GPU Teaching Kit

Accelerated Computing

Lecture 2.1 - Introduction to CUDA C

CUDA C vs. OpenACC vs. CUDA Libraries

Objective

- **To learn the main venues and developer resources for GPU computing**
  - Where CUDA C fits in the big picture

3 Ways to Accelerate Applications

Applications

Libraries	Compiler Directives	Programming Languages
Easy to use Most Performance	Easy to use Portable code	Most Performance Most Flexibility

Libraries: Easy, High-Quality Acceleration

- **Ease of use:** Using libraries enables GPU acceleration without in-depth knowledge of GPU programming
- **“Drop-in”:** Many GPU-accelerated libraries follow standard APIs, thus enabling acceleration with minimal code changes
- **Quality:** Libraries offer high-quality implementations of functions encountered in a broad range of applications

GPU Accelerated Libraries

Linear Algebra
FFT, BLAS,
SPARSE, Matrix

NVIDIA cuFFT, cuBLAS, cuSPARSE | CULA tools | MAGMA | CUSP

Numerical & Math
RAND, Statistics

IMSL Fortran Numerical Library | NVIDIA Math Lib | ArrayFire | NVIDIA cuRAND

Data Struct. & AI
Sort, Scan, Zero Sum

Thrust | GPU AI – Board Games | GPU AI – Path Finding

Visual Processing
Image & Video

NVIDIA NPP | NVIDIA Video Encode | Sundog Software

Vector Addition in Thrust

```
thrust::device_vector<float> deviceInput1(inputLength);
thrust::device_vector<float> deviceInput2(inputLength);
thrust::device_vector<float> deviceOutput(inputLength);

thrust::copy(hostInput1, hostInput1 + inputLength,
    deviceInput1.begin());
thrust::copy(hostInput2, hostInput2 + inputLength,
    deviceInput2.begin());

thrust::transform(deviceInput1.begin(), deviceInput1.end(),
    deviceInput2.begin(), deviceOutput.begin(),
    thrust::plus<float>());
```

Compiler Directives: Easy, Portable Acceleration

- **Ease of use:** Compiler takes care of details of parallelism management and data movement

- **Portable:** The code is generic, not specific to any type of hardware and can be deployed into multiple languages

- **Uncertain:** Performance of code can vary across compiler versions

OpenACC

– Compiler directives for C, C++, and FORTRAN

```
#pragma acc parallel loop
copyin(input1[0:inputLength],input2[0:inputLength]),
  copyout(output[0:inputLength])
  for(i = 0; i < inputLength; ++i) {
    output[i] = input1[i] + input2[i];
  }
```

Programming Languages: Most Performance and Flexible Acceleration

- **Performance:** Programmer has the best control of parallelism and data movement
- **Flexible:** The computation does not need to fit into a limited set of library patterns or directive types
- **Verbose:** The programmer often needs to express more details

GPU Programming Languages

Numerical analytics	MATLAB Mathematica, LabVIEW
Fortran	CUDA Fortran
C	CUDA C
C++	CUDA C++
Python	PyCUDA, Copperhead, Numba
F#	Alea.cuBase

CUDA - C

Applications

Libraries	Compiler Directives	Programming Languages
Easy to use Most Performance	Easy to use Portable code	**Most Performance** **Most Flexibility**

GPU Teaching Kit

Accelerated Computing

西南石油大學计算机科学学院

SCHOOL OF COMPUTER SCIENCE, SOUTHWEST PETROLEUM UNIVERSITY

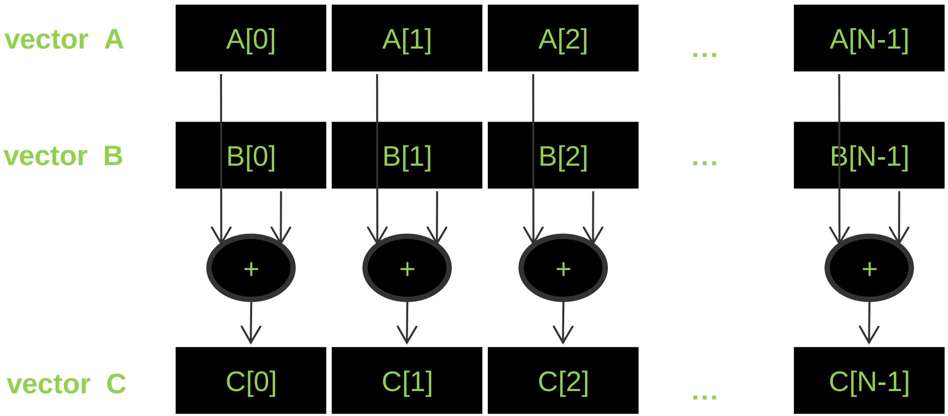
Lecture 2.2 - Introduction to CUDA C

Memory Allocation and Data Movement API Functions

Objective

- **To learn the basic API functions in CUDA host code**
  - Device Memory Allocation
  - Host-Device Data Transfer

Data Parallelism - Vector Addition Example

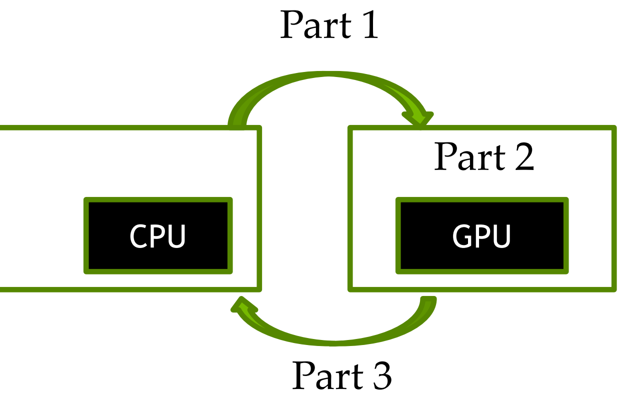


Vector Addition – Traditional C Code

```
// Compute vector sum C = A + B
void vecAdd(float *h_A, float *h_B, float *h_C, int n)
{
    int i;
    for (i = 0; i<n; i++) h_C[i] = h_A[i] + h_B[i];
}

int main()
{
    // Memory allocation for h_A, h_B, and h_C
    // I/O to read h_A and h_B, N elements
    …
    vecAdd(h_A, h_B, h_C, N);
}
```

Heterogeneous Computing vecAdd CUDA Host Code

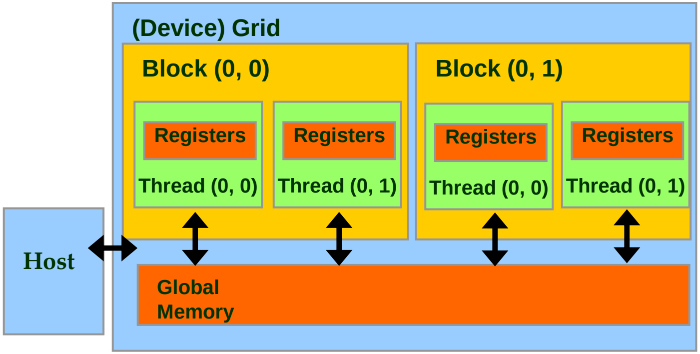



```
#include <cuda.h>
void vecAdd(float *h_A, float *h_B, float *h_C, int n)
{
   int size = n* sizeof(float);
  float *d_A, *d_B, *d_C;
  // Part 1
  // Allocate device memory for A, B, and C
  // copy A and B to device memory

  // Part 2
  // Kernel launch code – the device performs the actual vector addition

  // Part 3
  // copy C from the device memory
  // Free device vectors
}
```

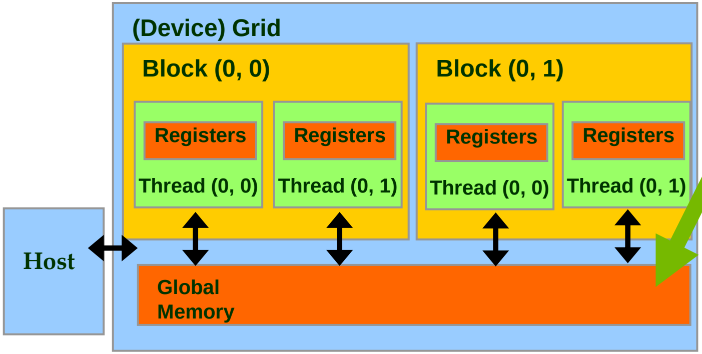
Partial Overview of CUDA Memories



- Device code can:
  - R/W per-thread registers
  - R/W all-shared global memory
- Host code can
  - Transfer data to/from per grid global memory

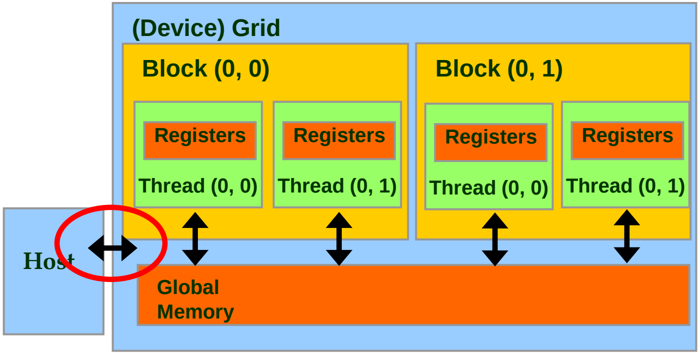
We will cover more memory types and more sophisticated memory models later.

CUDA Device Memory Management API functions



- cudaMalloc()
  - Allocates an object in the device <u>global memory</u>
  - Two parameters
    - **Address of a pointe**r to the allocated object
    - **Size of** allocated object in terms of bytes
- cudaFree()
  - Frees object from device global memory
  - One parameter
    - **Pointer** to freed object

Host-Device Data Transfer API functions



- cudaMemcpy()
  - memory data transfer
  - Requires four parameters
    - Pointer to destination
    - Pointer to source
    - Number of bytes copied
    - Type/Direction of transfer
  - Transfer to device is asynchronous

Vector Addition Host Code

```
void vecAdd(float *h_A, float *h_B, float *h_C, int n)
{
    int size = n * sizeof(float); float *d_A, *d_B, *d_C;

    cudaMalloc((void **) &d_A, size);
    cudaMemcpy(d_A, h_A, size, cudaMemcpyHostToDevice);
    cudaMalloc((void **) &d_B, size);
    cudaMemcpy(d_B, h_B, size, cudaMemcpyHostToDevice);
    cudaMalloc((void **) &d_C, size);

    // Kernel invocation code – to be shown later

    cudaMemcpy(h_C, d_C, size, cudaMemcpyDeviceToHost);
    cudaFree(d_A); cudaFree(d_B); cudaFree (d_C);
}
```

In Practice, Check for API Errors in Host Code

```
cudaError_t  err = cudaMalloc((void **) &d_A, size);

if (err != cudaSuccess)  {
   printf("%s in %s at line %d\n",   cudaGetErrorString(err), __FILE__,
   __LINE__);
   exit(EXIT_FAILURE);
}
```

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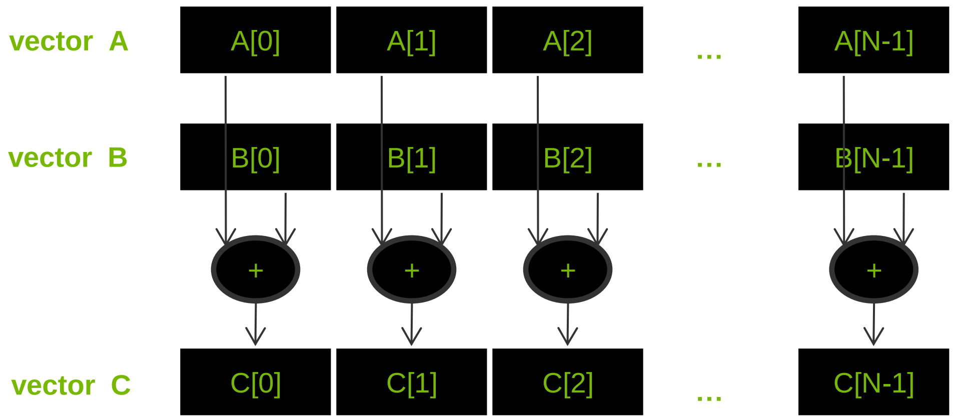
Lecture 2.3 – Introduction to CUDA C

Threads and Kernel Functions

Objective

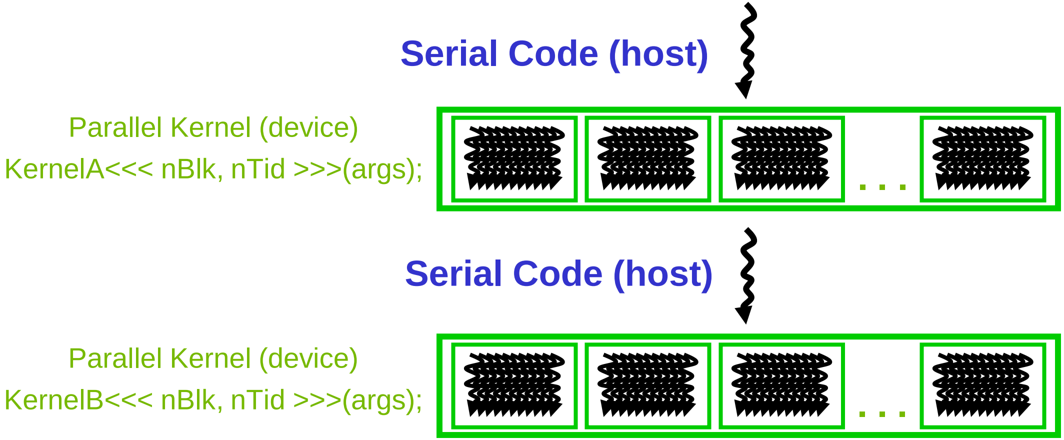
- **To learn about CUDA threads, the main mechanism for exploiting of data parallelism**
  - Hierarchical thread organization
  - Launching parallel execution
  - Thread index to data index mapping

Data Parallelism - Vector Addition Example



CUDA Execution Model

- Heterogeneous host (CPU) + device (GPU) application C program
  - Serial parts in **host** C code
  - Parallel parts in **device** SPMD kernel code



From Natural Language to Electrons

Natural Language (e.g, English)

Algorithm

High-Level Language (C/C++…)

Compiler →

Instruction Set Architecture

Microarchitecture

Circuits

Electrons

©Yale Patt and Sanjay Patel, *From bits and bytes to gates and beyond*

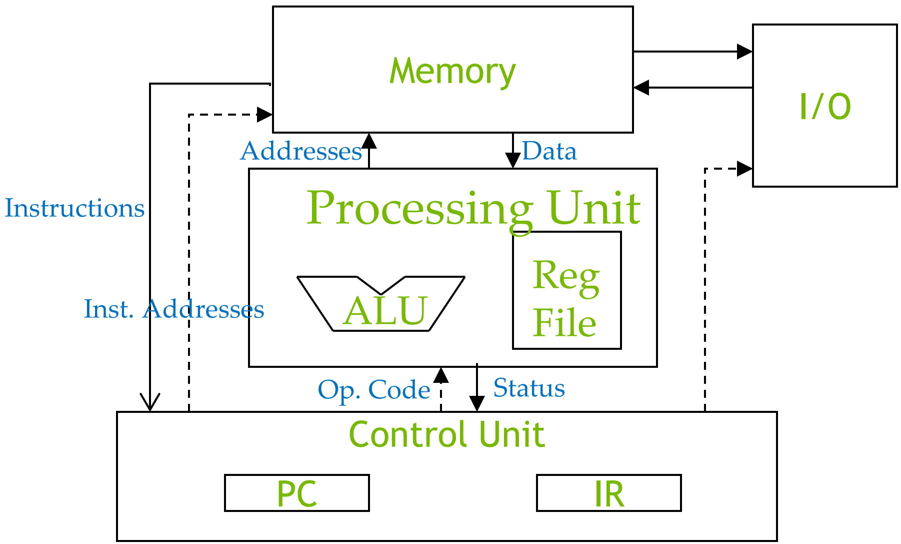
A program at the ISA level

- **A program** is a set of instructions stored in memory that can be read, interpreted, and executed by the hardware.
  - Both CPUs and GPUs are designed based on (different) instruction sets

- **Program instructions** operate on data stored in memory and/or registers.

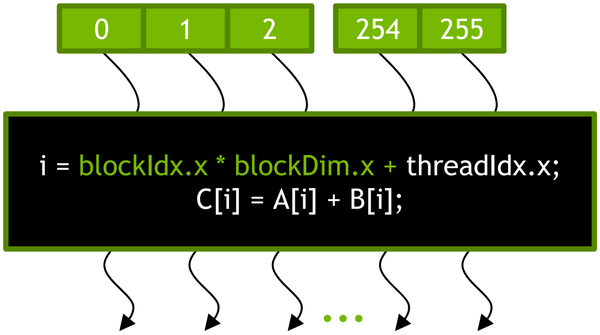
A Thread as a Von-Neumann Processor

A thread is a “virtualized” or “abstracted” Von-Neumann Processor

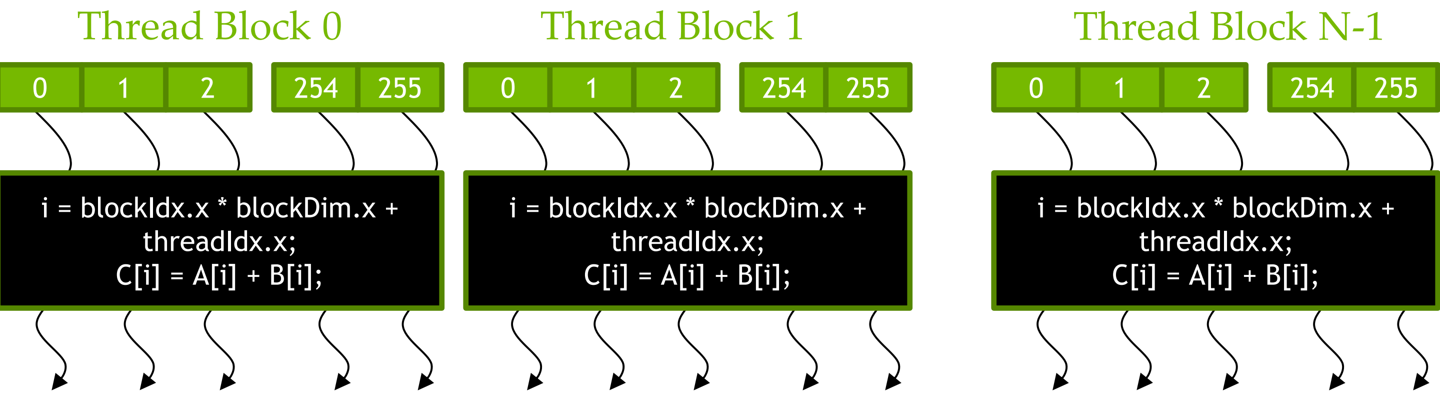


Arrays of Parallel Threads

- A CUDA kernel is executed by a grid (array) of threads
  - All threads in a grid run the same kernel code (**Single Program Multiple Data**)
  - Each thread has indexes that it uses to compute memory addresses and make control decisions



Thread Blocks: Scalable Cooperation

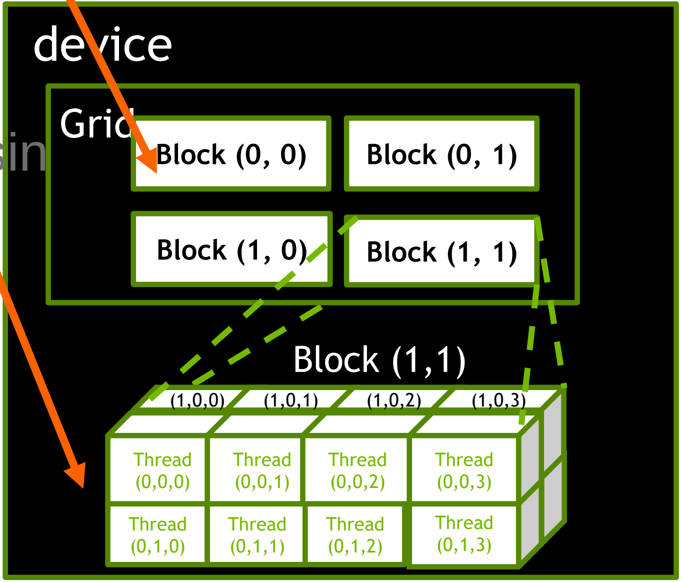


- Divide thread array into multiple blocks
  - Threads within a block cooperate via **shared memory, atomic operations** and **barrier synchronization**
  - Threads in different blocks do not interact

blockIdx and threadIdx

- Each thread uses indices to decide what data to work on
  - blockIdx: 1D, 2D, or 3D (CUDA 4.0)
  - threadIdx: 1D, 2D, or 3D

- Simplifies memory addressing when processing multidimensional data
  - Image processing
  - Solving PDEs on volumes
  - …



GPU Teaching Kit

Accelerated Computing

Lecture 2.4 – Introduction to CUDA C

Introduction to the CUDA Toolkit（Self–study）

Objective

- **To become familiar with some valuable tools and resources from the CUDA Toolkit**
  - Compiler flags
  - Debuggers
  - Profilers

GPU Programming Languages

Numerical analytics	MATLAB, Mathematica, LabVIEW
Fortran	CUDA Fortran
C	CUDA C
C++	CUDA C++
Python	PyCUDA, Copperhead, Numba, NumbaPro
F#	Alea.cuBase

CUDA - C

Applications

Libraries	Compiler Directives	Programming Languages
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NVIDIA

NVCC Compiler

- NVIDIA provides a CUDA-C compiler
  - nvcc
- NVCC compiles device code then forwards code on to the host compiler (e.g. g++)
- Can be used to compile & link host only applications

Example 1: Hello World

```
int main() {
   printf("Hello World!\n");
   return 0;
}
```

Instructions:

1. Build and run the hello world code
2. Modify Makefile to use nvcc instead of g++
3. Rebuild and run

CUDA Example 1: Hello World

```
__global__ void mykernel(void) {
}

int main(void) {
  mykernel<<<1,1>>>();
  printf("Hello World!\n");
  return 0;
}
```

Instructions:

1. Add kernel and kernel launch to main.cu
2. Try to build

CUDA Example 1: Build Considerations

- Build failed
  - Nvcc only parses .cu files for CUDA
- Fixes:
  - Rename main.cc to main.cu

  OR
  - nvcc –x cu
    - Treat all input files as .cu files

Instructions:
1. Rename main.cc to main.cu
2. Rebuild and Run

Hello World! with Device Code

```
__global__ void mykernel(void) {
}

int main(void) {
    mykernel<<<1,1>>>();
    printf("Hello World!\n");
    return 0;
}
```

Output:

```
$ nvcc main.cu
$ ./a.out
Hello World!
```

– `mykernel(`does nothing, somewhat anticlimactic!)

Developer Tools - Debuggers

NSIGHT

CUDA-GDB

CUDA MEMCHECK

NVIDIA Provided

allinea DDT

TotalView®

3rd Party

https://developer.nvidia.com/debugging-solutions

Compiler Flags

- Remember there are two compilers being used
  - NVCC: Device code
  - Host Compiler: C/C++ code
- NVCC supports some host compiler flags
  - If flag is unsupported, use –Xcompiler to forward to host
    - e.g. –Xcompiler –fopenmp
- Debugging Flags
  - -g: Include host debugging symbols
  - -G: Include device debugging symbols
  - -lineinfo: Include line information with symbols

CUDA-MEMCHECK

- Memory debugging tool
  - No recompilation necessary

    %> cuda-memcheck ./exe
- Can detect the following errors
  - Memory leaks
  - Memory errors (OOB, misaligned access, illegal instruction, etc)
  - Race conditions
  - Illegal Barriers
  - Uninitialized Memory
- For line numbers use the following compiler flags:
  - -Xcompiler -rdynamic -lineinfo

https://developer.nvidia.com/cuda-memcheck

Example 2: CUDA-MEMCHECK

Instructions:

1. Build & Run Example 2
   Output should be the numbers 0-9
   Do you get the correct results?
2. Run with cuda-memcheck
   %> cuda-memcheck ./a.out
3. Add nvcc flags "–Xcompiler –rdynamic –lineinfo"
4. Rebuild & Run with cuda-memcheck
5. Fix the illegal write

https://developer.nvidia.com/cuda-memcheck

CUDA-GDB

- cuda-gdb is an extension of GDB
  - Provides seamless debugging of CUDA and CPU code
- Works on Linux and Macintosh
  - For a Windows debugger use NSIGHT Visual Studio Edition

https://developer.nvidia.com/cuda-gdb

Example 3: cuda-gdb

Instructions:

1. Run exercise 3 in cuda-gdb

   %> cuda-gdb --args ./a.out

2. Run a few cuda-gdb commands:

```
(cuda-gdb) b main                                     //set break
point at main
(cuda-gdb) r                                              //run
application
(cuda-gdb) l                                              //print
line context
(cuda-gdb) b foo                                          //break
at kernel foo
(cuda-gdb) c
//continue
(cuda-gdb) cuda thread              //print current thread
(cuda-gdb) cuda thread 10           //switch to thread 10
(cuda-gdb) cuda block               //print current block
(cuda-gdb) cuda block 1                               //switch to
block 1
(cuda-gdb) d                                              //delete
all break points
(cuda-gdb) set cuda memcheck on     //turn on cuda memcheck
(cuda-gdb) r                                              //run
from the beginning
```

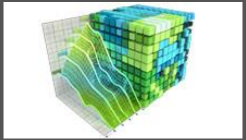
3. Fix Bug

https://developer.nvidia.com/cuda-gdb

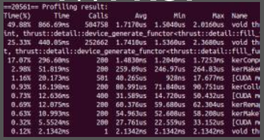
Developer Tools - Profilers

NSIGHT

NVVP



NVPROF



```
==20561== Profiling result:
Time(%)      Time     Calls       Avg       Min       Max  Name
 49.88%  866.69ms    504758  1.7170us  1.5040us  2.0160us  void th
int, thrust::detail::device_generate_functor<thrust::detail::fill_
 25.33%  440.05ms    252662  1.7410us  1.5360us  2.3680us  void th
t, thrust::detail::device_generate_functor<thrust::detail::fill_fu
 17.07%  296.60ms       200  1.4830ms  1.2040ms  1.7253ms  kerComp
  2.98%  51.819ms       200  259.09us  246.97us  264.83us  kerMake
  1.16%  20.173ms       501  40.265us     928ns  17.677ms  [CUDA m
  0.93%  16.198ms       200  80.991us  71.840us  90.751us  kerColl
  0.73%  12.636ms       400  31.589us  14.720us  50.432us  [CUDA m
  0.69%  12.075ms       200  60.376us  59.680us  62.304us  kerRema
  0.63%  10.993ms       200  54.963us  52.608us  58.208us  kerMake
  0.32%  5.5524ms       200  27.761us  22.559us  33.152us  [CUDA m
  0.12%  2.1342ms         1  2.1342ms  2.1342ms  2.1342ms  void th
```

NVIDIA Provided

TAU

VampirTrace

3rd Party

https://developer.nvidia.com/performance-analysis-tools

NVPROF

Command Line Profiler

- Compute time in each kernel
- Compute memory transfer time
- Collect metrics and events
- Support complex process hierarchy's
- Collect profiles for NVIDIA Visual Profiler
- No need to recompile

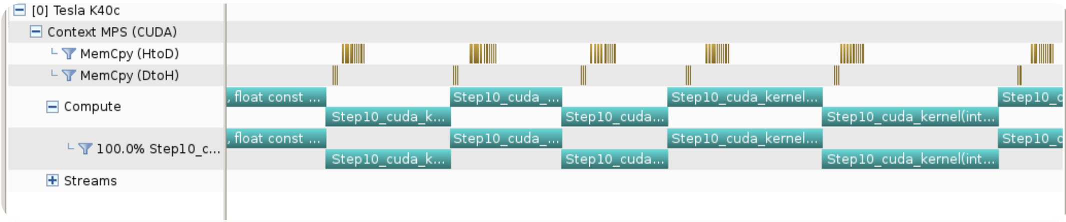
Example 4: nvprof

Instructions:

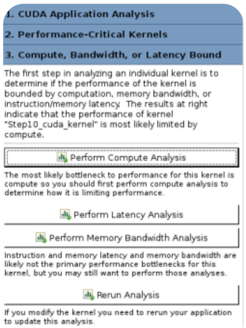
1. Collect profile information for the matrix add example
   %> nvprof ./a.out
2. How much faster is add_v2 than add_v1?
3. View available metrics
   %> nvprof --query-metrics
4. View global load/store efficiency
   %> nvprof --metrics gld_efficiency,gst_efficiency ./a.out
5. Store a timeline to load in NVVP
   %> nvprof –o profile.timeline ./a.out
6. Store analysis metrics to load in NVVP
   %> nvprof –o profile.metrics --analysis-metrics ./a.out

NVIDIA’s Visual Profiler (NVVP)

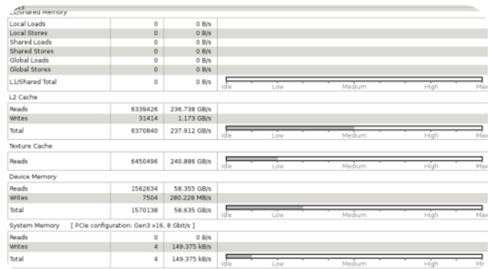
Timeline

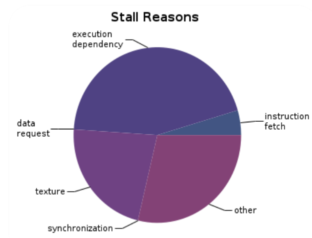


Guided System



Analysis





Example 4: NVVP

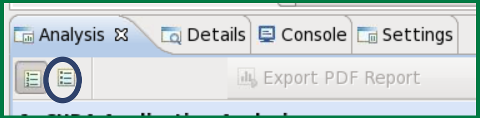
Instructions:

1. Import nvprof profile into NVVP
   - Launch nvvp
   - Click File/ Import/ Nvprof/ Next/ Single process/ Next / Browse
     - Select profile.timeline
   - Add Metrics to timeline
     - Click on 2nd Browse
     - Select profile.metrics
   - Click Finish
2. Explore Timeline
   - Control + mouse drag in timeline to zoom in
   - Control + mouse drag in measure bar (on top) to measure time

Example 4: NVVP

Instructions:

1. Click on a kernel
2. On Analysis tab click on the unguided analysis



2\. Click Analyze All

Explore metrics and properties

What differences do you see between the two kernels?

Note:

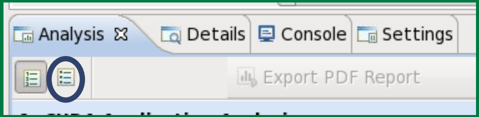
If kernel order is non-deterministic you can only load the timeline or the metrics but not both.

If you load just metrics the timeline looks odd but metrics are correct.

Example 4: NVVP

Let's now generate the same data within NVVP

1. Click File / New Session / Browse
   Select Example 4/a.out
   Click Next / Finish



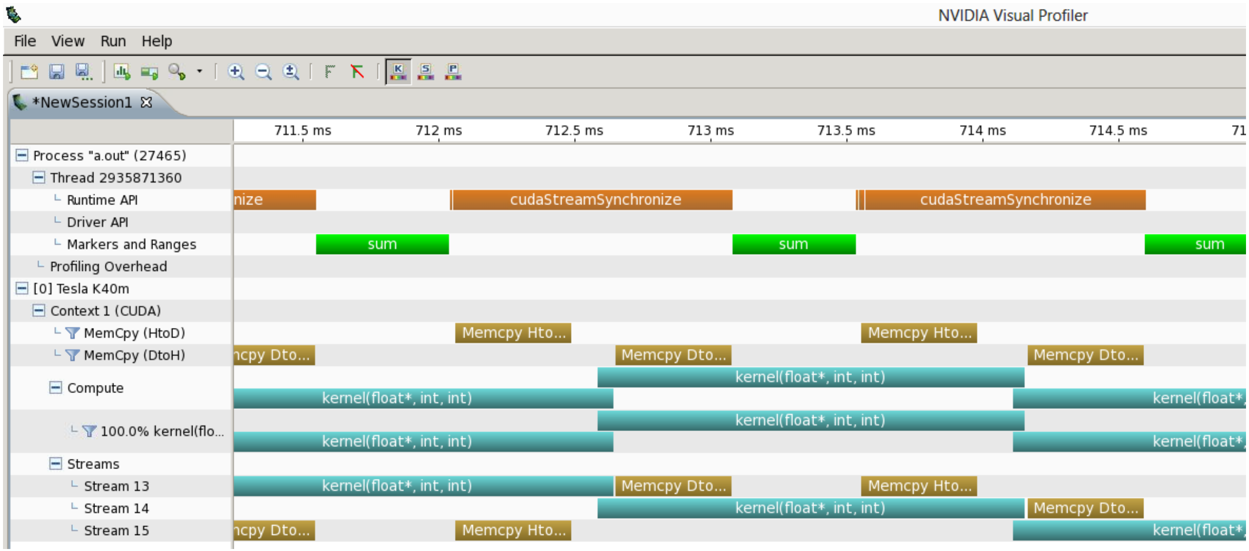
2. Click on a kernel
   Select Unguided Analysis
   Click Analyze All

NVTX

- Our current tools only profile API calls on the host
  - What if we want to understand better what the host is doing?
- The NVTX library allows us to annotate profiles with ranges
  - Add: #include <nvToolsExt.h>
  - Link with: -lnvToolsExt
- Mark the start of a range
  - nvtxRangePushA(“description”);
- Mark the end of a range
  - nvtxRangePop();
- Ranges are allowed to overlap

http://devblogs.nvidia.com/parallelforall/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx/

NVTX Profile



NSIGHT

- CUDA enabled Integrated Development Environment
  - Source code editor: syntax highlighting, code refactoring, etc
  - Build Manger
  - Visual Debugger
  - Visual Profiler
- Linux/Macintosh
  - Editor = Eclipse
  - Debugger = cuda-gdb with a visual wrapper
  - Profiler = NVVP
- Windows
  - Integrates directly into Visual Studio
  - Profiler is NSIGHT VSE

Example 4: NSIGHT

Let's import an existing Makefile project into NSIGHT

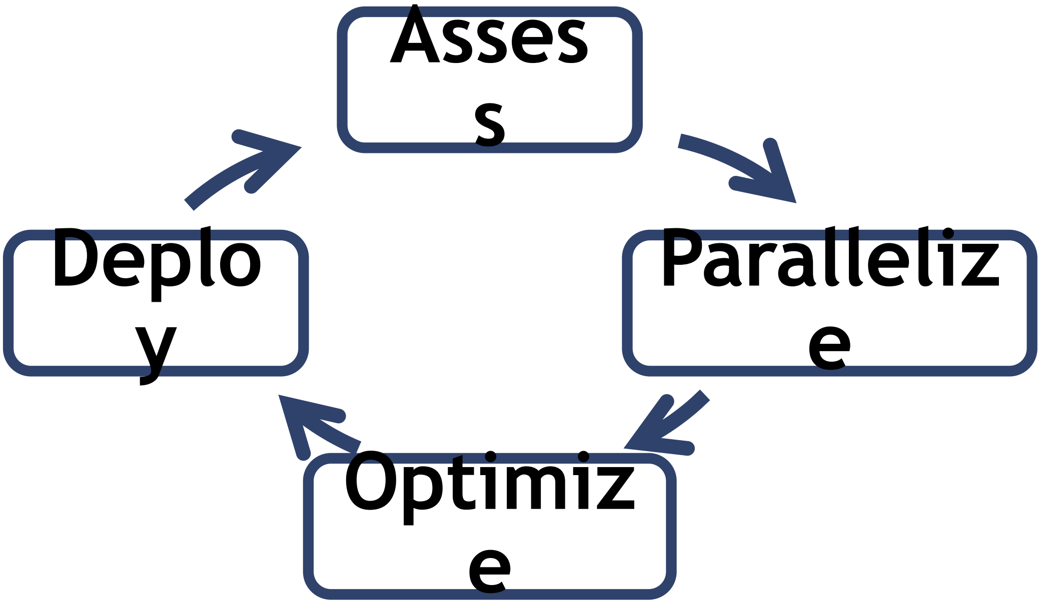
Instructions:

1. Run nsight
   Select default workspace
2. Click File / New / Makefile Project With Existing CodeTest
3. Enter Project Name and select the Example15 directory
4. Click Finish
5. Right Click On Project / Properties / Run Settings / New / C++ Application
6. Browse for Example 4/a.out
7. In Project Explorer double click on main.cu and explore source
8. Click on the build icon
9. Click on the run icon
10. Click on the profile icon

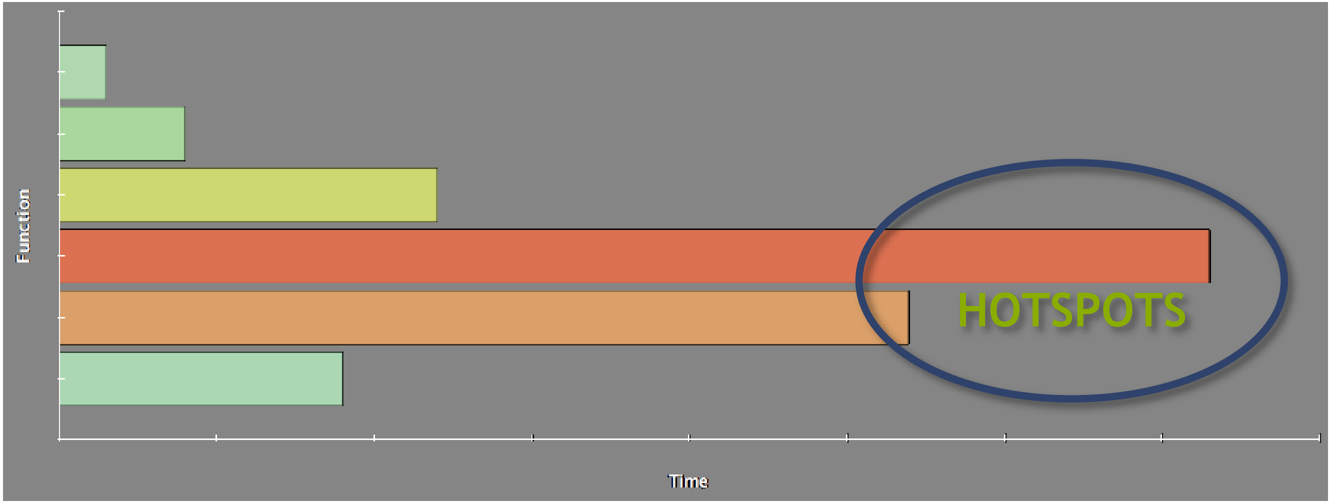
Profiler Summary

- Many profile tools are available
- NVIDIA Provided
  - NVPROF: Command Line
  - NVVP: Visual profiler
  - NSIGHT: IDE (Visual Studio and Eclipse)
- 3rd Party
  - TAU
  - VAMPIR

Optimization



Assess



– Profile the code, find the hotspot(s)
– Focus your attention where it will give the most benefit

Parallelize

Applications

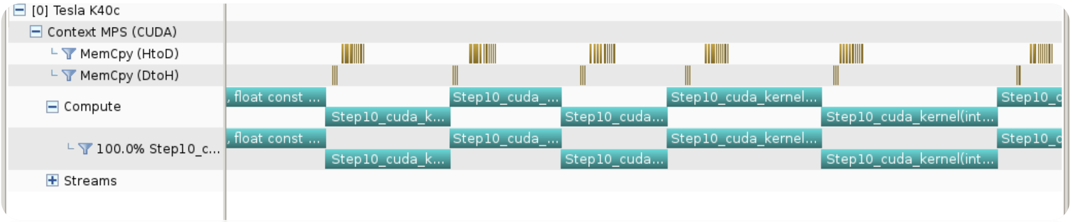
Libraries

Compiler Directives

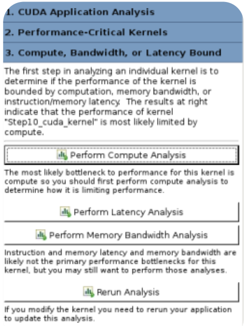
Programming Languages

Optimize

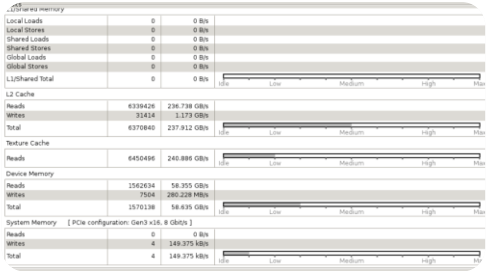
Timeline



Guided System



Analysis



L1/Shared Memory

Local Loads	0	0 B/s	
Local Stores	0	0 B/s	
Shared Loads	0	0 B/s	
Shared Stores	0	0 B/s	
Global Loads	0	0 B/s	
Global Stores	0	0 B/s	
L1/Shared Total	0	0 B/s	Idle Low Medium High Max

L2 Cache

Reads	6339426	236.738 GB/s	
Writes	31414	1.173 GB/s	
Total	6370840	237.912 GB/s	Idle Low Medium High Max

Texture Cache

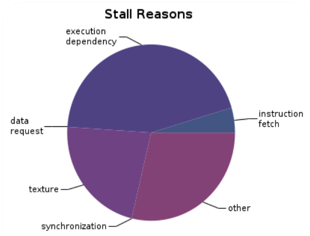
Reads	6450496	240.886 GB/s	Idle Low Medium High Max

Device Memory

Reads	1562634	58.355 GB/s	
Writes	7504	280.228 MB/s	
Total	1570138	58.635 GB/s	Idle Low Medium High Max

System Memory [PCIe configuration: Gen3 x16, 8 Gbit/s]

Reads	0	0 B/s	
Writes	4	149.375 kB/s	
Total	4	149.375 kB/s	Idle Low Medium High Max



Bottleneck Analysis

- Don’t assume an optimization was wrong
- Verify if it was wrong with the profiler

129 GB/s ➡ 84 GB/s

L1/Shared Memory

Local Loads	0	0 B/s	
Local Stores	0	0 B/s	
Shared Loads	2097152	1,351.979 GB/s	
Shared Stores	131072	84.499 GB/s	
Global Loads	131072	42.249 GB/s	
Global Stores	131072	42.249 GB/s	
Atomic	0	0 B/s	
L1/Shared Total	2490368	1,520.977 GB/s	Idle Low Medium

gpuTranspose_kernel(int, int, float const *, float*)	
Start	547.303 ms (5
End	547.716 ms (5
Duration	413.872 µs
Grid Size	[64,64,1]
Block Size	[32,32,1]
Registers/Thread	10
Shared Memory/Block	4 KiB
▽ Efficiency	
Global Load Efficiency	100%
Global Store Efficiency	100%
Shared Efficiency	⚠ 5.9%
Warp Execution Efficiency	100%
Non-Predicated Warp Execution Efficien	97.1%
▽ Occupancy	
Achieved	86.7%
Theoretical	100%
▽ Shared Memory Configuration	
Shared Memory Requested	48 KiB
Shared Memory Executed	48 KiB

⚠ **Shared Memory Alignment and Access Pattern**

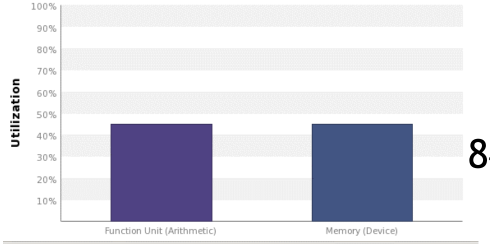
Memory bandwidth is used most efficiently when each shared memory load and store has proper alignment and access pattern.

Optimization: Select each entry below to open the source code to a shared load or store within the kernel with an inefficient alignment or access pattern. For each access pattern of the memory access.

▽ Line / File	main.cu - /home/jluitjens/code/CudaHandsOn/Example19
49	Shared Load Transactions/Access = 16, Ideal Transactions/Access = 1 [2097152 transactions for 131072 total executions]

Performance Analysis

gpuTranspose_kernel(int, int, float const *, float*	
Start	770.067
End	770.324
Duration	256.714
Grid Size	[64,64,1
Block Size	[32,32,1
Registers/Thread	10
Shared Memory/Block	4.125 Ki
Efficiency	
Global Load Efficiency	100%
Global Store Efficiency	100%
Shared Efficiency	50%
Warp Execution Efficiency	100%
Non-Predicated Warp Execution Efficien	97.1%
Occupancy	
Achieved	87.7%
Theoretical	100%
Shared Memory Configuration	
Shared Memory Requested	48 KiB
Shared Memory Executed	48 KiB



84 GB/s → 137 GB/s

L1/Shared Memory			
Local Loads	0	0 B/s	
Local Stores	0	0 B/s	
Shared Loads	131072	138.433 GB/s	
Shared Stores	131720	139.118 GB/s	
Global Loads	131072	69.217 GB/s	
Global Stores	131072	69.217 GB/s	
Atomic	0	0 B/s	
L1/Shared Total	524936	415.984 GB/s	Idle Low Medium
L2 Cache			
L1 Reads	524288	69.217 GB/s	
L1 Writes	524288	69.217 GB/s	
Texture Reads	0	0 B/s	
Atomic	0	0 B/s	
Noncoherent Reads	0	0 B/s	
Total	1048576	138.433 GB/s	Idle Low Medium
Texture Cache			
Reads	0	0 B/s	Idle Low Medium
Device Memory			
Reads	524968	69.306 GB/s	
Writes	524289	69.217 GB/s	
Total	1049257	138.523 GB/s	Idle Low Medium

NVIDIA

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西南石油大學计算机科学学院

SCHOOL OF COMPUTER SCIENCE, SOUTHWEST PETROLEUM UNIVERSITY

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