







Fundamentals of Accelerated Computing with CUDA C/C++

Dr. Momme Allalen LRZ | 07.11.2023

Fundamentals of Accelerated Computing with CUDA C/C++



- You learn the basics of CUDA C/C++ by:
 - Accelerating CPU-only applications to run their latent parallelism on GPUs.
 - Utilizing essential CUDA memory management techniques to optimize accelerated applications
 - Exposing accelerated application potential for concurrency and exploiting it with CUDA streams
 - Leveraging command line and visual profiling to guide and check your work.
 - Upon completion, you'll be able to accelerate and optimize existing C/C++ CPU-only
 applications using the most essential CUDA tools and techniques. You'll understand
 an iterative style of CUDA development that will allow you to ship accelerated
 applications fast.

Tentative Agenda



10:00-10:15 Intro@CUDA 10:15-12:00 Accelerating Applications with CUDA C/C++

12:00-13:00 Lunch break

13:00-14:20 Managing Accelerated Application Memory with CUDA Unified Memory and nsys

14:20-14:30 Coffee break

14:30-15:45 Asynchronous Streaming and Visual Profiling for Accelerated Applications with CUDA C/C++

15:45-16:00 Q&A, Final Remarks

Workshop Webpage



- Lecture material will be made available under:
 - https://tinyurl.com/hdli3w23
- Access CUDA C/C++ Code :
 - See the **Chat Window**

Training Setup



- To get started, follow these steps:
- Create an NVIDIA Developer account at <u>http://courses.nvidia.com/join</u> Select "Log in with my NVIDIA Account" and then "Create Account".
- If you use your own laptop, make sure that WebSockets works for you: Test your Laptop at <u>http://websocketstest.com</u>
 - Under ENVIRONMENT, confirm that "WebSockets" is checked yes.
 - Under WEBSOCKETS (PORT 80]. confirm that "Data Receive", "Send", and "Echo Test" are checked yes.
 - If there are issues with WebSockets, try updating your browser. We recommend Chrome, Firefox, or Safari for an optimal performance.
- Visit <u>http://courses.nvidia.com/dli-event</u> and enter the event code provided by the instructor.
- You're ready to get started.



And now

Enjoy the course !

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

Why do we need to program for GPU?

Moore's law is dead !

The long-held notion that the processing power of computers increases exponentially every couple of years has hit its limit....

The free lunch is over..

Future is parallel !





Typical example Intel chip: Core i7 Gen System Agent w/Display, Memory Control Kaby Lake processors 4*CPU cores With hyperthreading Each with 8-wide AVX instructions GPU with 1280 processing elements Programming on chip: - Serial C/C++ .. Code only takes advantage of a very small amount of the available resources of the chip - Using vectorisation allows you to fully utilise the resources of a single hyper-thread Graphics Core + **New Media Capabilities** GPU need to be used? Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

Why do we need to program for GPU?

 Using multi-threading allows you to fully utilise all CPU cores





Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@lrz.de

Why do we need to program for GPU?

GPU programming:

- -Limited only to a specific domain
- -Separate source solutions
- -Verbose low Levels APIs
- oneAPI & DPC++
- CUDA C/C++
- HIP
- SYCL
- OpenCL
- Kokkos
- HPX ...





Why do we need GPUs on HPC?

- Increase in parallelism
- Today almost a similar amount of efforts on using CPUs vs GPUs by real applications
- GPUs well-suited to deep learning.

NVIDIA Software uses CUDA

M/by do we pood "CDU cooplaratore"	Rank	System	Cores	Rmax (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
on HPC?	1	Frontier - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE D0E/SC/0ak Ridge National Laboratory United States	8,699,904	1,194.00	1,679.82	22,703
	2	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442.01	537.21	29,899
	3	LUMI - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE EuroHPC/CSC Finland	2,220,288	309.10	428.70	6,016
GPU-accelerated	4	Leonardo - BullSequana XH2000, Xeon Platinum 8358 32C 2.6GHz, NVIDIA A100 SXM4 64 GB, Quad-rail NVIDIA HDR100 Infiniband, Atos EuroHPC/CINECA Italy	1,824,768	238.70	304.47	7,404
systems	5	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148.60	200.79	10,096
	6	Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94.64	125.71	7,438
TOP 500	7	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93.01	125.44	15,371
The List.	8	Perlmutter - HPE Cray EX235n, AMD EPYC 7763 64C 2.45GHz, NVIDIA A100 SXM4 40 GB, Slingshot-10, HPE D0E/SC/LBNL/NERSC United States	761,856	70.87	93.75	2,589
www.top500.org	9	Selene - NVIDIA DGX A100, AMD EPYC 7742 64C 2.25GHz, NVIDIA A100, Mellanox HDR Infiniband, Nvidia NVIDIA Corporation United States	555,520	63.46	79.22	2,646
Fundamentals of Accelerated Computing with CUDA C/C++ LRZ 07.11.2023; Allalen@Irz.de	10	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000, NUDT National Super Computer Center in Guangzhou China	4,981,760	61.44	100.68	18,482

GPU vs CPU Architecture

ALU Control * Small number of large cores ALU ALU * More control structures and less processing units *Optimised for latency which Cache requires quite a lot of power DRAM DRAM CPU GPU Massively data parallel General purpose architecture

•GPU devotes more transistors data processing rather than data caching and flow control. Same problem executed on many data elements in parallel.

* Large number of small cores
* Less control structured and more processing units
*Less flexible program model
*There're more restrictions but Requires a lot less power

- Hopper GPU (H100) with over 80 Billion Transistors on an 814 mm²
- 89 GB memory
- First support PCIe gen5 and utilize the HBM3 enabling 3TB/s
- 30 Tflops of peak FP64, 60 Tflops with FP64 tensor-core or 32 FP performance

What and Why CUDA C/C++ ?

CUDA = "Compute Unified Device Architecture"

* Introduced and released in 2006 for the GeForce 8800 *

• GPU = massively data parallel - co-processor

C/C++ plus a few simple extensions - Compute oriented drivers, language, and tools

Documentations:

CUDA_C_Programming_Guide.pdf CUDA_C_Getting_Started.pdf CUDA_C_Toolkit_Release.pdf

CUDA Programming Model

- A kernel is executed as a grid of thread blocks
- All threads share data memory space
- A thread block is a batch of threads that can cooperate with each other by:
 - Synchronizing their execution
 - Efficiently sharing data through a low latency shared memory
- Tow threads from two different blocks cannot cooperate
- Sequential code launches asynchronously GPU kernels

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

CUDA C/C++

Host: The CPU and ist memory (host memory)

Host

memory (device memory)

Device

CUDA Devices and Threads Execution Model

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

CUDA C/C++

The CPU copies data from CPU to GPU The CPU launches kernels on the GPU The CPU copies data to CPU from GPU

The CPU allocates memory on the GPU

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

NVCC Compiler

- NVIDIA provides a CUDA-C compiler
- \rightarrow nvcc
- NVCC splits your code in 2: Host code and Device code.
- **Device** code sent to NVIDIA device compiler.

- nvcc is capable of linking together both host and device code into a single executable.
 - Convention: C++ source files containing CUDA syntax are typically given the extension .cu.

• For ".**cpp**" extension use: nvcc –x cu –arch=sm_70 –o exe code.cpp

DEEP LEARNIN(. INSTITUTI

Lab1: Accelerating Applications with CUDA C/C++ Dr. Momme Allalen Leibniz Computing Centre, Munich Germany - www.lrz.de Deep Learning Certified Instructor, NVIDIA Deep Learning Institute NVIDIA Corporation.

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

Lab1: Accelerating Applications with CUDA C/C++

You should already be able to:

- Declare variables, write loops, and use if / else statements in C.
- Define and invoke functions in C.
- Allocate arrays in C.
- No previous CUDA knowledge is required.

Objectives

•

By the time you complete this lab, you will be able to:

- Write, compile, and run C/C++ programs that both call CPU functions and launch GPU kernels.
 - Control parallel threadhierarchy using execution configuration.
 - Refactor serial loops to execute their iterations in parallel on a GPU.
 - Allocate and free memory available to both CPUs and GPUs.
 - Handle errors generated by CUDA code.
 - Accelerate CPU-only applications.

nvc :is a C11 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C compiler, assembler, and linker for the target processors with options derived from its command line arguments. **nvc** supports ISO C11, supports GPU programming with OpenACC, and supports multicore CPU programming with OpenACC and OpenMP.

nvc++ : is a C++17 compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the C++ compiler, assembler, and linker for the target processors with options derived from its command line arguments. **nvc++** supports ISO C++17, supports GPU and multicore CPU programming with C++17 parallel algorithms, OpenACC, and OpenMP.

nvfortran : is a Fortran compiler for NVIDIA GPUs and AMD, Intel, OpenPOWER, and Arm CPUs. It invokes the Fortran compiler, assembler, and linker for the target processors with options derived from its command line arguments. **nvfortran** supports ISO Fortran 2003 and many features of ISO Fortran 2008, supports GPU programming with CUDA Fortran, and GPU and multicore CPU programming with ISO Fortran parallel language features, OpenACC, and OpenMP.

nvcc : is the CUDA C and CUDA C++ compiler driver for NVIDIA GPUs. nvcc accepts a range of conventional compiler options, such as for defining macros and include/library paths, and for steering the compilation process. nvcc produces optimized code for NVIDIA GPUs and drives a supported host compiler for AMD, Intel, OpenPOWER, and Arm CPUs.

DEEP LEARNING INSTITUTE

Lab2: Managing Accelerated Application Memory with CUDA Unified Memory and nsys Dr. Momme Allalen Leibniz Computing Centre, Munich Germany - www.lrz.de Deep Learning Certified Instructor, NVIDIA Deep Learning Institute NVIDIA Corporation.

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

Lab2: Managing Accelerated Application Memory with CUDA Unified Memory and nsys

Prerequisites

You should already be able to:

- Write, compile, and run C/C++ programs that both call CPU functions and **launch** GPU **kernels**.
- Control parallel thread hierarchy using execution configuration.
- Refactor serial loops to execute their iterations in parallel on a GPU.
- Allocate and free Unified Memory.

DEEP LEARNING INSTITUTE

Objectives

By the time you complete this lab, you will be able to: Use the Nsight Systems command line tool (nsys) to profile accelerated application performance.
Laverage and understanding of Streaming
Multiprocessors to optimize execution configurations.
Understand the behavior of Unified Memory with regard to page faulting and data migrations.
Use asynchronous memory prefetching to reduce page faults and data migrations for increased performance.
Employ an iterative development cycle to rapidly

 Employ an iterative development cycle to rapidly accelerate and deploy applications. CUDA® PROFILING TOOLS

nvvc: NVIDIA visual profiler nvprof: toolto understand and optimize the performance of your CUDA, OpenACC or OpenMP applications, Application level opportunities Overall application performance Overlap CPU and CPU work, identify the bottlenecks (CPU or GPU) Overall GPU utilization and efficiency Overlap compute and memory copies Utilize compute and copy engines effectively.

Kernel level opportunities

Use memory bandwidth efficiently Use compute resources efficiently Hide instruction and memory latency

There are more features, example for Dependency Analysis Command: nvprof --dependency-analysis --cpu-thread-tracing on ./ executable_cuda

THE NSIGHT SUITE COMPONENTS

Figure 1. Flowchart describing working with new NVIDIA Nsight tools for performance optimization

nvprof replaced with nsys -profile....

https://developer.nvidia.com/nsight-systems

Nsight Systems GUI

Main timeline view, Events View

	Nsight Systems 2023.2.1							-		>
le <u>V</u> iew	Tools Help									
ale_repo	rt.qdrep ×									
≡ Timeli	ne View 🔻					ΞQ	1x	▲ <u>3 warning</u> :	s, 15 mes	essag
	0s 🝷	+520ms	+530ms		+540ms +550ms +	560ms	+57	70ms		
CPU (9	96)									
	HW (0000:03:00.0 -									_
- 64 50	Context 1				PETROPA CA CA					
- 100	00% Kanada				conletfleat fle					
• 100	.0% Kernels				scale(lioat, ilo					
▼ 10	0.0% scale				scale(float, flo					
1	100.0% scale(float, f				scale(float, flo					
▶ 35.59	6 Unified memory									
Thread	ds (7)									
- J M	8921 scale vector								l	L.
• [-re	552] Scale_vector, 1				المحفة علم المنافقة المناحية والتكاف المستحد والمستحد المناكر المنافقة والمنافقة والمنافقة والمنافقة والمنافقة					
OS	runtime libraries		sem_timedw	ait			sem_time	dwait)	
CUL	DA API	cudaN	/allocManaged		cudaDeviceSy	C				
CUL	DA API filer overhead	cudaN	/allocManaged		cudaDeviceSy	C	CUDA profiling	g data flush overh	nead	
Prot	DA API filer overhead	cudaM	AallocManaged		cudaDeviceSy	C	CUDA profiling	g data flush overh	nead	
Prot	filer overhead	cudaN	AallocManaged		cudaDeviceSy	C	CUDA profiling	g data flush overh	nead	•
CUI Proi	A API filer overhead	cudał	AallocManaged		cudaDeviceSy		CUDA profiling	g data flush overh	nead	•
CUI Proi	ew	cuda	AallocManaged		cudaDeviceSy	C	CUDA profiling	g data flush overh	nead	•
CUI Proi Events Vi	A API filer overhead ew	cuda	AallocManaged	Duration	TID	[C]]	CUDA profiling Name Description:	g data flush overh	nead	•
CUI Pro: Events Vi # 1	A API filer overhead ew Name b cudaMallocManaged	cuda	AallocManaged Start 0,27528s	Duration 265,216 ms	TID 4892	<u>C</u>	CUDA profiling	g data flush overh	nead	
CUI Pro- Events Vi # 1 227	A API filer overhead ew Name CudaMallocManaged cudaMallocManaged	cuda	AallocManaged Start 0,27528s 0,540498s	Duration 265,216 ms 23,380 µs	TID 4892 4892	<u>C</u>	CUDA profiling	g data flush overh	nead	•
CUI Pro Events Vi # 1 227 229	A API filer overhead ew Name CudaMallocManaged cudaMallocManaged scale_vector_um!main	cudaM	Start 0,27528s 0,540498s 0,540807s	Duration 265,216 ms 23,380 μs -	TID 4892 4892 4892	<u>C</u>	CUDA profiling	g data flush overh	nead	•
CUI Pro Events Vi # 1 227 229 230	A API filer overhead ew Name CudaMallocManaged cudaMallocManaged scale_vector_um!main scale_vector_um!main	cudaM	Start 0,27528s 0,540498s 0,540807s 0,541117s	Duration 265,216 ms 23,380 μs - -	TID 4892 4892 4892 4892 4892	<u>C</u>	CUDA profiling	g data flush overh	nead	
CUI Pro Events Vi # 1 227 229 230 231	A API filer overhead w v Name CudaMallocManaged scale_vector_um!main scale_vector_um!main scale_vector_um!main	cuda	Start 0,27528s 0,540498s 0,540498s 0,540807s 0,541117s 0,541227s	Duration 265,216 ms 23,380 μs - - -	TID 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892		CUDA profiling	g data flush overh	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 232	A API filer overhead w w v Name CudaMallocManaged scale_vector_um!mail scalevector_um!mail scalevector_um	cudah	Start 0,27528s 0,540498s 0,540498s 0,540498s 0,540807s 0,541117s 0,541127s 0,541227s 0,541486s 0,54186s	Duration 265,216 ms 23,380 μs - - - -	TID 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 233 233	A API filer overhead w w v Name CudaMallocManaged scale_vector_um!main	cudah	Start 0.27528s 0.540498s 0.540498s 0.540498s 0.541117s 0.541127s 0.541127s 0.541486s 0.541486s 0.541596s 0.54159658 0.541596s 0.	Duration 265,216 ms 23,380 μs - - - - - -	TID 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 234 234	A API filer overhead ew Name CudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged scale_vector_um!mail scale_vector_um!mail scale_vector_um!mail scale_vector_um!mail	cudah	Start 0,27528s 0,540498s 0,540498s 0,541175s 0,54127s 0,54127s 0,54127s 0,54127s 0,54127s 0,54127s 0,541205s 0,541205s	Duration 265,216 ms 23,380 μs - - - - - - - -	Image: CudaDeviceSy TID 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 234 235 234	A API filer overhead ew Name CudaMallocManaged CudaMallocManaged CudaMallocManaged CudaMallocManaged CudaMallocManaged Scale_vector_um!maii Scale_vector_um!maii Scale_vector_um!maii Scale_vector_um!maii Scale_vector_um!maii	cuda 	Start 0,27528s 0,540498s 0,540498s 0,541117s 0,54127s 0,54127s 0,54186s 0,541596s 0,541706s 0,5419395	Duration 265,216 ms 23,380 μs - - - - - - - - - - - - -	Indicator Indicator TID 1 4892 1		CUDA profiling	g data flush overh	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 234 235 236 237	A API filer overhead ew Name CudaMallocManaged CudaMallocManaged cudaMallocManaged scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii	cuda 	AallocManaged Start 0,27528s 0,540498s 0,540498s 0,54127s 0,54127s 0,54127s 0,54126s 0,541996s 0,541995s 0,541999s 0,5421055	Duration 265,216 ms 23,380 µs - - - - - - - - - - - - - - - - - - -	TID 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 233 234 235 236 237	A API filer overhead filer overhead ew Aname CudaMallocManaged c	cuda 	Start 0,27528s 0,540498s 0,540498s 0,541117s 0,541227s 0,541246s 0,541596s 0,541596s 0,541939s 0,542105s 0,542297s	Duration 265,216 ms 23,380 μs - - - - - - - - - - - - - - - - - - -	TID 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 233 234 235 236 237 238	A API filer overhead filer overhead ew Aname CudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii	cuda 	Start 0,27528s 0,540498s 0,540498s 0,541117s 0,541275 0,541486s 0,541596s 0,541706s 0,541205s 0,542207s 0,542207s 0,542205s 0,542505s	Duration 265,216 ms 23,380 μs - - - - - - - - - - - - - - - - - - -	TID 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 233 233 234 235 236 237 238 239	A API filer overhead filer overhead w w Aname CudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged scale_vector_um!maii	cuda 	Start 0,27528s 0,540498s 0,540498s 0,541227s 0,541117s 0,541486s 0,541596s 0,541706s 0,542105s 0,54227s 0,54226s 0,54226s 0,5428s	Duration 265,216 ms 23,380 μs - - - - - - - - - - - - - - - - - - -	TID 4892		CUDA profiling	g data flush over	nead	
CUI Pro Events Vi # 1 227 229 230 231 232 233 233 233 234 235 234 235 236 237 238 239 240	A API filer overhead ew Name CudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged cudaMallocManaged scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii scale_vector_um!maii	cuda 	Start 0,27528s 0,540498s 0,540498s 0,541227s 0,541227s 0,541706s 0,541706s 0,541205s 0,541205s 0,541205s 0,541205s 0,541205s 0,541205s 0,541205s 0,54205s 0,54205s 0,542269s 0,54268s 0,542789s	Duration 265,216 ms 23,380 μs - - - - - - - - - - - - - - - - - - -	TID 4892		CUDA profiling	g data flush over	nead	

- Nsight Systems is an extremely low overhead profiling Tool across any number of CPUs and GPUs.
- Nsight System is your first stop on your profiling workflow, inspect your algorithm timing and GPU interaction and identify a large number of opportunities for optimization.

NSIGHT SYSTEMS

- Provides users with a more complete view of how their codes balance workload across multiple CPUs and GPUs
- Locate optimization opportunities, helps and allows to identify issues such as:
 - GPU starvation
 - Insufficient CPU parallelisation or pipelining
 - Unexpectedly expensive CPU or GPU algorithm
 - Unnecessary GPU synchronization
- The tool uses low overhead tracing and sampling techniques to collect process and thread activity and visualize millions of events on a very fast GUI timeline
- Correlates that data across CPU cores and GPU streams, allowing users to investigate bottlenecks.
- Multi-platform: Linux & Windows, x86-64, Tegra, Power, MacOSX (host only)

GPU Starvation Investigations

https://developer.nvidia.com/nsight-systems

Unnecessary GPU Synchronisation Calls

	51s +197.395ms +197.4ms +197.405ms +197.41ms +197.415ms +197.4	42ms +197.425ms +197.43ms +197.435ms +197.44ms +19	97.445ms +197.45ms +197.455ms +197.	46ms +197.465ms +197.47ms +197.47 51s 197.47817m
CPU (12)				
cuDNN	cudnnBatchNormalizationForwardTraining [1			
CUDA API	bn_fw_tr_1C11_kerne	cudaStreamSynchronize	cudaMemcpyAsync	cudaStreamSynchronize
Profiler overhead				
23 threads hidden				
✓ CUDA (TITAN X (Pascal))				
> Stream 47				
✓ Stream 13				
✓ Memory				
Memset				
HtoD memcpy				
DtoH memcpy				
DtoD memcpy				Memcpy
✓ Kernels		bn_fw_tr_1C11_kernel_new		

https://developer.nvidia.com/nsight-systems

NVIDIA NSIGHT SYSTEMS

- Support: MPI, OpenACC, OpenMP
- Complex data mining capabilities, enables to go beyond basic statistics.
- Support multiple simultaneous sessions.
- MPI trace feature enables to analyse when the threads are busy or blocked in long-running functions of the MPI standard, available on OpenMPI, MPICH and NVShmem.
- OpenACC trace enables to see where code has been offload and parallelized onto the GPU, which helps you to analyse the activities executing on the CPUs and GPUs in parallel.
- Tracing OpenMP code is available for compilers supporting OpenMP5 and OMPT interface. This capability enables tracing of the parallel regions of code that are distributed either across multiple threads or to the GPU.
- Provides support for CUDA graphs. To understand the execution of the source of CUDA kernels and execution of CUDA graphs, kernels can be correlated back through the graph lunch, instantiation, and all the way back to the code creation, to identify the origin of the kernel execution on the GPU.

Command Line Options nsys

Command	Description
profile	A fully formed profiling description requiring and accepting no further input. The command switch options used (see below table) determine when the collection starts, stops, what collectors are used (e.g. API trace, IP sampling, etc.), what processes are monitored, etc.
start	Start a collection in interactive mode. The start command can be executed before or after a launch command.
stop	Stop a collection that was started in interactive mode. When executed, all active collections stop, the CLI process terminates but the application continues running.
cancel	Cancels an existing collection started in interactive mode. All data already collected in the current collection is discarded.
launch	In interactive mode, launches an application in an environment that supports the requested options. The launch command can be executed before or after a start command.
shutdown	Disconnects the CLI process from the launched application and forces the CLI process to exit. If a collection is pending or active, it is cancelled
export	Generates an export file from an existing .nsys-rep file. For more information about the exported formats see the /documentation/nsys- exporter directory in your Nsight Systems installation directory.
stats	Post process existing Nsight Systems result, either in .nsys-rep or SQLite format, to generate statistical information.
analyze	Post process existing Nsight Systems result, either in .nsys-rep or SQLite format, to generate expert systems report.
status	Reports on the status of a CLI-based collection or the suitability of the profiling environment.
sessions	Gives information about all sessions running on the system.

https://docs.nvidia.com/nsight-systems/UserGuide/index.html

NSIGHT COMPUTE (ncu)

Interactive CUDA Kernel profiler

- Targeted metric sections for various performance aspects (Debug/&Profile)
- API debugging via a user interface command line tool
- Very high freq. GPU perf counter, customizable data collection and presentation (tables, charts ..,)
- Python-based rules for guided analysis (or postprocessing)
- Provides a customizable and data-driven user interface and metric collection and can be extended with analysis scripts for post-processing results.

NVIDIA NSIGHT COMPUTE Important Features

- Result comparison across one or multiple reports within the tool
- Graphical profile report
- Interactive kernel profiler and API debugger: debugging CPU and GPU simultaneously and capable of handling thousands of simultaneous threads.
- Fast data collection
- GUI and command line interface
- Fully customizable reports and analysis rules

Nsight Compute Feature Spotlight in CUDA Toolkit 11 and A100

Roofline Analysis

Arithmetic intensity= Compute/Memory FLOPS = Floating Points Ops/Second

- Asynchronous copy _
- Sparse Data Compression –

Shows the amount of data compressed through this feature and the compression ratio, helps on kernels with bandwidth or cache issues.

Docs/product: https://developer.nvidia.com/nsight-compute

NVIDIA® Tools Extension SDK (NVTX)

- C-based Application Programming Interface (API) for annotating events, code ranges, and resources in your applications
- Codes which integrate NVTX can use NVIDIA Nsight, Tegra System Profiler, and Visual Profiler to capture and visualize these events and ranges.

[[allalen1@jwlogin22 v2]\$ ncu -h grep	nvtx
nvtx	Enable NVTX support.
nvtx -include arg	Adds include statement to the NVTX filter, which allows selecting kernels to
nvtx -exclude arg	Adds exclude statement to the NVTX filter, which allows selecting kernels to
print- <mark>nvtx</mark> -rename arg (=none)	Select how NVTX should be used for renaming:
	per- <mark>nvtx</mark>
Usage ofnvtx-include andnvtx-excl	.ude:
ncu nvtxnvtx -include "Domain A@R	lange A"
ncu nvtxnvtx -exclude "Range A]"	
ncu nvtxnvtx -include "Range A" -	nvtx-exclude "Range B"

https://docs.nvidia.com/nsight-visual-studio-edition/nvtx/index.html


```
#include <nvToolsExt.h>
#include <sys/syscall.h>
#include <unistd.h>
static void wait(int seconds) {
                                              nsys profile –t nvtx --stats=true …
    nvtxRangePush(___FUNCTION___);
                                              Or for Julia code:
    nvtxMark("Waiting...");
                                              nsys profile -t nvtx,cuda -o output_file.qdrep
    sleep(seconds);
                                              julia --project=../../ script.jl
    nvtxRangePop();
int main(void) {
    nvtxNameOsThread(syscall(SYS_gettid), "Main Thread");
    nvtxRangePush(___FUNCTION___);
    wait(1);
    nvtxRangePop();
                                                           https://docs.nvidia.com/nsight-visual-studio-edition/2020.1/nvtx/index.html
```

A First (I)Nsight Recording with the CLI

- Use the command line
 - srun nsys profile --trace=cuda,nvtx,mpi --force-overwrite=true --output=my_report.%q{SLURM_PROCID} \
 ./jacobi -niter 10
- Inspect results: Open the report file in the GUI
 - Also possible to get details on command line
 - Either add --stats to profile command line, or: nsys stats --help
- Runs set of reports on command line, customizable (sqlite + Python):
 - Useful to check validity of profile, identify important kernels

	Running	[/reports,	/gpukernsi	um.py jaco	obi_metric	cs_more-r	vtx.0. <mark>sq</mark>	lite]	
	Time (0)	Tatal Time (na)	Tustanas	Aug. (22)	Mad (ma)	Min (no)	Mary (ma)		
1	lime(%)	lotal lime (ns)	Instances	avg (ns)	Med (ns)	Min (ns)	max (ns)	StaDev (ns)	Name
	99.9	36750359	20	1837518.0	1838466.5	622945	3055044	1245121.7	void jacobi_kernel
	0.1	22816	2	11408.0	11408.0	7520	15296	5498.5	initialize_boundaries
	\smile								

System-level Profiling with Nsight Systems

- Global timeline view
 - CUDA HW: streams, kernels, memory
- Different traces, e.g. CUDA, MPI
 - correlations API <-> HW
- Stack samples
 - bottom-up, top-down for CPU code
- GPU metrics
- Events View
 - Expert Systems
- looks at single process (tree)
 - correlate multi-process reports in single timeline

<u>View</u> <u>T</u> ools	<u>H</u> elp										
obi_metrics_no	-nvtx.0.nsys-rep ×										
Timeline View	v •				[22]	Q 1x .	1 1	<u>A</u> 2v	varnings	s, 16 me	ssag
	1s • +85	Oms	+900ms	+950ms	2s		+50ms		+ 100r	ms	
GPU (0000:03:0	00.0 - NVIDIA										
CUDA HW (00	00:03:00.0 -		7		1.1	1	T	11 1	1	<u>1</u>	
[All Streams]	ĩ	ñ		Memcpy DtoH	11.1	1				M	
61.4% Defaul	t stream 7	i.	, 🗖	Memcpy DtoH							
31.8% Stream	n 13 🖡										
6.5% Stream	16									M	1
5 streams hid	lden – +							1 1			
Threads (8)				\frown							
• • [10309] M						andarada 🗖 keel o 🔺 ke	- Millelere	4 144	-	-	
MPI CUDA API	cudaHost	Nioc CudaM)	,	cudaMemcpy	MPI_Sen	drecv [41,692]MPI_S C	. M MPI_S	MPI_Sen	1PI) MPI	L) , [MPI	_S)
MPI CUDA API Profiler ove	cudaHost	Niloc cudaM	, ,	cudaMemcpy	(MPLSen	drecv [41,692] MPI_S	MMPI_S.	(MPI_Sen)(N	IPI) MPI	I) <u>, (MPI</u>	_S)
MPI CUDA API Profiler ove	rhead	Nioc cudaM	2	cudaMemcpy	MPLSen	drecv [41,692) MPI_S	. M MPI_S	MPI_Sen)N	IPI)(MPI	I) _{in} (MPI	_5)
MPI CUDA API Profiler ove	rhead	Klioc CudaM	,	cudaMemcpy	MPI_Sen	drecv [41,692) MPI_S	M MPI_S.) MPI_Sen) N	IPI)MPI) <u> (MPI</u>	_S)
MPI CUDA API Profiler ove (10367) jac 6 threads hid	rhead cobi ~	Nioc cudaM	2	cudaMemcpy	MPLSen	drecv [41,692) MPI_S	. M MPLS.) MPI_Sen) (N	IPI)MPI	I) _{in} (MPI	_S)
MPI CUDA API Profiler ove (10367) jau 6 threads hid	rhead	Viloc CudaM		cudaMemcpy	MPLSen	drecv [41,692) MPI_S C)	. M MPI_S.	(MPI_Sen)(N	IPI)(MPI	IIII) _{III} (MPI	_S)
MPI CUDA API Profiler ove (10367) jac 6 threads hid	rhead cobi ~	Viloc CudaM		cudaMemcpy	MPLSen	drecv [41,692) MPI_S C)			1000	I) , (MPI	
MPI CUDA API Profiler ove (10367) jau 6 threads hid	cudaHost rhead cobi ~ iden +	Nioc cudaM	Duration	cudaMemcpy	GPU	drecv [41,692) MPI_S []	me		191)(MPI) <u>, (MP</u> I	_S)
MPI CUDA API Profiler ove I [10367] jac 6 threads hid	cudaHosta rhead cobi ~ den +	Klioc cudaM	Duration 3,200 μs	CudaMemcpy	GPU 0	drecv [41,692] MPI_S C]	me	MPI_Sen)N	IPI) (MPI	<(int)32	 2,
MPI CUDA API Profiler ove I [10367] ja 6 threads hid	 Pi Kank U * cudaHost/ cudaHost/ cobi * den + Mame Memset void jacobi_ke 	Klioc cudaM	2 Duration 3,200 μs 3,056 ms	CudaMemcpy	GPU 0 GPU 0	drecv [41,692) MPI_S C Nar Context Stream 13 Stream 13	me	MPI_SenN Description: void jacobi (int)32> (flo	_kernel	<(int)32	
MPI CUDA API Profiler ove I (10367) jau 6 threads hid	Ank o CudaHost/ cudaHost/ cobi ~ den + Name Memset void jacobi_ke Memcpy DtoD	Nioc cudaM	Duration 3,200 μs 3,056 ms 5,024 μs	CudaMemcpy CudaMemcpy	GPU GPU 0 GPU 0 GPU 0 GPU 0	drecv [41,692] MPI_S C] Nar Context Stream 13 Stream 13 Stream 14	me	MPI_SenN Description: void jacobi (int)32>(flut *, float *, ir Begins: 1.88	_kernel- pat *, co it, int, in 259s	<(int)32 onst floa nt, bool	 2, at])

Discovering Optimization Potential

- Using Jacobi solver example*
- Spot kernels lots of whitespace
 - Which part is "bad"?
 - Enhance!
- MPI calls
 - Memory copies
 - We know: This is CUDA-aware MPI
- Even without knowing source, insight
- Too complicated for repeated/reliable usage
 - How to simplify navigating and comparing reports?

Adding NVTX Simple range-based API

- #include "nvtx3/nvToolsExt.h"
 - NVTX v3 is header-only, needs just -ldl
 - C++ and Python APIs
- Fortran: <u>NVHPC compilers include module</u>
 - Just use nvtx and -lnvhpcwrapnvtx
 - Other compilers: See blog posts linked below
- Definitely: Include PUSH/POP macros (see links below)

PUSH_RANGE(name, color_idx)

- Sprinkle them strategically through code
 - Use hierarchically: Nest ranges
- Not shown: Advanced usage (domains, ...)
- Similar range-based annotations exist for other tools
 - e.g. <u>SCOREP_USER_REGION_BEGIN</u>

https://github.com/NVIDIA/NVTX and https://nvidia.github.io/NVTX/#how-do-i-use-nvtx-in-my-code

https://developer.nvidia.com/blog/cuda-pro-tip-generate-custom-application-profile-timelines-nvtx/ https://developer.nvidia.com/blog/customize-cuda-fortran-profiling-nvtx/

```
int main(int argc, char** argv) {
    PUSH_RANGE("main", 0)
    PUSH_RANGE("init", 1)
    do_initialization();
    POP_RANGE
    /* ... */
    PUSH_RANGE("computation", 2)
    jacobi_kernel<<</* ... */, compute_stream>>>(...);
    cudaStreamSynchronize(compute_stream);
    POP_RANGE
    /* ... */
    POP_RANGE
}
```

Minimizing Profile Size

Shorter time, smaller files = quicker progress

- Only profile what you need all profilers have some overhead
 - Example: Event that occurs after long-running setup phase
- Bonus: lower number of events leads to smaller file size
- Add to nsys command line:
 - --capture-range=nvtx --nvtx-capture=any_nvtx_marker_name \
 --env-var=NSYS_NVTX_PROFILER_REGISTER_ONLY=0 --kill none
 - Use NVTX registered strings for best performance
- Alternatively: cudaProfilerStart() and -Stop()
 - --capture-range=cudaProfilerApi

Nsight Systems Workflow with NVTX

Repeating the analysis

NVIDIA Nsight S	Systems 2021.4.1								-		×
<u>File</u> <u>V</u> iew <u>⊺</u> ools	Help										
jacobi_metrics_mor	e-nvtx.0.nsys-rep ×										
= Timeline View	-					📼 Q 1x 🖵	1	-	<u> A</u> 2 warning	is, 16 messag	ies
	2s - +660,4m	ns +660,5ms 2s 660,6070	ms +660,7	ms +660,8ms	+660,9m	s +661ms		+661,1m	s +661,	2ms	
 CPU (96) 											
GPU (0000:03:0)	0.0 - NVIDIA										
CUDA HW (000)	0:03:00.0 - N						1		r i i i i		
 Threads (8) 											
▼ ✔ [17825] MP	PI Rank 0 👻										
MPI	1						MPI_Ser	ndrecv [MP	I	duce [
				Jacobi solve [7,8	10 ms]						
NVTX		i	kemel (682.252	it_000 [917,263	3 µs]		MPI	[105,391 usl	norm [128	150 usi	
CUDA API	c (cuda)		cudaEve	ntSynchronize							
Profiler over	head										
✓ [17878] jac	obi 👻	2									
6 threads hide	ien — +										-
	4									Þ	•
Events View	•										
						1	Vame	-			Q
#	Name		Start	Duration	TID	Category		Descripti	on:		
1	▶ init		0,17077s	2,490 s	17825			it_000			
5	 Jacobi solve 		2,66034s	7,810 ms	17825			Begins: 2	,66035s	52 uc)	
6	▼ <mark> </mark> it_000		2,66035s	917,263 μs	17825			Thread: 1	7825	55 μs)	
7	kernel		2,66035s	682,252 μs	17825						
8	MPI		2,66103s	105,391 µs	17825						
9	norm		2,66114s	128,150 µs	17825						
10	• it_001		2,66127s	75 1 ,182 μs	17825						
14	it_002		2,66202s	767,433 μs	17825						
18	it_003		2,66279s	752,632 μs	17825						
22	it_004		2,66354s	762,572 μs	17825		Ŧ				
•							•				

Q

GPU Metrics in Nsight Systems

...and other traces you can activate

- Valuable low-overhead insight into HW usage:
 - SM instructions
 - DRAM Bandwidth, PCIe Bandwith (GPUDirect)
- Also: Memory usage, Page Faults (higher overhead)
 - CUDA Programming guide: <u>Unified Memory</u>
 Programming
- Can save kernel-level profiling effort!

```
    nsys profile

            --gpu-metrics-device=0
            --cuda-memory-usage=true
            --cuda-um-cpu-page-faults=true
```

--cuda-um-gpu-page-faults=true
./app

Unified Memory movement

Observing transfers in Nsight Systems

NSIGHT SYSTEMS

System-wide application algorithm tuning Multi-process tree support Locate optimization opportunities Visualize millions of events on a very fast GUI timeline Or gaps of unused CPU and GPU time

Balance your workload across multiple CPUs and GPUs CPU algorithms, utilization, and thread state GPU streams, kernels, memory transfers, etc

Multi-platform: Linux & Windows, x86-64, Te g r a, Power, MacOSX(host only)

GPUs: Volta, Turing

Docs/product: https://developer.nvidia.com/nsight-systems

CUDA Kernel profiler

Targeted metric sections for various performance aspects (Debug/&Profile)

Very high freq GPU perf counter, customizable data collection and presentation (tables, charts ...,)

Python-based rules for guided analysis (or postprocessing)

GPUs: Volta, Turing, Amper...

Docs/product: https://developer.nvidia.com/nsight-systems

NVIDIA Tools Extension API Library (NVTX)

The NVIDIA Tools Extension SDK (NVTX) is a C-based Application Programming Interface (API) for annotating events, code ranges, and resources in your applications. Applications which integrate NVTX can use NVIDIA Nsight VSE to capture and visualize these events and ranges.

IS

DEEP LEARNING INSTITUTE

Lab3: Asynchronous Streaming, and Visual Profiling with CUDA C/C++

Dr. Momme Allalen Leibniz Computing Centre, Munich Germany - www.lrz.de Deep Learning Certified Instructor, NVIDIA Deep Learning Institute NVIDIA Corporation.

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de

Lab2: Managing Accelerated Application Memory with CUDA Unified Memory and nvprof

Prerequisites

To get the most out of this lab you should already be able to:

- Write, compile, and run C/C++ programs that both call CPU functions and launch GPU kernels.
- Control parallel thread hierarchy using execution configuration.
- Refactor serial loops to execute their iterations in parallel on a GPU.
- Allocate and free CUDA Unified Memory.
- Understand the behavior of Unified Memory with regard to page faulting and data migrations.
- Use asynchronous memory prefetching to reduce page faults and data migrations.

Objectives

By the time you complete this lab you will be able to:

- Use the Nsight Systems to visually profile the timeline of GPU-accelerated CUDA applications.
- Use **Nsight Systems** to identify, and exploit, optimization opportunities in GPUaccelerated CUDA applications.
- Utilize CUDA streams for concurrent kernel execution in accelerated applications.
- (Optional Advanced Content) Use manual memory allocation, including allocating pinned memory, in order to asynchronously transfer data in concurrent CUDA streams.

Multiple Streams

Overlap copy with kernel

	Stream 0	Stream 1
	memcpy A to GPU	
	memcpy B to GPU	
	kernel	memcpy A to GPU
		memcpy B to GPU
me	memcpy C from GPU	kernel
F		memcpy C from GPU
	memcpy A to GPU	
	memcpy B to GPU	
	kernel	memcpy A to GPU
		memcpy B to GPU
¥	memcpy C from GPU	kernel
		memcpy C from GPU

Multiple Streams

for (int i=0; i<FULL_SIZE; i+= N*2) {</pre>

// copy the locked memory to the device, async cudaMemcpyAsync(dev_a0, host_a+i, N * sizeof(int),cudaMemcpyHostToDevice, stream0); cudaMemcpyAsync(dev b0, host b+i, N * sizeof(int),cudaMemcpyHostToDevice, stream0);

kernel << <N/256,256,0,stream0>>> (dev a0, dev b0, dev c0);

// copy the data from device to locked memory
cudaMemcpyAsync(host_c+i, dev_c0, N * sizeof(int),cudaMemcpyDeviceToHost, stream0);
// copy the locked memory to the device, async
cudaMemcpyAsync(dev_a1,host_a+i+N, N * sizeof(int),cudaMemcpyHostToDevice, stream1);
cudaMemcpyAsync(dev_b1,host_b+i+N, N * sizeof(int),cudaMemcpyHostToDevice, stream1);

kernel <<< N/256,256,0,stream1>>> (dev_a1, dev_b1, dev_c1);

// copy the data from device to locked memory
cudaMemcpyAsync(host_c+i+N,dev_c1, N * sizeof(int),cudaMemcpyDeviceToHost, stream1);
}

DEEP LEARNING INSTITUTE

THANK YOU

Instructor: Dr. Momme Allalen www.nvidia.com/dli

Fundamentals of Accelerated Computing with CUDA C/C++| LRZ | 07.11.2023; Allalen@Irz.de