



COMPUTING WITH GPUS AT JSC

ESM SYMPOSIUM JSC 2019

28 May 2019 | Andreas Herten | Forschungszentrum Jülich *Handout Version*

Outline

GPUs at JSC

JUWELS

JURECA

JURON

GPU Architecture

Empirical Motivation

Comparisons

3 Core Features

Memory

Asynchronicity

Summary

Programming GPUs

Libraries

Directives

Languages

Tools

Advanced Topics

Using GPUs on JURECA & JUWELS

Compiling

Resource Allocation



JUWELS – Jülich's New Large System

- 2500 nodes with Intel Xeon CPUs (2×24 cores)
- 46 + 10 nodes with 4 NVIDIA Tesla V100 cards
- 10.4 (CPU) + 1.6 (GPU) PFLOP/s peak performance (Top500: #26)



JURECA – Jülich's Multi-Purpose Supercomputer

- 1872 nodes with Intel Xeon E5 CPUs (2×12 cores)
- 75 nodes with 2 NVIDIA Tesla K80 cards (look like 4 GPUs)
- JURECA Booster: 1640 nodes with Intel Xeon Phi *Knights Landing*
- 1.8 (CPU) + 0.44 (GPU) + 5 (KNL) PFLOP/s peak performance (Top500: #44)
- Mellanox EDR InfiniBand



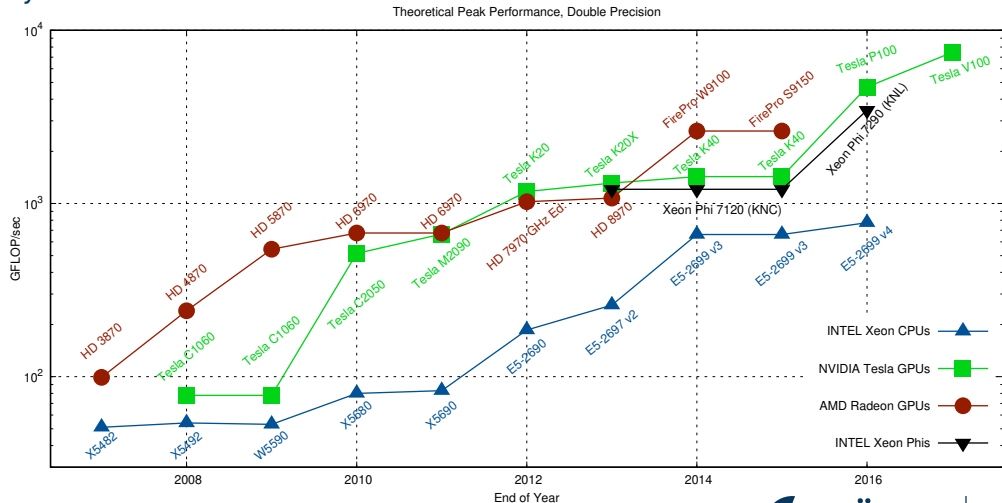
JURON – A Human Brain Project *Pilot System*

- 18 nodes with IBM POWER8NVL CPUs (2×10 cores)
- Per Node: 4 NVIDIA Tesla P100 cards (16 GB HBM2 memory), connected via NVLink
- GPU: 0.38 PFLOP/s peak performance

Why?

Status Quo Across Architectures

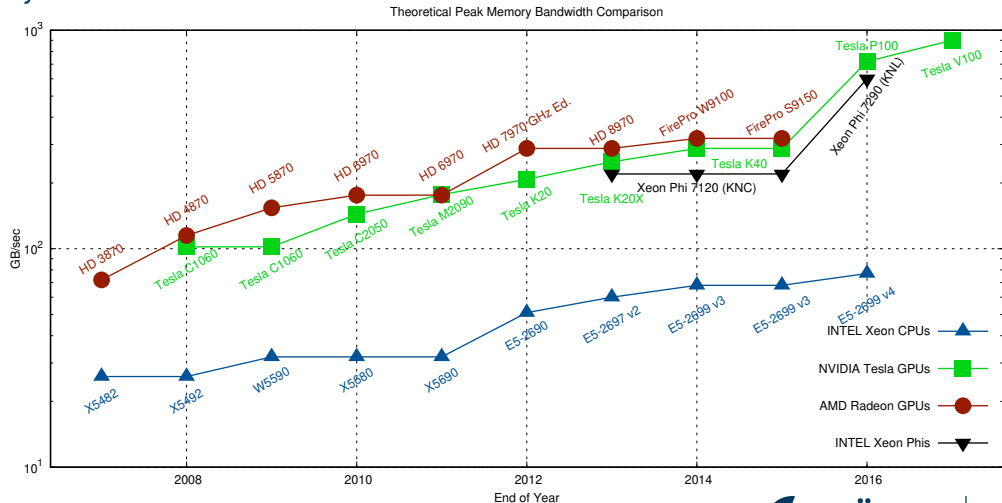
Memory Bandwidth



Graphic: Rupp [2]

Status Quo Across Architectures

Memory Bandwidth



Graphic: Rupp [2]

CPU vs. GPU

A matter of specialties



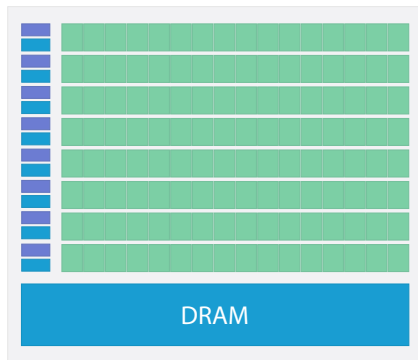
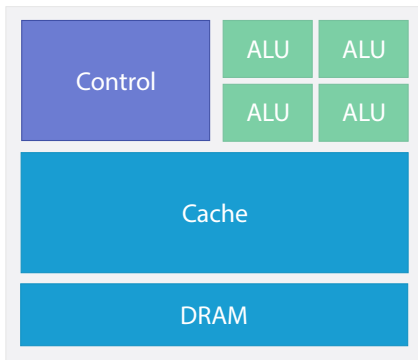
Transporting one



Transporting many

CPU vs. GPU

Chip



GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

Memory

GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

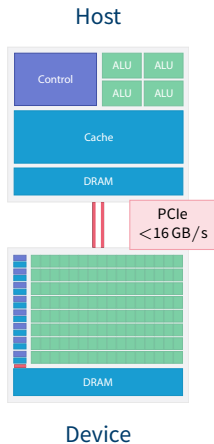
Asynchronicity

Memory

Memory

GPU memory ain't no CPU memory

- GPU: accelerator / extension card
- Separate device from CPU
- **Separate memory**
- Memory transfers need special consideration!
Do as little as possible!
- Formerly: Explicitly copy data to/from GPU
Now: Done automatically (performance...?)



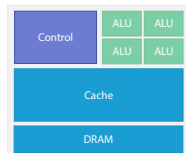
Memory

GPU memory ain't no CPU memory

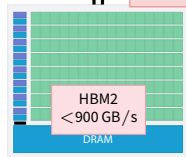
- GPU: accelerator / extension card
- Separate device from CPU
 - **Separate memory but Unified Memory**
 - Memory transfers need special consideration!
Do as little as possible!
 - Formerly: Explicitly copy data to/from GPU
Now: Done automatically (performance...?)
 - P100: 16 GB RAM, 720 GB/s; V100: 16 (32) GB RAM, 900 GB/s



Host



NVLink
≈ 80 GB/s



Device

GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

Memory

Async

Following different streams

- Problem: Memory transfer is comparably slow
Solution: Do something else in meantime (**computation**)!

→ Overlap tasks

- Copy and compute engines run separately (*streams*)



- GPU needs to be fed: Schedule many computations
- CPU can do other work while GPU computes; synchronization

GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

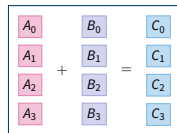
Memory

SIMT

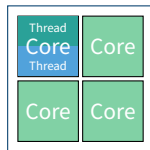
Of threads and warps

- CPU:
 - Single Instruction, Multiple Data (SIMD)
 - Simultaneous Multithreading (SMT)
- GPU: Single Instruction, Multiple Threads (SIMT)
 - CPU core $\cong$ GPU multiprocessor (SM)
 - Working unit: set of threads (32, a *warp*)
 - Fast switching of threads (large register file)
 - Branching 

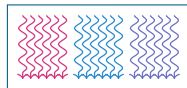
Vector



SMT



SIMT



SIMT

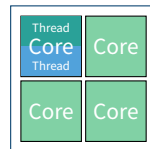
of 1



Vector

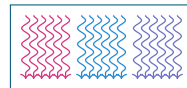
$$\begin{matrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{matrix} + \begin{matrix} B_0 \\ B_1 \\ B_2 \\ B_3 \end{matrix} = \begin{matrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{matrix}$$

SMT



Graphics: volta-pictures

SIMT



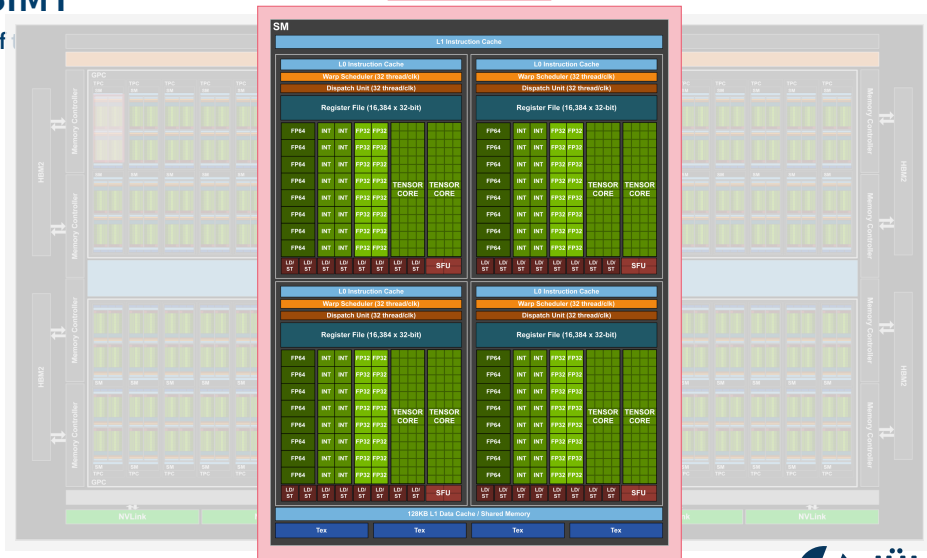
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CENTRE

SIMT

of 1

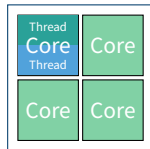
Multiprocessor



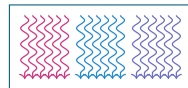
Vector

$$\begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{bmatrix} + \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ B_3 \end{bmatrix} = \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix}$$

SMT



SIMT



Graphics: volta-pictures



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SIMT

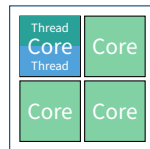
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Vector

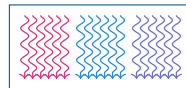
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SMT



Graphics: volta-pictures

SIMT



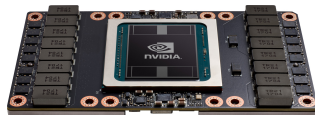
CPU vs. GPU

Let's summarize this!



Optimized for **low latency**

- + Large main memory
- + Fast clock rate
- + Large caches
- + Branch prediction
- + Powerful ALU
- Relatively low memory bandwidth
- Cache misses costly
- Low performance per watt



Optimized for **high throughput**

- + High bandwidth main memory
- + Latency tolerant (parallelism)
- + More compute resources
- + High performance per watt
- Limited memory capacity
- Low per-thread performance
- Extension card

Programming GPUs

Preface: CPU

A simple CPU program as reference!

SAXPY: $\vec{y} = a\vec{x} + \vec{y}$, with single precision

Part of LAPACK BLAS Level 1

```
void saxpy(int n, float a, float * x, float * y) {  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}
```

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
saxpy(n, a, x, y);
```

Libraries

Programming GPUs is easy: **Just don't!**

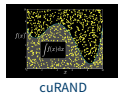
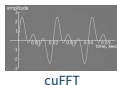
Use applications & libraries



Libraries

Programming GPUs is easy: **Just don't!**

Use applications & libraries



Numba



theano



- GPU-parallel BLAS (all 152 routines)
- Single, double, complex data types
- Constant competition with Intel's MKL
- Multi-GPU support

→ <https://developer.nvidia.com/cublas>
<http://docs.nvidia.com/cuda/cublas>

cuBLAS

Code example

```
int a = 42;  int n = 10;
float x[n], y[n];
// fill x, y

cublasHandle_t handle;
cublasCreate(&handle);

float * d_x, * d_y;
cudaMallocManaged(&d_x, n * sizeof(x[0]));
cudaMallocManaged(&d_y, n * sizeof(y[0]));
cublasSetVector(n, sizeof(x[0]), x, 1, d_x, 1);
cublasSetVector(n, sizeof(y[0]), y, 1, d_y, 1);

cublasSaxpy(n, a, d_x, 1, d_y, 1);

cublasGetVector(n, sizeof(y[0]), d_y, 1, y, 1);

cudaFree(d_x); cudaFree(d_y);
cublasDestroy(handle);
```


cuBLAS

Code example

```
int a = 42; int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
cublasHandle_t handle;  
cublasCreate(&handle);
```

Initialize

```
float * d_x, * d_y;  
cudaMallocManaged(&d_x, n * sizeof(x[0]));  
cudaMallocManaged(&d_y, n * sizeof(y[0]));  
cublasSetVector(n, sizeof(x[0]), x, 1, d_x, 1);  
cublasSetVector(n, sizeof(y[0]), y, 1, d_y, 1);
```

Allocate GPU memory

Copy data to GPU

```
cublasSaxpy(n, a, d_x, 1, d_y, 1);
```

Call BLAS routine

```
cublasGetVector(n, sizeof(y[0]), d_y, 1, y, 1);
```

Copy result to host

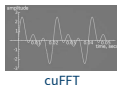
```
cudaFree(d_x); cudaFree(d_y);  
cublasDestroy(handle);
```

Finalize

Libraries

Programming GPUs is easy: **Just don't!**

Use applications & libraries



Numba



theano

Thrust

Iterators! Iterators everywhere! 

- $\frac{\text{Thrust}}{\text{CUDA}} = \frac{\text{STL}}{\text{C++}}$
- Template library
- Based on iterators
- Data-parallel primitives (`scan()`, `sort()`, `reduce()`, ...)
- Fully compatible with plain CUDA C (comes with **CUDA** Toolkit)
- Great with `[]()`{} lambdas!

→ <http://thrust.github.io/>
<http://docs.nvidia.com/cuda/thrust/>

Thrust

Code example with lambdas

```
int a = 42;
int n = 10;
thrust::host_vector<float> x(n), y(n);
// fill x, y

thrust::device_vector d_x = x, d_y = y;

using namespace thrust::placeholders;
thrust::transform(
    d_x.begin(), d_x.end(), // Input 1
    d_y.begin(),           // Input 2
    d_y.begin(),           // Output
    a * _1 + _2            // Operation
);
```

Thrust

Code example with lambdas

```
#include <thrust/for_each.h>
#include <thrust/execution_policy.h>
constexpr int gGpuThreshold = 10000;
void saxpy(float *x, float *y, float a, int N) {
    auto r = thrust::counting_iterator<int>(0);

    auto lambda = [=] __host__ __device__ (int i) {
        y[i] = a * x[i] + y[i];};

    if(N > gGpuThreshold)
        thrust::for_each(thrust::device, r, r+N, lambda);
    else
        thrust::for_each(thrust::host, r, r+N, lambda);}
```

Source

Programming GPUs

Directives

GPU Programming with Directives

Keepin' you portable

- Annotate usual source code by directives

```
#pragma acc loop
```

```
for (int i = 0; i < 1; i++) {};
```

- Also: Generalized API functions

```
acc_copy();
```

- Compiler interprets directives, creates according instructions

Pro

- Portability
 - Other compiler? No problem! To it, it's a serial program
 - Different target architectures from same code
- Easy to program

Con

- Compilers support limited
- Raw power hidden
- Somewhat harder to debug

GPU Programming with Directives

The power of... two.

OpenMP Standard for multithread programming on CPU, GPU since 4.0, better since 4.5

```
#pragma omp target map(tofrom:y), map(to:x)
#pragma omp teams num_teams(10) num_threads(10)
#pragma omp distribute
for ( ) {
    #pragma omp parallel for
    for ( ) {
        // ...
    }
}
```

OpenACC Similar to OpenMP, but more specifically for GPUs
Might eventually be re-merged into OpenMP standard

OpenACC

Code example

```
void saxpy_acc(int n, float a, float * x, float * y) {  
    #pragma acc kernels  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}
```

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
saxpy_acc(n, a, x, y);
```



OpenACC

Code example

```
void saxpy_acc(int n, float a, float * x, float * y) {  
    #pragma acc parallel loop copy(y) copyin(x)  
    for (int i = 0; i < n; i++)  
        y[i] = a * x[i] + y[i];  
}
```

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
saxpy_acc(n, a, x, y);
```

OpenACC

Code example

```
void saxpy_acc(int n, float a, float * x, float * y) {  
    #pragma acc parallel loop copy(y) copyin(x)  
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        y[i] = a * x[i] + y[i];  
}
```

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y
```

```
saxpy_acc(n, a, x, y);
```

GPU hands-on
later!

Programming GPUs

Languages

Programming GPU Directly

Finally...

- Two solutions:

OpenCL Open Computing Language by Khronos Group (Apple, IBM, NVIDIA, ...) 2009

- Platform: Programming language (OpenCL C/C++), API, and compiler
- Targets CPUs, GPUs, FPGAs, and other many-core machines
- Fully open source
- Different compilers available

CUDA NVIDIA's GPU platform 2007

- Platform: Drivers, programming language (CUDA C/C++), API, compiler, debuggers, profilers, ...
- Only NVIDIA GPUs
- Compilation with `nvcc` (free, but not open)
`clang` has CUDA support, but CUDA needed for last step
- Also: CUDA Fortran

- Choose what flavor you like, what colleagues/collaboration is using
- **Hardest: Come up with parallelized algorithm**



CUDA SAXPY

With runtime-managed data transfers

```
__global__ void saxpy_cuda(int n, float a, float * x, float * y) {  
    int i = blockIdx.x * blockDim.x + threadIdx.x;  
    if (i < n)  
        y[i] = a * x[i] + y[i];  
}
```

Specify kernel

ID variables

Guard against
too many threads

```
int a = 42;  
int n = 10;  
float x[n], y[n];
```

```
// fill x, y
```

```
cudaMallocManaged(&x, n * sizeof(float));
```

```
cudaMallocManaged(&y, n * sizeof(float));
```

Allocate GPU-capable
memory

Call kernel
2 blocks, each 5 threads

```
saxpy_cuda<<<2, 5>>>(n, a, x, y);
```

Wait for
kernel to finish

```
cudaDeviceSynchronize();
```

Programming GPUs

Tools

GPU Tools

The helpful helpers helping helpless (and others)

- NVIDIA

- `cuda-gdb` GDB-like command line utility for debugging

- `cuda-memcheck` Like Valgrind's memcheck, for checking errors in memory accesses

- `Nsight` IDE for GPU developing, based on Eclipse (Linux, OS X) or Visual Studio (Windows)

- `nvprof` Command line profiler, including detailed performance counters

- Visual Profiler** Timeline profiling and annotated performance experiments

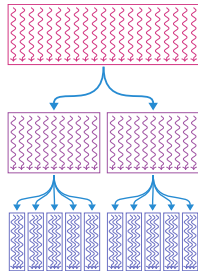
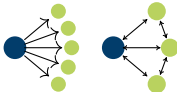
- See appendix

- OpenCL: `CodeXL` (Open Source, GPUOpen/AMD) – debugging, profiling.

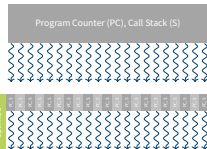
Advanced Topics

So much more interesting things to show!

- Memory spaces (shared, pinned, ...); memory transfer optimization
- Atomic  operations
- Optimize applications for GPU architecture (access patterns, streams)
- Drop-in BLAS acceleration with NVBLAS (`$LD_PRELOAD`)
- Cooperative groups, independent thread progress
- Tensor Cores for Deep Learning (→ [Appendix](#))
- Libraries, Abstractions: [Kokkos](#) (→ [Appendix](#)), [Alpaka](#), [SYCL](#), [HIP](#) ...
- Half precision FP16
- Use multiple GPUs
 - On one node
 - Across many nodes → MPI
- ...
- Some of that: Addressed at **dedicated training courses**



Cooperative Groups



Independent
Thread Progress

Using GPUs on JURECA & JUWELS

Compiling

CUDA

- Module: `module load CUDA/10.1.105`
- Compile: `nvcc file.cu`
Default host compiler: `g++`; use `nvcc_pgc++` for PGI compiler
- cuBLAS: `g++ file.cpp -I$CUDA_HOME/include -L$CUDA_HOME/lib64 -lcublas -lcudart`

OpenACC

- Module: `module load PGI/19.3-GCC-8.3.0`
- Compile: `pgc++ -acc -ta=tesla file.cpp`

MPI

- Module: `module load MVAPICH2/2.3.1-GDR` (also needed: `gcc/8.3.0`)
Enabled for CUDA (*CUDA-aware*); no need to copy data to host before transfer

Running

- Dedicated GPU partitions

JUWELS

`--partition=gpus` 46 nodes (Job limits: <1 d)
`--partition=develgpus` 10 nodes (Job limits: <2 h, ≤ 2 nodes)

JURECA

`--partition=gpus` 70 nodes (Job limits: <1 d, ≤ 32 nodes)
`--partition=develgpus` 4 nodes (Job limits: <2 h, ≤ 2 nodes)

- Needed: Resource configuration with `--gres`

`--gres=gpu:4`

`--gres=mem1024,gpu:2 --partition=vis` *only JURECA*

→ See [online documentation](#)

Example

- 96 tasks in total, running on 4 nodes
- Per node: 4 GPUs

```
#!/bin/bash -x
#SBATCH --nodes=4
#SBATCH --ntasks=96
#SBATCH --ntasks-per-node=24
#SBATCH --output=gpu-out.%j
#SBATCH --error=gpu-err.%j
#SBATCH --time=00:15:00
```

```
#SBATCH --partition=gpus
#SBATCH --gres=gpu:4
```

```
srun ./gpu-prog
```

Conclusion, Resources

- GPUs provide highly-parallel computing power
- We have many devices installed at JSC, ready to be used!
- Training courses by JSC
 - CUDA Course April 2020
 - OpenACC Course 28 - 29 October 2019
- Generally: see [online documentation](#) and sc@fz-juelich.de
- Further consultation via our lab: *NVIDIA Application Lab*

Thank you
for your attention!
a.herten@fz-juelich.de

APPENDIX

Appendix

Further Reading & Links

GPU Performances

GPU Architecture: Tensor Cores

GPU Programming: Abstraction Libraries/DSL

NVIDIA GPU Tools

Glossary

References

Further Reading & Links

More!

- A discussion of SIMD, SIMT, SMT by Y. Kreinin.
- NVIDIA's documentation: docs.nvidia.com
- NVIDIA's [Parallel For All](#) blog

Volta Performance

Tesla Product	Tesla K40	Tesla M40	Tesla P100	Tesla V100
GPU	GK180 (Kepler)	GM200 (Maxwell)	GP100 (Pascal)	GV100 (Volta)
SMs	15	24	56	80
TPCs	15	24	28	40
FP32 Cores / SM	192	128	64	64
FP32 Cores / GPU	2880	3072	3584	5120
FP64 Cores / SM	64	4	32	32
FP64 Cores / GPU	960	96	1792	2560
Tensor Cores / SM	NA	NA	NA	8
Tensor Cores / GPU	NA	NA	NA	640
GPU Boost Clock	810/875 MHz	1114 MHz	1480 MHz	1462 MHz
Peak FP32 TFLOPS ¹	5	6.8	10.6	15
Peak FP64 TFLOPS ¹	1.7	.21	5.3	7.5
Peak Tensor TFLOPS ¹	NA	NA	NA	120
Texture Units	240	192	224	320
Memory Interface	384-bit GDDR5	384-bit GDDR5	4096-bit HBM2	4096-bit HBM2
Memory Size	Up to 12 GB	Up to 24 GB	16 GB	16 GB
L2 Cache Size	1536 KB	3072 KB	4096 KB	6144 KB
Shared Memory Size / SM	16 KB/32 KB/48 KB	96 KB	64 KB	Configurable up to 96 KB
Register File Size / SM	256 KB	256 KB	256 KB	256KB
Register File Size / GPU	3840 KB	6144 KB	14336 KB	20480 KB
TDP	235 Watts	250 Watts	300 Watts	300 Watts
Transistors	7.1 billion	8 billion	15.3 billion	21.1 billion
GPU Die Size	551 mm ²	601 mm ²	610 mm ²	815 mm ²
Manufacturing Process	28 nm	28 nm	16 nm FinFET+	12 nm FFN
¹ Peak TFLOPS rates are based on GPU Boost Clock				

Figure: Tesla V100 performance characteristics in comparison [volta-pictures]

Appendix

GPU Architecture: Tensor Cores

Tensor Cores

New since Volta

- 8 Tensor Cores per Streaming Multiprocessor (SM) (640 total for V100)
 - Performance: 125 TFLOP/s (half precision)
 - Calculate $\mathbf{A} \times \mathbf{B} + \mathbf{C} = \mathbf{D}$ (4×4 matrices; $\mathbf{A}$, $\mathbf{B}$: half precision)
- 64 floating-point FMA operations per clock (mixed precision)
- Turing architecture: int-based Tensor Cores



Appendix

GPU Programming: Abstraction Libraries/DSL

Abstraction Libraries & DSLs

- Libraries with ready-programmed abstractions; partly compiler/transpiler necessary
- Have different backends to choose from for targeted accelerator
- Between Thrust, OpenACC, and CUDA
- Examples: **Kokkos**, Alpaka, Futhark, HIP, C++AMP, ...

An Alternative: Kokkos

From Sandia National Laboratories

- C++ library for *performance* portability
- Data-parallel patterns, architecture-aware memory layouts, ...

```
Kokkos::View<double*> x("X", length);  
Kokkos::View<double*> y("Y", length);  
double a = 2.0;
```

```
// Fill x, y
```

```
Kokkos::parallel_for(length, KOKKOS_LAMBDA (const int& i) {  
    x(i) = a*x(i) + y(i);  
});
```

→ <https://github.com/kokkos/kokkos/>

Appendix

NVIDIA GPU Tools

nvprof

Command that line

Usage: nvprof ./app

```
$ nvprof ./matrixMul -wA=1024 -hA=1024 -wB=1024 -hB=1024
==37064== Profiling application: ./matrixMul -wA=1024 -hA=1024 -wB=1024 -hB=1024
==37064== Profiling result:
Time(%)   Time      Calls      Avg      Min      Max  Name
99.19%    262.43ms    301    871.86us    863.88us    882.44us  void matrixMulCUDA<int=32>(float*, float*, float*, int, int)
0.58%     1.5428ms     2    771.39us    764.65us    778.12us  [CUDA memcpy HtoD]
0.23%     599.40us     1    599.40us    599.40us    599.40us  [CUDA memcpy DtoH]

==37064== API calls:
Time(%)   Time      Calls      Avg      Min      Max  Name
61.26%    258.38ms     1    258.38ms    258.38ms    258.38ms  cudaEventSynchronize
35.68%    150.49ms     3    50.164ms    914.97us    148.65ms  cudaMalloc
0.73%     3.0774ms     3    1.0258ms    1.0097ms    1.0565ms  cudaMemcpy
0.62%     2.6287ms     4    657.17us    655.12us    660.56us  cuDeviceTotalMem
0.56%     2.3408ms    301    7.7760us    7.3810us    53.103us  cudaLaunch
0.48%     2.0111ms    364    5.5250us      235ns    201.63us  cuDeviceGetAttribute
0.21%     872.52us     1    872.52us    872.52us    872.52us  cudaDeviceSynchronize
```

nvprof

Command that line

With metrics: `nvprof --metrics flop_sp_efficiency ./app`

```
$ nvprof --metrics flop_sp_efficiency ./matrixMul -wA=1024 -hA=1024 -wB=1024 -hB=1024
[Matrix Multiply Using CUDA] - Starting...
==37122== NVPROF is profiling process 37122, command: ./matrixMul -wA=1024 -hA=1024 -wB=1024 -hB=1024
GPU Device 0: "Tesla P100-SXM2-16GB" with compute capability 6.0
```

```
MatrixA(1024,1024), MatrixB(1024,1024)
Computing result using CUDA Kernel...
==37122== Some kernel(s) will be replayed on device 0 in order to collect all events/metrics.
done122== Replaying kernel "void matrixMulCUDA<int=32>(float*, float*, float*, int, int)" (0 of 2)...
Performance= 26.61 GFlop/s, Time= 80.697 msec, Size= 2147483648 Ops, WorkgroupSize= 1024 threads/block
Checking computed result for correctness: Result = PASS
```

```
==37122== Profiling application: ./matrixMul -wA=1024 -hA=1024 -wB=1024 -hB=1024
```

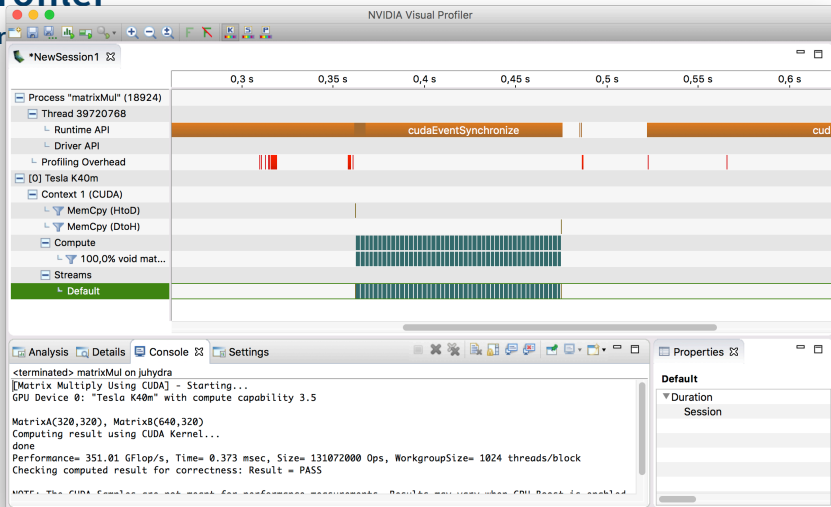
```
==37122== Profiling result:
```

```
==37122== Metric result:
```

Invocations	Metric Name	Metric Description	Min	Max	Avg
Device "Tesla P100-SXM2-16GB (0)"					
Kernel: void matrixMulCUDA<int=32>(float*, float*, float*, int, int)					
301	flop_sp_efficiency	FLOP Efficiency(Peak Single)	22.96%	23.40%	23.15%

Visual Profiler

Your new favor



Appendix

Glossary & References

Glossary I

API A programmatic interface to software by well-defined functions. Short for application programming interface. [35](#), [41](#)

CUDA Computing platform for [GPUs](#) from NVIDIA. Provides, among others, CUDA C/C++. [31](#), [41](#), [42](#), [47](#), [50](#), [58](#), [67](#)

DSL A Domain-Specific Language is a specialization of a more general language to a specific domain. [52](#), [57](#), [58](#)

JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. [2](#), [50](#), [65](#)

JURECA A multi-purpose supercomputer with 1800 nodes at JSC. [2](#), [4](#), [46](#), [48](#)

Glossary II

JURON One of the two HBP pilot system in Jülich; name derived from Juelich and Neuron. 5

JUWELS Jülich's new supercomputer, the successor of JUQUEEN. 2, 3, 46, 48

MPI The Message Passing Interface, a API definition for multi-node computing. 45, 47

NVIDIA US technology company creating GPUs. 3, 4, 5, 41, 44, 50, 52, 53, 60, 65, 66, 67, 68

NVLink NVIDIA's communication protocol connecting CPU ↔ GPU and GPU ↔ GPU with high bandwidth. 5, 67

OpenACC Directive-based programming, primarily for many-core machines. 36, 37, 38, 39, 47, 50, 58

Glossary III

OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (**CPU**, **GPU**, DSP, FPGA). The alternative to **CUDA**. 41, 44

OpenMP Directive-based programming, primarily for multi-threaded machines. 36

P100 A large **GPU** with the **Pascal** architecture from **NVIDIA**. It employs **NVLink** as its interconnect and has fast *HBM2* memory. 5

Pascal **GPU** architecture from **NVIDIA** (announced 2016). 67

POWER **CPU** architecture from IBM, earlier: PowerPC. See also POWER8. 67

POWER8 Version 8 of IBM's **POWER**processor, available also under the OpenPOWER Foundation. 5, 67

SAXPY Single-precision $A \times X + Y$. A simple code example of scaling a vector and adding an offset. 24, 42

Glossary IV

Tesla The GPU product line for general purpose computing computing of NVIDIA. 3, 4, 5

Thrust A parallel algorithms library for (among others) GPUs. See <https://thrust.github.io/>. 31

Volta GPU architecture from NVIDIA (announced 2017). 56

References I

- [2] Karl Rupp. *Pictures: CPU/GPU Performance Comparison*. URL: <https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characteristics-over-time/> (pages 7, 8).
- [6] Wes Breazell. *Picture: Wizard*. URL: <https://thenounproject.com/wes13/collection/its-a-wizards-world/> (pages 25, 26, 30).

References: Images, Graphics I

- [1] Igor Ovsyannykov. *Yarn*. Freely available at Unsplash. URL: <https://unsplash.com/photos/hvILKk7SlH4>.
- [3] Mark Lee. *Picture: kawasaki ninja*. URL: <https://www.flickr.com/photos/pochacco20/39030210/>. License: Creative Commons BY-ND 2.0 (page 9).
- [4] Bob Adams. *Picture: Hylton Ross Mercedes Benz Irizar coach*. URL: <https://www.flickr.com/photos/satransport/13197324714/>. License: Creative Commons BY-SA 2.0 (page 9).
- [5] Nvidia Corporation. *Pictures: Volta GPU*. Volta Architecture Whitepaper. URL: <https://images.nvidia.com/content/volta-architecture/pdf/Volta-Architecture-Whitepaper-v1.0.pdf>.