Accelerating Molecular Modeling using GPUs

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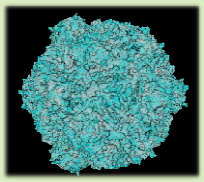
Motivation & Approach

Electrostatic Interactions

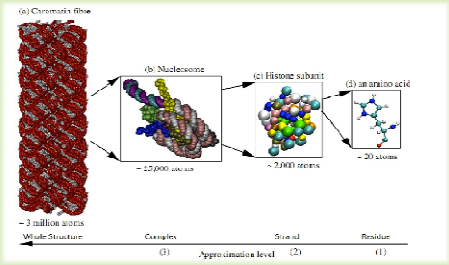
1. Critical to the analysis of
   - Biomolecular structure [1]
   - Biomolecular function
     - Ligand binding
     - Complex formation
     - Proton transport
2. Contribute to rational drug design.



Viral Capsid

Stopping AIDS Epidemic

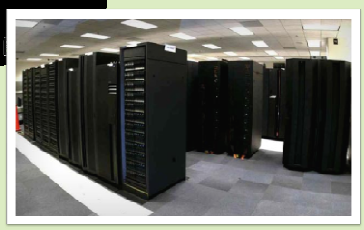
Approximation Levels for Biomolecules



Hierarchical Charge Partitioning (HCP)

- Our approach to electrostatic surface potential calculation [2].
  - An approximation algorithm that exploits the natural partitioning of biomolecules.
  - Certain benefits over particle-mesh Ewald (PME) and spherical cut-off methods.
  - Belongs to n-body class of problems, known to map extremely well on a GPU.

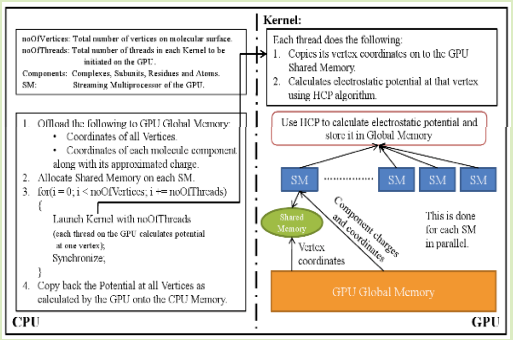
GTX 480
"Fastest commodity GPU in the world" for our electrostatics calculation



Roadrunner
3rd fastest supercomputer in the world, according to the TOP500 List [3]

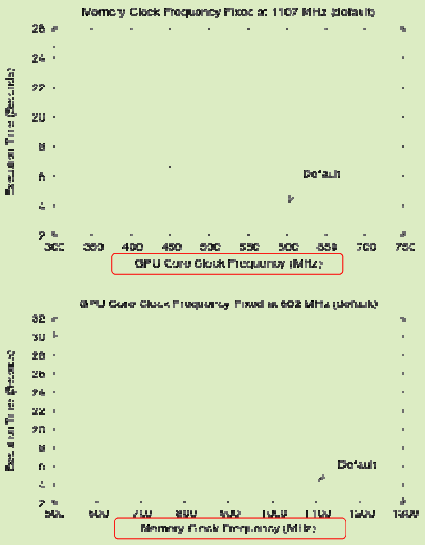
	GPU	Roadrunner
Cost	$350 - $450	$133M
Peak Performance	1.35 TFLOPS	1457 TFLOPS
Performance/Price Ratio	3857 MFLOPS/$	11 MFLOPS/$

Algorithmic Mapping



Mapping of HCP onto GPU

HCP on GPU: Memory Bound



High-Level Algorithmic Mapping

1. Determine the nature of the application
   - Memory bound or compute bound
2. Apply appropriate optimizations

Memory Optimizations for HCP on GPU

- Reduction of the # of kernel parameters per launch
- Reduction of the # of global load and store transactions via memory-access coalescing
- Judicious use of constant memory
- Optimized use of shared memory

Most Effective Optimization

- Optimized use of shared memory, as shown below

% Reduction in the Number of Global Memory Loads

Structure	Without HCP	With HCP
H Helix myoglobin	50%	32%
nucleosome core paricle	50%	62%
chaperonin GroEL	50%	84%
virus capsid	50%	96%

Next Most Effective Optimizations

- Reduction of the # of global load and store transactions via memory-access coalescing
  → 47% to 120% improvement in performance
- Judicious use of constant memory
  → 20% improvement in performance

Results

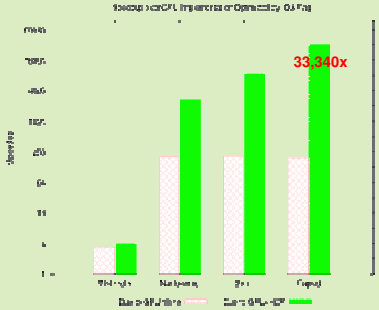
Four Different Structures

1. Mb.Hhelix 382 atoms
2. Nucleosome 25,086 atoms
3. 2eu1 109,802 atoms
4. Capsid 476,040 atoms

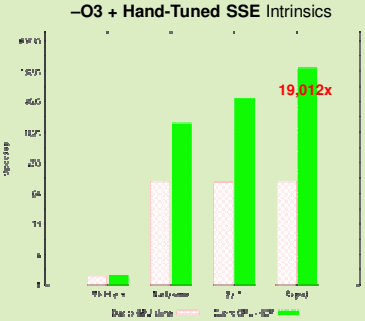
Compute Environment

- GPU: NVIDIA GTX 280
- CPU: Intel E8200 quad-core
- Memory: 4 GB

Speedup over CPU Optimized with **–O3**



Speedup over CPU Optimized with **–O3 + Hand-Tuned SSE** Intrinsics



Accuracy

Structure	Version	Relative RMSE
H helix myoglobin, 1MBO	CPU with HCP	0.215821
	GPU	0.000030
	GPU with HCP	0.236093
nucleosome core particle, 1KX5	CPU with HCP	0.022950
	GPU	0.000062
	GPU with HCP	0.022853
chaperonin GroEL, 2EU1	CPU with HCP	0.008799
	GPU	0.000042
	GPU with HCP	0.008816
virus capsid, 1A6C	CPU with HCP	0.015376
	GPU	0.000173
	GPU with HCP	0.015273

References

[1] M. Perutz, Electrostatic Effect in Proteins, 1978.
[2] R. Anandakrishnan and A.O. Onufriev, An N-log(N) Approximation Based on the Natural Organization of Biomolecules for Speeding Up the Computation of Long Range Interactions, *Journal of Computational Chemistry*, in press, 2009.
[3] The TOP500 List, http://www.top500.org/

Acknowledgements

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