Supercomputing in Plain English Part X: GPGPU: Number Crunching Inside Your GPU

Henry Neeman, Director

OU Supercomputing Center for Education & Research University of Oklahoma Information Technology Tuesday April 28 2009





This is an experiment!

It's the nature of these kinds of videoconferences that FAILURES ARE GUARANTEED TO HAPPEN! NO PROMISES!

- So, please bear with us. Hopefully everything will work out well enough.
- If you lose your connection, you can retry the same kind of connection, or try connecting another way.
- Remember, if all else fails, you always have the toll free phone bridge to fall back on.







This week's Access Grid (AG) venue: Cactus.

If you aren't sure whether you have AG, you probably don't.

Tue Apr 28	Cactus
Tue May 5	Titan

Many thanks to John Chapman of U Arkansas for setting these up for us.





If you want to use H.323 videoconferencing – for example, Polycom – then dial

69.77.7.203##12345

any time after 2:00pm. Please connect early, at least today.

For assistance, contact Andy Fleming of <u>KanREN</u>/Kan-ed (<u>afleming@kanren.net</u> or 785-230-2513).

KanREN/Kan-ed's H.323 system can handle up to 40 simultaneous H.323 connections. If you cannot connect, it may be that all 40 are already in use.

Many thanks to Andy and KanREN/Kan-ed for providing H.323 access.





We have unlimited simultaneous iLinc connections available.

- If you're already on the SiPE e-mail list, then you should already have an e-mail about iLinc. Your personal URL will always be the same.
- If you want to use iLinc, please follow the directions in the iLinc e-mail.
- For iLinc, you <u>MUST</u> use either Windows (XP strongly preferred) or MacOS X with Internet Explorer.
- To use iLinc, you'll need to download a client program to your PC. It's free, and setup should take only a few minutes.
- Many thanks to Katherine Kantardjieff of California State U Fullerton for providing the iLinc licenses.





QuickTime Broadcaster

If you cannot connect via the Access Grid, H.323 or iLinc, then you can connect via QuickTime:

rtsp://129.15.254.141/test_hpc09.sdp

We recommend using QuickTime Player for this, because we've tested it successfully.

We recommend upgrading to the latest version at:

http://www.apple.com/quicktime/

When you run QuickTime Player, traverse the menus

File -> Open URL

Then paste in the rstp URL into the textbox, and click OK. Many thanks to Kevin Blake of OU for setting up QuickTime Broadcaster for us.





Phone Bridge

If all else fails, you can call into our toll free phone bridge:

1-866-285-7778, access code 6483137#

Please mute yourself and use the phone to listen.

Don't worry, we'll call out slide numbers as we go.

- Please use the phone bridge <u>ONLY</u> if you cannot connect any other way: the phone bridge is charged per connection per minute, so our preference is to minimize the number of connections.
- Many thanks to Amy Apon and U Arkansas for providing the toll free phone bridge.





No matter how you connect, please mute yourself, so that we cannot hear you.

- At OU, we will turn off the sound on all conferencing technologies.
- That way, we won't have problems with echo cancellation.
- Of course, that means we cannot hear questions.
- So for questions, you'll need to send some kind of text.

Also, if you're on iLinc: **SIT ON YOUR HANDS! Please DON'T touch ANYTHING!**





Questions via Text: iLinc or E-mail

Ask questions via text, using one of the following:

- iLinc's text messaging facility;
- e-mail to <u>sipe2009@gmail.com</u>.

All questions will be read out loud and then answered out loud.





Thanks for helping!

- OSCER operations staff (Brandon George, Dave Akin, Brett Zimmerman, Josh Alexander)
- OU Research Campus staff (Patrick Calhoun, Josh Maxey, Gabe Wingfield)
- Kevin Blake, OU IT (videographer)
- Katherine Kantardjieff, CSU Fullerton
- John Chapman and Amy Apon, U Arkansas
- Andy Fleming, KanREN/Kan-ed
- This material is based upon work supported by the National Science Foundation under Grant No. OCI-0636427, "CI-TEAM Demonstration: Cyberinfrastructure Education for Bioinformatics and Beyond."





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Supercomputing Exercises

Want to do the "Supercomputing in Plain English" exercises?

• The first several exercises are already posted at:

http://www.oscer.ou.edu/education.php

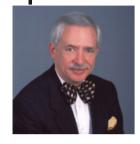
 If you don't yet have a supercomputer account, you can get a temporary account, just for the "Supercomputing in Plain English" exercises, by sending e-mail to:

hneeman@ou.edu

Please note that this account is for doing the <u>exercises only</u>, and will be shut down at the end of the series.



OK Supercomputing Symposium 2009



2003 Keynote: Peter Freeman NSF Computer & Information Science & Engineering Assistant Director

2009 Keynote: **Ed Seidel** Director **NSF** Office of Cyberinfrastructure





2004 Keynote: Sangtae Kim **NSF** Shared Cyberinfrastructure **Division** Director





2005 Keynote: Walt Brooks NASA Advanced Supercomputing **Division Director**



2006 Keynote: Dan Atkins Head of NSF's Office of Cvberinfrastructure



2007 Keynote: Jay Boisseau Director Texas Advanced **Computing Center** U. Texas Austin



2008 Keynote: José Munoz **Deputy Office** Director/ Senior Scientific Advisor Office of Cyberinfrastructure National Science Foundation

is **OPEN**!

FREE! Wed Oct 7 2009 @ OU http://symposium2009.oscer.ou.edu/

Registration Parallel Programming Workshop FREE! Tue Oct 6 2009 @ OU **Sponsored by SC09 Education Program** FREE! Symposium Wed Oct 7 2009 @ OU Supercomputing in Plain English: GPGPU

Tuesday April 28 2009



SC09 Summer Workshops

This coming summer, the SC09 Education Program, part of the SC09 (Supercomputing 2009) conference, is planning to hold two weeklong supercomputing-related workshops in Oklahoma, for **FREE** (except you pay your own transport):

- <u>At OSU Sun May 17 the May 23</u>: <u>FREE</u> Computational Chemistry for Chemistry Educators (2010 TENTATIVE: Computational Biology)
- <u>At OU Sun Aug 9 Sat Aug 15</u>:
 <u>FREE</u> Parallel Programming & Cluster Computing
- We'll alert everyone when the details have been ironed out and the registration webpage opens.
- Please note that you must <u>apply</u> for a seat, and acceptance <u>CANNOT</u> be guaranteed.





SC09 Summer Workshops

- 1. May 17-23: Oklahoma State U: Computational Chemistry
- 2. May 25-30: Calvin Coll (MI): Intro to Computational Thinking
- 3. June 7-13: U Cal Merced: Computational Biology
- 4. June 7-13: Kean U (NJ): Parallel Progrmg & Cluster Comp
- 5. June 14-20: Widener U (PA): Computational Physics
- 6. July 5-11: Atlanta U Ctr: Intro to Computational Thinking
- 7. July 5-11: Louisiana State U: Parallel Progrmg & Cluster Comp
- 8. July 12-18: U Florida: Computational Thinking Grades 6-12
- 9. July 12-18: Ohio Supercomp Ctr: Computational Engineering
- 10. Aug 2-8: U Arkansas: Intro to Computational Thinking
- 11. Aug 9-15: U Oklahoma: Parallel Progrmg & Cluster Comp





Outline

- What is GPGPU?
- GPU Programming
- Digging Deeper: CUDA on NVIDIA
- CUDA Thread Hierarchy and Memory Hierarchy
- CUDA Example: Matrix-Matrix Multiply





What is GPGPU?



Accelerators

No, not this



http://gizmodo.com/5032891/nissans-eco-gas-pedal-fights-back-to-help-you-save-gas





- In HPC, an accelerator is hardware component whose role is to speed up some aspect of the computing workload.
- In the olden days (1980s), supercomputers sometimes had <u>array processors</u>, which did vector operations on arrays, and PCs sometimes had <u>floating point accelerators</u>: little chips that did the floating point calculations in hardware rather than software.
- More recently, *Field Programmable Gate Arrays* (FPGAs) allow reprogramming deep into the hardware.





Why Accelerators are Good

Accelerators are good because:

• they make your code run faster.





Why Accelerators are Bad

Accelerators are bad because:

- they're expensive;
- they're hard to program;
- your code on them isn't portable to other accelerators, so the labor you invest in programming them has a very short half-life.





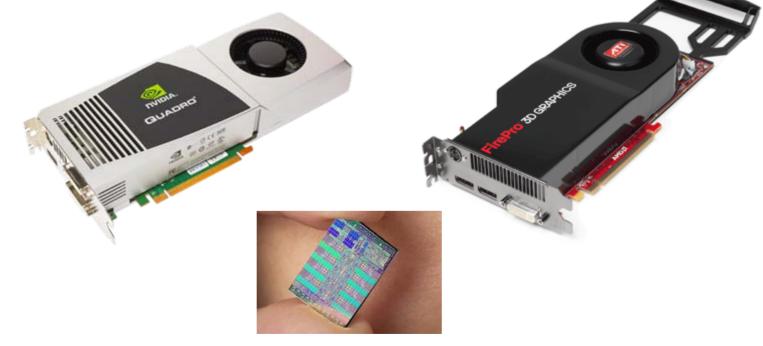
The King of the Accelerators

The undisputed champion of accelerators is:

the graphics processing unit.

http://www.amd.com/us-en/assets/content_type/DigitalMedia/46928a_01_ATI-FirePro_V8700_angled_low_res.gif

http://images.nvidia.com/products/quadro_fx_5800/Quadro_FX5800_low_3qtr.png



http://www.gamecyte.com/wp-content/uploads/2009/01/ibm-sony-toshiba-cell.jpg





Why GPU?

- Graphics Processing Units (GPUs) were originally designed to accelerate graphics tasks like image rendering.
- They became very very popular with videogamers, because they've produced better and better images, and lightning fast.
- And, prices have been extremely good, ranging from three figures at the low end to four figures at the high end.





GPUs are Popular

- Chips are expensive to design (hundreds of millions of \$\$\$), expensive to build the factory for (billions of \$\$\$), but cheap to produce.
- In 2006 2007, GPUs sold at a rate of about 80 million cards per year, generating about \$20 billion per year in revenue.

http://www.xbitlabs.com/news/video/display/20080404234228_Shipments_of_Discrete_Graphi cs_Cards_on_the_Rise_but_Prices_Down_Jon_Peddie_Research.html

• This means that the GPU companies have been able to recoup the huge fix costs.





GPU Do Arithmetic

- GPUs mostly do stuff like rendering images.
- This is done through mostly floating point arithmetic the same stuff people use supercomputing for!





GPU Programming



Hard to Program?

- In the olden days that is, until just the last few years programming GPUs meant either:
 - using a graphics standard like OpenGL (which is mostly meant for rendering), or
 - getting fairly deep into the graphics rendering pipeline.
- To use a GPU to do general purpose number crunching, you had to make your number crunching pretend to be graphics.
- This was hard. So most people didn't bother.





More recently, GPU manufacturers have worked hard to make GPUs easier to use for general purpose computing.

This is known as *General Purpose Graphics Processing Units*.





- Proprietary programming language or extensions
 - NVIDIA: CUDA (C/C++)
 - AMD/ATI: StreamSDK/Brook+ (C/C++)
- OpenCL (Open Computing Language): an industry standard for doing number crunching on GPUs.
- Portland Group Fortran and C compilers with accelerator directives.





NVIDIA CUDA

- NVIDIA proprietary
- Formerly known as "Compute Unified Device Architecture"
- Extensions to C to allow better control of GPU capabilities
- Modest extensions but major rewriting of the code
- No Fortran version available





CUDA Example Part 1

```
| |
```

```
#include "stdafx.h"
```

```
#include <stdio.h>
#include <cuda.h>
```

```
// Kernel that executes on the CUDA device
__global__ void square_array(float *a, int N)
{
    int idx = blockIdx.x * blockDim.x + threadIdx.x;
    if (idx<N) a[idx] = a[idx] * a[idx];
}</pre>
```

http://llpanorama.wordpress.com/2008/05/21/my-first-cuda-program/





CUDA Example Part 2

// main routine that executes on the host
int main(void)

```
float *a h, *a d; // Pointer to host & device arrays
const int N = 10; // Number of elements in arrays
size t size = N * sizeof(float);
cudaMalloc((void **) &a_d, size); // Allocate array on device
// Initialize host array and copy it to CUDA device
for (int i=0; i<N; i++) a h[i] = (float)i;
cudaMemcpy(a d, a h, size, cudaMemcpyHostToDevice);
// Do calculation on device:
int block size = 4;
int n blocks = N/block size + (N%block size == 0 ? 0:1);
square array <<< n blocks, block size >>> (a d, N);
// Retrieve result from device and store it in host array
cudaMemcpy(a h, a d, sizeof(float)*N, cudaMemcpyDeviceToHost);
// Print results
for (int i=0; i<N; i++) printf("%d %f\n", i, a h[i]);</pre>
// Cleanup
free(a h); cudaFree(a d);
```





AMD/ATI Brook+

- AMD/ATI proprietary
- Formerly known as "Close to Metal" (CTM)
- Extensions to C to allow better control of GPU capabilities
- No Fortran version available





{

Brook+ Example Part 1

float4 matmult_kernel (int y, int x, int k,
 float4 M0[], float4 M1[])

```
float4 total = 0;
for (int c = 0; c < k / 4; c++)
{
    total += M0[y][c] * M1[x][c];
}
return total;</pre>
```

http://developer.amd.com/gpu_assets/Stream_Computing_Overview.pdf





Brook+ Example Part 2

```
void matmult (float4 A[], float4 B'[], float4 C[])
ł
    for (int i = 0; i < n; i++)
    ł
        for (j = 0; j < m / 4; j+)
            launch_thread{
                C[i][j] =
                    matmult_kernel(j, i, k, A, B');}
    sync_threads{}
```





OpenCL

- Open Computing Language
- Open standard developed by the Khronos Group, which is a consortium of many companies (including NVIDIA, AMD and Intel, but also lots of others)
- Initial version of OpenCL standard released in Dec 2008.
- Many companies will create their own implementations.
- Apple expects to be first to market, with an OpenCL implementation included in Mac OS X v10.6 ("Snow Leopard"), expected in 2009.





```
// create a compute context with GPU device
context = clCreateContextFromType(0, CL DEVICE TYPE GPU, NULL, NULL,
   NULL);
// create a work-queue
queue = clCreateWorkOueue(context, NULL, NULL, 0);
// allocate the buffer memory objects
memobjs[0] =
    clCreateBuffer(context,
                   CL MEM READ ONLY | CL MEM COPY HOST PTR,
                   sizeof(float)*2*num entries, srcA);
memobjs[1] =
    clCreateBuffer(context, CL_MEM_READ_WRITE,
                   sizeof(float)*2*num entries, NULL);
// create the compute program
program =
    clCreateProgramFromSource(context, 1, &fft1D_1024_kernel_src, NULL);
// build the compute program executable
clBuildProgramExecutable(program, false, NULL, NULL);
// create the compute kernel
kernel = clCreateKernel(program, "fft1D 1024");
```









```
// This kernel computes FFT of length 1024. The 1024 length FFT
// is decomposed into calls to a radix 16 function, another
// radix 16 function and then a radix 4 function
kernel void fft1D 1024 (
    global float2 *in, global float2 *out,
    local float *sMemx, local float *sMemy)
{
    int tid = get_local_id(0);
    int blockIdx = get group id(0) * 1024 + tid;
    float2 data[16];
    // starting index of data to/from global memory
    in = in + blockIdx;
    out = out + blockIdx;
    globalLoads(data, in, 64); // coalesced global reads
```





fftRadix16Pass(data); // in-place radix-16 pass twiddleFactorMul(data, tid, 1024, 0); // local shuffle using local memory localShuffle(data, sMemx, sMemy, tid, (((tid & 15) * 65) + (tid >> 4))); fftRadix16Pass(data); // in-place radix-16 pass twiddleFactorMul(data, tid, 64, 4); // twiddle factor multiplication localShuffle(data, sMemx, sMemy, tid, (((tid >> 4) * 64) + (tid & 15))); // four radix-4 function calls fftRadix4Pass(data); fftRadix4Pass(data + 4); fftRadix4Pass(data + 8); fftRadix4Pass(data + 12); // coalesced global writes globalStores(data, out, 64);



Portland Group Accelerator Directives

- Proprietary directives in Fortran and C
- Similar to OpenMP in structure
- Currently in beta release
- If the compiler doesn't understand these directives, it ignores them, so the same code can work with an accelerator or without, and with the PGI compilers or other compilers.
- In principle, this will be able to work on a variety of accelerators, but the first instance will be NVIDIA; PGI recently announced a deal with AMD/ATI.
- The directives tell the compiler what parts of the code happen in the accelerator; the rest happens in the regular hardware.





PGI Accelerator Example

!\$acc region do k = 1, n1do i = 1, n3c(i,k) = 0.0do j = 1, n2c(i,k) = c(i,k) +a(i,j) * b(j,k) δ enddo enddo enddo !\$acc end region http://www.pgroup.com/resources/accel.htm





Digging Deeper: CUDA on NVIDIA



NVIDIA Tesla

- NVIDIA now offers a GPU platform named Tesla.
- It consists of their highest end graphics card, minus the video out connector.
- This cuts the cost of the GPU card roughly in half: Quadro FX 5800 is ~\$3000, Tesla C1060 is ~\$1500.





NVIDIA Tesla C1060 Card Specs

- 240 GPU cores
- 1.296 GHz



- Single precision floating point performance: 933 GFLOPs (3 single precision flops per clock per core)
- Double precision floating point performance: 78 GFLOPs (0.25 double precision flops per clock per core)
- Internal RAM: 4 GB
- Internal RAM speed: 102 GB/sec (compared 21-25 GB/sec for regular RAM)
- Has to be plugged into a PCIe slot (at most 8 GB/sec)





NVIDIA Tesla S1070 Server Specs

- 4 C1060 cards inside a 1U server (looks like a Sooner node)
- Available in both 1.296 GHz and 1.44 GHz
- Single Precision (SP) floating point performance:
 3732 GFLOPs (1.296 GHz) or 4147 GFLOPs (1.44 GHz)
- Double Precision (DP) floating point performance:
 311 GFLOPs (1.296 GHz) or 345 GFLOPs (1.44 GHz)
- Internal RAM: 16 GB total (4 GB per GPU card)
- Internal RAM speed: 408 GB/sec aggregate
- Has to be plugged into two PCIe slots (at most 16 GB/sec)





Compare x86 vs S1070

Let's compare the best dual socket x86 server today vs S1070.

	Dual socket, Intel 2.66 hex core	NVIDIA Tesla S1070	
Peak DP FLOPs	128 GFLOPs DP	345 GFLOPs DP (2.7x)	
Peak SP FLOPS	256 GFLOPs SP	4147 GFLOPs SP (16.2x)	
Peak RAM BW	17 GB/sec	408 GB/sec (24x)	
Peak PCIe BW	N/A	16 GB/sec	
Needs x86 server to attach to?	No	Yes	
Power/Heat	~400 W	$\sim 800 \text{ W} + \sim 400 \text{ W} (3x)$	
Code portable?	Yes	No (CUDA)	
		Yes (PGI, OpenCL)	





Compare x86 vs S1070

Here are some interesting measures:

	Dual socket, Intel 2.66 hex core	NVIDIA Tesla S1070
DP GFLOPs/Watt	~0.3 GFLOPs/Watt	~0.3 GFLOPs/Watt (same)
SP GFLOPS/Watt	0.64 GFLOPs/Watt	~3.5 GFLOPs (~5x)
DP GFLOPs/sq ft	~340 GFLOPs/sq ft	~460 GFLOPs/sq ft (1.3x)
SP GFLOPs/sq ft	~680 GFLOPs/sq ft	~5500 GFLOPs/sq ft (8x)
Racks per PFLOP DP	244 racks/PFLOP DP	181 racks/PFLOP (3/4) DP
Racks per PFLOP SP	122 racks/PFLOP SP	15 racks/PFLOP (1/8) SP

OU's Sooner is 65 TFLOPs SP, which is <u>1 rack</u> of S1070.





What Are the Downsides?

- You have to rewrite your code into CUDA or OpenCL or PGI accelerator directives.
 - CUDA: Proprietary, C/C++ only
 - OpenCL: portable but cumbersome
 - PGI accelerator directives: not clear whether you can have most of the code live inside the GPUs.





Programming for Performance

The biggest single performance bottleneck on GPU cards today is the PCIe slot:

- PCIe 2.0 x16: 8 GB/sec
- 1600 MHz Front Side Bus: 25 GB/sec
- GDDR3 GPU card RAM: 102 GB/sec per card

Your goal:

- At startup, move the data from x86 server RAM into GPU RAM.
- Do almost all the work inside the GPU.
- Use the x86 server only for I/O and message passing, to minimize the amount of data moved through the PCIe slot.





Does CUDA Help?

Example Applications	URL	Speedup
Seismic Database	http://www.headwave.com	66x – 100x
Mobile Phone Antenna Simulation	http://www.accelware.com	45x
Molecular Dynamics	http://www.ks.uiuc.edu/Research/vmd	21x – 100x
Neuron Simulation	http://www.evolvedmachines.com	100x
MRIProcessing	http://bic-test.beckman.uiuc.edu	245x – 415x
Atmospheric Cloud Simulation	http://www.cs.clemson.edu/~jesteel/clouds.html	50x

http://www.nvidia.com/object/IO_43499.html



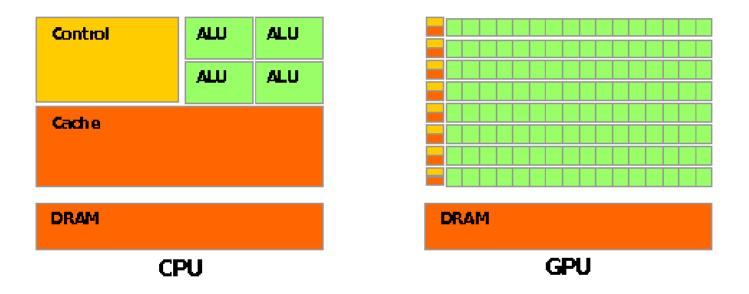


CUDA Thread Hierarchy and Memory Hierarchy

Some of these slides provided by Paul Gray, University of Northern Iowa



CPU vs GPU Layout



Source: Nvidia CUDA Programming Guide





Buzzword: Kernel

In CUDA, a *kernel* is code (typically a function) that can be run inside the GPU.

Typically, the kernel code operates in lock-step on the stream processors inside the GPU.





Buzzword: Thread

In CUDA, a *thread* is an execution of a kernel with a given index.

Each thread uses its index to access a specific subset of the elements of a target array, such that the collection of all threads cooperatively processes the entire data set.

So these are very much like threads in the OpenMP or pthreads sense – they even have shared variables and private variables.





Buzzword: Block

In CUDA, a *block* is a group of threads.

- Just like OpenMP threads, these could execute concurrently or independently, and in no particular order.





Buzzword: Grid

In CUDA, a *grid* is a group of (thread) blocks, with no synchronization at all among the blocks.



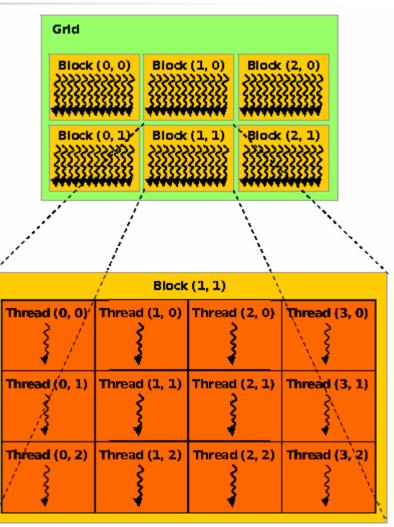


NVIDIA GPU Hierarchy

- <u>Grids</u> map to GPUs
- <u>Blocks</u> map to the MultiProcessors (MP)
 - Blocks are never split across MPs, but an MP can have multiple blocks
- <u>Threads</u> map to Stream Processors (SP)
- <u>Warps</u> are groups of (32) threads that execute simultaneously

Image Source: Nvidia CUDA Programming Guide







CUDA Built-in Variables

- **blockIdx.x, blockIdx.y, blockIdx.z** are built-in variables that returns the block ID in the x-axis, y-axis and z-axis of the block that is executing the given block of code.
- threadIdx.x, threadIdx.y, threadidx.z are built-in variables that return the thread ID in the x-axis, y-axis and z-axis of the thread that is being executed by this stream processor in this particular block.
- So, you can express your collection of blocks, and your collection of threads within a block, as a 1D array, a 2D array or a 3D array.

These can be helpful when thinking of your data as 2D or 3D.





_global___ Keyword

- In CUDA, if a function is declared with the **___global___** keyword, that means that it's intended to be executed inside the GPU.
- In CUDA, the term for the GPU is <u>*device*</u>, and the term for the x86 server is <u>*host*</u>.
- So, a kernel runs on a device, while the main function and so on run on the host.
- Note that a host can play host to multiple devices; for example, an S1070 server contains 4 C1060 GPU cards, and if a single host has two PCIe slots, then both of the PCIe plugs of the S1070 can be plugged into that same host.





Copying Data from Host to Device

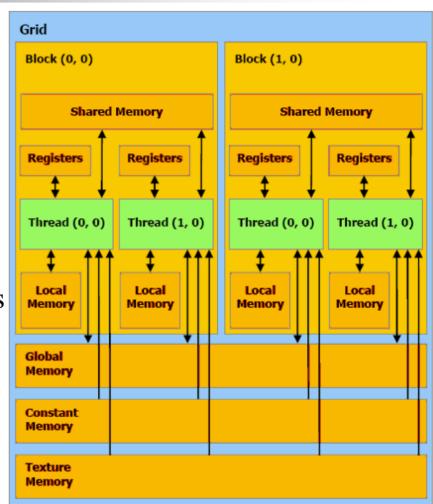
- If data need to move from the host (where presumably the data are initially input or generated), then a copy has to exist in both places.
- Typically, what's copied are arrays, though of course you can also copy a scalar (the address of which is treated as an array of length 1).





CUDA Memory Hierarchy #1

- CUDA has a hierarchy of several kinds of memory:
- Host memory (x86 server)
- Device memory (GPU)
 - <u>Global</u>: visible to all threads in all blocks – largest, slowest
 - <u>Shared</u>: visible to all threads in a particular block – medium size, medium speed
 - *Local*: visible only to a particular thread smallest, fastest



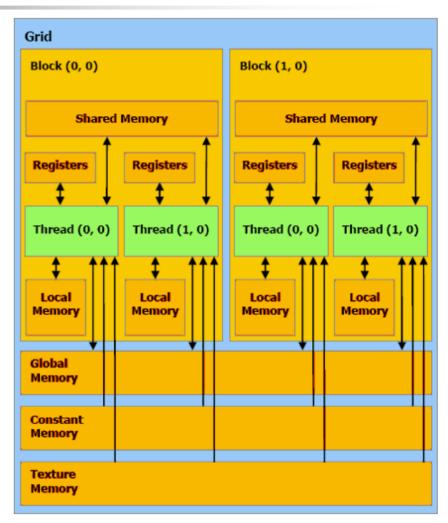




CUDA Memory Hierarchy #2

CUDA has a hierarchy of several kinds of memory:

- Host memory (x86 server)
- Device memory (GPU)
 - <u>Constant</u>: visible to all threads in all blocks; read only
 - <u>Texture</u>: visible to all threads in all blocks; read only







CUDA Example: Matrix-Matrix Multiply



Matrix-Matrix Multiply Main Part 1

float* host_B;
float* host_B;
float* device_A;
float* device_B;
float* device_C;
host_A = (float*) malloc(mem_size_A);

float* host A;

host_B = (float*) malloc(mem_size_B); host C = (float*) malloc(mem_size_C);

```
cudaMalloc((void**) &device_A, mem_size_A);
cudaMalloc((void**) &device_B, mem_size_B);
cudamalloc((void**) &device_C, mem_size_C);
```

 $\ensuremath{{\prime}}\xspace$ // Set up the initial values of A and B here.

// Henry says: I've oversimplified this a bit from
// the original example code.





Matrix-Matrix Multiply Main Part 2



Q

Matrix Matrix Multiply Kernel Part 1

_global___ void matrixMul(float* C, float* A, float* B, int wA, int wB)

```
// Block index
int bx = blockIdx.x;
int by = blockIdx.v;
// Thread index
int tx = threadIdx.xi
int ty = threadIdx.y;
// Index of the first sub-matrix of A processed by the block
int aBegin = wA * BLOCK SIZE * by;
// Index of the last sub-matrix of A processed by the block
           = aBegin + wA - 1;
int aEnd
// Step size used to iterate through the sub-matrices of A
int aStep = BLOCK SIZE;
// Index of the first sub-matrix of B processed by the block
int bBegin = BLOCK SIZE * bx;
// Step size used to iterate through the sub-matrices of B
int bStep = BLOCK SIZE * wB;
// Csub is used to store the element of the block sub-matrix
// that is computed by the thread
float Csub = 0;
```



Matrix Matrix Multiply Kernel Part 2

```
// Loop over all the sub-matrices of A and B
// required to compute the block sub-matrix
for (int a = aBegin, b = bBegin;
         a \leq a \in a \in d;
         a += aStep, b += bStep) {
    // Declaration of the shared memory array As used to
    // store the sub-matrix of A
   shared float As[BLOCK SIZE][BLOCK SIZE];
    // Declaration of the shared memory array Bs used to
    // store the sub-matrix of B
    shared float Bs[BLOCK SIZE][BLOCK SIZE];
    // Load the matrices from device memory
    // to shared memory; each thread loads
    // one element of each matrix
   AS(ty, tx) = A[a + wA * ty + tx];
   BS(ty, tx) = B[b + wB * ty + tx];
    // Synchronize to make sure the matrices are loaded
    syncthreads();
```



Matrix Matrix Multiply Kernel Part 3

```
// Multiply the two matrices together;
// each thread computes one element
// of the block sub-matrix
for (int k = 0; k < BLOCK_SIZE; ++k)
        Csub += AS(ty, k) * BS(k, tx);
```

// Synchronize to make sure that the preceding
// computation is done before loading two new
// sub-matrices of A and B in the next iteration
____syncthreads();

```
// Write the block sub-matrix to device memory;
// each thread writes one element
int c = wB * BLOCK_SIZE * by + BLOCK_SIZE * bx;
C[c + wB * ty + tx] = Csub;
```



}



We wouldn't really do matrix-matrix multiply this way.

- NVIDIA has developed a CUDA implementation of the BLAS libraries, which include a highly tuned matrix-matrix multiply routine.
- (We'll learn about BLAS next time.)
- There's also a CUDA FFT library, if your code needs Fast Fourier Transforms.



But What If I Have a Fortran Code?

Here are your options for Fortran:

- Rewrite part or all of your code in C or C++.
- Use the PGI accelerator directives.



OK Supercomputing Symposium 2009



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2009 Keynote: **Ed Seidel** Director **NSF** Office of Cyberinfrastructure





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SC09 Summer Workshops

This coming summer, the SC09 Education Program, part of the SC09 (Supercomputing 2009) conference, is planning to hold two weeklong supercomputing-related workshops in Oklahoma, for **FREE** (except you pay your own transport):

- <u>At OSU Sun May 17 the May 23</u>: <u>FREE</u> Computational Chemistry for Chemistry Educators (2010 TENTATIVE: Computational Biology)
- <u>At OU Sun Aug 9 Sat Aug 15</u>: <u>FREE</u> Parallel Programming & Cluster Computing
- We'll alert everyone when the details have been ironed out and the registration webpage opens.
- Please note that you must <u>apply</u> for a seat, and acceptance <u>CANNOT</u> be guaranteed.





SC09 Summer Workshops

- 1. May 17-23: Oklahoma State U: Computational Chemistry
- 2. May 25-30: Calvin Coll (MI): Intro to Computational Thinking
- June 7-13: U Cal Merced: Computational Biology
- 4. June 7-13: Kean U (NJ): Parallel, Distributed & Grid
- 5. June 14-20: Widener U (PA): Computational Physics
- 6. July 5-11: Atlanta U Ctr: Intro to Computational Thinking
- 7. July 5-11: Louisiana State U: Parallel, Distributed & Grid
- 8. July 12-18: U Florida: Computational Thinking Pre-college
- 9. July 12-18: Ohio Supercomp Ctr: Computational Engineering
- 10. Aug 2-8: U Arkansas: Intro to Computational Thinking
- 11. Aug 9-15: U Oklahoma: Parallel, Distributed & Grid





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Thanks for your attention!

