Klaus Schulten
Department of Physics and Theoretical and Computational Biophysics Group
University of Illinois at Urbana-Champaign

GTC, San Jose Convention Center, CA | Sept. 20–23, 2010
GPU and the Computational Microscope

Investigation of drug (Tamiflu) resistance of the “swine” flu virus demanded fast response!

Accuracy • Speed-up • Unprecedented Scale
The Computational Microscope Views at Atomic Resolution...

...how living cells maintain health and battle disease
Our Microscope is Made of...

Chemistry

\[ U(\vec{R}) = \sum_{\text{bonds}} k_i^\text{bond}(r_i - r_0)^2 + \sum_{\text{angles}} k_i^\text{angle}(\theta_i - \theta_0)^2 + \sum_{\text{dihedrals}} k_i^\text{dihedral}[1 + \cos(n_i\phi_i + \delta_i)] + \sum_{\text{improper}} U^\text{improper} \]

Physics

\[ m_i \frac{d^2 \vec{r}_i}{dt^2} = \vec{F}_i = -\nabla U(\vec{R}) \]

Math

\[ \vec{r}_i(t + \Delta t) = 2\vec{r}_i(t) - \vec{r}_i(t - \Delta t) + \frac{\Delta t^2}{m_i} \vec{F}_i(t) \]

(repeat one billion times = microsecond)
Our Microscope is a “Tool to Think”

140,000 Registered Users

Physics
- Atomic coordinates

Genetics
- Ribosomes in whole cell

Graphics, Geometry
- VMD Analysis Engine

- HDL Lipoprotein particle
- 0.0 us

- T. Martinez, Stanford U.
Science 1: Poliovirus Infection

**How does this work?**
Answer requires 100 million atom long-time simulation
Science 1: Virus Capsid Mechanics
Atomic Force Microscope

— Hepatitis B Virus —

![Image of Hepatitis B Virus]

![Graph showing indentation vs. force with Experiment and Simulation data points]

- Force (pN)
- Indentation (Å)

-500 -400 -300 -200 -100 0 100 200 300 400 500
-40 -20 0 20 40 60

- Experiment
- Simulation
• Thousands of trajectory frames
• **1.5 hour** job reduced to **3 min**
• GPU Speedup: **25.5x**
• Per-node power consumption on NCSA GPU cluster:
  – CPUs-only: 448 Watt-hours
  – CPUs+GPUs: 43 Watt-hours
• Power efficiency gain: **10x**
Science 2: How Nature Harvesets Sun Light
95% of the energy in the biosphere comes from this energy source

Purple Photosynthetic Bacterium

Chromatophore (70 nm)

LIGHT

ADP

ATP

20

200

6

1
Science 2: How Nature Harvests Sun Light

Electrostatic field calculated with multilevel summation method

~10M atoms
Electrostatic field calculated with multilevel summation method

1 CPU core: 1 hr 10 min
3 GPUs (G80): ~90 seconds
GPU Solution 2: Multilevel Summation Method for Electrostatics on the GPU

Multilevel summation method has linear time complexity well suited for GPUs; more flexible than other methods.
Science 3: How Proteins are Made from Genetic Blueprint

- **Ribosome** — Decodes genetic information from mRNA
- Important target of many antibiotics
- Static structures of crystal forms led to 2009 Nobel Prize
- But one needs structures of ribosomes in action!
Science 3: How Proteins Are Made from Genetic Blueprint

Low-resolution Data

High-resolution Structure

Close-up of Nascent Protein
GPU Solution 3: Molecular Dynamics Simulations

Molecular dynamics simulation of protein insertion process

NCSA Lincoln Cluster performance (8 Intel cores and 2 NVIDIA Tesla GPUs per node, 1 million atoms)

GPUs reduced time for simulation from two months to two weeks!
Science 4: Nanopore Sensors

**Genetics:** Genes control our bodies and experiences!

**Epigenetics:** Our bodies and experiences control the genes!

Epigenetics made possible through DNA methylation

- Related pathologies: obesity, depression, cancer
New materials, new problems: Nanoprecipitation

Radial distribution functions identify nanoprecipitation

nanoprecipitation of ions

Precipitate

Liquid
GPU Solution 4: Computing Radial Distribution Functions

- 4.7 million atoms
- 4-core Intel X5550 CPU: **15 hours**
- 4 NVIDIA C2050 GPUs: **10 minutes**
- Fermi GPUs ~3x faster than GT200

GPUs: larger on-chip shared memory

![Graph showing comparison of computing times for different architectures](image)

- **Faster**

![Graph showing Radial Distribution Functions](image)
Science 5: Quantum Chemistry Visualization

• Chemistry is the result of atoms sharing electrons
• Electrons occupy “clouds” in the space around atoms
• Calculations for visualizing these “clouds” are costly: tens to hundreds of seconds on CPUs – non-interactive
• GPUs enable the dynamics of electronic structures to be animated interactively for the first time

Taxol: Cancer Drug
VMD enables interactive display of QM simulations, e.g. Terachem, GAMESS
Science 5: Quantum Chemistry Visualization

Rendering of electron “clouds” achieved on GPUs as quickly as you see this movie! CPUs: One working day!

Simulation: Terachem Interactive Visualization: VMD
Courtesy T. Martinez, Stanford
GPU Solution 5: Computing $C_{60}$ Molecular Orbitals

<table>
<thead>
<tr>
<th>Device</th>
<th>CPUs, GPUs</th>
<th>Runtime (s)</th>
<th>Speedup</th>
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</table>

3-D orbital lattice: millions of points

Lattice slices computed on multiple GPUs

2-D CUDA grid on one GPU

CUDA thread blocks

GPU threads each compute one point
Science 6: Protein Folding

• Protein **misfolding** responsible for diseases:
  – Alzheimer’s
  – Parkinson’s
  – Huntington
  – Mad cow
  – Type II diabetes
  – ...

Observe folding process in unprecedented detail
Science 6: Protein Folding

• Some simulations still fail to fold proteins due to inaccurate modeling of interatomic forces!
• Protein folding demands more accurate model which leads to more expensive computation
GPU Solution 6: Computing More Accurate Simulation Models

- Atomic polarizability increases computation by 2x...
- ...but, the additional computations are perfectly suited to the GPU!
- For now, NAMD calculates atomic polarizability on CPUs only...soon we will also use GPUs

NAMD CPU performance scaling

Atomic polarizability of water, highly accurately simulated through additional particles (shown in green)
Since our technique is a native GPU algorithm, no optimized CPU version exists by which to measure its performance.

<table>
<thead>
<tr>
<th>Calculation</th>
<th>FX5600</th>
<th>GTX280</th>
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<tr>
<td>Total</td>
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2010 Workshop on GPU Computing for Molecular Modeling

- Spread the benefits of GPU computing to solve new problems in molecular modeling
- Intensive 2-day workshop after 1-week GPU workshop at NCSA
- Participants present their work and exchange ideas and GPU solutions
Three of our GPU Heroes

Our GPU Biomedical Science Computing Goals:

– More accurate simulations
– Speed-up: simulations now take minutes instead of weeks
– Make previously unreachable scales accessible

Acknowledgements

• Theoretical and Computational Biophysics Group, University of Illinois at Urbana-Champaign
• Wen-mei Hwu and the IMPACT group at University of Illinois at Urbana-Champaign
• L. Kale and the Center for Parallel Computing at University of Illinois at Urbana-Champaign
• NVIDIA CUDA Center of Excellence, University of Illinois at Urbana-Champaign
• Ben Levine, Axel Kohlmeyer at Temple University
• NCSA Innovative Systems Lab
• The CUDA team at NVIDIA
• Zan Luthey-Schulten and Elija Roberts (E. coli whole cell simulations)
• NIH support: P41-RR05969
Thank You