

# CUDA INTRODUCTION PART I GSP GPU COURSE 2018

8 August 2018 | Andreas Herten | Forschungszentrum Jülich



## **Outline**

Introduction

GPU History

**Architecture Comparison** 

Jülich Systems

App Showcase

The GPU Platform

3 Core Features

Memory

Asynchronicity

**SIMT** 

**High Throughput** 

Summary

**Programming GPUs** 

Libraries

**About CUDA Alternatives** 

**Directives** 

Thrust

CUDA C/C++



50 Shaders of Gray

1999 Graphics computation pipeline implemented in dedicated *graphics hardware*Computations using OpenGL graphics library [2]
»GPU« coined by NVIDIA [3]

Slide 2144



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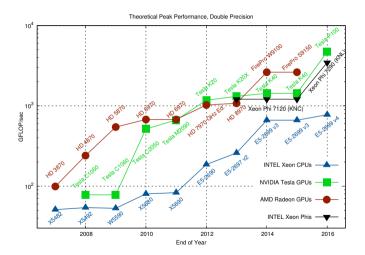
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- 2007 CUDA
- 2009 OpenCL
- 2016 Top 500: > 1/10 with GPUs [4], Green 500:  $\approx 2/3$  of top 50 with GPUs [5]

# **Status Quo Across Architectures**

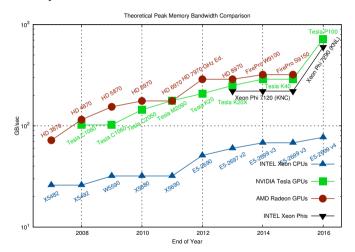
#### Performance





# **Status Quo Across Architectures**

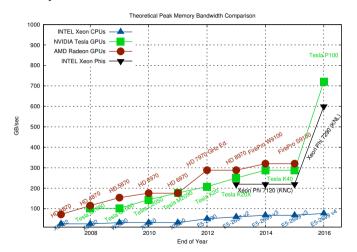
#### **Memory Bandwidth**





# **Status Quo Across Architectures**

### **Memory Bandwidth**







## 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 (#29)
- Mellanox EDR InfiniBand





### JURON - A Human Brain Project Prototype

- 18 nodes with IBM POWER8NVL CPUs (2  $\times$  10 cores)
- Per Node: 4 NVIDIA Tesla P100 cards, connected via NVLink
- GPU: 0.38 PFLOP/s peak performance





## JURON – A Human Brain Project *Prototype*

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- GPU: 0.38 PFLOP/s peak performance





JUWELS – Jülich's New Large System just went online

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



# **Getting GPU-Acquainted**



**Some Applications** 

Location of Code: 1-Basics/exercises/tasks/getting\_started/

See Instructions.rst for hints.

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**Some Applications** 

GEMM N-Body

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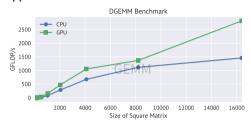
Mandelbrot

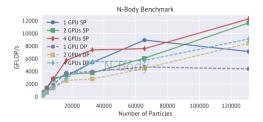
**Dot Product** 

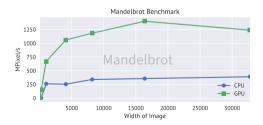
## **Getting GPU-Acquainted**

## TASK

### **Some Applications**









## The GPU Platform



## CPU vs. GPU

### A matter of specialties





### CPU vs. GPU

#### A matter of specialties



Transporting one

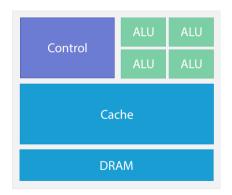


**Transporting many** 

aphics: Lee [7] and Shearings Holida

## CPU vs. GPU

Chip







## **GPU** Architecture

Overview

Aim: Hide Latency Everything else follows



## **GPU** Architecture

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SIMT

Asynchronicity

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## **GPU** Architecture

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SIMT

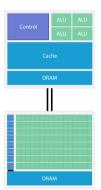
Asynchronicity

**Memory** 



#### **GPU** memory ain't no **CPU** memory

- GPU: accelerator / extension card
- $\rightarrow$  Separate device from CPU



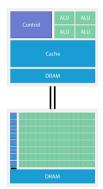
Device



#### GPU memory ain't no CPU memory

Unified Virtual Addressing

- GPU: accelerator / extension card
- → Separate device from CPŲ
   Separate memory, but UVA

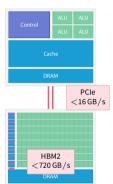


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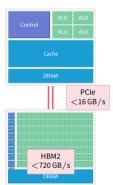


Device



#### GPU memory ain't no CPU memory

- GPU: accelerator / extension card
- → Separate device from CPU Separate memory, but UVA
  - Memory transfers need special consideration! Do as little as possible!



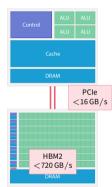
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  - Formerly: Explicitly copy data to/from GPU Now: Done automatically (performance...?)



Device



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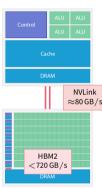
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- GPU: accelerator / extension card
- → Separate device from CPU Separate memory, but UVA and UM
  - Memory transfers need special consideration! Do as little as possible!
  - Formerly: Explicitly copy data to/from GPU
     Now: Done automatically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





Host



Device

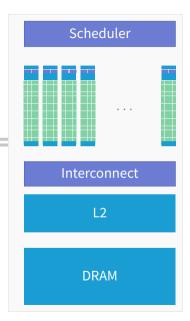


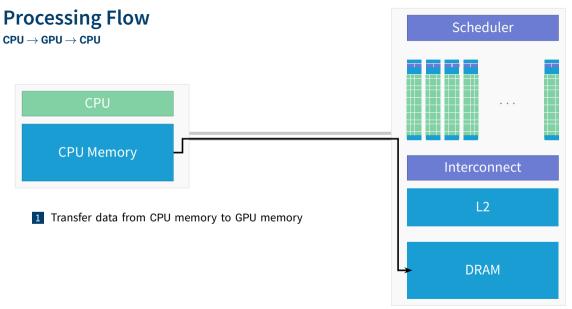
# **Processing Flow**

 $CPU \rightarrow GPU \rightarrow CPU$ 

CPU

**CPU Memory** 

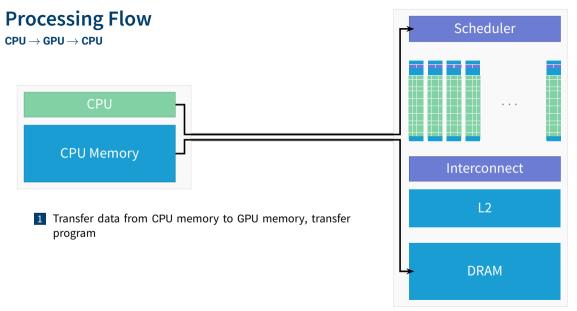




Member of the Helmholtz Association

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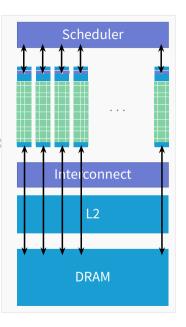
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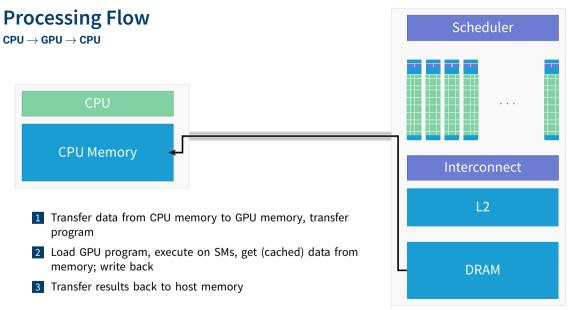
 $CPU \rightarrow GPU \rightarrow CPU$ 

### CPU

## **CPU Memory**

- Transfer data from CPU memory to GPU memory, transfer program
- 2 Load GPU program, execute on SMs, get (cached) data from memory; write back





# **GPU** Architecture

Overview

Aim: Hide Latency Everything else follows

SIMT

Asynchronicity

**Memory** 



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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

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# **GPU** Architecture

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Memory



### $\mathbf{SIMT} = \mathbf{SIMD} \oplus \mathbf{SMT}$

- CPU:
  - Single Instruction, Multiple Data (SIMD)

### Scalar

 $\mathbf{SIMT} = \mathbf{SIMD} \oplus \mathbf{SMT}$ 

- CPU:
  - Single Instruction, Multiple Data (SIMD)

### Vector



### $\mathbf{SIMT} = \mathbf{SIMD} \oplus \mathbf{SMT}$

- CPU:
  - Single Instruction, Multiple Data (SIMD)
  - Simultaneous Multithreading (SMT)

### Vector





Slide 17144

### $\mathbf{SIMT} = \mathbf{SIMD} \oplus \mathbf{SMT}$

- CPU:
  - Single Instruction, Multiple Data (SIMD)
  - Simultaneous Multithreading (SMT)

### Vector



### SMT



### $SIMT = SIMD \oplus SMT$

- CPU:
  - Single Instruction, Multiple Data (SIMD)
  - Simultaneous Multithreading (SMT)
- GPU: Single Instruction, Multiple Threads (SIMT)

### Vector



### SMT



Slide 17144

### $SIMT = SIMD \oplus SMT$

- CPU:
  - Single Instruction, Multiple Data (SIMD)
  - Simultaneous Multithreading (SMT)
- GPU: Single Instruction, Multiple Threads (SIMT)

### Vector



### **SMT**



### SIMT



### $SIMT = SIMD \oplus SMT$

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

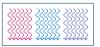
#### Vector



### SMT



### SIMT





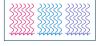
### Vector



SMT



SIMT







### Vector



SMT

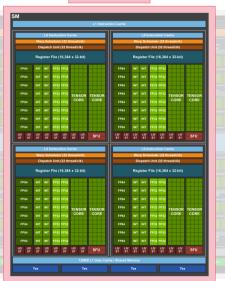


SIMT





Multiprocessor



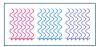
### Vector



### SMT



### SIMT





# Low Latency vs. High Throughput

Maybe GPU's ultimate feature

CPU Minimizes latency within each thread

GPU Hides latency with computations from other thread warps



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CPU Minimizes latency within each thread

GPU Hides latency with computations from other thread warps

**CPU Core: Low Latency** 





# Low Latency vs. High Throughput

Maybe GPU's ultimate feature

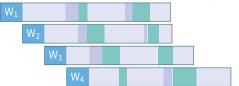
CPU Minimizes latency within each thread

GPU Hides latency with computations from other thread warps

### **CPU Core: Low Latency**



### GPU Streaming Multiprocessor: High Throughput







# 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!

```
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++)
    v[i] = a * x[i] + v[i]:
int a = 42;
int n = 10:
float x[n], y[n];
// fill x, v
saxpv(n, a, x, y);
```

# **Libraries**

Programming GPUs is easy: Just don't!



# Libraries

Programming GPUs is easy: Just don't!

Use applications & libraries!



# **Libraries**

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

Use applications & libraries!



/izard: Breazell [10]























Numba

theano

























Numba









### Parallel algebra



- 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

### Code example

```
int a = 42: int n = 10:
float x[n], y[n]:
// fill x. v
cublasHandle t handle:
cublasCreate(&handle):
float * d x. * d v:
cudaMallocManaged(\delta d \times n * sizeof(x[0]):
cudaMallocManaged(\delta d \ v. \ n \ * \ sizeof(v[0]):
cublasSetVector(n, sizeof(x[0]), x, 1, d x, 1);
cublasSetVector(n, sizeof(y[0]), y, 1, d y, 1);
cublasSaxpv(n. a. d x. 1. d v. 1):
cublasGetVector(n, sizeof(v[0]), d v, 1, v, 1);
cudaFree(d x): cudaFree(d v):
cublasDestrov(handle):
```

### Code example

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```

Allocate GPU memory

Copy data to GPU

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```



### Implement a matrix-matrix multiplication

- Location of code: 1-Basics/excercises/tasks/cublas/
- Look at Instructions.rst for instructions
  - 1 Implement call to double-precision GEMM of cuBLAS
  - 2 Build with make (CUDA needs to be loaded!)
  - 3 Run with make run

```
Orsrun ./dgemm_um N, where N=100, 200, ...
```

Check cuBLAS documentation for details on cublasDgemm()

### **JUWELS Getting Started**

```
module load CUDA/9.1.85
salloc --partition=gpus --gres=mem192,gpu:4 -n 1
srun hostname
srun --pty --forward-x bash -i
```



# Programming GPUs About CUDA Alternatives





Libraries are not enough?

You think you want to write your own GPU code?



Amdahl's Law

Total Time 
$$t = t_{serial} + t_{parallel}$$



Amdahl's Law

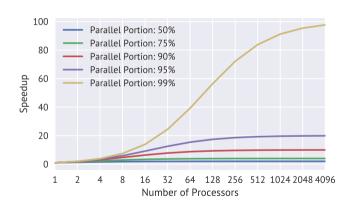
Total Time 
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 $N$  Processors  $t(N) = t_{s} + t_{p}/N$ 

Amdahl's Law

Total Time 
$$t = t_{\text{serial}} + t_{\text{parallel}}$$
  
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Speedup  $s(N) = t/t(N) = \frac{t_{\text{s}} + t_{\text{p}}}{t_{\text{s}} + t_{\text{p}}/N}$ 

Amdahl's Law

Total Time 
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 $N$  Processors  $t(N)=t_{\mathsf{s}}+t_{\mathsf{p}}/N$   
Speedup  $s(N)=t/t(N)=\frac{t_{\mathsf{s}}+t_{\mathsf{p}}}{t_{\mathsf{s}}+t_{\mathsf{p}}/N}$ 







Parallel programming is not easy!

#### Things to consider:

- Is my application computationally intensive enough?
- What are the levels of parallelism?
- How much data needs to be transferred?
- Is the gain worth the pain?



### **Alternatives**

#### The twilight

There are alternatives to CUDA C, which can ease the pain...

- OpenACC
- Thrust
- PyCUDA

Other alternatives (for completeness)

- CUDA Fortran
- OpenMP
- OpenCL



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The twilight

There are alternatives to CUDA C, which can ease the pain...

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# **Programming GPUs Directives**



#### Keepin' you portable

Annotate serial source code by directives

```
#pragma acc loop
for (int i = 0; i < 1; i+*) {};</pre>
```



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Annotate serial source code by directives

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- Also: Generalized API functions acc\_copy();
- Compiler interprets directives, creates according instructions



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#pragma acc loop
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```

- 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

- Only few compilers
- Not all the raw power available
- Harder to debug
- Easy to program wrong



The power of... two.

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

OpenACC Similar to OpenMP, but more specifically for GPUs For C/C++ and Fortran



```
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);</pre>
```

```
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];
}
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float x[n], y[n];
// fill x, y
saxpy_acc(n, a, x, y);</pre>
```

```
DASK
```

```
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];
}

Tommorrow!

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

saxpy_acc(n, a, x, y);</pre>
```



# Programming **GPUs**Thrust



### **Thrust**

Iterators! Iterators everywhere! 🚀

- $\frac{\mathsf{Thrust}}{\mathsf{CUDA}} = \frac{\mathsf{STL}}{\mathsf{C++}}$
- Template library
- Based on iterators
- Data-parallel primitives (scan(), sort(), reduce(),...)
- Fully compatible with plain CUDA C (comes with CUDA Toolkit)
- → http://thrust.github.io/ http://docs.nvidia.com/cuda/thrust/

### **Thrust**

```
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(), d_y.begin(), d_y.begin(), a * _1 + _2);
x = d_x;
```



### **Thrust Task**



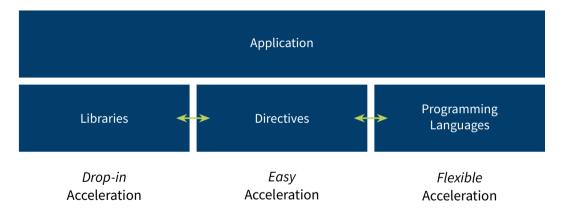
#### Let's sort some randomness

- Location of code: 1-Basics/excercises/tasks/thrust/
- Look at Instructions.rst for instructions
  - Sort random numbers with Thrust on CPU and GPU
  - 2 Build with make (CUDA needs to be loaded!)
  - 3 Run with make run

```
Orsrun -p gpus --gres=gpu:1 ./ThrustSort
```

Check Thrust documentation for details on thrust::sort()

# **Summary of Acceleration Possibilities**



# **Programming GPUs** CUDA C/C++



#### **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)
    v[i] = a * x[i] + v[i]:
int a = 42:
int n = 10:
float x[n], y[n];
// fill x, v
cudaMallocManaged(&x, n * sizeof(float));
cudaMallocManaged(&v, n * sizeof(float));
saxpv cuda<<<2. 5>>>(n. a. x. v):
```

In software: Threads, Blocks

• Methods to exploit parallelism:



- Methods to exploit parallelism:
  - Thread



- Methods to exploit parallelism:
  - Threads





- Methods to exploit parallelism:
  - $\blacksquare \quad \underline{\mathsf{Threads}} \to \underline{\mathsf{Block}}$



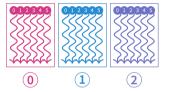


- Methods to exploit parallelism:
  - $\bullet \quad \text{Threads} \rightarrow \quad \text{Block}$
  - Block

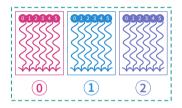




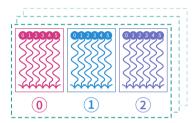
- Methods to exploit parallelism:
  - lacktriangle Threads ightarrow Block
  - Blocks



- Methods to exploit parallelism:
  - Threads → Block
  - lacks ightarrow Grid

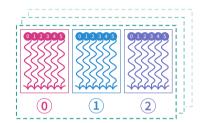


- Methods to exploit parallelism:
  - $\blacksquare \quad \underbrace{\mathsf{Threads}}_{} \to \underbrace{\mathsf{Block}}_{}$
  - lacks ightarrow Grid
  - Threads & blocks in 3D



In software: Threads, Blocks

- Methods to exploit parallelism:
  - Threads  $\rightarrow$  Block
  - Blocks  $\rightarrow$  Grid
  - Threads & blocks in 30



- Parallel function: kernel
  - \_\_global\_\_ kernel(int a, float \* b) { }
  - Access own ID by global variables threadIdx.x, blockIdx.y,...
- Execution entity: threads
  - Lightweight → fast switchting!
  - 1000s threads execute simultaneously → order non-deterministic!

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?!?

# $\rightarrow$ Jan!



### **Conclusions**

...of Part 1

- GPUs achieve performance by specialized hardware
- Acceleration can be done by different means
- Libraries are the easiest
- Thrust, OpenACC can give first entry point
- Full power with CUDA
- CUDA parallelizes for GPUs with many threads



### **Conclusions**

...of Part 1

- GPUs achieve performance by specialized hardware
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- CUDA parallelizes for GPUs with many threads





### **APPENDIX**



Appendix Glossary References



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# Glossary I

- API A programmatic interface to software by well-defined functions. Short for application programming interface. 82, 83, 84, 106, 113
- ATI Canada-based GPUs manufacturing company; bought by AMD in 2006. 3, 4, 5, 6, 7
- CUDA Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 2, 3, 4, 5, 6, 7, 79, 80, 91, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 106, 107, 108, 112
  - JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. 111
- JURECA A multi-purpose supercomputer with 1800 nodes at JSC. 11



# **Glossary II**

- JURON One of the two HBP pilot system in Jülich; name derived from Juelich and Neuron. 12, 13
- JUWELS Jülich's new supercomputer, the successor of JUQUEEN. 14, 71
  - NVIDIA US technology company creating GPUs. 3, 4, 5, 6, 7, 11, 12, 13, 14, 111, 112, 113, 114
  - NVLink NVIDIA's communication protocol connecting CPU  $\leftrightarrow$  GPU and GPU  $\leftrightarrow$  GPU with high bandwidth. 12, 13, 113
- OpenACC Directive-based programming, primarily for many-core machines. 79, 80, 85, 86, 87, 88, 89, 107, 108
  - OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 3, 4, 5, 6, 7, 79, 80



# **Glossary III**

- OpenGL The *Open Graphics Library*, an API for rendering graphics across different hardware architectures. 3, 4, 5, 6, 7
- OpenMP Directive-based programming, primarily for multi-threaded machines. 79, 80, 85
  - P100 A large GPU with the Pascal architecture from NVIDIA. It employs NVLink as its interconnect and has fast *HBM2* memory. 12, 13
  - Pascal GPU architecture from NVIDIA (announced 2016). 113
  - POWER CPU architecture from IBM, earlier: PowerPC. See also POWER8. 113
- POWER8 Version 8 of IBM's POWERprocessor, available also under the OpenPOWER Foundation. 12, 13, 113
  - SAXPY Single-precision  $A \times X + Y$ . A simple code example of scaling a vector and adding an offset. 57, 96



# **Glossary IV**

- Tesla The GPU product line for general purpose computing computing of NVIDIA. 11, 12, 13, 14
- Thrust A parallel algorithms library for (among others) GPUs. See https://thrust.github.io/. 79, 80, 91, 93, 107, 108
  - CPU Central Processing Unit. 11, 12, 13, 14, 19, 20, 21, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 57, 85, 93, 112, 113
  - GPU Graphics Processing Unit. 2, 3, 4, 5, 6, 7, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 56, 58, 59, 60, 61, 62, 63, 72, 73, 81, 82, 83, 84, 85, 90, 93, 95, 107, 108, 111, 112, 113, 114

HBP Human Brain Project. 112



# **Glossary V**

SIMD Single Instruction, Multiple Data. 42, 43, 44, 45, 46, 47, 48, 49, 50, 51

SIMT Single Instruction, Multiple Threads. 22, 23, 24, 37, 38, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51

SM Streaming Multiprocessor. 42, 43, 44, 45, 46, 47, 48, 49, 50, 51

SMT Simultaneous Multithreading. 42, 43, 44, 45, 46, 47, 48, 49, 50, 51

### References I

- [2] Kenneth E. Hoff III et al. "Fast Computation of Generalized Voronoi Diagrams Using Graphics Hardware". In: Proceedings of the 26th Annual Conference on Computer Graphics and Interactive Techniques. SIGGRAPH '99. New York, NY, USA: ACM Press/Addison-Wesley Publishing Co., 1999, pp. 277–286. ISBN: 0-201-48560-5. DOI: 10.1145/311535.311567. URL: http://dx.doi.org/10.1145/311535.311567 (pages 3-7).
- [3] Chris McClanahan. "History and Evolution of GPU Architecture". In: A Survey Paper (2010). URL: http://mcclanahoochie.com/blog/wp-content/uploads/2011/03/gpu-hist-paper.pdf (pages 3-7).
- [4] Jack Dongarra et al. *TOP500*. Nov. 2016. URL: https://www.top500.org/lists/2016/11/(pages 3-7).



### References II

- [5] Jack Dongarra et al. *Green500*. Nov. 2016. URL: https://www.top500.org/green500/lists/2016/11/(pages 3-7).
- [6] Karl Rupp. *Pictures: CPU/GPU Performance Comparison*. URL: https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardwarecharacteristics-over-time/(pages 8-10).
- Wes Breazell Picture: Wizard URL: [10] https://thenounproject.com/wes13/collection/its-a-wizards-world/ (pages 58-62).

# References: Images, Graphics I

- [1] Igor Ovsyannykov. *Yarn*. Freely available at Unsplash. URL: https://unsplash.com/photos/hvILKk7SlH4.
- [7] Mark Lee. *Picture: kawasaki ninja*. URL: https://www.flickr.com/photos/pochacco20/39030210/ (pages 19, 20).
- [8] Shearings Holidays. *Picture: Shearings coach 636*. URL: https://www.flickr.com/photos/shearings/13583388025/(pages 19, 20).
- [9] Nvidia Corporation. Pictures: Volta GPU. Volta Architecture Whitepaper. URL: https://images.nvidia.com/content/volta-architecture/pdf/Volta-Architecture-Whitepaper-v1.0.pdf (pages 49-51).

