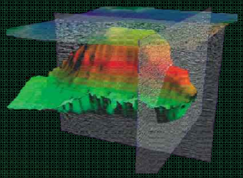
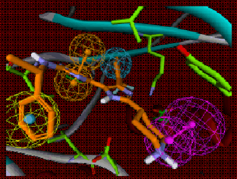
Parallel Computing: What has changed lately?

David B. Kirk

Future Science and Engineering Breakthroughs Hinge on Computing

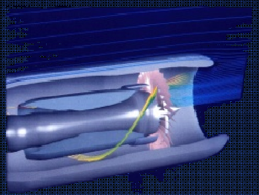


Computational Geoscience

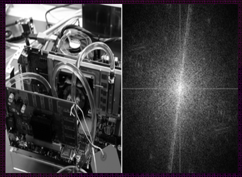


Computational Chemistry

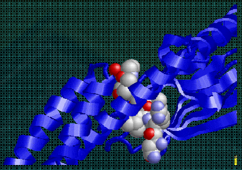
Computational Medicine



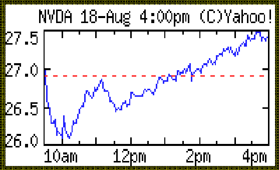
Computational Modeling



Computational Physics



Computational Biology



Computational Finance

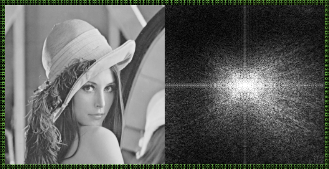
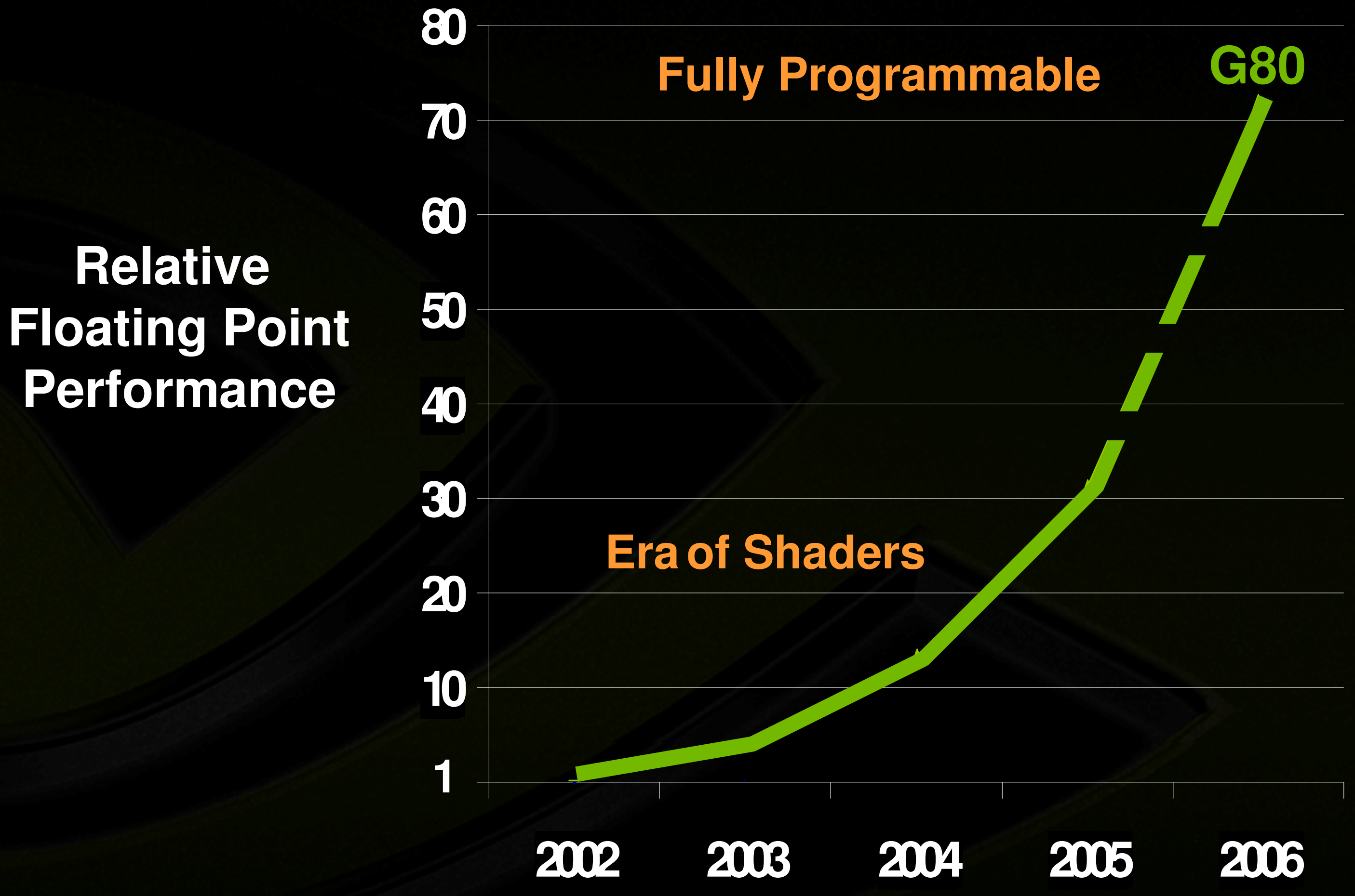


Image Processing

Faster is not “just Faster”

- 2-3X faster is “just faster”
  - Do a little more, wait a little less
  - Doesn’t change how you work
- 5-10x faster is “significant”
  - Worth upgrading
  - Worth re-writing (parts of) the application
- 100x+ faster is “fundamentally different”
  - Worth considering a new platform
  - Worth re-architecting the application
  - Makes new applications possible
  - Drives “time to discovery” and creates fundamental changes in Science

The GPU is a New Computation Engine



CPU

Powerful Multi-core Control Processor

- Operating system
- Database
- Productivity
- Temporal compression
- Recursive algorithms

GPU

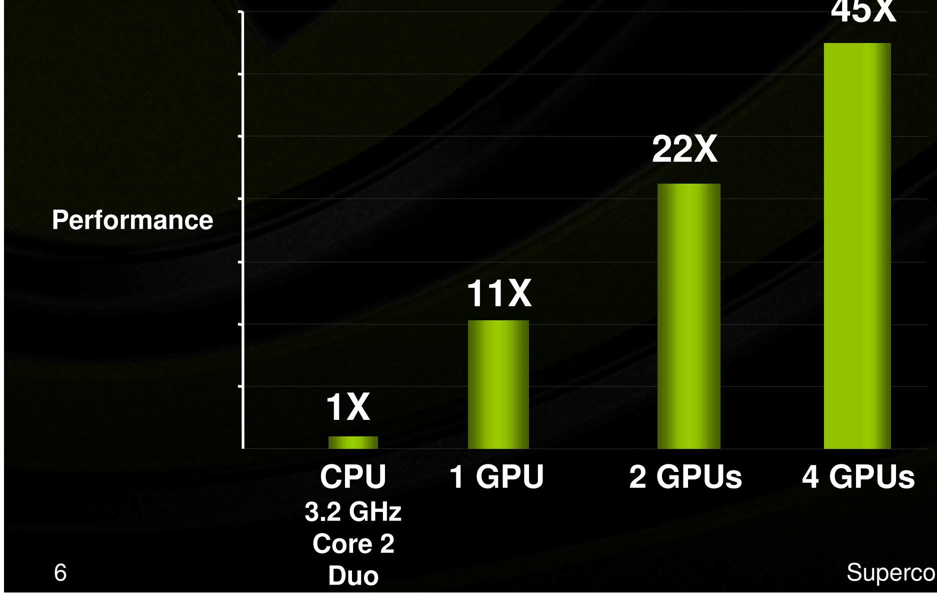
Powerful Massively Parallel Computation Processor

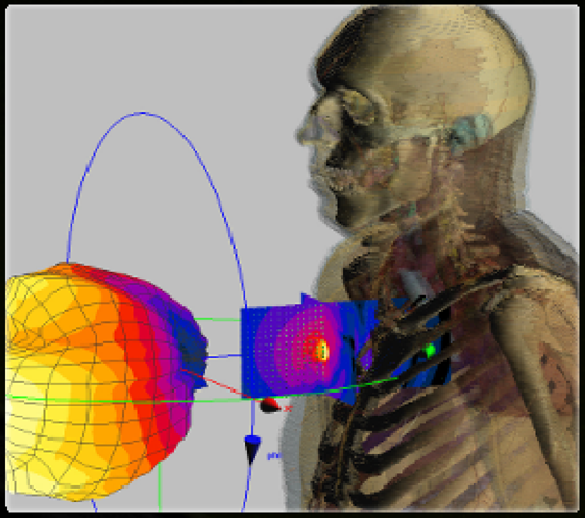
- Oil and gas seismic
- Financial risk modeling
- Medical Imaging
- Finite element computing
- Genetic pattern match

Data to Design

Acceleware EM Field simulation technology for the GPU

- 3D Finite-Difference and Finite-Element (FDTD)
- Modeling of:
  - Cell phone irradiation
  - MRI Design / Modeling
  - Printed Circuit Boards
  - Radar Cross Section (Military)



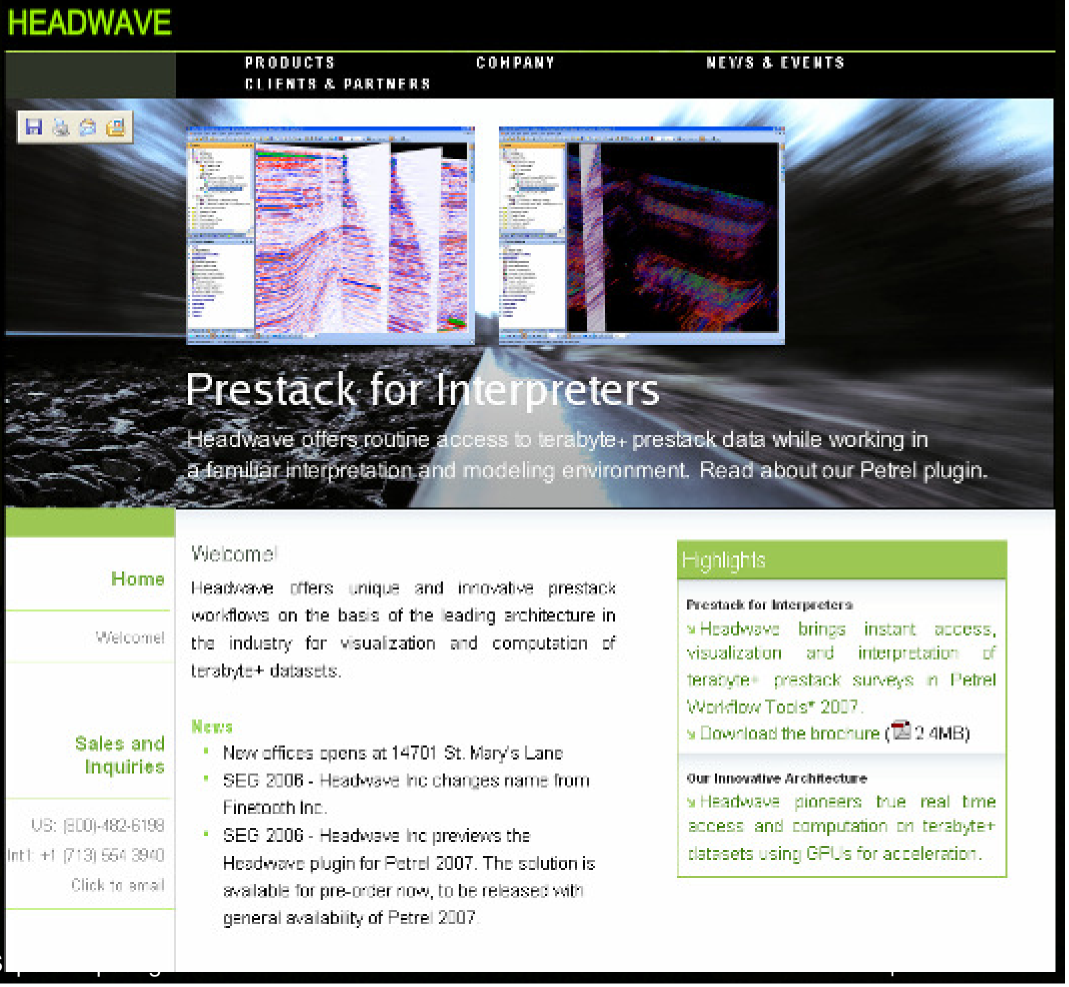


Pacemaker with Transmit Antenna

Terabyte Data to Drilling Decision

- Visualize Terabytes of data
- Interactive data processing and analysis

HEADWAVE



Prestack for Interpreters

Headwave offers routine access to terabyte+ prestack data while working in a familiar interpretation and modeling environment. Read about our Petrel plugin.

Welcome!

Headwave offers unique and innovative prestack workflows on the basis of the leading architecture in the industry for visualization and computation of terabyte+ datasets.

News

- New offices opens at 14701 St. Mary's Lane
- SEG 2006 - Headwave Inc changes name from Finetooth Inc.
- SEG 2006 - Headwave Inc previews the Headwave plugin for Petrel 2007. The solution is available for pre-order now, to be released with general availability of Petrel 2007.

US: (800)-482-6198
Intl: +1 (713) 554 3940

Highlights

Prestack for Interpreters

Headwave brings instant access, visualization and interpretation of terabyte+ prestack surveys in Petrel Workflow Tools* 2007.

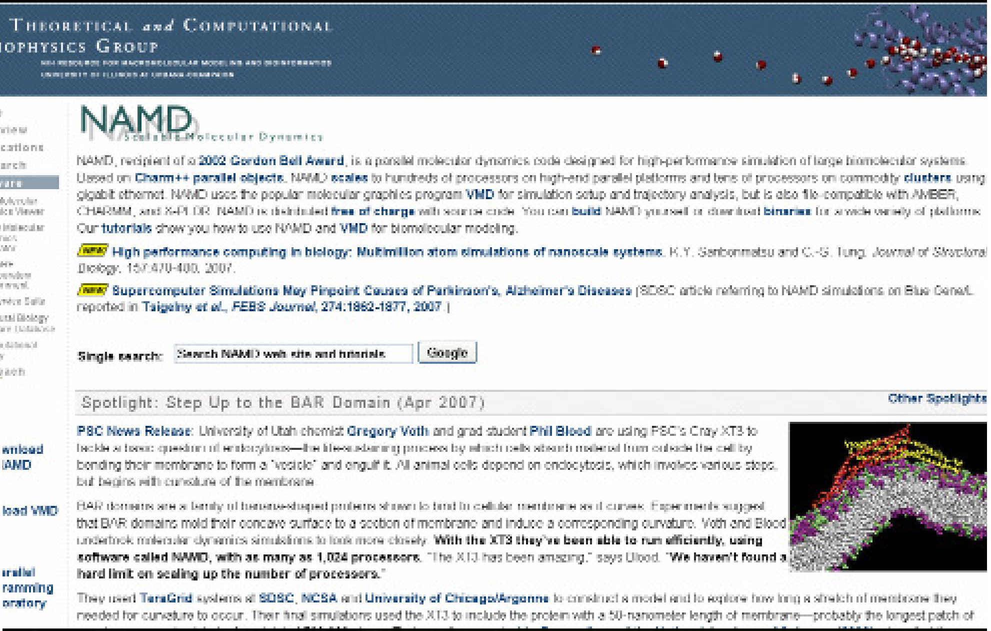
Download the brochure (2.4MB)

Our Innovative Architecture

Headwave pioneers true real time access and computation on terabyte+ datasets using GPUs for acceleration.

VMD/NAMD Molecular Dynamics

- 240X speedup
- Computational biology



THEORETICAL and COMPUTATIONAL BIOPHYSICS GROUP

Home
Overview
Publications
Research
Software
VMD Molecular Graphics Viewer
NAMD Molecular Dynamics Simulator
MD Service Suite
Structural Biology Software Database
Computational Facility
Outreach

NAMD Scalable Molecular Dynamics

NAMD, recipient of a **2002 Gordon Bell Award**, is a parallel molecular dynamics code designed for high-performance simulation of large biomolecular systems. Based on **Charm++ parallel objects**, NAMD **scales** to hundreds of processors on high-end parallel platforms and tens of processors on commodity **clusters** using gigabit ethernet. NAMD uses the popular molecular graphics program **VMD** for simulation setup and trajectory analysis, but is also file-compatible with AMBER, CHARMM, and X-PLOR. NAMD is distributed **free of charge** with source code. You can **build** NAMD yourself or download **binaries** for a wide variety of platforms. Our **tutorials** show you how to use NAMD and **VMD** for biomolecular modeling.

NEW **High performance computing in biology: Multimillion atom simulations of nanoscale systems.** K.Y. Sanbonmatsu and C.-S. Tung. *Journal of Structural Biology*, 157:470-480, 2007.

NEW **Supercomputer Simulations May Pinpoint Causes of Parkinson's, Alzheimer's Diseases** (SDSC article referring to NAMD simulations on Blue Gene/L reported in **Tsigelny et al., *FEBS Journal*, 274:1862-1877, 2007**.)

Single search: Search NAMD web site and tutorials [Google]

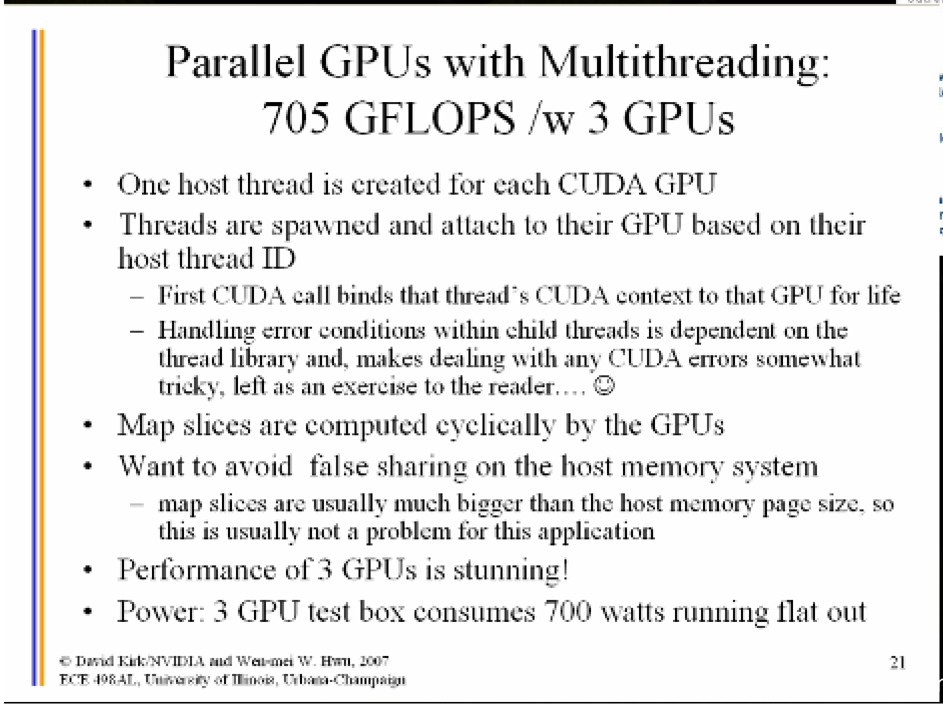
Spotlight: Step Up to the BAR Domain (Apr 2007) — Other Spotlights

PSC News Release: University of Utah chemist **Gregory Voth** and grad student **Phil Blood** are using PSC's Cray XT3 to tackle a basic question of endocytosis—the life-sustaining process by which cells absorb material from outside the cell by bending their membrane to form a "vesicle" and engulf it. All animal cells depend on endocytosis, which involves various steps, but begins with curvature of the membrane.

BAR domains are a family of banana-shaped proteins shown to bind to cellular membrane as it curves. Experiments suggest that BAR domains mold their concave surface to a section of membrane and induce a corresponding curvature. Voth and Blood undertook molecular dynamics simulations to look more closely. **With the XT3 they've been able to run efficiently, using software called NAMD, with as many as 1,024 processors.** "The XT3 has been amazing," says Blood. "**We haven't found a hard limit on scaling up the number of processors.**"

They used **TeraGrid** systems at **SDSC**, **NCSA** and **University of Chicago/Argonne** to construct a model and to explore how long a stretch of membrane they needed for curvature to occur. Their final simulations used the XT3 to include the protein with a 50-nanometer length of membrane—probably the longest patch of

wnload
NAMD
load VMD
rallel
ramming
oratory



Parallel GPUs with Multithreading: 705 GFLOPS /w 3 GPUs

- One host thread is created for each CUDA GPU
- Threads are spawned and attach to their GPU based on their host thread ID
  - First CUDA call binds that thread's CUDA context to that GPU for life
  - Handling error conditions within child threads is dependent on the thread library and, makes dealing with any CUDA errors somewhat tricky, left as an exercise to the reader…. ☺
- Map slices are computed cyclically by the GPUs
- Want to avoid false sharing on the host memory system
  - map slices are usually much bigger than the host memory page size, so this is usually not a problem for this application
- Performance of 3 GPUs is stunning!
- Power: 3 GPU test box consumes 700 watts running flat out

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ECE 498AL, University of Illinois, Urbana-Champaign

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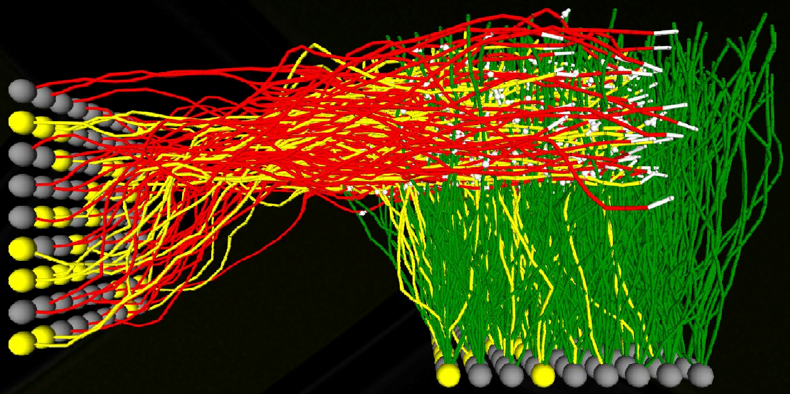
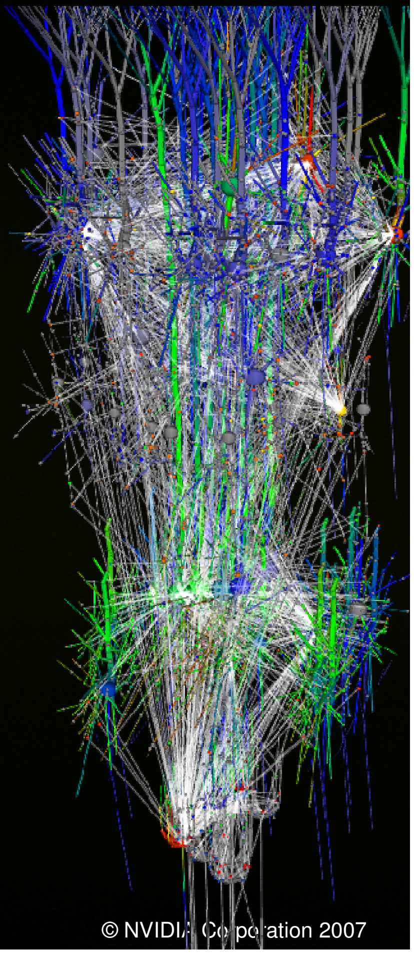
http://www.ks.uiuc.edu/Research/vmd/projects/ece498/lecture/

EvolvedMachines

- Simulate the brain circuit
- Sensory computing: vision, olfactory
- 130X Speed up



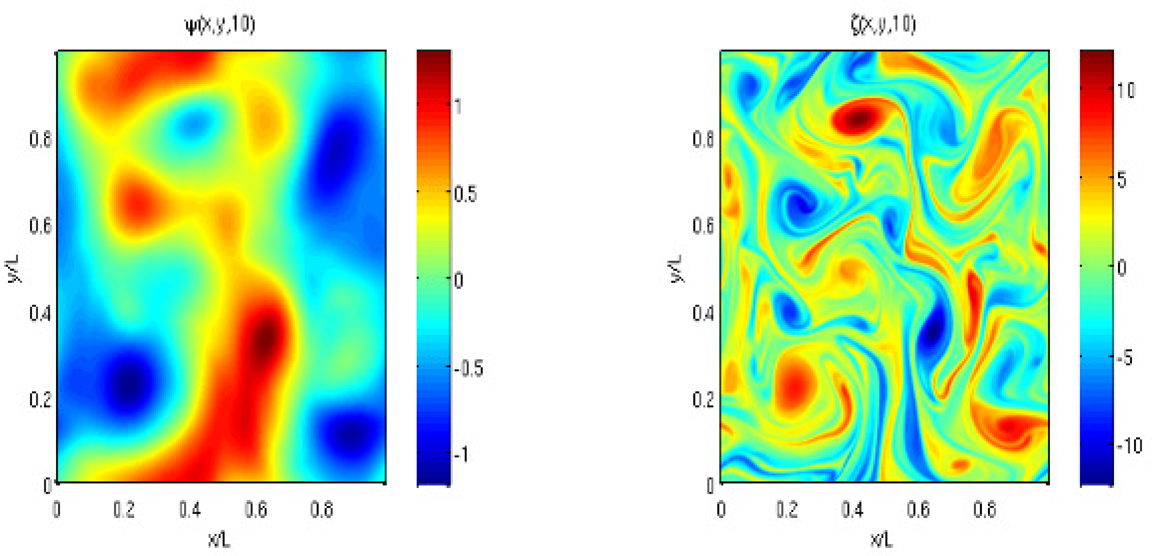


EvolvedMachines

Matlab: Language of Science

15X with MATLAB CPU+GPU

http://developer.nvidia.com/object/matlab_cuda.html



Pseudo-spectral simulation of 2D Isotropic turbulence

http://www.amath.washington.edu/courses/571-winter-2006/matlab/FS_2Dturb.m

Other Links

- Astrophysics
  Astrophysical simulations based on smoothed particle hydrodynamics: Fourier Volume Rendering
  Andrew Corrigan and John Wallin: Computational and Data Sciences, George Mason University
  http://cds.gmu.edu/~acorriga/pubs/meshless_fvr

- Astrophysics
  Astrophysical N-body simulation: The Chamomile Scheme
  Tsuyoshi Hamada and Toshiaki Iitaka: Computational Astrophysics Lab, RIKEN
  http://progrape.jp/cs/

- Financial Simulation
  Computational Finance: Swaption volatility
  Level 3 Finance
  http://www.level3finance.com/index.html

- Financial Simulation
  Quantita
  tive Risk Analysis and Algorithmic Trading Systems
  Hanweck Associates
  http://www.hanweckassoc.com/home.html

- Medial Imaging
  National Library of Medicine Insight Segmentation and Registration Toolkit (ITK)
  Won-Ki Jeong: Scientific Computing & Imaging Institute, University of Utah
  http://www.itk.org/

- Physical Simulation
  Simulation Open Framework Architecture for real-time simulation with an emphasis on medical simulation
  http://www-evasion.imag.fr/%7EFrancois.Faure/Sofa/web/home

- Video Capture
  3D Surface Image Capture and “4D Capture” of Stereo Video Time Sequencing
  Dimensional Imaging
  http://www.di3d.com/

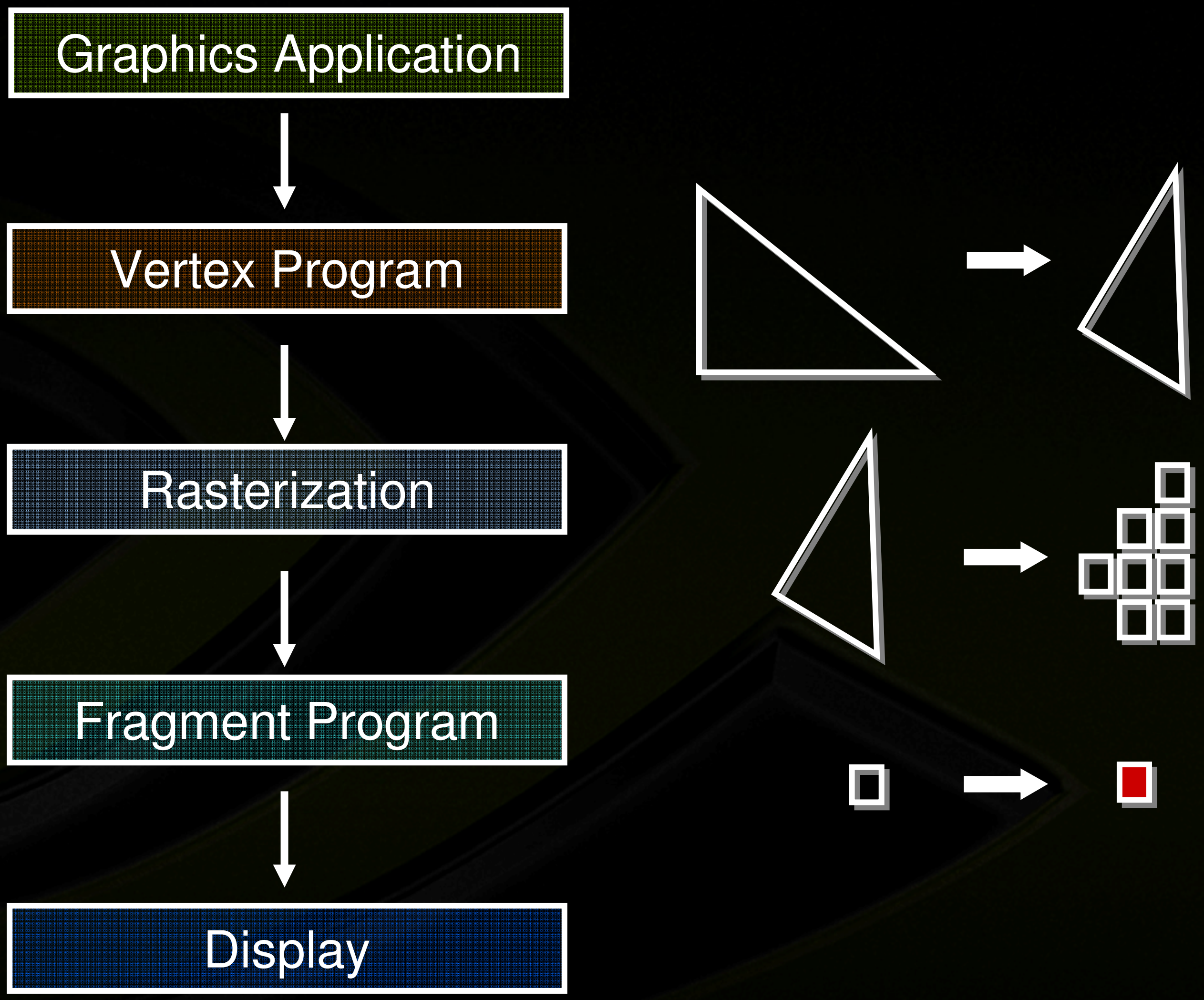
- GIS
  Geographic Information System (GIS) and Mapping products
  Manifold
  http://www.manifold.net/

- Bioscience
  Computational biology string matching: CMATCH
  Michael C. Schatz and Cole Trapnell: Center for Bioinformatics & Computational Biology
  University of Maryland
  http://www.cbcb.umd.edu/software/cmatch/

- Gene Sequence Analysis
  Genomic Data Sequence Analysis: SWBoost (Smith-Waterman Boost)
  Genboost
  http://www.genboost.com/swboost.php

CUDA Programming Model

Graphics Programming Model



Graphics Application

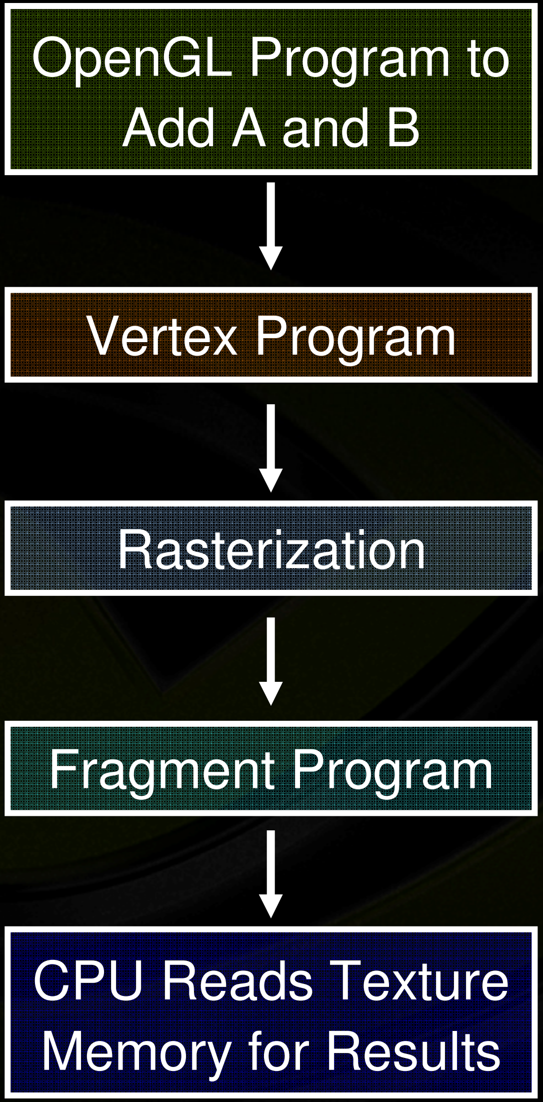
Vertex Program

Rasterization

Fragment Program

Display

Streaming GPGPU Programming



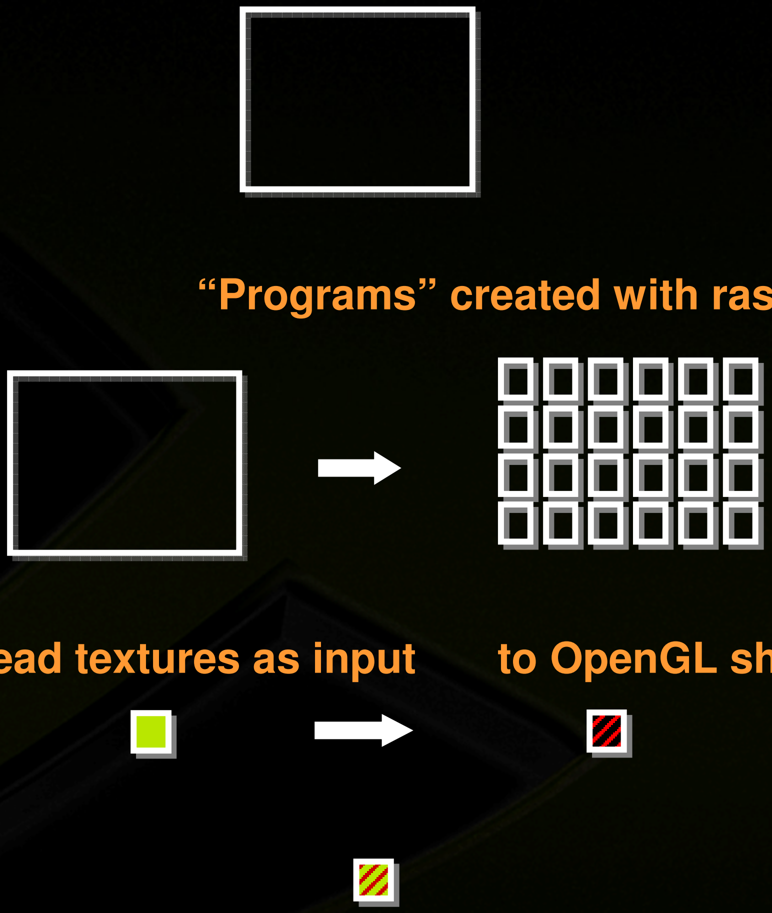
OpenGL Program to Add A and B

Vertex Program

Rasterization

Fragment Program

CPU Reads Texture Memory for Results



Start by creating a quad

“Programs” created with raster operation

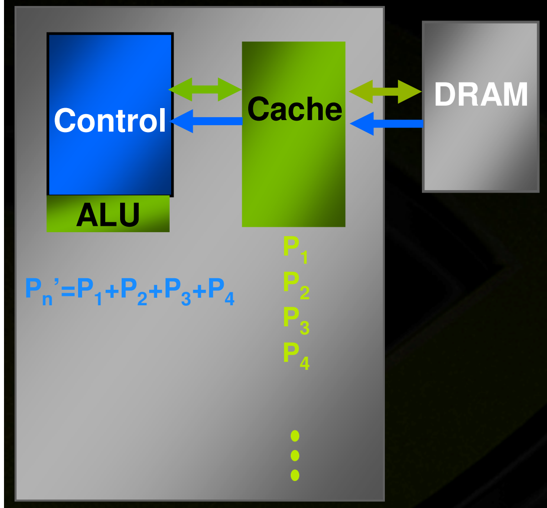
Read textures as input to OpenGL shader program

Write answer to texture memory as a “color”

All this just to do A + B

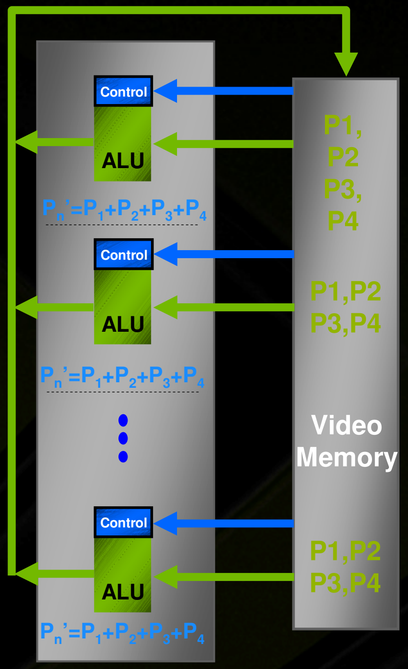
Example Fluid Algorithm

CPU

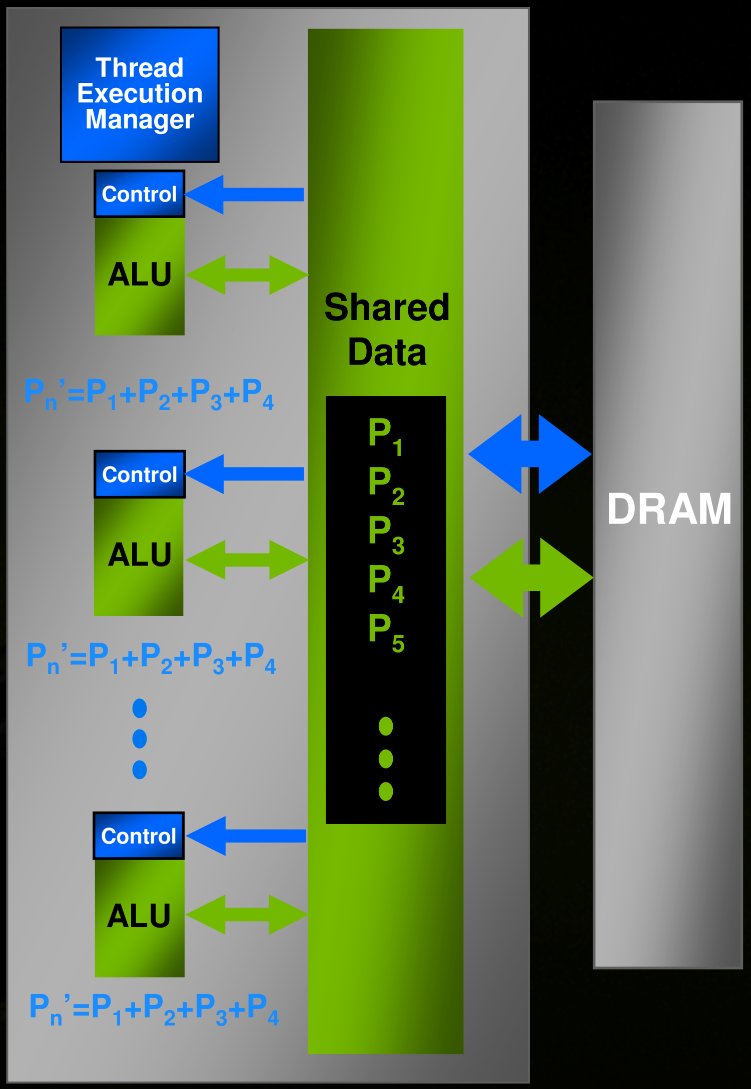


Single thread out of cache

GPGPU


Control
ALU
$P_n' = P_1 + P_2 + P_3 + P_4$
Control
ALU
$P_n' = P_1 + P_2 + P_3 + P_4$
⋮
Control
ALU
$P_n' = P_1 + P_2 + P_3 + P_4$
P1, P2 P3, P4
P1,P2 P3,P4
Video Memory
P1,P2 P3,P4

Multiple passes through video memory

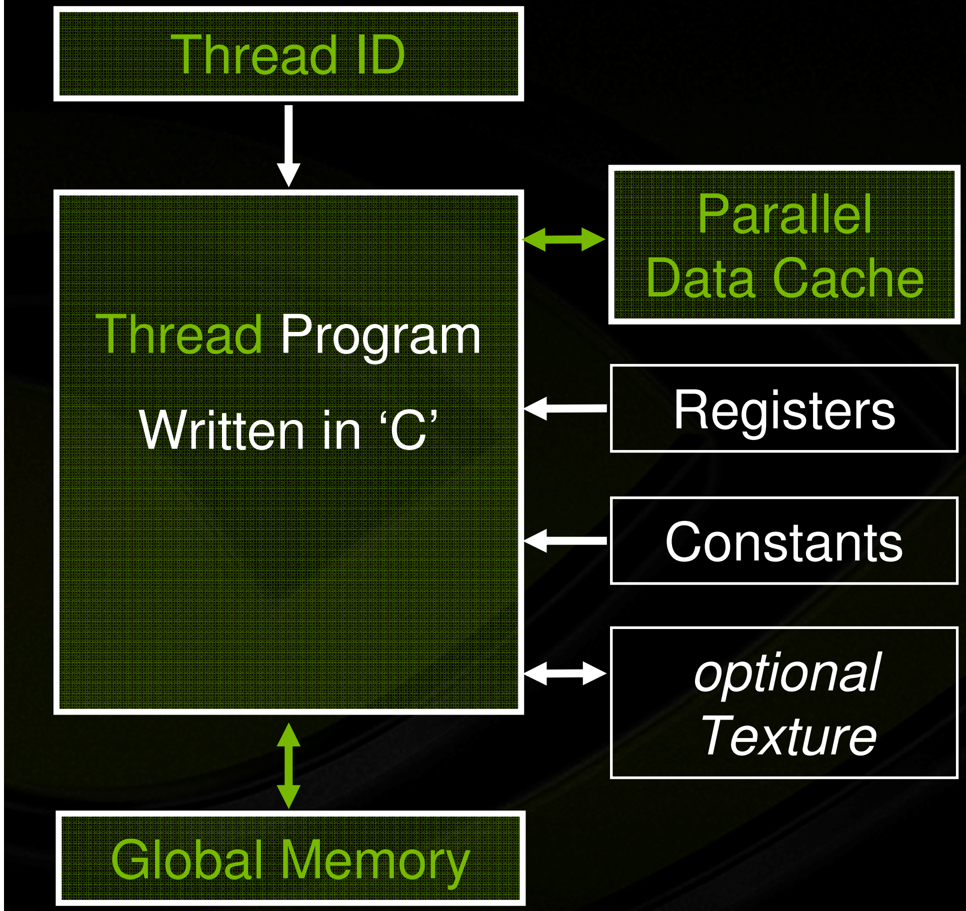


Parallel execution on-chip

🟩 Data/Computation

🟦 Program/Control

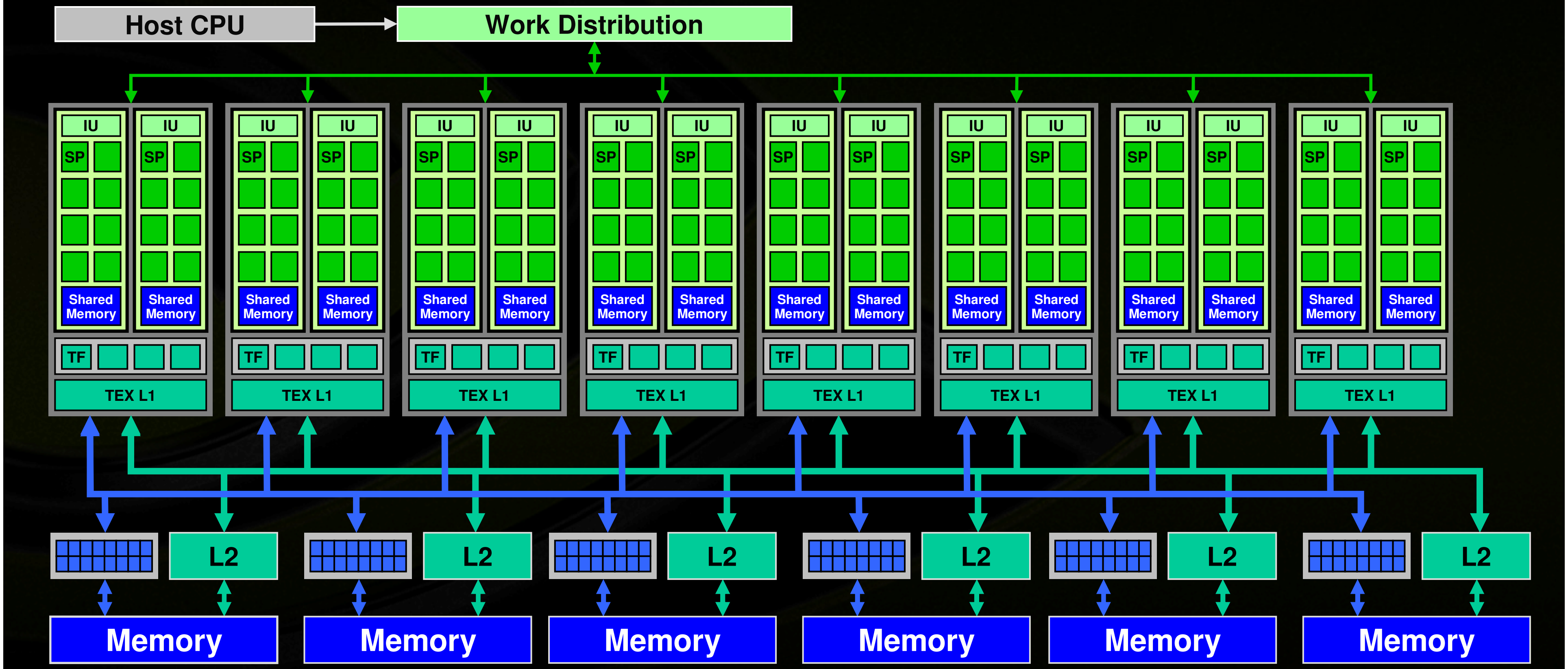
New GPU Computing Model



- **Dedicated computing mode**
- **Thread programs use 'C'**
- **On-chip shared memory**
- **General load/store**

The Future of Computing is Parallel

- CPU clock rate growth is slowing, future speed growth will be from parallelism
- GeForce-8 Series is a massively parallel computing platform
  - 12,288 concurrent threads, hardware managed
  - 128 SP Thread Processor cores at 1.35 GHz == 518 GFLOPS peak
  - GPU Computing features enable C on Graphics Processing Unit



Host CPU

Work Distribution

IU

SP

Shared Memory

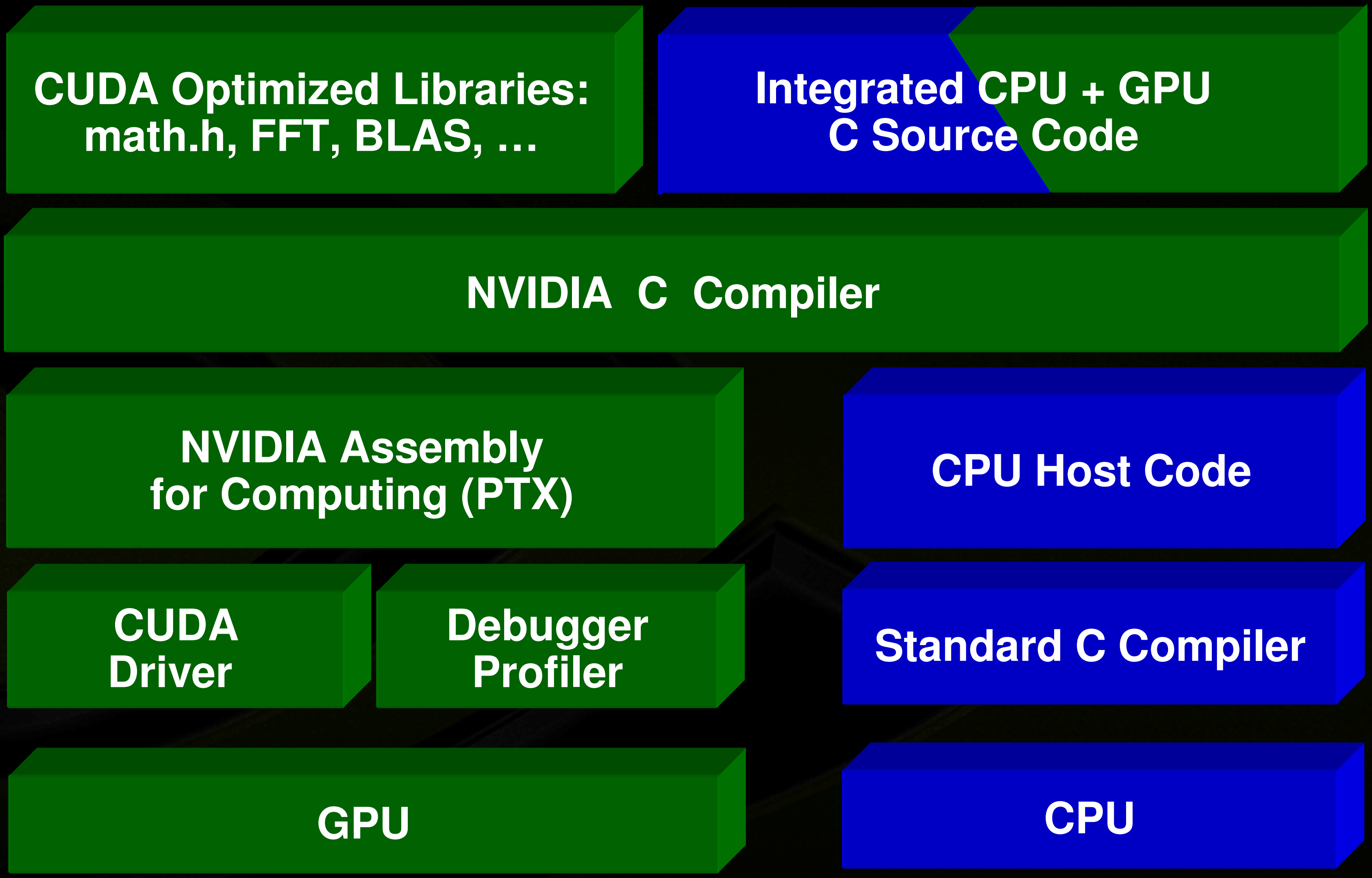
TF

TEX L1

L2

Memory

CUDA Software Development Kit



CUDA Optimized Libraries: math.h, FFT, BLAS, …

Integrated CPU + GPU C Source Code

NVIDIA C Compiler

NVIDIA Assembly for Computing (PTX)

CPU Host Code

CUDA Driver

Debugger Profiler

Standard C Compiler

GPU

CPU

CUDA: C on the GPU

- A simple, explicit programming language solution
- Extend only where necessary

```
__global__ void KernelFunc(...);

__shared__ int SharedVar;

KernelFunc<<< 500, 128 >>>(...);
```

- Explicit GPU memory allocation
  - `cudaMalloc()`, `cudaFree()`
- Memory copy from host to device, etc.
  - `cudaMemcpy()`, `cudaMemcpy2D()`, ...

C-Code Example to Add Arrays

CPU C program

```
void add_matrix_cpu
                (float *a, float *b, float *c, int N)
{
      int i, j, index;
    for (i=0;i<N;i++) {
     for (j=0;j<N;j++) {
        index =i+j*N;
        c[index]=a[index]+b[index];
        }
    }
}
void main()
{
   .....
       add_matrix(a,b,c,N);
}
```

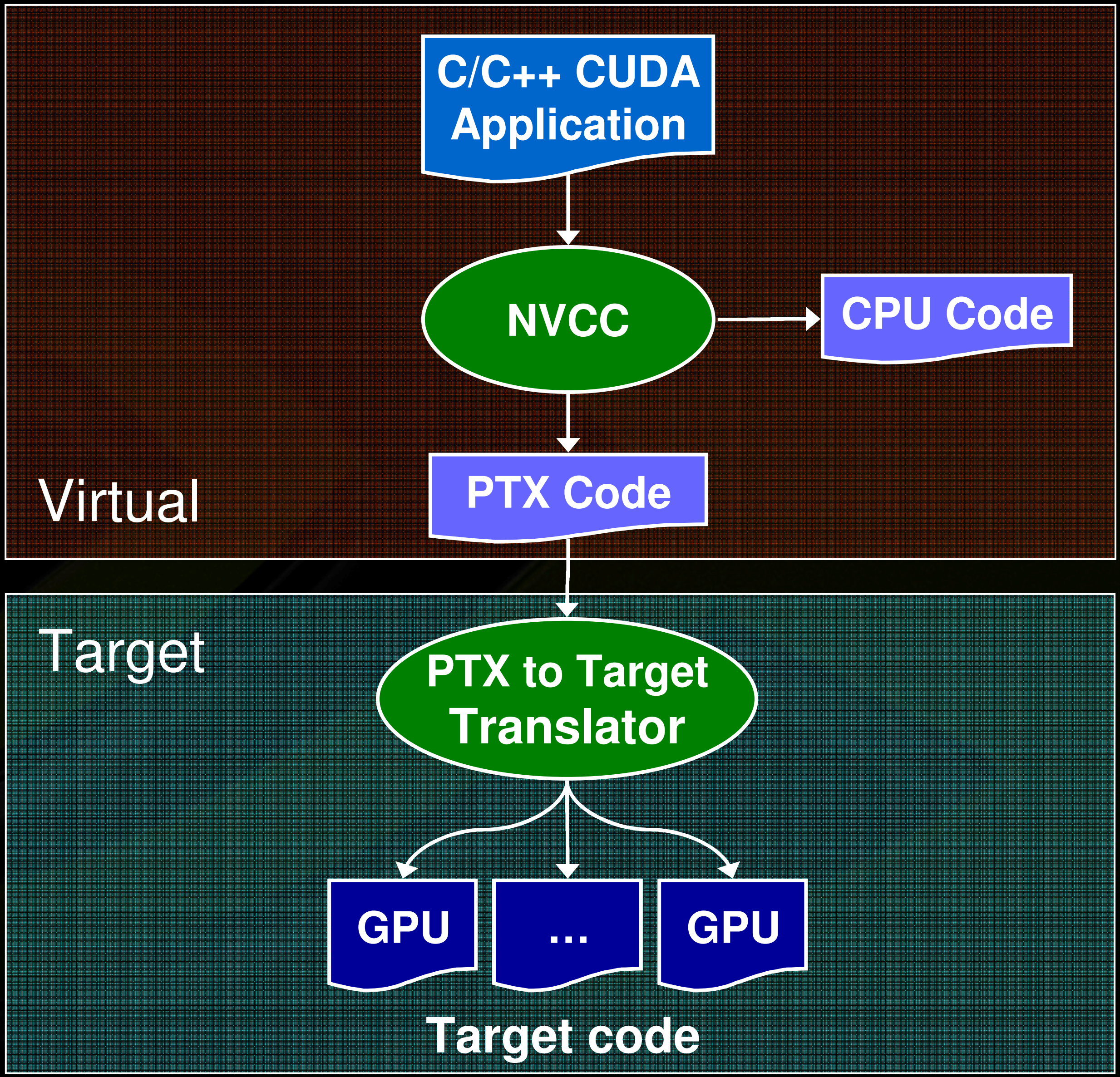
CUDA C program

```
__global__ void add_matrix_gpu
                (float *a, float *b, float *c, int N)
{
    int i=blockIdx.x*blockDim.x+threadIdx.x;
    int j=blockIdx.y*blockDim.y+threadIdx.y;
    int index =i+j*N;
    if( i <N && j <N) c[index]=a[index]+b[index];
}



void main()
{
    dim3 dimBlock (blocksize,blocksize);
    dim3 dimGrid (N/dimBlock.x,N/dimBlock.y);
    add_matrix_gpu<<<dimGrid,dimBlock>>>(a,b,c,N);
}
```

Compiling CUDA

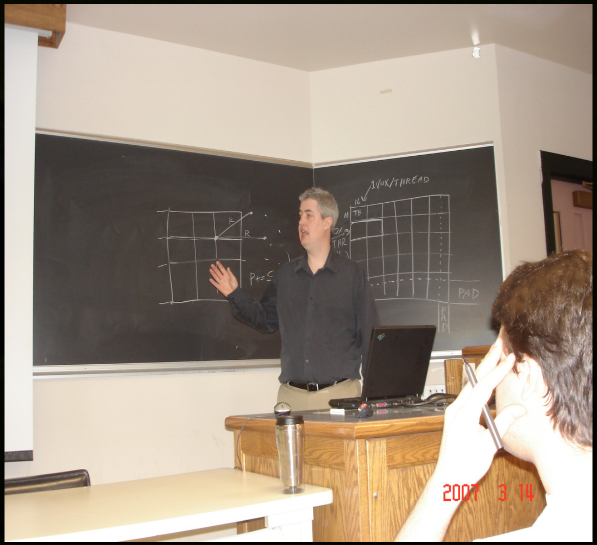


CUDA Stable Fluids Demo

CUDA port of:
Jos Stam, "Stable Fluids", In SIGGRAPH 99
Conference Proceedings, Annual
Conference Series, August 1999, 121-128.

Come visit the class!

- UIUC ECE498AL – Programming Massively Parallel Processors (http://courses.ece.uiuc.edu/ece498/al/)
  - David Kirk (NVIDIA) and Wen-mei Hwu (UIUC) co-instructors
  - CUDA programming, GPU computing, lab exercises, and projects
  - Lecture slides and voice recordings



Implications and Opportunities

- Massively parallel computing allows
  - Drastic reduction in “time to discovery”
  - New, 3rd paradigm for research: computational experimentation
  - The “democratization of supercomputing”
    - $2,000/Teraflop SPFP in personal computers today
    - $5,000,000/Petaflops DPFP in clusters in two years
    - HW cost will no longer be the main barrier for big science
  - This is once-in-a-career opportunity for many!
- Call to Action
  - Research in Parallel Programming models and Parallel Architecture
  - Teach massively parallel programming to CS/ECE students, scientists and other engineers.

http://www.nvidia.com/Tesla

http://developer.nvidia.com/CUDA

Questions?