



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



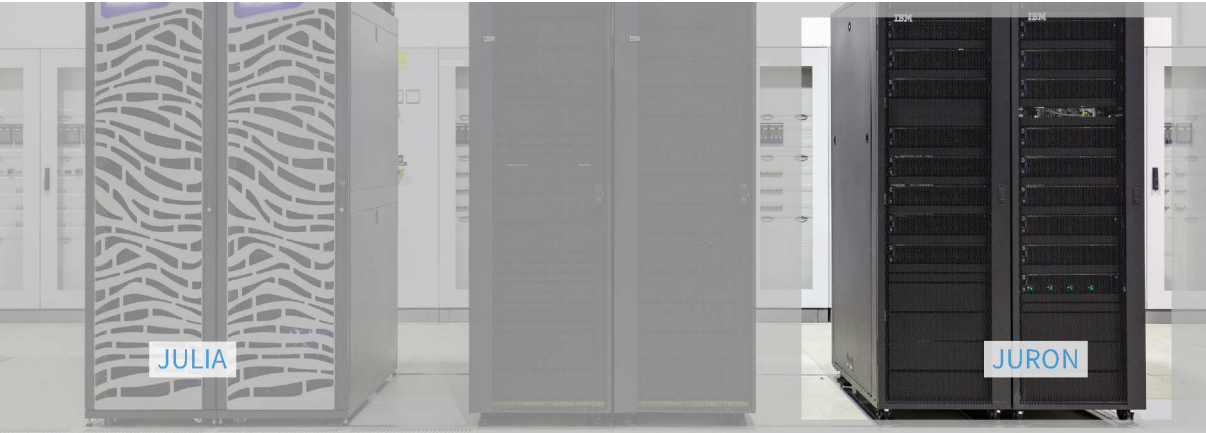
JUWELS – Jülich's New Large System

- 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



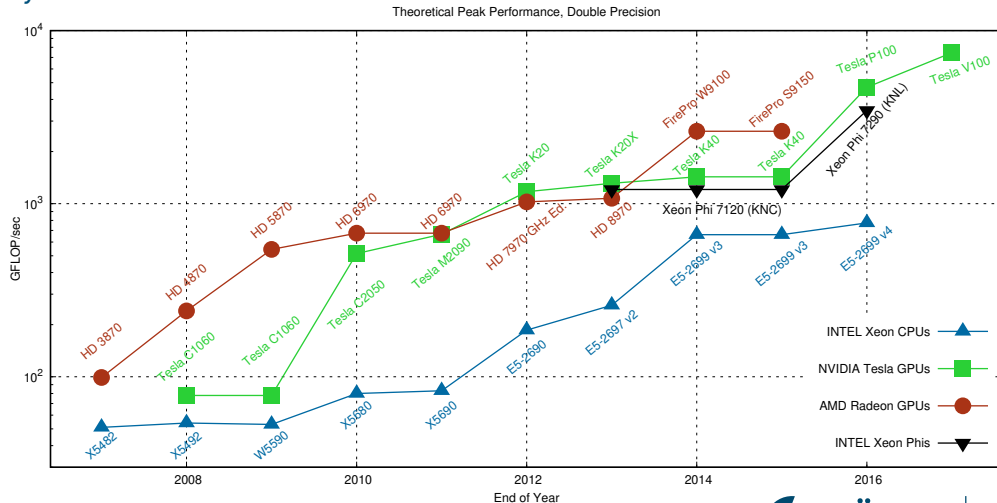
JURON – A Human Brain Project *Pilot System*

- 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

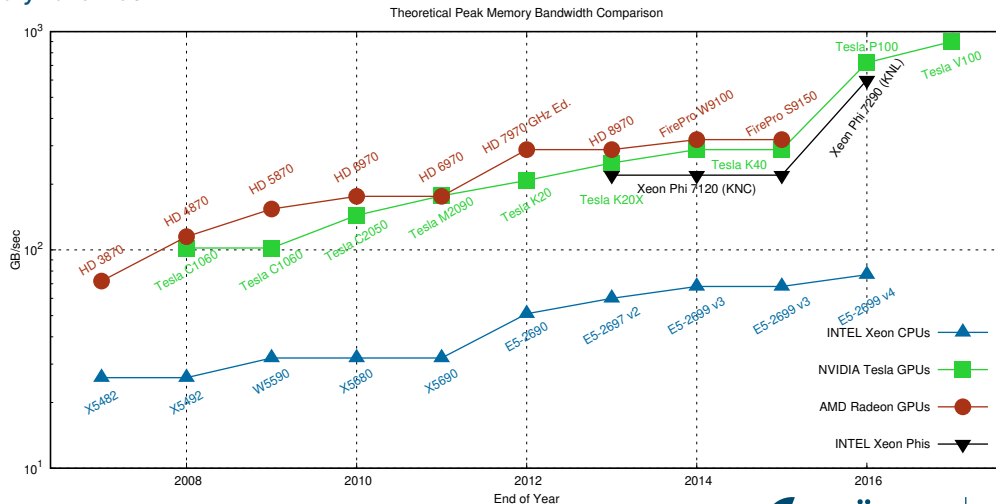
Memory Bandwidth



Graphic: Rupp [2]

Status Quo Across Architectures

Memory Bandwidth



Graphic: Rupp [2]

CPU vs. GPU

A matter of specialties



Transporting one

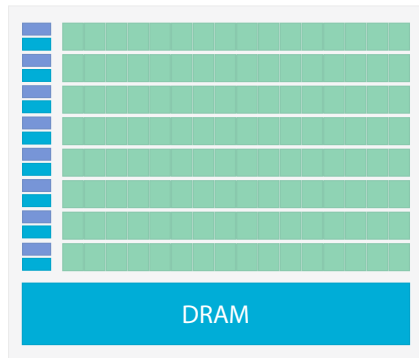
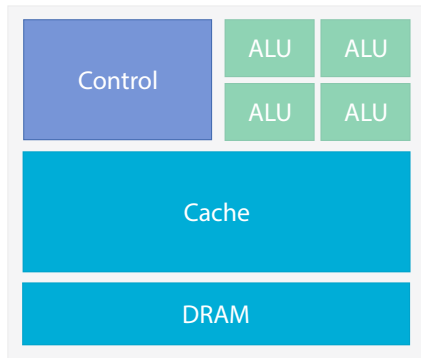


Transporting many

Graphics: Lee [3] and Bob Adams [4]

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

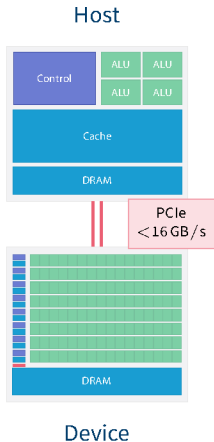
Asynchronicity

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...?)



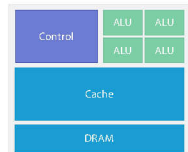
Memory

GPU memory ain't no CPU memory

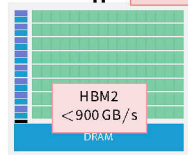
- GPU: accelerator / extension card
- Separate device from CPU
 - Separate memory but **Unified Memory**
- Memory transfers need special consideration!
Do as little as possible!
- Formerly: Explicitly copy data to/from GPU
Now: Done automatically (performance...?)
- P100: 16 GB RAM, 720 GB/s; V100: 16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

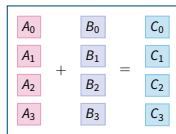
Memory

SIMT

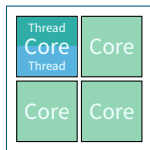
Of threads and warps

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

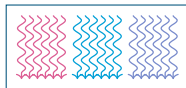
Vector



SMT



SIMT



SIMT

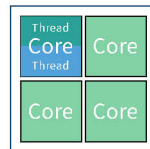
Of t



Vector

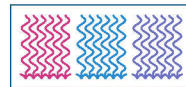
$$\begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ A_3 \end{bmatrix} + \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ B_3 \end{bmatrix} = \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \end{bmatrix}$$

SMT



Graphics: volta-pictures

SIMT



SIMT

of

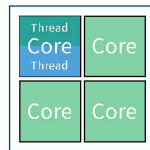
Multiprocessor



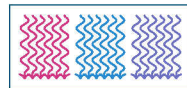
Vector

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

SMT



SIMT



Graphics: volta-pictures

SIMT

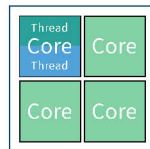
Of t



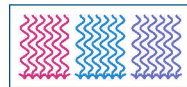
Vector

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

SMT



SIMT



Graphics: volta-pictures

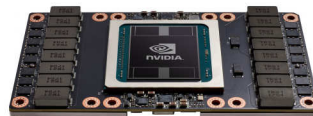
CPU vs. GPU

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!**

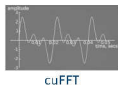
Use applications & libraries



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

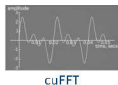
```
cudaFree(d_x); cudaFree(d_y);  
cublasDestroy(handle);
```

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
);
```

```
x = d_x;
```

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)  
    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);
```

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
```

Allocate GPU-capable
memory

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

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

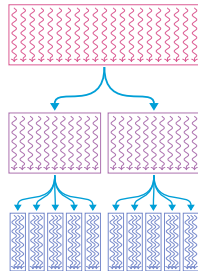
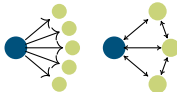
- [See appendix](#)

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

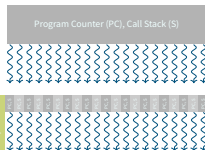
Advanced Topics

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

9-@ >+3/2	9-@ 00	9-@ E 00	9-@ &100	9-@ V100
GPU	GK180 (Kepler)	GM200 (Maxwell)	GP100 (Pascal)	GV100 (Volta)
SMs	15	24	56	80
TPCs	15	24	28	40
FP32 Cores / SM	1B2	128	64	64
FP32 Cores / GPU	2880	30C2	3584	5120
FP64 Cores / SM	64	4	32	32
FP64 Cores / GPU	B60	B6	1CB2	2560
TeDxor Cores / SM	EF	EF	EF	8
TeDxor Cores / GPU	EF	EF	EF	640
GPU Boost ClcH	810/8C5 MI J	1114 MI J	1480 MI J	1462 MI J
PeaHFP32 TFMLPS ¹	5	6M	10M	15
PeaHFP64 TFMLPS ¹	1M	M1	5M	OM
PeaHTeDxor TFMLPS ¹	EF	EF	EF	120
TextNe UDD	240	1B2	224	320
MeP or QDter Sice	384 TUDGVVW	384 TUDGVVW	40B6 TUD1 GM2	40B6 TUD1 GM2
MeP or QSe	Up to 12 GG	Up to 24 GG	16 GG	16 GG
K2 CacXe SOe	1536 KG	30C2 KG	40B6 KG	6144 KG
SXareYMeP or QSe / SM	16 KG/32 KG/48 KG	B6 KG	64 KG	CoDSNaUe Np to B6 KG
WZer FQe SOe / SM	256 KG	256 KG	256 KG	256KG
WZer FQe SOe / GPU	3840 KG	6144 KG	14336 KG	20480 KG
TVP	235 [atts	250 [atts	300 [atts	300 [atts
TradGtors	OM UDD	8 UDD	15M UDD	21M UDD
GPU VQSe	551 P P\	601 P P\	610 P P\	815 P P\
MaDSctNDE Process	28 DP	28 DP	16 DP FQI T^	12 DP FFE

¹ PeaHTFMLPS rates are UseY oDGPU Boost ClcH

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

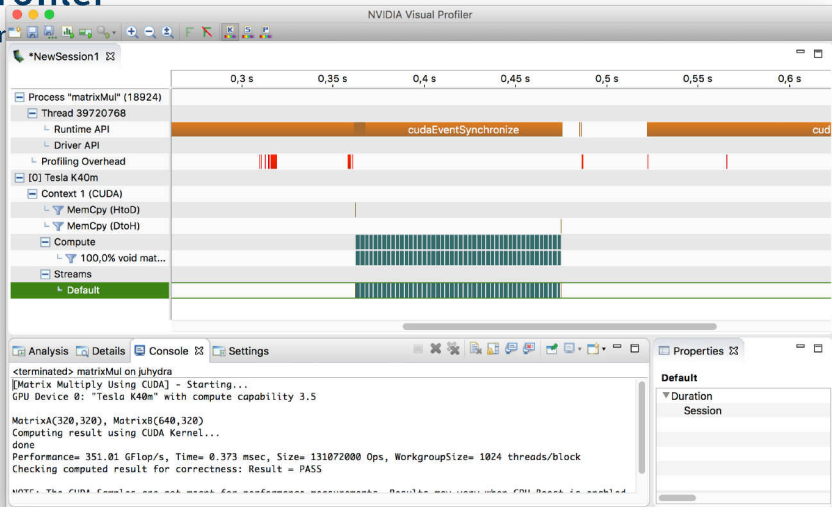
With metrics: `nvprof --metrics flop_sp_efficiency ./app`

```
$ 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 POWERprocessor, 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>.