General Purpose Computation on Graphics Processors (GPGPU)

Mike Houston, Stanford University

A little about me

- http://graphics.stanford.edu/~mhouston
- Education:
  - UC San Diego, Computer Science BS
  - Stanford University, Computer Science MS
  - Currently a PhD candidate at Stanford University
- Research
  - Parallel Rendering
  - High performance computing
    - Sequoia
  - Computation on graphics processors (GPGPU)
    - Brook, Folding@Home (GPU)

The world changed over the last year…

- Multiple GPGPU initiatives
  - Vendors without GPGPU talking about it
- A few big apps:
  - Game physics
  - Folding@Home
  - Video processing
  - Finance modeling
  - Biomedical
  - Real-time image processing
- Courses
  - UIUC – ECE 498
  - Supercomputing 2006
  - SIGGRAPH 2006/2007
- Lots of academic research
- Actual GPGPU companies
  - PeakStream
  - RapidMind
  - Accelware
  - …

What can you do on GPUs other than graphics?

- Large matrix/vector operations (BLAS)
- Protein Folding (Molecular Dynamics)
- Finance modeling
- FFT (SETI, signal processing)
- Ray Tracing
- Physics Simulation [cloth, fluid, collision,…]
- Sequence Matching (Hidden Markov Models)
- Speech/Image Recognition (Hidden Markov Models, Neural nets)
- Databases
- Sort/Search
- Medical Imaging (image segmentation, processing)
- And many, many, many more…

GPGPU

http://www.gpgpu.org

Why use GPUs?

- Commodity off the shelf (COTS)
  - In every machine
- Performance
  - Intel Core2 Duo
    - 48 GFLOPS peak
    - 10 GB/s to main memory
  - AMD HD2900XT
    - 475 GFLOPS peak
    - 100 GB/s to video memory
- Lots of Perf/Watt and Perf/$

Rolling your own GPGPU apps

- Lots of information on GPGPU.org
- Use graphics APIs (old way)
- High level languages and systems to make GPGPU easier
  - PeakStream
  - RapidMind
  - Brook
  - CUDA
- Mid-level
  - CTM (CAL)
- Low-level
  - Full control over hardware – CTM (HAL)

GPGPU/Streaming Languages

- Why do you want them?
  - Make programming GPUs easier!
    - Don't need to know OpenGL, DirectX, or ATI/NV extensions
    - Simplify common operations
    - Focus on the algorithm, not on the implementation
- PeakStream
  http://www.peakstreaminc.com
- RapidMind
  Commercial follow-on to Sh
  http://www.rapidmind.net
- Accelerator
  - Microsoft Research
  http://research.microsoft.com/downloads
- Brook
  - Stanford University
  http://brook.sourceforge.net
- CUDA
  - NVIDIA
- CTM
  - AMD

BrookGPU

- History
  - Developed at Stanford University
  - Goal: allow non-graphics users to use GPUs for computation
  - Lots of GPGPU apps written in Brook
- Design
  - C based language with streaming extensions
  - Compiles kernels to DX9, OpenGL, CTM
  - Runtimes (DX9/OpenGL/CTM) handle GPU interaction
- Used for Folding@Home GPU code
  - Large, real application

Streams

- Collection of records requiring similar computation
  - particle positions, voxels, FEM cell, …

```
Ray r<200>;
float3 velocityfield<100,100,100>;
```

- Similar to arrays, but…
  - index operations disallowed: `position[i]`
  - read/write stream operators

```
streamRead (r, r_ptr);
streamWrite (velocityfield, v_ptr);
```

Kernels

- Functions applied to streams
  - similar to for_all construct
  - no dependencies between stream elements

```
kernel void foo (float a<>, float b<>,
                 out float result<>) {
  result = a + b;
}

float a<100>;
float b<100>;
float c<100>;

foo(a,b,c);
```

```
for (i=0; i<100; i++)
      c[i] = a[i]+b[i];
```

Kernels

- Kernel arguments
  - input/output streams

```
kernel void foo (float a<>,
                 float b<>,
                 out float result<>) {
   result = a + b;
}
```

Kernels

- Kernel arguments
  - input/output streams
  - gather streams

```
kernel void foo (..., float array[] ) {
      a = array[i];
}
```

Kernels

- Kernel arguments
  - input/output streams
  - gather streams
  - constant parameters

```
kernel void foo (..., float c ) {
      a = c + b;
}
```

Brook for GPUs

- Open source - Sourceforge
  - CVS tree *much* more up to date (includes CTM support)
- Project Page
  - http://graphics.stanford.edu/projects/brook
- Source
  - http://www.sourceforge.net/projects/brook
- **Paper:**

Brook for GPUs: Stream Computing on Graphics Hardware

Ian Buck, Tim Foley, Daniel Horn, Jeremy Sugerman, Kayvon Fatahalian, Mike Houston, Pat Hanrahan

Fly-fishing fly images from The English Fly Fishing Shop

PeakStream

- http://www.peakstreaminc.com
- C/C++ library based
- Extended operators
  - Array constructs
- Just-in-time compilation/optimization
  - Really amazing vectorization and scheduling
- Fairly easy switch for Fortan/Matlab users
- GPUs and multi-core

RapidMind

- http://www.rapidmind.net/
- Embedded within Standard C++
  - No new tools, compilers, preprocessors, etc.
- Portable core
  - Exposes platform specific functionality to also allow tuning for specific platforms
- Integrates with existing programming models
  - Wrap your compute heavy code in extensions
  - Leave rest of the code alone
- GPUs, multi-core, Cell

CUDA - NVIDIA

- C with extensions/limitations
- Similar to Brook, but better matched to G80 hardware
- Complete toolchain
  - Compiler/profiler/debugger
- Standard provided libraries
  - BLAS, FFT
- Support for G80+
- Programmer's guide and lots of hardware information available

- Exposed hardware traits
  - Shared memory
  - Multiple memory levels
  - Register limits
- Data-parallel + multi-threading
  - Exposes the steaming model as data-parallel at the top
  - Exposes multi-threading at the bottom
    - Threads/Warps/Blocks

AMD CTM

- HAL – low level
  - Streaming processor ISA
  - Command buffer control
  - Full memory layout
    - Tiling
    - Addressing
  - Full processor scheduling
- Basically a low level driver interface

- CAL – mid level
  - Stream processor compilers
    - HLSL/PS3/PS4
  - Command buffer assistance
  - Memory management
    - Allocation
    - Layout
  - Multi-GPU handling
- Similar to DX/GL GPGPU programming but semantics to match computation and without the overheads of graphics APIs

AMD + Stream Processing Future

- Brook
  - AMD actively supporting CTM Brook backend for R5XX/R6XX
- CTM – CAL is open platform
  - http://sourceforge.net/projects/amdctm
  - Sits atop HAL for each target
- Streaming extensions to current programming languages
  - Brook-like at first, then expanding
- Multiple platforms
  - GPUs and multi-core with same abstraction through CAL
- Support multiple abstraction levels
  - High-level – Brook support and streaming extensions to standard languages
  - Mid-level (CAL) – memory management, command buffers, etc
  - Low-level (HAL) – direct access to hardware, including ISA

Sequoia – Programming the memory system

- Hierarchical stream programming
  - Similar to multi-level Brook
  - Performance is about programming the memory system
    - Compute is “free”
    - Fast application have data locality at all levels
- We can run on “difficult” systems
  - Cell/PS3
  - Clusters
  - Multi-core/SMP
  - Cluster of Cells in SMP
- http://sequoia.stanford.edu

GPGPU and the HD 2900XT

GPGPU on the HD 2900XT

- 32-bit floating point
  - Tighter IEEE conformance compared to last generation
  - ½ ULP on MUL/ADD,

    1 ULP on MAD
  - Denorm/underflow treated as 0
  - No exception support
- Integer support
  - Much more natural stream addressing
- Scalar floating-point engines
  - 320 of them
- Long programs
  - No instruction limits (up to available memory)
- Branching and Looping
  - Low overhead branching and looping
  - Fine branch granularity:

    ~64 fragments

GPGPU on the HD 2900XT, cont.

- Advanced memory controller
  - Latency hiding for streaming reads and writes to memory
    - With enough math ops you can hide all memory access!
  - Large bandwidth improvement over previous generation
    - Fetch4 performance without the pain
- Large memory addressing
  - 40-bit address space
- Faster upload/download
  - DMA engine

GPGPU on the HD 2900XT, cont.

- Read/Write cache
  - 8KB of on-chip storage
  - Spill to memory
  - Lots of interesting uses
    - Reduction buffer
    - Unlimited writes
    - Register spill
    - …
- Flexibility
  - Unlimited texture reads
  - Scalar engines
  - ***Lots*** of latency hiding
  - Heavy register usage without penalty
    - Fewer threads in flight, but you should have more math

Performance basics for GPGPU – HD 2900XT

- Compute (DX/CTM)
  - 470 GFLOPS (MAD – observed)
    - No games, just a giant MAD kernel
- Offload to GPU (DX)
  - Readback (GPU→CPU): 1.4 GB/s
  - Download (CPU→GPU): 2.4GB/s
- Branch granularity (DX/CTM)
  - ~64 threads

- Memory (CTM)
  - 180 GB/s cache bandwidth
  - 60 GB/s streaming bandwidth
  - 8 GB/s random access
  - 1 cycle latency for a float4 fetch (cache hit)

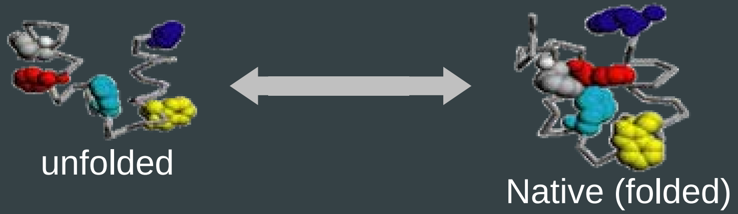
    4 cycle latency for a float4 fetch (streaming)

    1 cycle = 5 four-way MADs

Folding@Home

What is protein folding

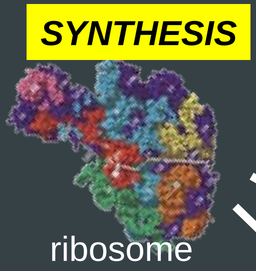
Protein folding: a fundamental biophysical problem

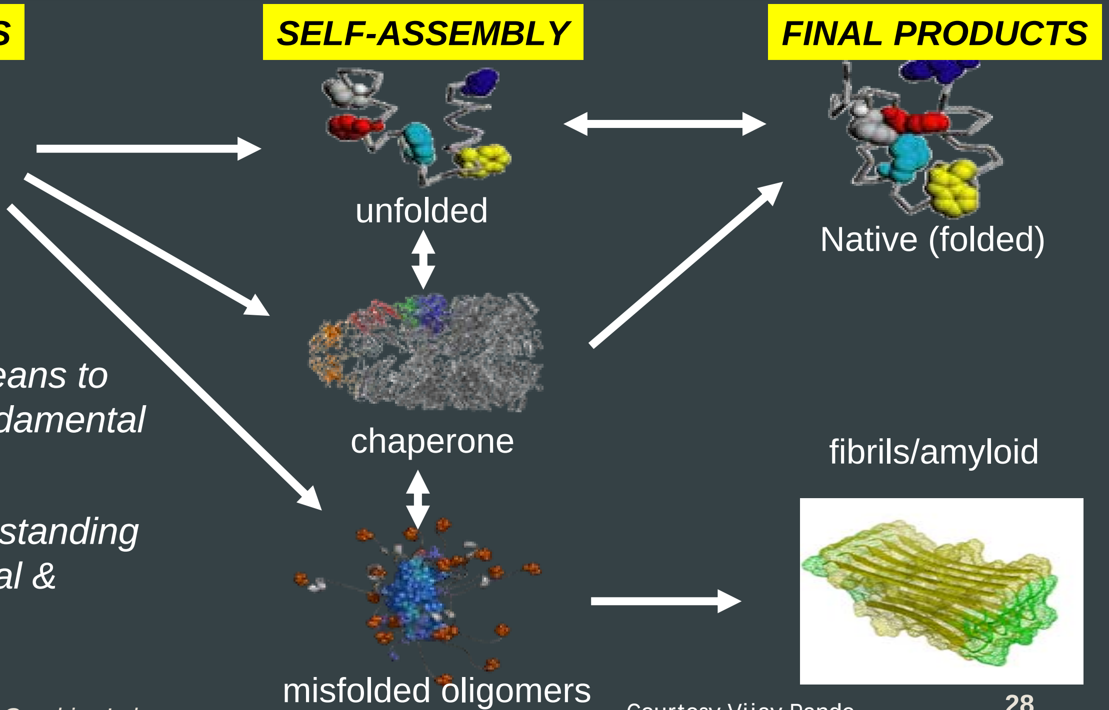


- What are proteins and why do they “fold”?
  - Proteins are molecules in the body which carries out many important functions, such as enzymes and antibodies
  - Before proteins can carryout their function, they must first assemble themselves or “fold”

- Potential impact
  - Design of novel proteins & protein-like heteropolymers
  - Understanding protein misfolding related diseases

Protein folding in the cell





Our goals:

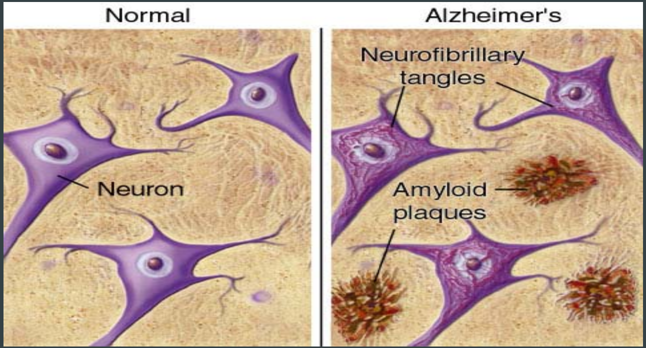
(1) To develop new means to characterize these fundamental biophysical processes

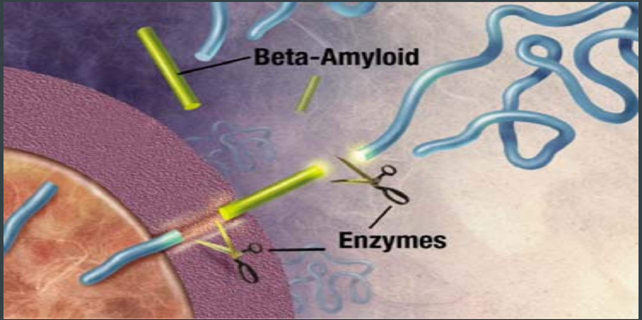
(2) To apply this understanding to challenging biological & biomedical problems

Courtesy Vijay Pande

Molecular nature of Alzheimer’s Disease

- Molecular nature
  - Brain tissue contains deposits of beta-Amyloid peptide (Aβ)
  - amphipathic 39-42 residue fragment of a membrane protein cleaved by secretases
  - Aggregate first into oligomers, then fibrils
- Intrinsically unstructured protein
  - Important new class of proteins
  - Common issue in many protein misfolding related diseases
  - Very different paradigm for structural study

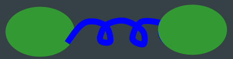




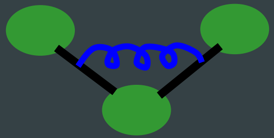
Courtesy Vijay Pande

The 25+ year old dream: use the laws of physics to study biomolecules

- Biomolecules obey the laws of physics
  - Use physical chemistry theory and simulation techniques to study biomolecules
  - All atom model with physical interactions
- Physics-based model: Molecular Dynamics
  - Numerically integrate Newton's equations
  - Choose δt to match timescale ($\delta t \sim 10^{-15}$ sec)
  - Classical model, with parameters to match experiment and/or quantum mechanics calculation
- Comparison to informatic approaches
  - Not limited by protein experiment: examine structures not in PDB (eg aggregates)
  - Possibility to include non-protein molecules (eg small molecules)
  - **<u>BUT, very, very computationally demanding</u>**
  -



bond stretching



angle bending

van der Waals

electrostatics

The 25 year old nightmare- ***The challenge of long timescales***

- Fundamental problem for simulation
  - Proteins fold in micro- to milliseconds
  - Computers can simulate nanoseconds
  - **How can we break this impasse?**

Natural idea: Use multiple processors

- Natural first idea: use multiple CPU's
  - Typical calculation needed requires 1,000,000 days on 1 fast processor
  - How about running on 100,000 CPU's?
  - "Linear scaling" would suggest this would take just 10 days with 100,000 CPU's

- Life isn't that easy
  - Most codes can't scale this way
  - In 2000, we suggested a method to solve this problem
  - Newest version (2005), allows for a very efficient use of 100K CPU's

Can 2000 grad students complete a PhD's worth of research in 1 day?

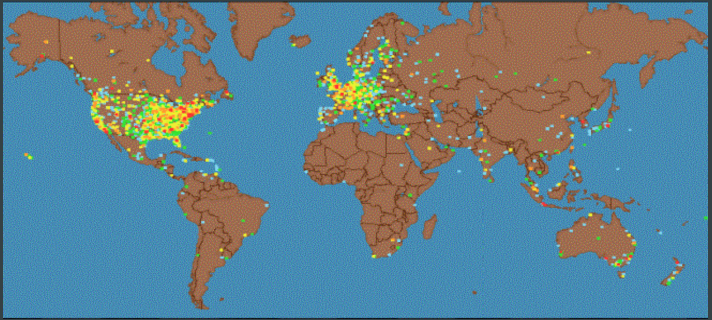
Most likely not! One must design novel ways to utilize large scale resources in efficient ways.

Courtesy Vijay Pande

Folding@Home: Computational resources from the future, realized today

- Very powerful computational resource
  - ~700 Teraflops sustained performance
  - >2,000,000 total processors; ~250,000 active
- Big impact
  - Break the micro- to millisecond barrier
  - What used to take 1M days, now takes a week or two
  - Enables key research previously impossible
  - These new methods are also starting to be used by other groups for folding study

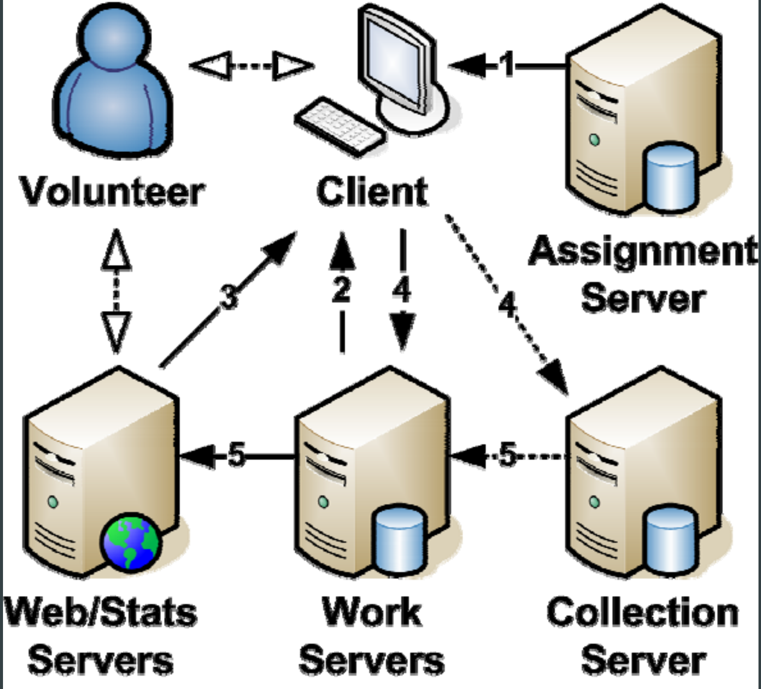
Folding@home distributed computing



>250,000 active CPUs over the world (CPU locations from IP address)

Courtesy Vijay Pande

How does this all work?

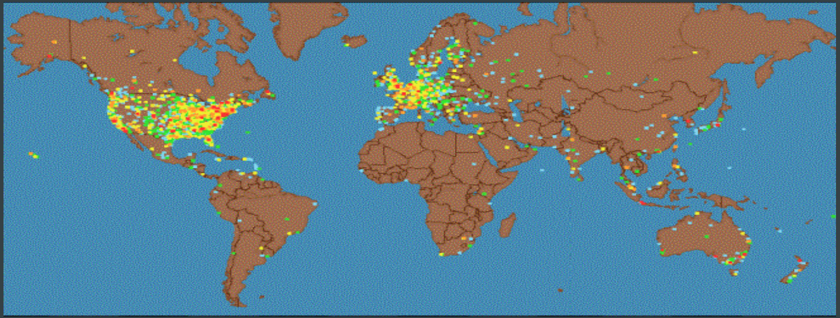


Courtesy Vijay Pande

Who’s Folding?

Folding@Home

~100,000 CPUs over the world (CPU locations from IP address)



Earth@Night

Electricity as distributed in the world (from NASA satellite data)

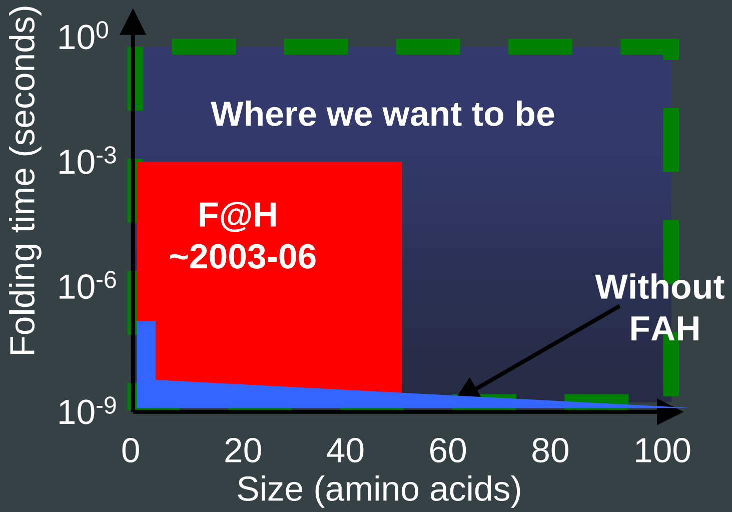
Courtesy Vijay Pande

Folding@Home communities – small subset

Next steps: new challenges

- What we can do
  - Somewhat long timescales (microseconds to milliseconds)
  - Somewhat large peptides & proteins (30-50 residues)
  - Allows us to directly test the relevant chemical detail in these biophysical problems

- Where we want to be
  - Longer timescales (seconds?)
  - Larger systems (~100 residues)
  - Yet not sacrificing details



Streaming processors on FAH

- New processors
  - Originally special purpose (eg for graphics, games)
  - High flops: ~500GFLOPS peak programmable, 32-bit FLOPs

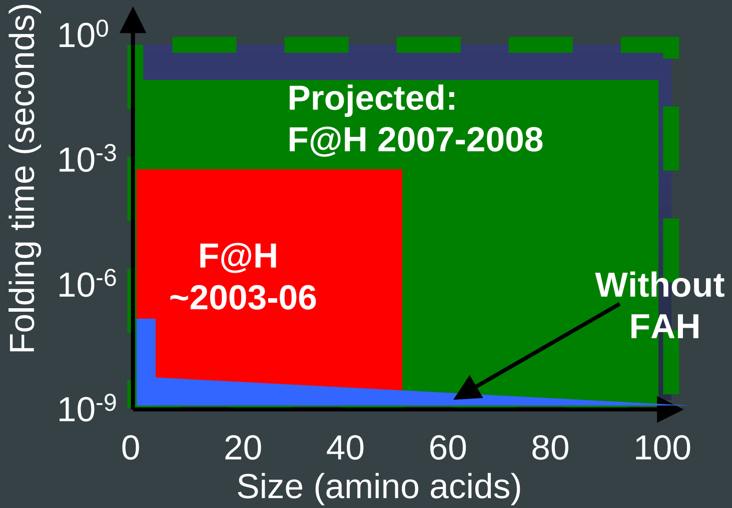
- Utilize for scientific computing
  - We have ported our MD code to GPUs & Cell (PS3)
  - Partnership with Sony and AMD
  - 20x to 40x speed increase

- Impact on calculations
  - Critical for MSM's: *longer trajectories, not just more of them*
  - Tackle more complex systems

Courtesy Vijay Pande

Folding@Home's next steps

- New methods
  - New processors and new advances in implicit solvation models allow for a ~20x to 500x speedup
  - Achieve simulations on the second timescale
- Impact: sampling may soon not be a problem
  - "@Home" not needed to simulate sub-millisecond timescale
  - More complex problems would be in reach with distributed computing
  - Turn our attention to further improving models (experiment key for these next steps)



With these new capabilities, we would be able to simulate the folding of a significant fraction of protein domains

Courtesy Vijay Pande

GPUs, SMPs, PS3s (oh my!)

- Performance
  - GPU > PS3 > SMP > Single-core
- Flexibility
  - Single-core > SMP > PS3 > GPU

- GPUs are ***really*** fast
  - 20-40x a single core P4
- But they can only run a subset of the research
  - Implicit water models

- Points are awarded with this in consideration

Current status – April 20, 2007

http://fah-web.stanford.edu/cgi-bin/main.py?qtype=osstats

Client type	Current TFLOPS*	Active Processors
Windows	177	185870
Mac OS X/PPC	8	10394
Mac OS X/Intel	14	4600
Linux	47	27373
GPU	56	947
Playstation3	409	31217
Total	711	260401

*TFLOPS is actual flops from software cores, **not** peak values

For More Information

- Main site
  - http://folding.stanford.edu
- GPU information
  - http://folding.stanford.edu/FAQ-ATI.html
- Petaflop Initiative
  - Stream processors
    - GPUs
    - PS3 (Cell)
  - http://folding.stanford.edu/FAQ-FPI.html

Folding on HD 2900XT

- Support will ship with next release
- Force calculation 2.2X(!) faster than R580
- Overall application ~45% faster
  - Amdahl's law strikes again
    - Supporting kernels unoptimized
    - CPU overhead
  - Little tuning time so far on R6XX
- We can now explore more complex algorithms
  - Larger register requirements
  - Integer support – random number generation
  - More bandwidth

Future Folding@Home GPGPU

- Improvements
  - Lower CPU overhead
    - Brook DX9 backend + core changes
  - CTM through Brook
    - Lower overhead/finer tuning
    - Linux support much easier
    - Better stability – users can upgrade drivers for games without breaking anything
  - More GPUs supported
- New cores
  - Back-port some of what we learned from Cell ports
  - Several new models
  - Many more work units
  - Revisit other models running well on SMP/Cell

Acknowledgements – Folding@Home research group

Current members:
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Making GPGPU easier

What GPGPU needs from vendors – what we got

- More information
  - Shader ISA ★
  - Latency information
  - GPGPU Programming guide (floating point) ★
- Direct access to the hardware/Compute APIs ★
- Fast transfer to and from GPU
  - Non-blocking
- Consistent graphics drivers ★
  - Some optimizations for games hurt GPGPU performance

What GPGPU needs from vendors

- More information
  - Latency information
  - Memory system information
- Fast transfer to and from GPU
  - Non-blocking
  - DMA driven
- Consistent drivers
  - Stable drivers for games AND computation
- High-level <u>and</u> low-level access
  - High-level: get more people using GPUs, make it easy to approach
  - Low-level: let us tune to our heart's content!
    - Remove shader compiler and game optimizations from breaking our code
- More software companies
  - PeakStream and RapidMind a good start

What GPGPU needs from the community

- Data Parallel programming languages
  - Need more exploration
- “GCC” for GPUs/streaming processors
  - We almost have enough information for this
- Parallel data structures
  - Still really hard…
- More applications
  - What will make the average user care about GPGPU?
    - Folding@Home! ;-)
  - What else can we make data parallel and run fast?

Questions?

- I'll also be around after the talk
- Email: mhouston@stanford.edu
- Web: http://graphics.stanford.edu/~mhouston

- For lots of great GPGPU information:
  - GPGPU.org (http://www.gpgpu.org)