Introduction and Welcome

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

Workshop on GPU Programming for Molecular Modeling , University of Illinois at Urbana-Champaign, August 6, 2010

Announcements and Reminders

- Hotel provides continental breakfast: make sure you eat before you arrive on Saturday and Sunday mornings.
- Lunch: will be provided on Saturday (Pizza) and Sunday (Jimmy John's)
- Saturday dinner: Ad hoc

Announcements and Reminders (2)

- Please arrive between 8:30am and 9:00am on Sat./Sun. so we can start on time
- Let us know if you do not have an account on the NCSA GPU cluster or have trouble accessing it and we will make other arrangements for your lab time access.
- Please use the provided ethernet cable or WiFi to access the internet.
- The workshop agenda page has been updated with new links to CUDA and OpenCL example code, and PDFs of relevant papers and book chapters.

Overview of Daily Agenda

- Lectures are intended to be in an informal format. Questions are welcome at any time!
- Participant presentations and discussions are intended to be in an informal "clinic" format, where we learn about each participant's problem and discuss potential GPU solutions.
- You may use scheduled lab time and any other free time to work on your own projects on the GPU cluster.

Introductions

- Everyone introduce yourself and tell us:
  - Your name and institution
  - Length of time and level of experience you have working with CUDA or OpenCL so far
  - What do you hope to learn from this workshop?
  - Any topics from VSCSE workshop that you would like to know more about?

Participant Presentations, Group Discussions, GPU "clinic"

- Friday night (tonight after opening lecture)
- Saturday afternoon
- Sunday afternoon

- Any unused presentation time will be used to allow participants extra "lab" time.

A Brief Introduction to GPU Computing in Molecular Modeling

John Stone

Programmable Graphics Hardware

Groundbreaking research systems:

AT&T Pixel Machine (1989):

82 x DSP32 processors

UNC PixelFlow (1992-98):

64 x (PA-8000 +

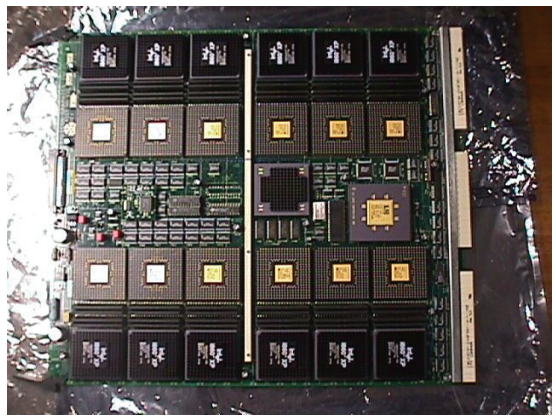
8,192 bit-serial SIMD)

SGI RealityEngine (1990s):

Up to 12 i860-XP processors perform vertex operations (*u*code), fixed-func. fragment hardware

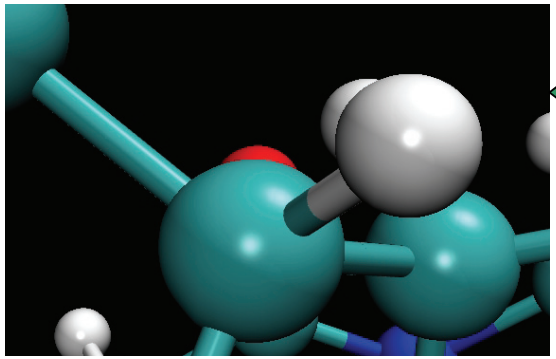
All mainstream GPUs now incorporate fully programmable processors

UNC PixelFlow Rack



SGI Reality Engine i860 Vertex Processors

GLSL Sphere Fragment Shader



- Written in OpenGL Shading Language
- High-level C-like language with vector types and operations
- Compiled dynamically by the graphics driver at *runtime*
- Compiled machine code executes on GPU

```
//
// VMD Sphere Fragment Shader (not for normal geometry)
//
void main(void) {
  vec3 raydir = normalize(V);
  vec3 spheredir = spherepos - rayorigin;

  // Perform ray-sphere intersection tests based on the code in Tachyon
  float b = dot(raydir, spheredir);
  float temp = dot(spheredir, spheredir);
  float disc = b*b + sphereradsq - temp;

  // only calculate the nearest intersection, for speed
  if (disc <= 0.0)
    discard; // ray missed sphere entirely, discard fragment

  // calculate closest intersection
  float tnear = b - sqrt(disc);

  if (tnear < 0.0)
    discard;

  // calculate hit point and resulting surface normal
  vec3 pnt = rayorigin + tnear * raydir;
  vec3 N = normalize(pnt - spherepos);

  // Output the ray-sphere intersection point as the fragment depth
  // rather than the depth of the bounding box polygons.
  // The eye coordinate Z value must be transformed to normalized device
  // coordinates before being assigned as the final fragment depth.
  if (vmdprojectionmode == 1) {
    // perspective projection = 0.5 + (hfpn + (f * n / pnt.z)) / diff
    gl_FragDepth = 0.5 + (vmdprojparms[2] + (vmdprojparms[1] * vmdprojparms[0
3];
  } else {
    // orthographic projection = 0.5 + (-hfpn - pnt.z) / diff
    gl_FragDepth = 0.5 + (-vmdprojparms[2] - pnt.z) / vmdprojparms[3];
  }

#ifdef TEXTURE
  // perform texturing operations for volumetric data
  // The only texturing mode that applies to the sphere shader
```

Origins of Computing on GPUs

- Widespread support for programmable shading led researchers to begin experimenting with the use of GPUs for general purpose computation, “GPGPU”
- Early GPGPU efforts used existing graphics APIs to express computation in terms of drawing
- As expected, expressing general computation problems in terms of triangles and pixels and “drawing the answer” is obfuscating and painful to debug…
- Soon researchers began creating dedicated GPU programming tools, starting with Brook and Sh, and ultimately leading to a variety of commercial tools such as RapidMind, CUDA, OpenCL, and others...

GPU Computing

- Commodity devices, omnipresent in modern computers (over a **million** sold per **week**)
- Massively parallel hardware, hundreds of processing units, throughput oriented architecture
- Standard integer and floating point types supported
- 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 data-parallel work decomposition

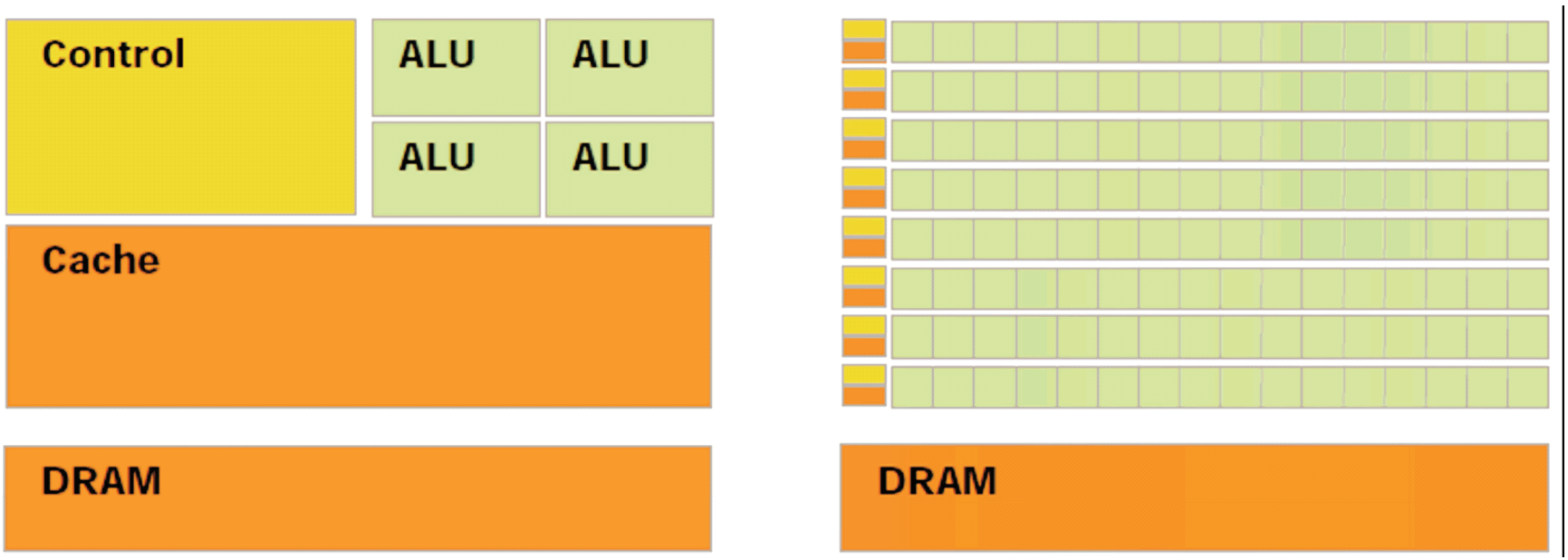
What Speedups Can GPUs Achieve?

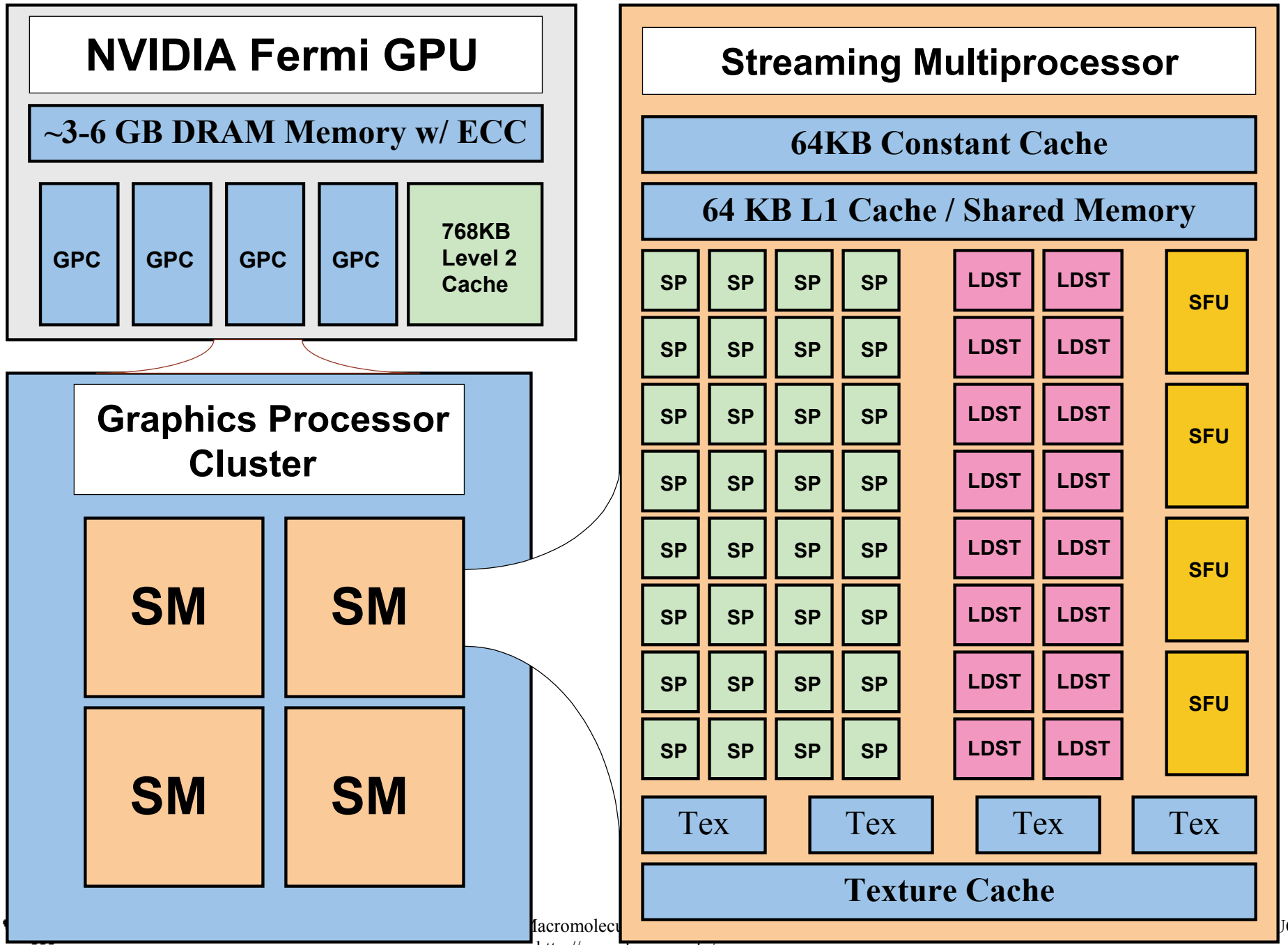
- Single-GPU speedups of **10x** to **30x** vs. one CPU core are common
- Best speedups can reach **100x** or more, attained on codes dominated by floating point arithmetic, especially native GPU machine instructions, e.g. expf(), rsqrtf(), …
- Amdahl's Law can prevent legacy codes from achieving peak speedups with shallow GPU acceleration efforts

Comparison of CPU and GPU Hardware Architecture

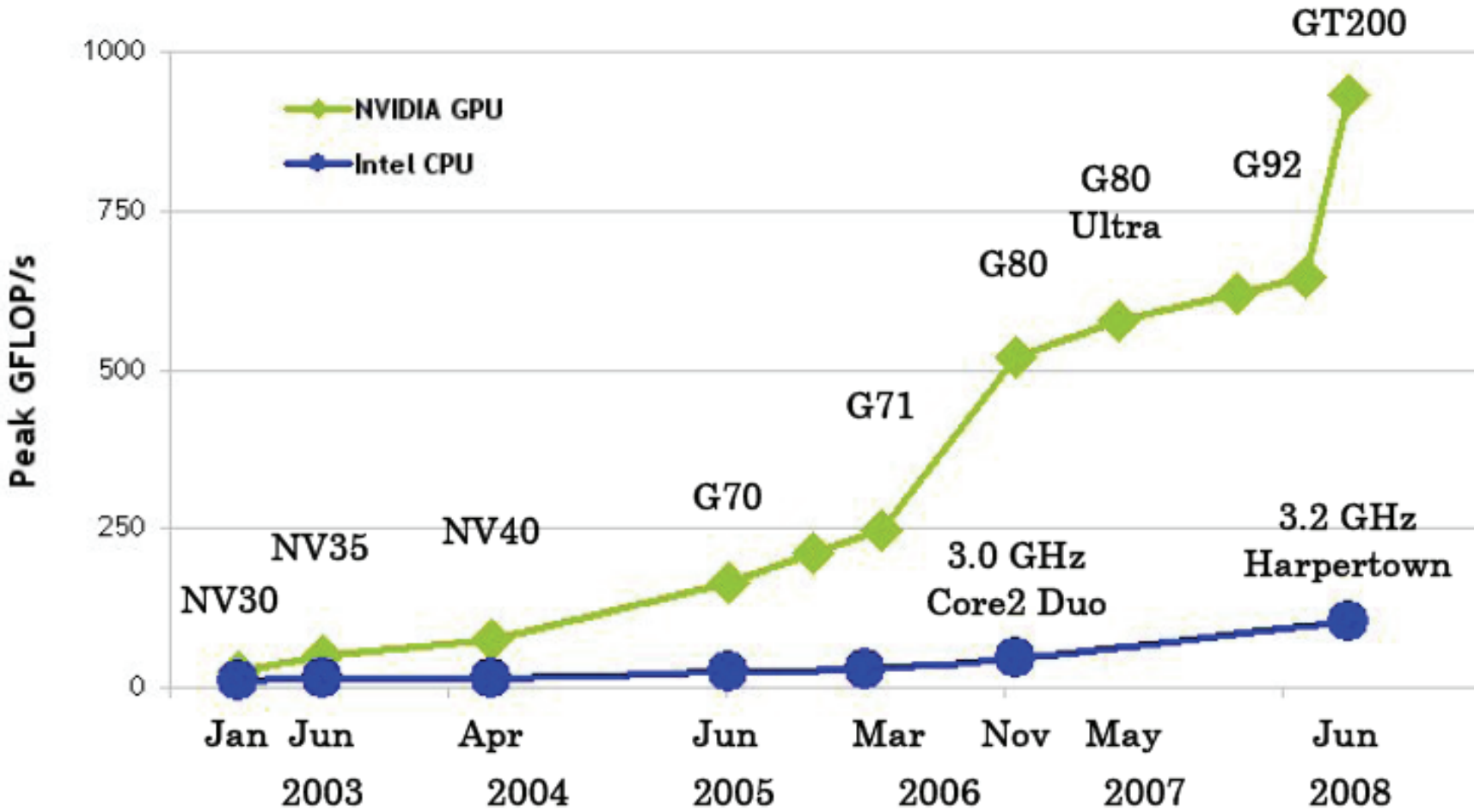
CPU: Cache heavy, focused on individual thread performance

GPU: ALU heavy, massively parallel, throughput oriented

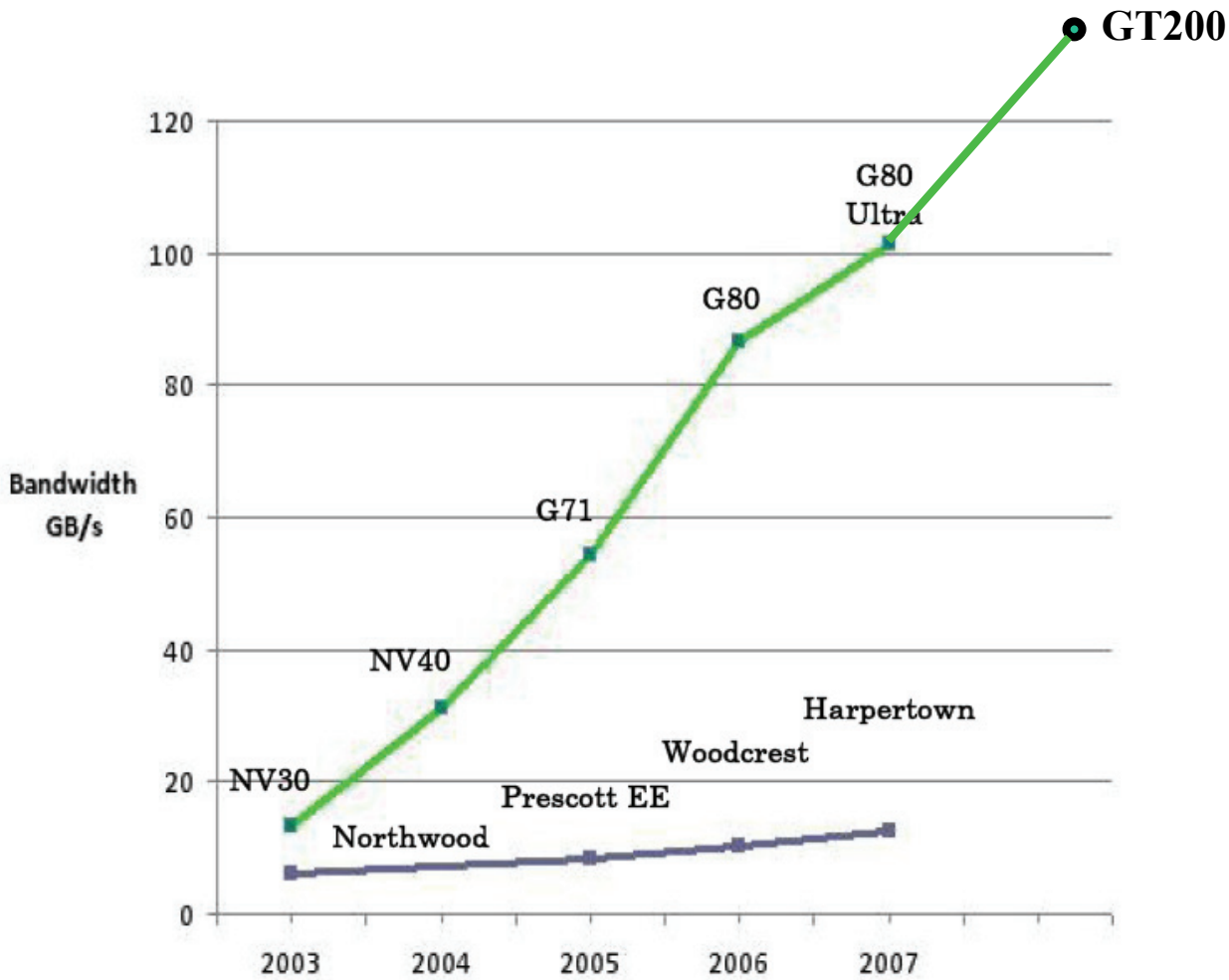



NVIDIA Fermi GPU
~3-6 GB DRAM Memory w/ ECC
GPC
GPC
GPC
GPC
768KB Level 2 Cache
Graphics Processor Cluster
SM
SM
SM
SM
Streaming Multiprocessor
64KB Constant Cache
64 KB L1 Cache / Shared Memory
SP
LDST
SFU
Tex
Texture Cache

GPU Peak Single-Precision Performance: **Exponential Trend**



GPU Peak Memory Bandwidth: **Linear Trend**

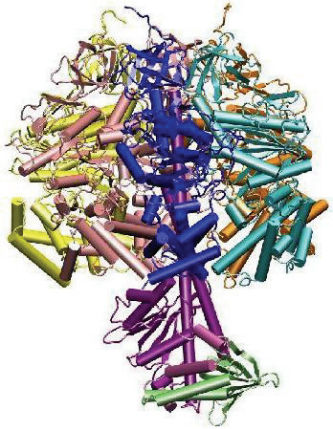


Examples of GPU Accelerated Molecular Modeling Applications

- Molecular dynamics
- Quantum chemistry
- Docking
- Molecular visualization
- MD trajectory analysis
- Simulation preparation
- Many more, see mini-review:
  "GPU-accelerated molecular modeling coming of age"
  (posted on workshop web site)

NAMD: Parallel Molecular Dynamics

2002 Gordon Bell Award



ATP synthase

PSC Lemieux

34,000 Users, 1200 Citations

Computational Biophysics Summer School

Blue Waters Target Application

Illinois Petascale Computing Facility

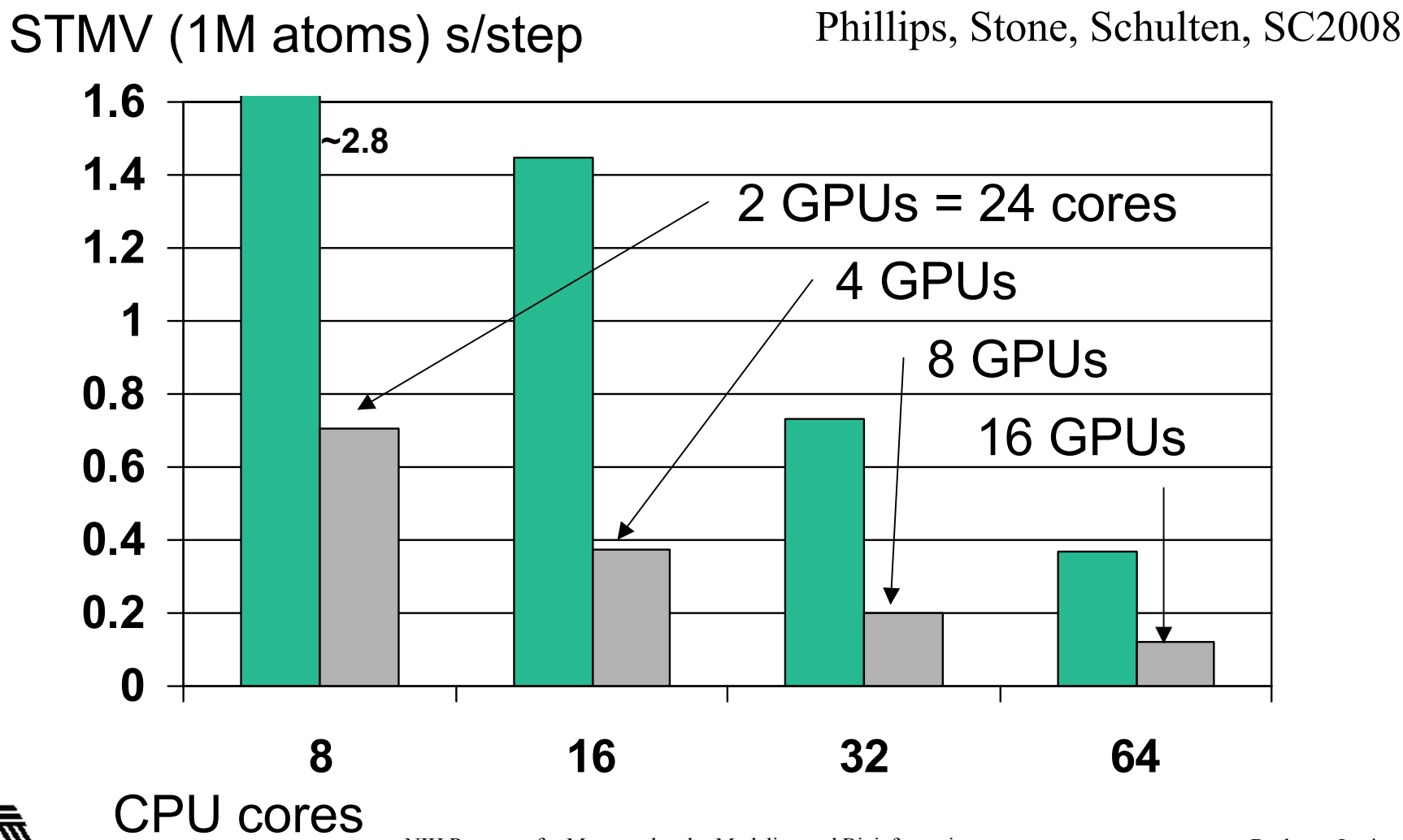
GPU Acceleration

NVIDIA Tesla

NCSA Lincoln

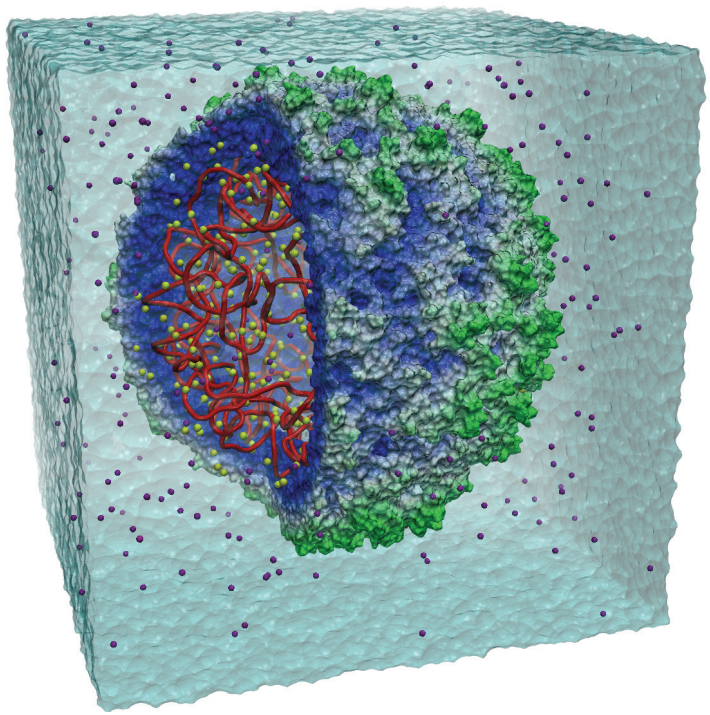
NCSA Lincoln Cluster Performance

(8 Intel cores and 2 NVIDIA Telsa GPUs per node)



NAMD 2.7b3 w/ CUDA Released

- CUDA-enabled NAMD binaries for 64-bit Linux are available on the NAMD web site now!
  http://www.ks.uiuc.edu/Research/namd/2.7b3/announce.html
- Direct download link:
  http://www.ks.uiuc.edu/Development/Download/download.cgi?PackageName=NAMD

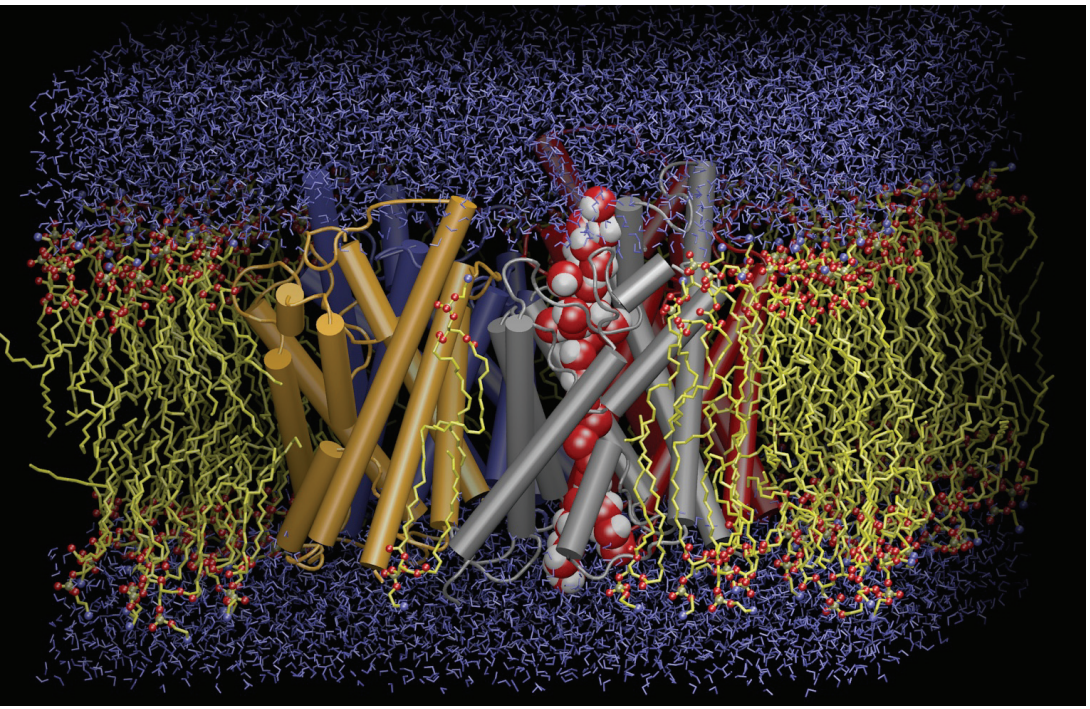


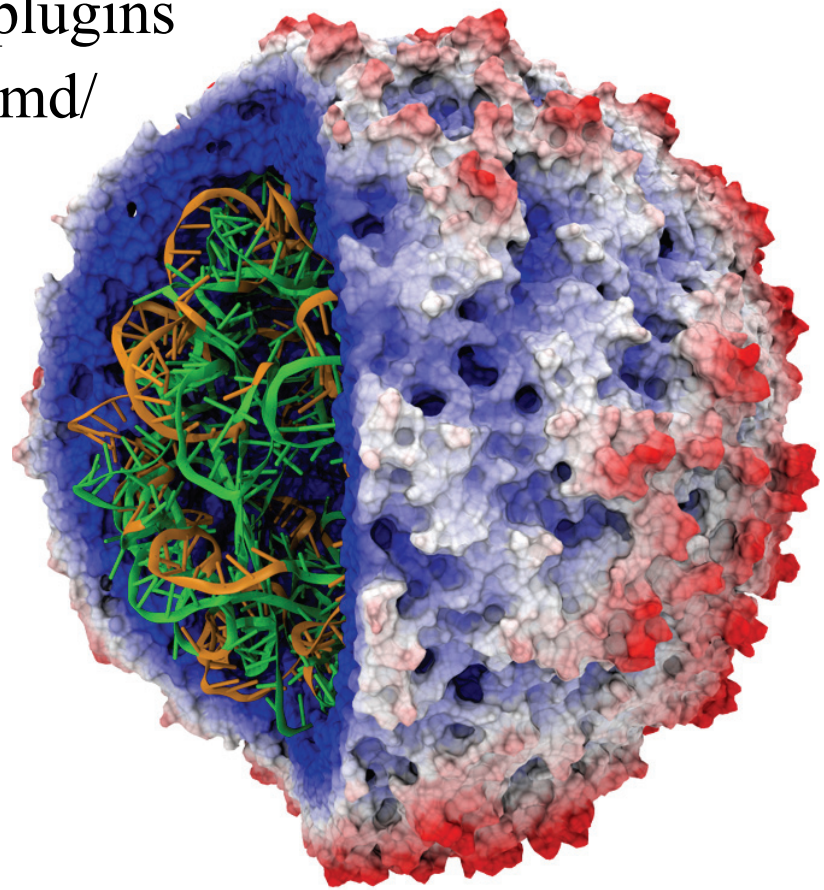
National Center for Research Resources

Beckman Institute, UIUC

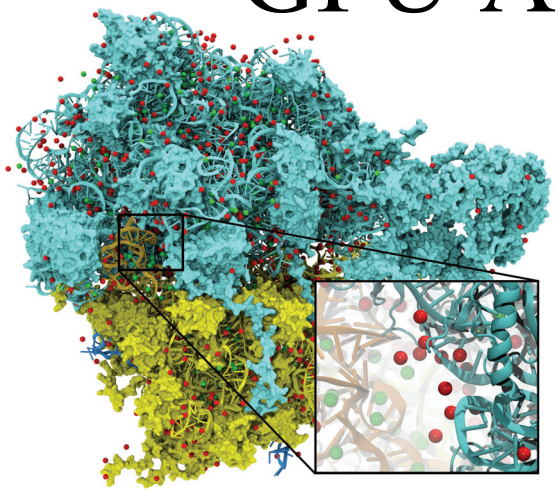
VMD – "Visual Molecular Dynamics"

- Visualization and analysis of molecular dynamics simulations, sequence data, volumetric data, quantum chemistry calculations, particle systems, …
- User extensible with scripting and plugins
- http://www.ks.uiuc.edu/Research/vmd/



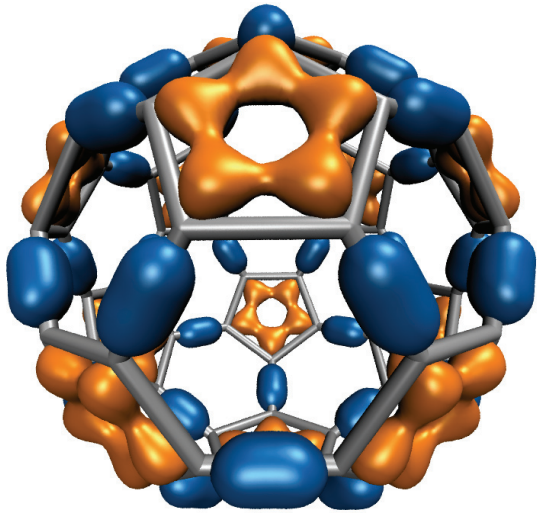


GPU Acceleration in VMD 1.8.7



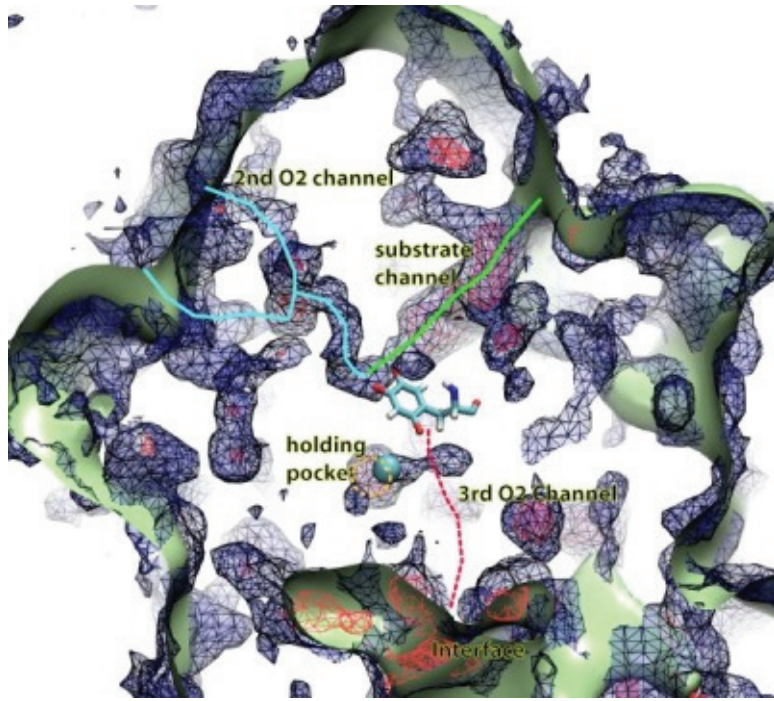
Electrostatic field calculation, ion placement

20x to 44x faster



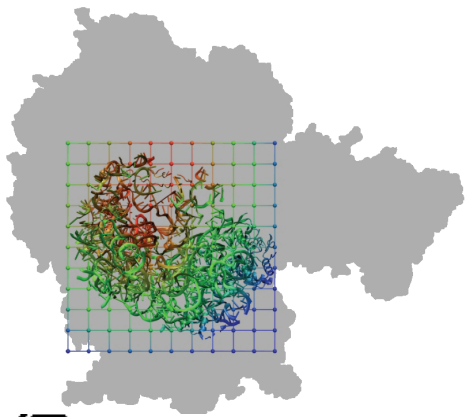
Molecular orbital calculation and display

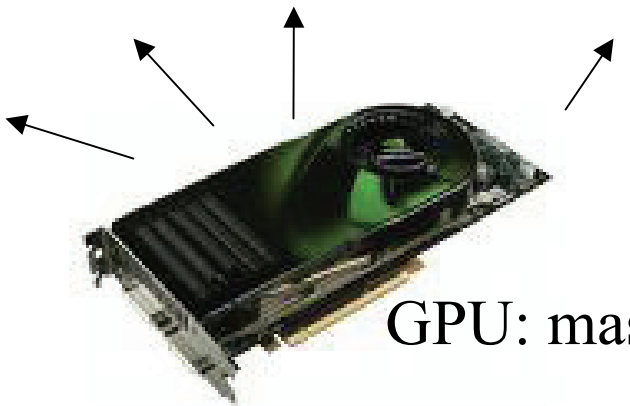
100x to 120x faster



Imaging of gas migration pathways in proteins with implicit ligand sampling

20x to 30x faster





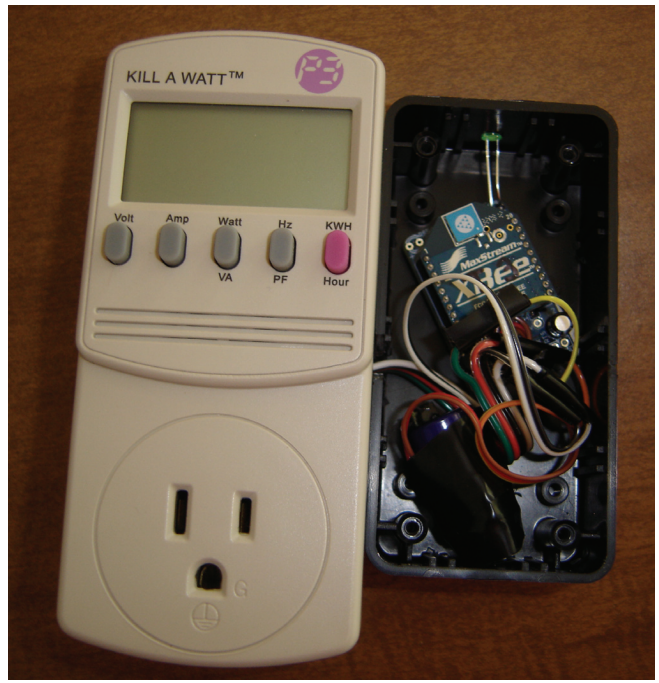
GPU: massively parallel co-processor

Motivation for GPU Acceleration in VMD

- Increases in supercomputing resources at NSF centers such as NCSA enable increased simulation complexity, fidelity, and longer time scales…
- Drives need for more visualization and analysis capability at the desktop and on clusters
- Desktop use is the most compute-limited scenario, where **GPUs can make a big impact**…
- GPU acceleration provides an opportunity to make some **slow, or batch** calculations capable of being run **interactively, or on-demand…**

Trajectory Analysis on GPU Cluster with MPI-enabled VMD

- Short time-averaged electrostatic field test case (few hundred frames, 700,000 atoms)
- 1:1 CPU/GPU ratio
- Power measured on a single node w/ NCSA monitoring tools
- CPUs-only: 1465 sec, 299 watts
- CPUs+GPUs: 57 sec, 742 watts
- Speedup 25.5 x
- Power efficiency gain: 10.5 x



NCSA Tweet-a-watt power monitoring device

Acknowledgements

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