X component:

  potentialA += charge[i] / (distanceA to atom[i])

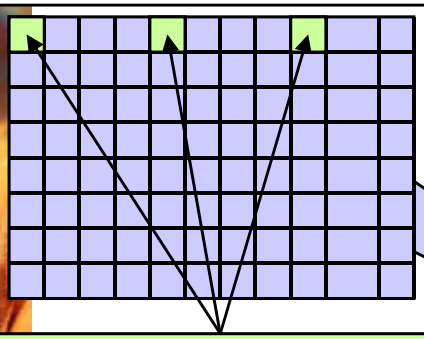
  potentialB += charge[i] / (distanceB to atom[i]) …



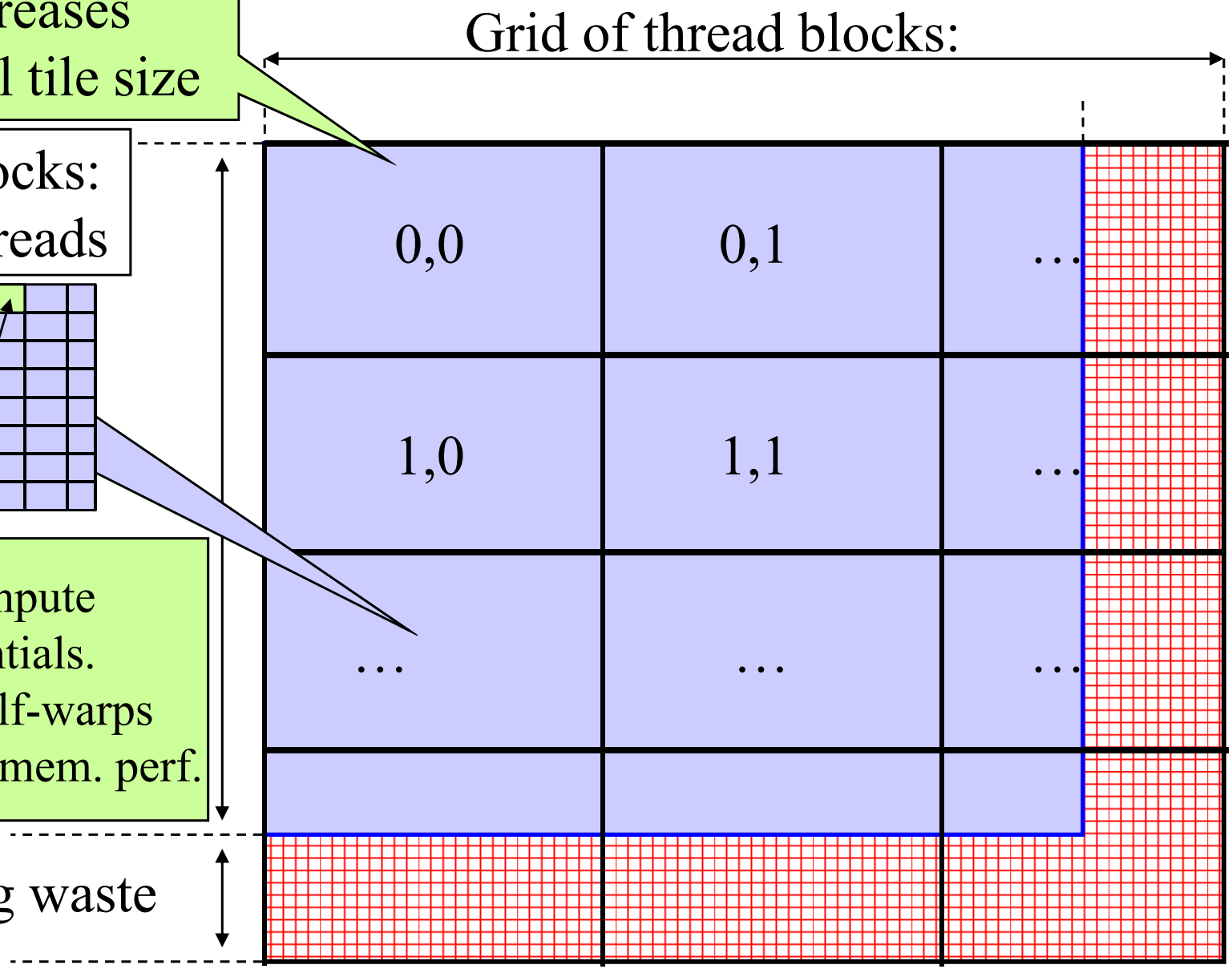
CUDA Block/Grid Decomposition

Unrolling increases computational tile size

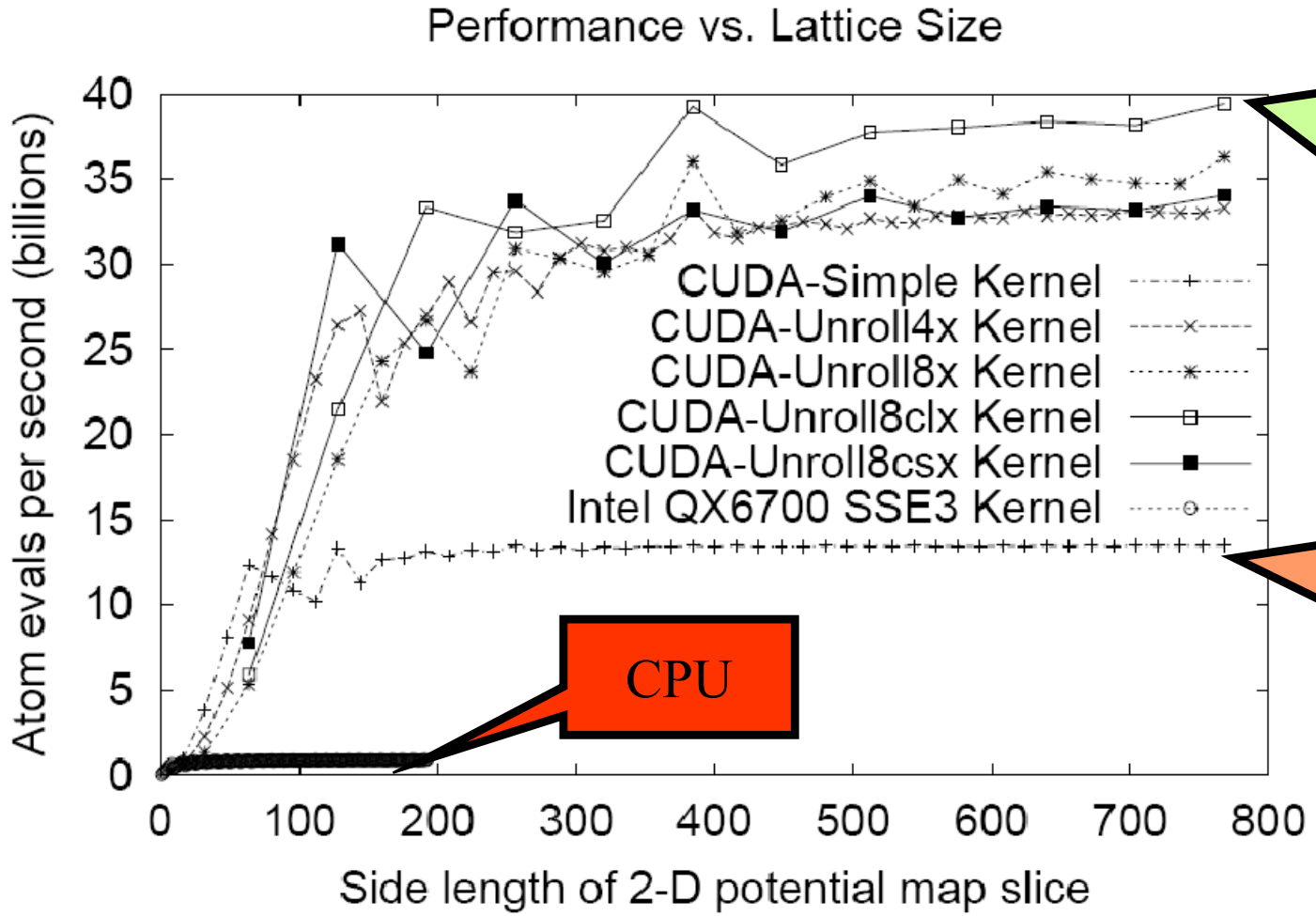
Thread blocks: 64-256 threads



Threads compute up to 8 potentials. Skipping by half-warps optimizes global mem. perf.



Direct Coulomb Summation Performance



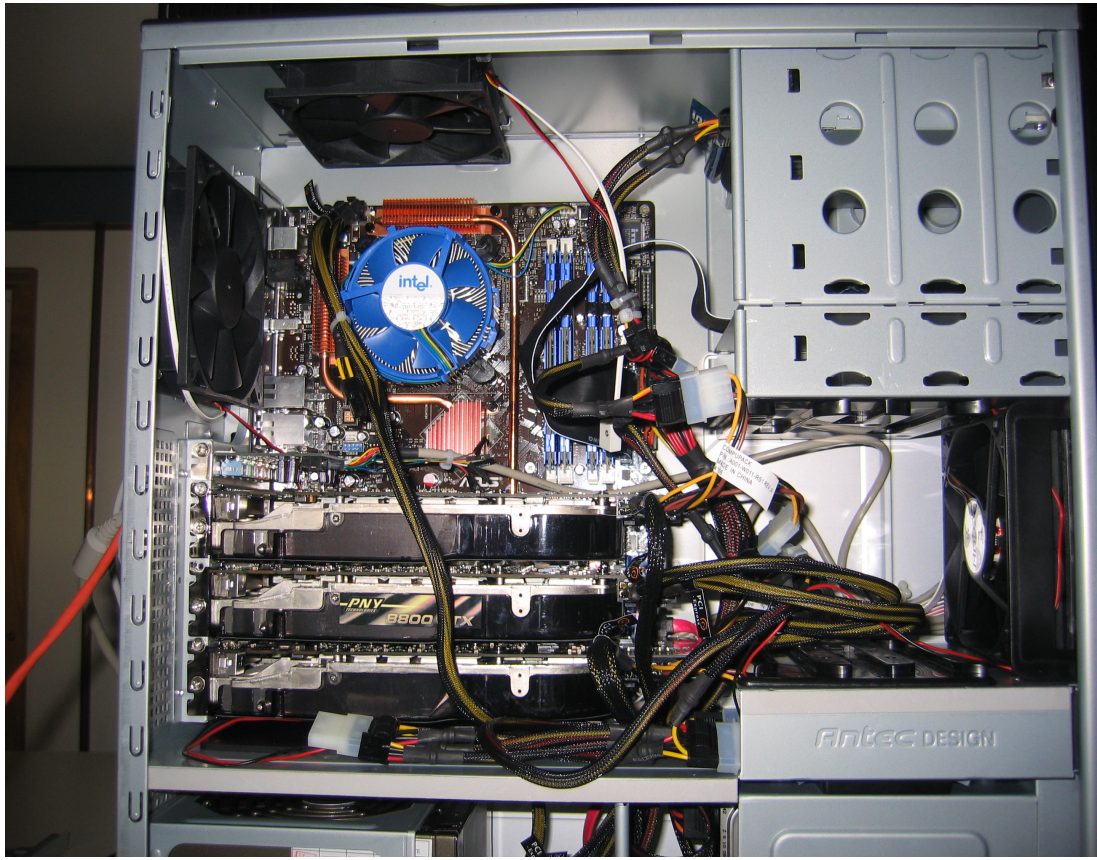
CUDA-Unroll8clx: fastest GPU kernel, 44x faster than CPU, 291 GFLOPS on GeForce 8800GTX

CUDA-Simple: 14.8x faster, 33% of fastest GPU kernel

GPU computing. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.

Multi-GPU Direct Coulomb Summation

- Effective memory bandwidth scales with the number of GPUs utilized
- PCIe bus bandwidth not a bottleneck for this algorithm
- 117 billion evals/sec
- 863 GFLOPS
- 131x speedup vs. CPU core
- Power: 700 watts during benchmark



Quad-core Intel QX6700

Three NVIDIA GeForce 8800GTX

Multi-GPU Direct Coulomb Summation

- 4-GPU (2 Quadroplex) Opteron node at NCSA
- 157 billion evals/sec
- 1.16 TFLOPS
- 176x speedup vs. Intel QX6700 CPU core w/ SSE

- 4-GPU (GT200)
- 241 billion evals/sec
- 1.78 TFLOPS
- 271x speedup vs. Intel QX6700 CPU core w/ SSE

NCSA GPU Cluster

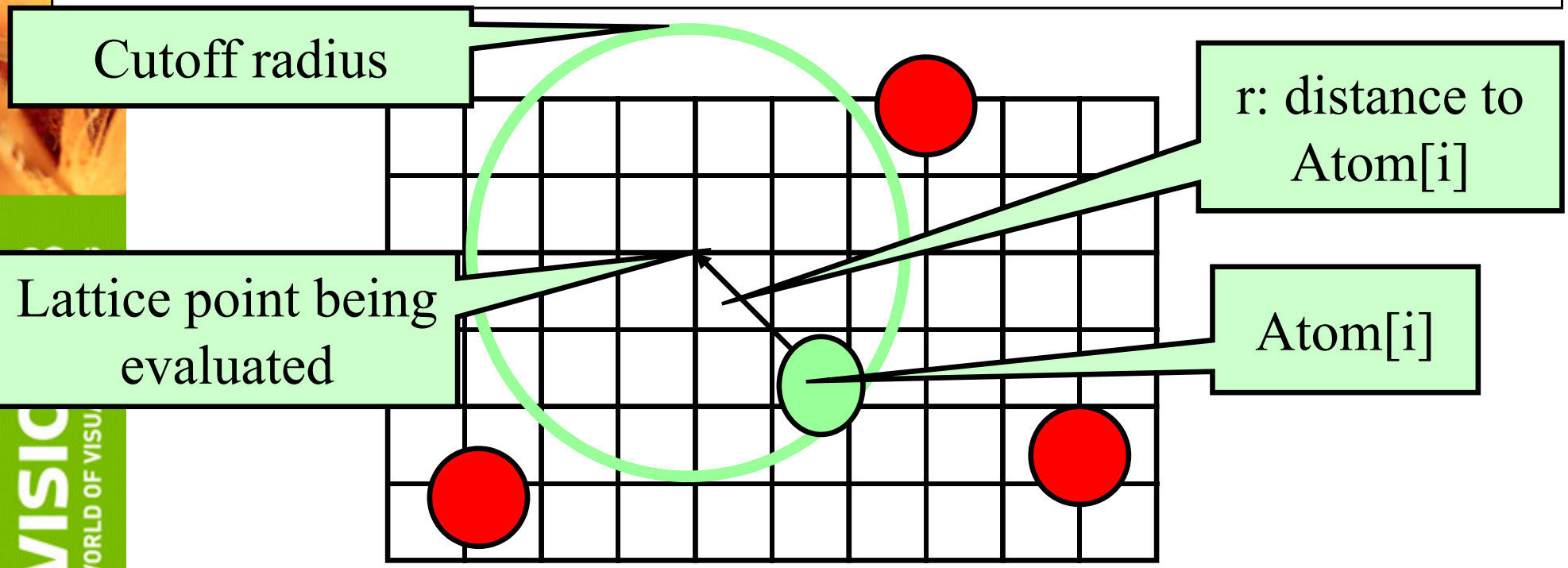
http://www.ncsa.uiuc.edu/Projects/GPUcluster/

Cutoff Summation

- At each lattice point, sum potential contributions for atoms within cutoff radius:

```
if (distance to atom[i] < cutoff)
  potential += (charge[i] / r) * s(r)
```

- Smoothing function s(r) is algorithm dependent



Infinite vs. Cutoff Potentials

- Infinite range potential:
  - All atoms contribute to all lattice points
  - Summation algorithm has quadratic complexity
- Cutoff (range-limited) potential:
  - Atoms contribute within cutoff distance to lattice points
  - Summation algorithm has linear time complexity
  - Has many applications in molecular modeling:
    - Replace electrostatic potential with shifted form
    - Short-range part for fast methods of approximating full electrostatics
    - Used for fast decaying interactions (e.g. Lennard-Jones, Buckingham)

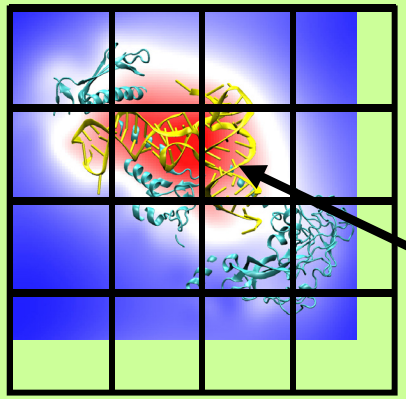
Cutoff Summation on the GPU

Atoms spatially hashed into fixed-size "bins" in global memory

Atoms

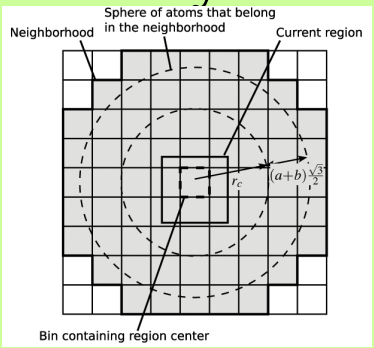
Global memory

Potential map regions



Constant memory

Bin-Region neighborlist



Shared memory

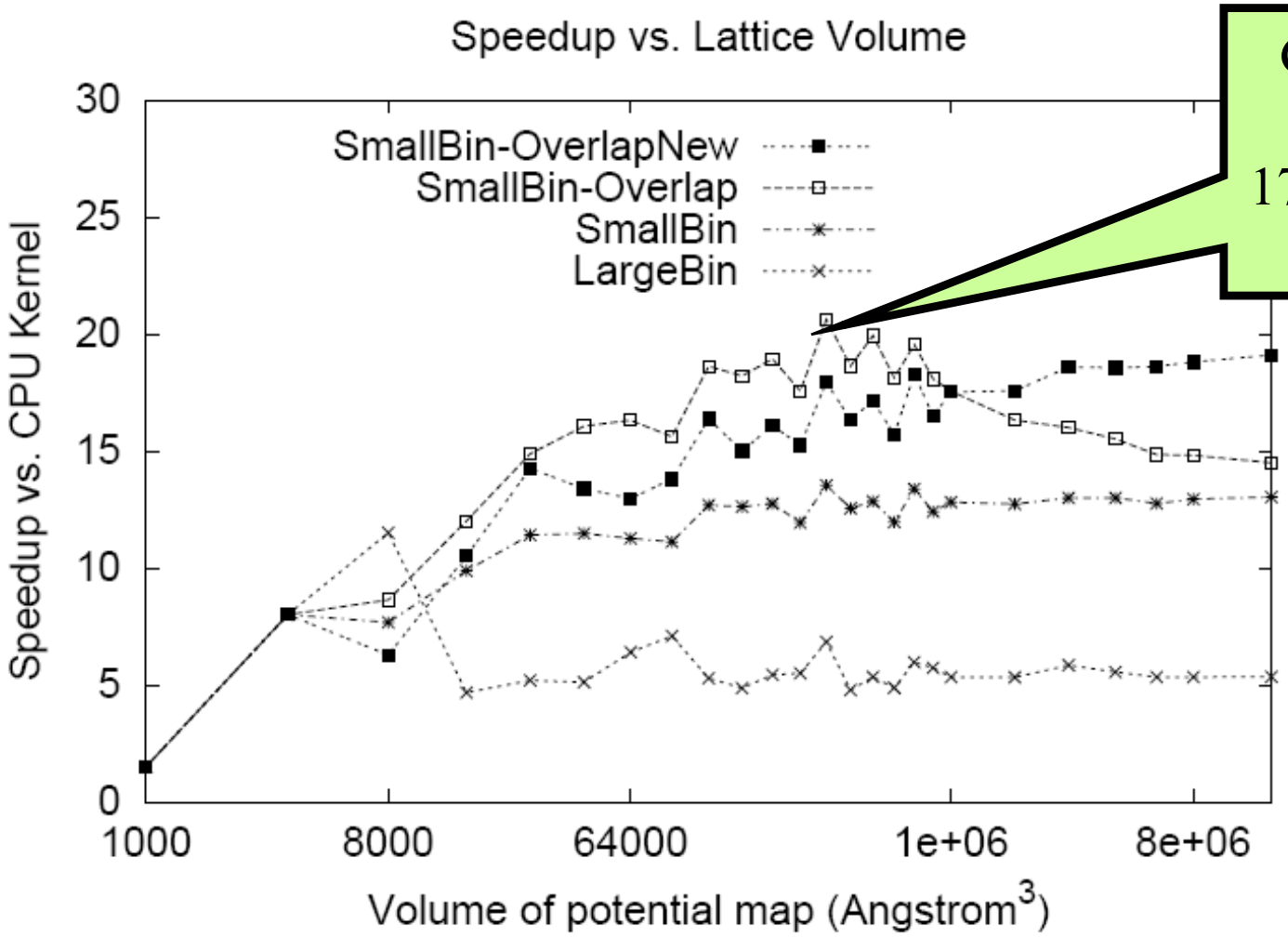
Atom bin

Process atom bins for current potential map region

Using the CPU to Improve GPU Performance

- GPU performs best when the work evenly divides into the number of threads/processing units
- Optimization strategy:
  - Use the CPU to “regularize” the GPU workload
  - Handle exceptional or irregular work units on the CPU while the GPU processes the bulk of the work
  - On average, the GPU is kept highly occupied, attaining a much higher fraction of peak performance

Cutoff Summation Runtime



GPU cutoff with CPU overlap: 17x-21x faster than CPU core

GPU acceleration of cutoff pair potentials for molecular modeling applications. C. Rodrigues, D. Hardy, J. Stone, K. Schulten, W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.

NAMD Parallel Molecular Dynamics

Kale *et al., J. Comp. Phys.* **151**:283-312, 1999.

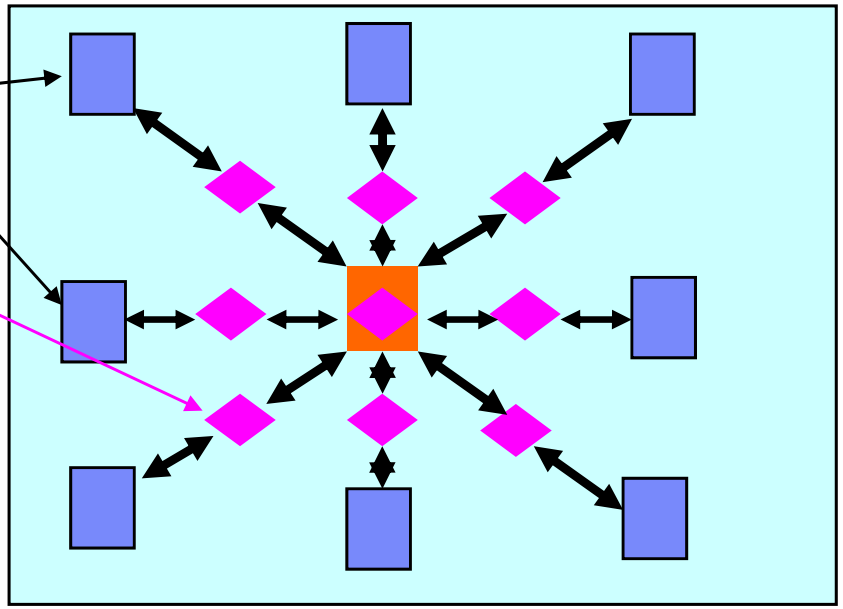
- Designed from the beginning as a parallel program
- Uses the Charm++ idea:
  - Decompose the computation into a large number of objects
  - Have an Intelligent Run-time system (of Charm++) assign objects to processors for dynamic load balancing with minimal communication

Hybrid of spatial and force decomposition:

•Spatial decomposition of atoms into cubes (called patches)

•For every pair of interacting patches, create one object for calculating electrostatic interactions

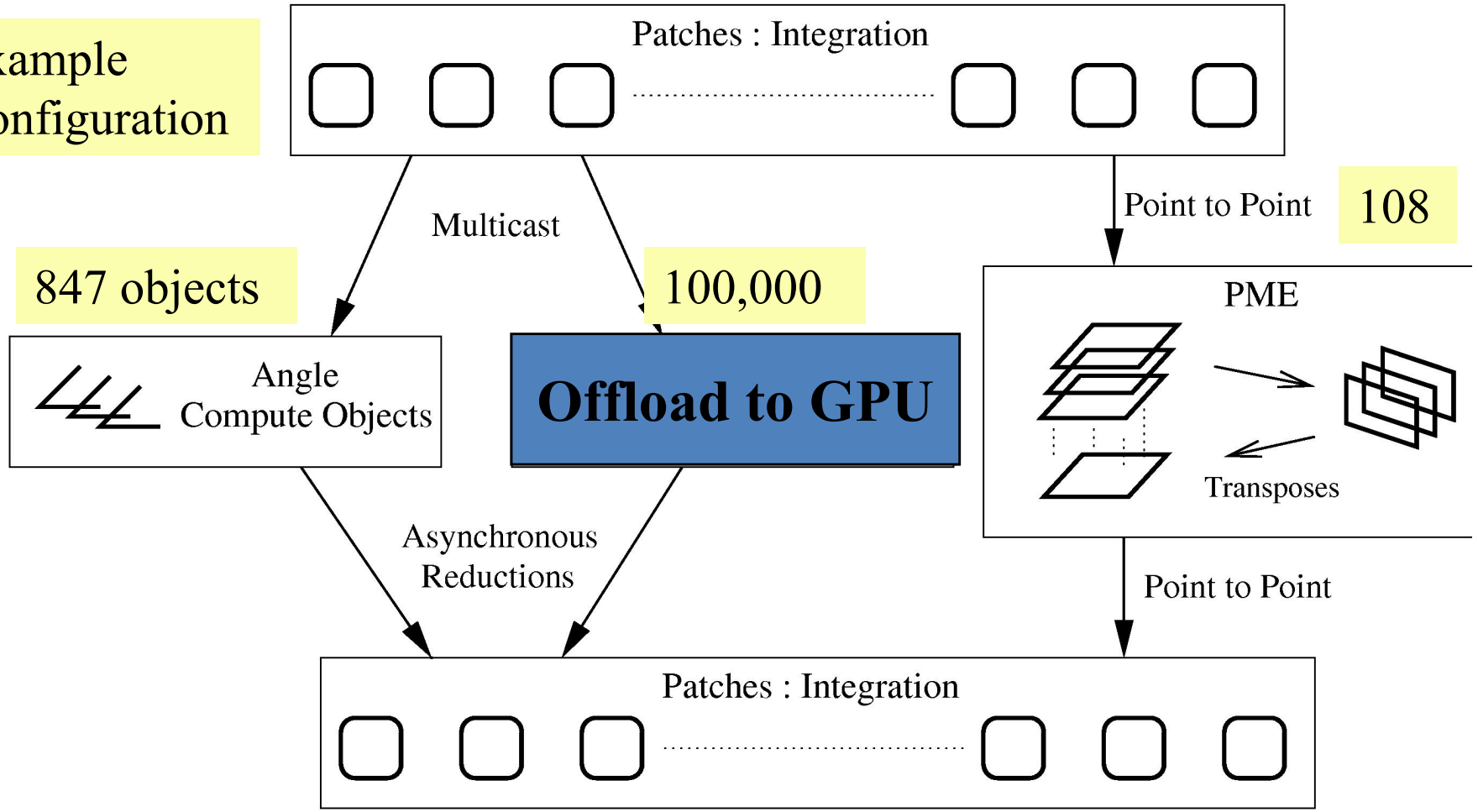
•Recent: Blue Matter, Desmond, etc. use this idea in some form



NAMD Overlapping Execution

Phillips *et al., SC2002.*

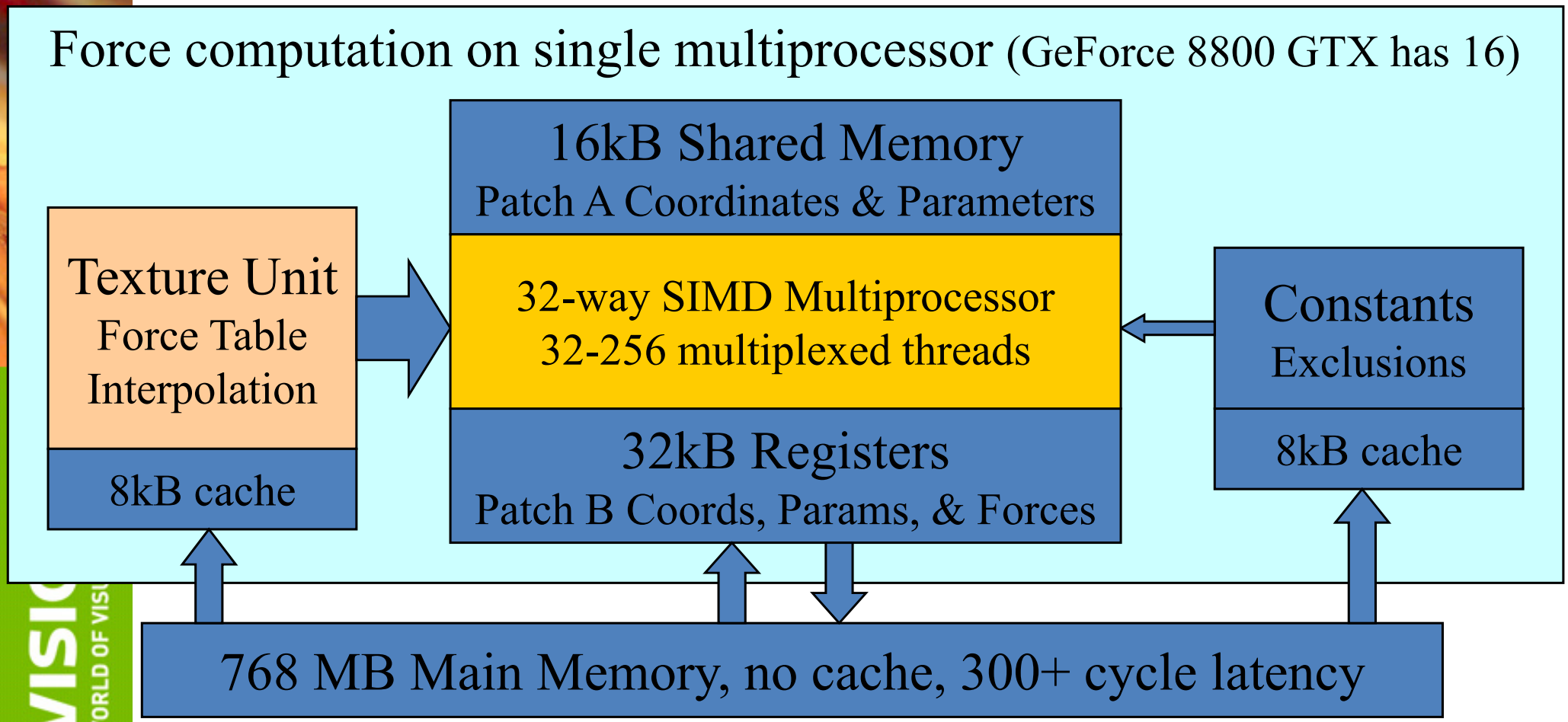
Example Configuration



Objects are assigned to processors and queued as data arrives.

Nonbonded Forces on G80 GPU

- Start with most expensive calculation: direct nonbonded interactions.
- Decompose work into pairs of patches, identical to NAMD structure.
- GPU hardware assigns patch-pairs to multiprocessors dynamically.



Stone *et al.*, *J. Comp. Chem.* **28**:2618-2640, 2007.

Nonbonded Forces CUDA Code

```
texture<float4> force_table;
__constant__ unsigned int exclusions[];
__shared__ atom jatom[];
atom iatom;      // per-thread atom, stored in registers
float4 iforce;   // per-thread force, stored in registers
for ( int j = 0; j < jatom_count; ++j ) {
  float dx = jatom[j].x - iatom.x;   float dy = jatom[j].y - iatom.y;  float dz = jatom[j].z - iatom.z;
  float r2 = dx*dx + dy*dy + dz*dz;
  if ( r2 < cutoff2 ) {
    float4 ft = texfetch(force_table, 1.f/sqrt(r2));
    bool excluded = false;
    int indexdiff = iatom.index - jatom[j].index;
    if ( abs(indexdiff) <= (int) jatom[j].excl_maxdiff ) {
      indexdiff += jatom[j].excl_index;
      excluded = ((exclusions[indexdiff>>5] & (1<<(indexdiff&31))) != 0);
    }
    float f = iatom.half_sigma + jatom[j].half_sigma;  // sigma
    f *= f*f;  // sigma^3
    f *= f;  // sigma^6
    f *= ( f * ft.x + ft.y );  // sigma^12 * fi.x - sigma^6 * fi.y
    f *= iatom.sqrt_epsilon * jatom[j].sqrt_epsilon;
    float qq = iatom.charge * jatom[j].charge;
    if ( excluded ) { f = qq * ft.w; }  // PME correction
    else { f += qq * ft.z; }  // Coulomb
    iforce.x += dx * f;   iforce.y += dy * f;    iforce.z += dz * f;
    iforce.w += 1.f;  // interaction count or energy
  }
}
```

Force Interpolation

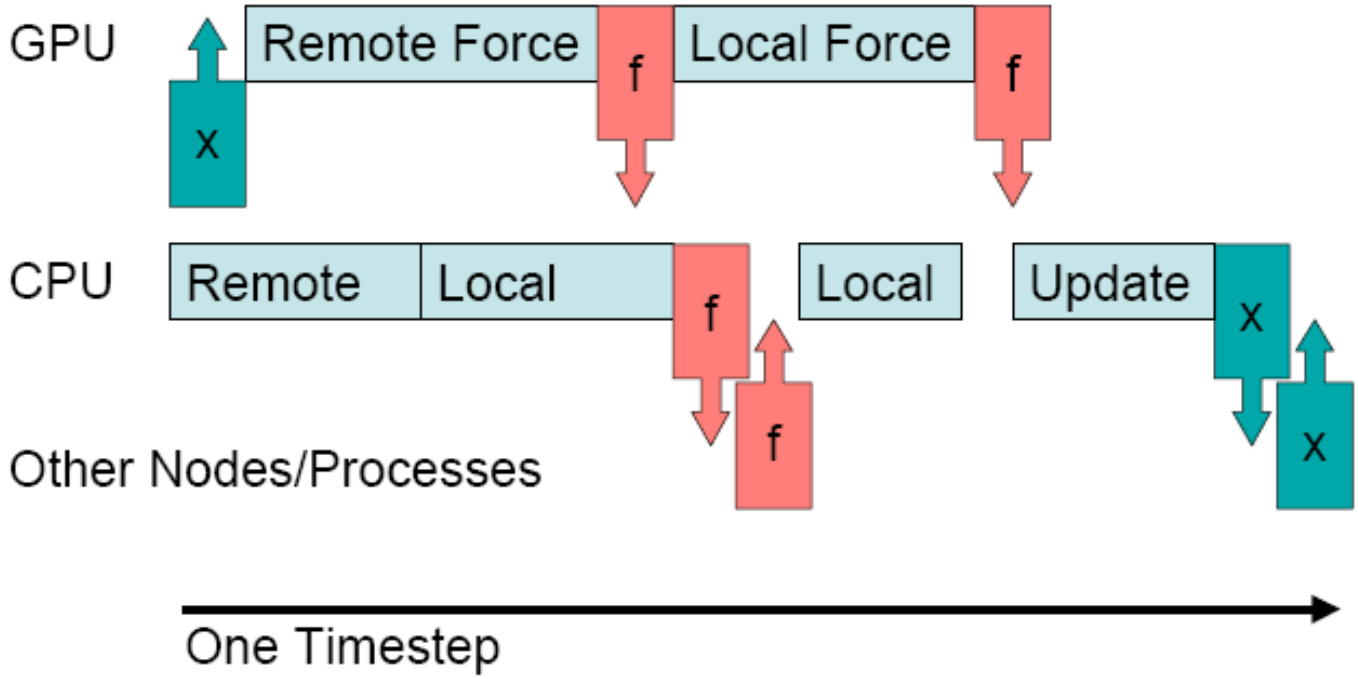
Exclusions

Parameters

Accumulation

Stone *et al.*, *J. Comp. Chem.* **28**:2618-2640, 2007.

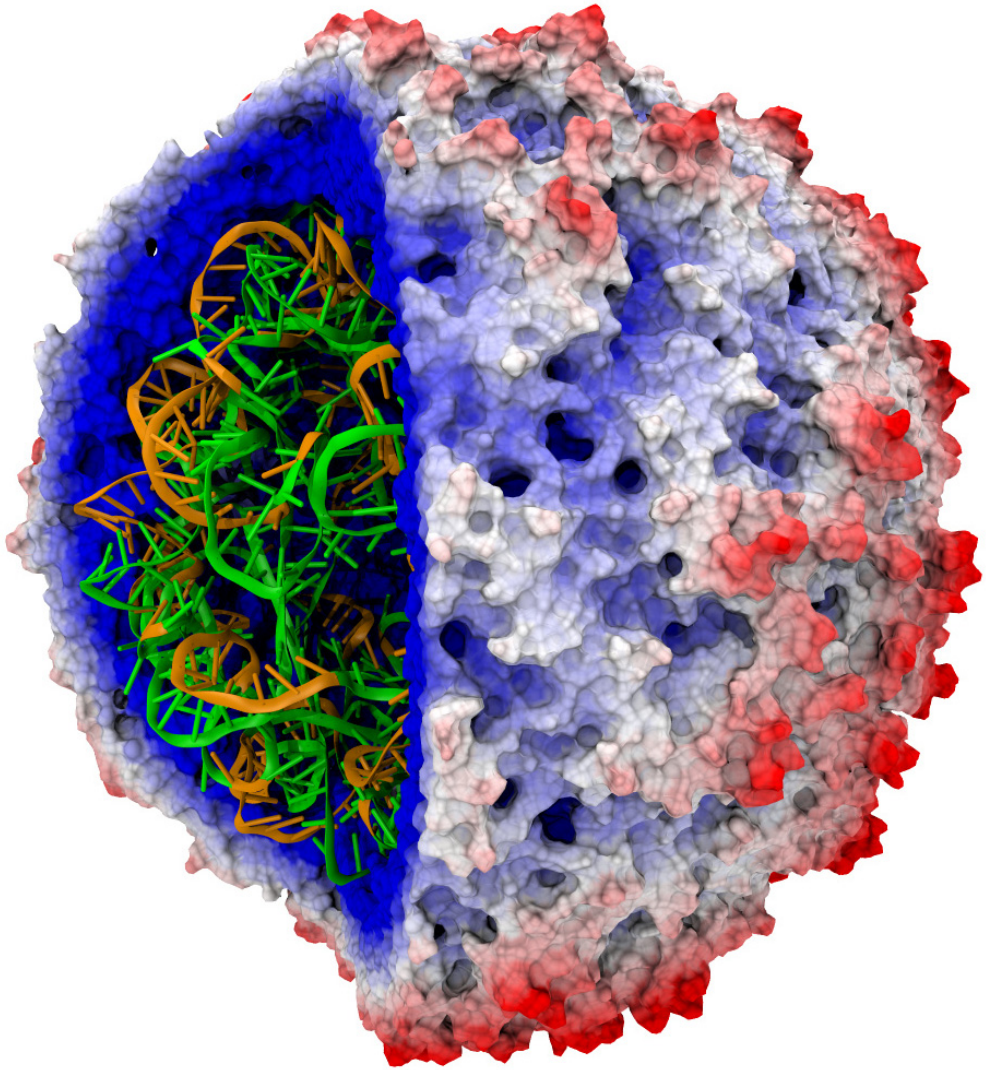
NAMD Overlapping Execution with Asynchronous CUDA kernels



GPU kernels are launched asynchronously, CPU continues with its own work, polling for GPU completion periodically. Forces needed by remote nodes are explicitly scheduled to be computed ASAP to improve overall performance.

Molecular Simulations: Virology

- Simulations lead to better understanding of the mechanics of viral infections
- Better understanding of infection mechanics at the molecular level may result in more effective treatments for diseases
- Since viruses are large, their computational “viewing” requires tremendous resources, in particular large parallel computers
- GPUs can significantly accelerate the simulation, analyses, and visualization of such structures



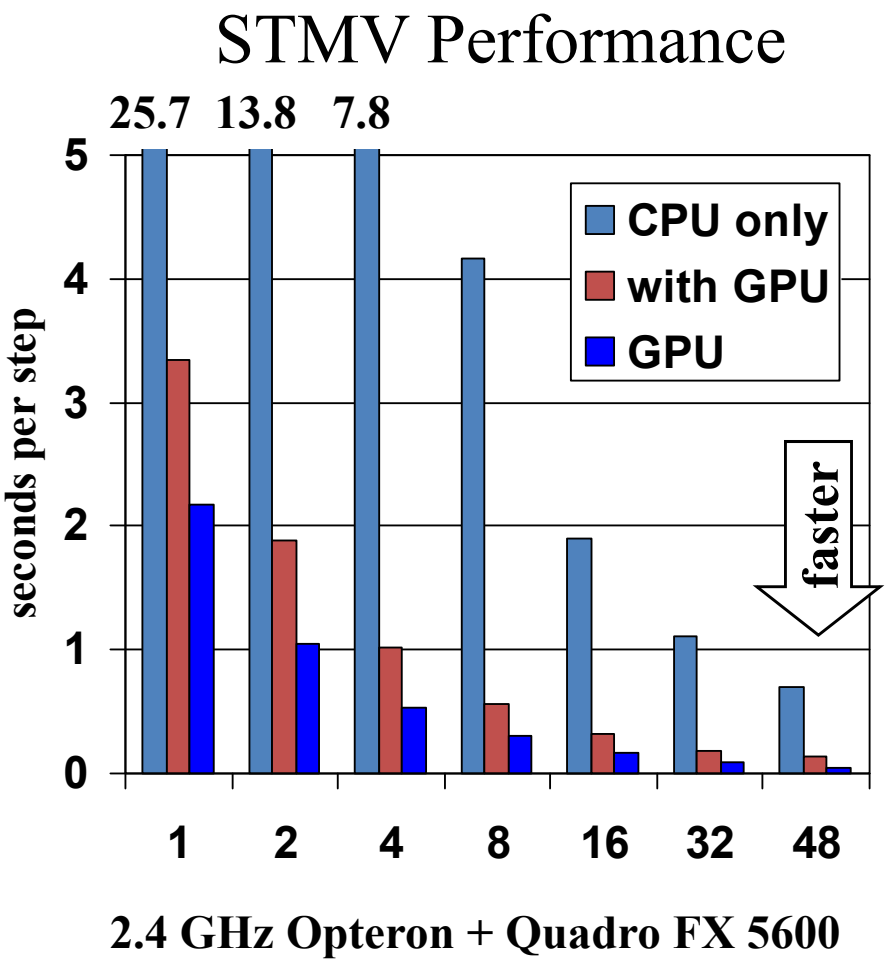
NAMD Performance on NCSA GPU Cluster, April 2008

CPU Cores & GPUs	4	8	16	32	60
GPU-accelerated performance					
Local blocks/GPU	13186	5798	2564	1174	577
Remote blocks/GPU	1644	1617	1144	680	411
GPU s/step	0.544	0.274	0.139	0.071	0.040
Total s/step	0.960	0.483	0.261	0.154	0.085
Unaccelerated performance					
Total s/step	6.76	3.33	1.737	0.980	0.471
Speedup from GPU acceleration					
Factor	7.0	6.9	6.7	6.4	5.5

STMV benchmark, 1M atoms,12A cutoff,
PME every 4 steps, running on
2.4 GHz AMD Opteron + NVIDIA Quadro FX 5600

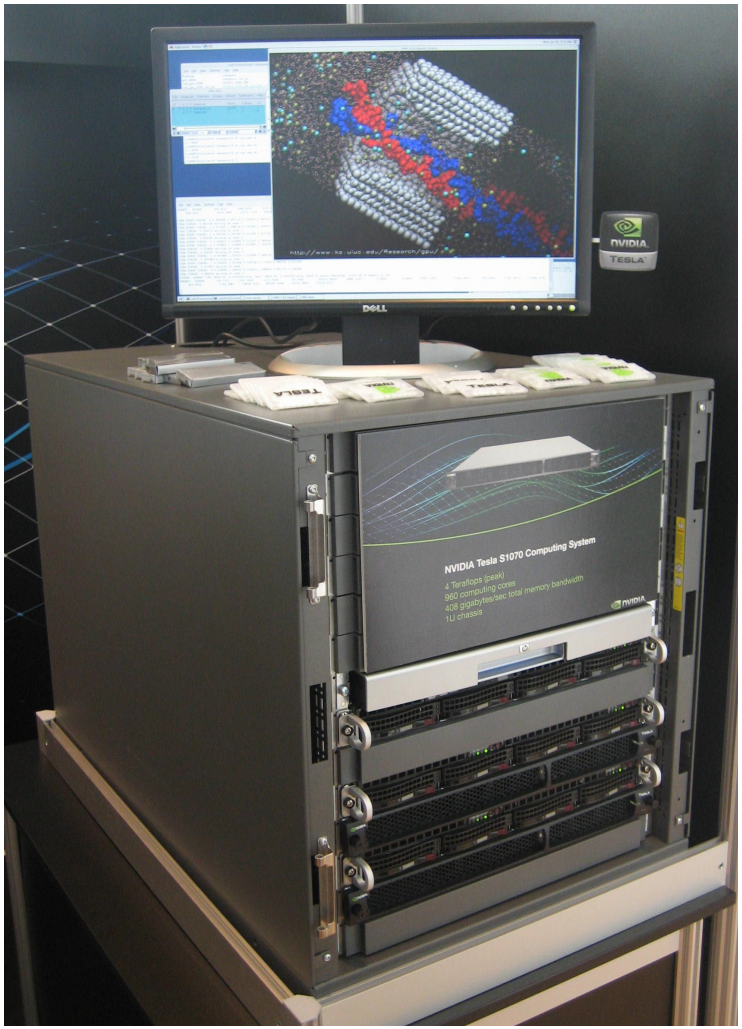
NAMD Performance on NCSA GPU Cluster, April 2008

- 5.5-7x overall application speedup w/ G80-based GPUs
- STMV virus (1M atoms)
- Overlap with CPU
- Off-node results done first
- Infiniband scales well
- Plans for better performance
  - Tune or port remaining work
  - Balance GPU load



NAMD Performance on GT200 GPU Cluster, August 2008

- 8 GT200s, 240 SPs @ 1.3GHz:
  - 72x faster than a single CPU core
  - 9x overall application speedup vs. 8 CPU cores
  - 32% faster overall than 8 nodes of G80 cluster
  - GT200 CUDA kernel is 54% faster
  - ~8% variation in GPU load
- Cost of double-precision for force accumulation is minimal: only 8% slower than single-precision



GPU Kernel Performance, May 2008

GeForce 8800GTX w/ CUDA 1.1, Driver 169.09

http://www.ks.uiuc.edu/Research/gpu/

Calculation / Algorithm	Algorithm class	Speedup vs. Intel QX6700 CPU core
Fluorescence microphotolysis	Iterative matrix / stencil	12x
Pairlist calculation	Particle pair distance test	10-11x
Pairlist update	Particle pair distance test	5-15x
Molecular dynamics non-bonded force calc.	N-body cutoff force calculations	10x 20x (w/ pairlist)
Cutoff electron density sum	Particle-grid w/ cutoff	15-23x
MSM short-range	Particle-grid w/ cutoff	24x
MSM long-range	Grid-grid w/ cutoff	22x
Direct Coulomb summation	Particle-grid	44x

Lessons Learned

- GPU algorithms need fine-grained parallelism and sufficient work to fully utilize the hardware
- Fine-grained GPU work decompositions compose well with the comparatively coarse-grained decompositions used for multicore or distributed memory programing
- Much of GPU algorithm optimization revolves around efficient use of multiple memory systems and latency hiding

Lessons Learned (2)

- The host CPU can potentially be used to “regularize” the computation for the GPU, yielding better overall performance
- Amdahl’s Law can prevent applications from achieving peak speedup with shallow GPU acceleration efforts
- Overlapping CPU work with GPU can hide some communication and unaccelerated computation

Ongoing and Future Work

- Visualization of multi-million atom biomolecular complexes
  - Migrate structural geometry and volumetric computations to the GPU
  - GPU accelerated ray tracing, ambient occlusion lighting, …
- GPU acceleration of long running molecular dynamics trajectory analyses
- More opportunities available than time to pursue them!

Acknowledgements

- Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
- Prof. Wen-mei Hwu, Chris Rodrigues, John Stratton, IMPACT Group, University of Illinois at Urbana-Champaign
- The CUDA team at NVIDIA
- NVIDIA, NCSA (GPU clusters)
- NIH support: P41-RR05969

Publications

http://www.ks.uiuc.edu/Research/gpu/

- Adapting a message-driven parallel application to GPU-accelerated clusters. J. Phillips, J. Stone, K. Schulten. *Proceedings of the 2008 ACM/IEEE Conference on Supercomputing, (in press)*
- GPU acceleration of cutoff pair potentials for molecular modeling applications. C. Rodrigues, D. Hardy, J. Stone, K. Schulten, W. Hwu. *Proceedings of the 2008 Conference On Computing Frontiers*, pp. 273-282, 2008.
- GPU computing. J. Owens, M. Houston, D. Luebke, S. Green, J. Stone, J. Phillips. *Proceedings of the IEEE*, 96:879-899, 2008.
- Accelerating molecular modeling applications with graphics processors. J. Stone, J. Phillips, P. Freddolino, D. Hardy, L. Trabuco, K. Schulten. *J. Comp. Chem.*, 28:2618-2640, 2007.
- Continuous fluorescence microphotolysis and correlation spectroscopy. A. Arkhipov, J. Hüve, M. Kahms, R. Peters, K. Schulten. *Biophysical Journal*, 93:4006-4017, 2007.