

GPU ACCELERATORS AT JSC OF THREADS AND KERNELS

28 May 2018 | Andreas Herten | Forschungszentrum Jülich



Outline

GPUs at JSC

GPU Architecture

Empirical Motivation

Comparisons

3 Core Features

Memory

Asynchronicity

SIMT

High Throughput

Summary

Programming GPUs

Libraries

OpenACC/ OpenMP

CUDA C/C++

Performance Analysis

Advanced Topics

Using GPUs on JURECA

Compiling

Resource Allocation





JURECA – Jülich's Multi-Purpose Supercomputer

- 1872 nodes with Intel Xeon E5 2680 v3 Haswell CPUs (2 × 12 cores)
- ullet 75 nodes with 2 NVIDIA Tesla K80 cards (look like 4 GPUs); each 2 imes 12 GB RAM

Slide 2141

- JURECA Booster: 1640 nodes with Intel Xeon Phi Knights Landing
- 1.8 (CPU) + 0.44 (GPU) + 5 (KNL) PFLOP/s peak performance (#29)





JURON – A Human Brain Project Prototype

- \blacksquare 18 nodes with IBM POWER8NVL CPUs (2 \times 10 cores)
- Per Node: 4 NVIDIA Tesla P100 cards (16 GB HBM2 memory), connected via NVLink

Slide 3141

■ GPU: 0.38 PFLOP/s peak performance





JUWELS - Jülich's New Large System currently under construction

- 2500 nodes with Intel Xeon CPUs (2 × 24 cores)
- 48 nodes with 4 NVIDIA Tesla V100 cards (16 GB HBM2 memory)
- 10.4 (CPU) + 1.6 (GPU) + PFLOP/s peak performance

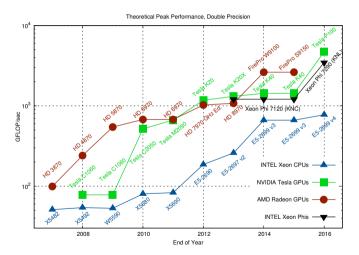




Why?

Status Quo Across Architectures

Performance

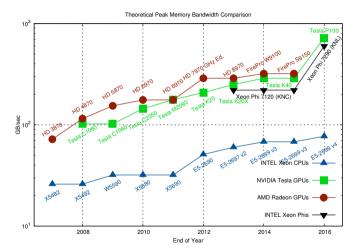




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Status Quo Across Architectures

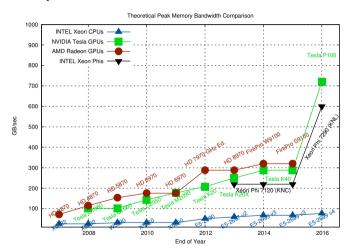
Memory Bandwidth





Status Quo Across Architectures

Memory Bandwidth





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CPU vs. GPU

A matter of specialties





raphics: Lee [3] and Shearings Holidays [4

CPU vs. GPU

A matter of specialties



Transporting one

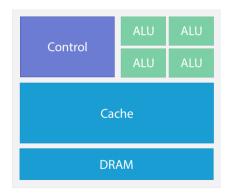


Transporting many

raphics: Lee [3] and Shearings Holiday

CPU vs. GPU

Chip







Overview

Aim: Hide Latency Everything else follows



Overview

Aim: Hide Latency Everything else follows

SIMT

Asynchronicity

Memory



Overview

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SIMT

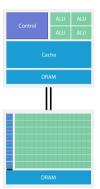
Asynchronicity

Memory



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

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



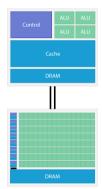
Device



GPU memory ain't no CPU memory

Unified Virtual Addressing

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

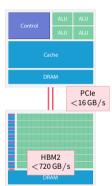


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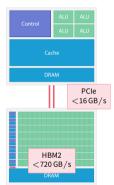


Device



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 - Memory transfers need special consideration! Do as little as possible!

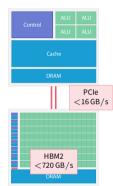


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GPU memory ain't no CPU memory

- GPU: accelerator / extension card
- → Separate device from CPU
 Separate memory, but UVA and UM
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 - Formerly: Explicitly copy data to/from GPU Now: Done automatically (performance...?)



Device



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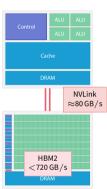


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- → Separate device from CPU Separate memory, but UVA and UM
 - Memory transfers need special consideration! Do as little as possible!
 - Formerly: Explicitly copy data to/from GPU Now: Done automatically (performance...?)
 - P100: 16 GB RAM, 720 GB/s;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







Device

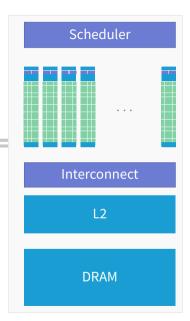


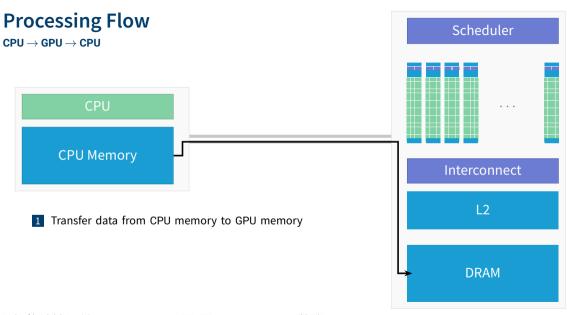
Processing Flow

 $CPU \rightarrow GPU \rightarrow CPU$

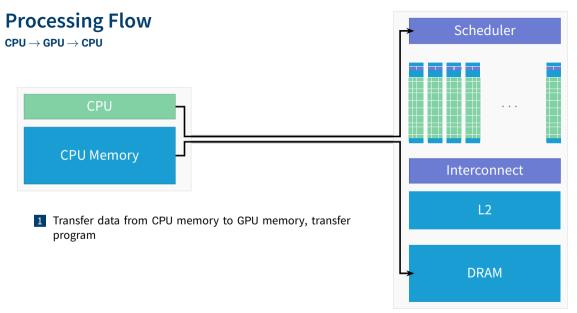
CPU

CPU Memory





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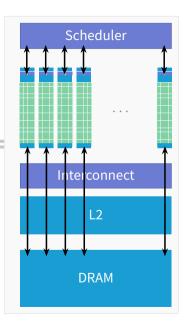
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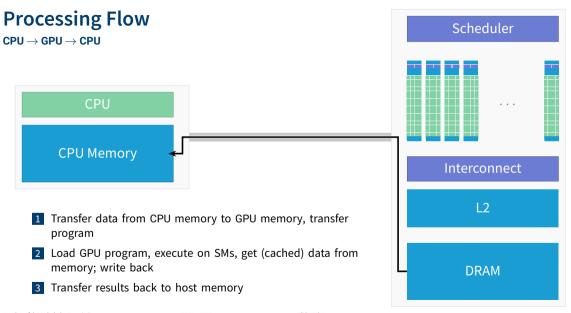
CPU o GPU o CPU

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





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Overview

Aim: Hide Latency Everything else follows

SIMT

Asynchronicity

Memory



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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

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SIMT

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

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

Scalar

SIMT

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

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

Vector



SIMT

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

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

Vector







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- CPU:
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SMT



$SIMT = SIMD \oplus SMT$

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

Vector



SMT



$SIMT = SIMD \oplus SMT$

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

Vector



SMT





$SIMT = SIMD \oplus SMT$

- 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





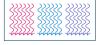


Vector



SMT







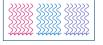


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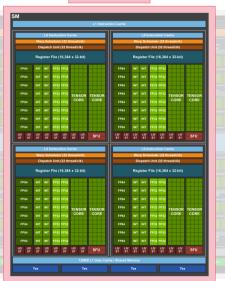
SMT







Multiprocessor

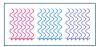


Vector



SMT







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



Low Latency vs. High Throughput

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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

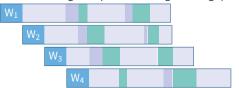
CPU Minimizes latency within each thread

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

Programming GPUs Libraries



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!



Wizard: Breazell [6]















Numba





CUDA Math



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

```
float 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):
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Allocate GPU memory

Copy data to GPU



Code example

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Programming GPUs OpenACC/ OpenMP



GPU Programming with Directives

Keepin' you portable

Annotate serial source code by directives

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#pragma acc loop
for (int i = 0; i < 1; i++) {};</pre>
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- OpenACC: Especially for GPUs; OpenMP: Has GPU support (in theory...)
- Compiler interprets directives, creates according instructions



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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

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];
}

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

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

OpenACC

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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];
}

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Programming GPUs CUDA C/C++



Programming GPU Directly

Finally...

Two solutions:



Programming GPU Directly

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- 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



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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



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- Hardest: Come up with parallelized algorithm



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In software: Threads, Blocks

• Methods to exploit parallelism:



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 - Thread



- Methods to exploit parallelism:
 - Threads





In software: Threads, Blocks

• Methods to exploit parallelism:

 $\blacksquare \quad \underline{\mathsf{Threads}} \to \underline{\mathsf{Block}}$

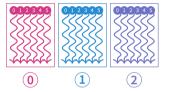


- Methods to exploit parallelism:
 - $\blacksquare \quad \text{Threads} \rightarrow \quad \text{Block}$
 - Block

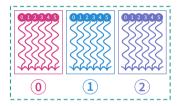




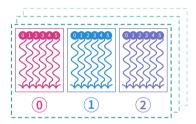
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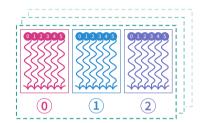
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 - Threads & blocks in 3D



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

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]:
float 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):
```

cudaDeviceSvnchronize():



Programming **GPUs**Performance Analysis



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

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



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nvprof Command line profiler, including detailed performance counters Visual Profiler Timeline profiling and annotated performance experiments

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



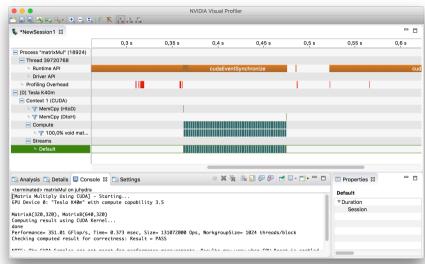
nvprof

Command that line

```
. . .
$ nyprof ./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 memcpv HtoD]
  0.23% 599.40us
                            599.40us 599.40us 599.40us
                                                         [CUDA memcpy DtoH]
==37064== APT calls:
Time(%)
             Time
                     Calls
                                 Avg
                                          Min
                                                    Max Name
 61.26% 258.38ms
                            258.38ms 258.38ms 258.38ms
                                                         cudaEventSynchronize
 35.68% 150.49ms
                            50.164ms 914.97us 148.65ms
                                                         cudaMalloc
  0.73% 3.0774ms
                         3 1.0258ms 1.0097ms 1.0565ms cudaMemony
  0.62% 2.6287ms
                            657, 17us 655, 12us 660, 56us
                                                         cuDeviceTotalMem
  0.56% 2.3408ms
                       301 7,7760us 7,3810us 53,103us cudal aunch
  0.48% 2.0111ms
                       364 5.5250us
                                         235ns 201.63us cuDeviceGetAttribute
  A 21% 872 52us
                            872.52us 872.52us 872.52us
                                                         cudaDeviceSynchronize
  0.15% 612.20us
                               406ns
                                         361ns 1.1970us
                                                         cudaSetupArgument
  0.12% 499.01us
                         3 166.34us 140.45us 216.16us
                                                         cudaFree
```



Visual Profiler

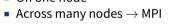




Advanced Topics

So much more interesting things to show!

- Optimize memory transfers to reduce overhead
- Optimize applications for GPU architecture
- Drop-in BLAS acceleration with NVBLAS (\$LD_PRELOAD)
- Tensor Cores for Deep Learning
- Use multiple GPUs
 - On one node







- Most of that: Addressed at dedicated training courses



Using GPUs on JURECA



Compiling on JURECA

CUDA

- Module: module load CUDA/9.1.85
- 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/17.10-GCC-5.5.0
- Compile: pgc++ -acc -ta=tesla file.cpp

MPI

Module: module load MVAPICH2/2.3a-GDR
 Enabled for CUDA (CUDA-aware); no need to copy data to host before transfer



Running on JURECA

- Dedicated GPU partitions: gpus and develgpus (+ vis)
 - --partition=develgpus Total 4 nodes (Job: <2 h, ≤ 2 nodes)
 - --partition=gpus Total 70 nodes (Job: $<1 \, d, \le 32 \, nodes$)
- Needed: Resource configuration with --gres

```
--gres=gpu:2
--gres=gpu:4
--gres=mem1024,gpu:2 --partition=vis
```

→ 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
```

Slide 40141

- GPUs provide highly-parallel computing power
- We have many devices installed at JSC, ready to be used!



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 CUDA Course April 2019
 OpenACC Course 29 30 October 2018
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APPENDIX



Appendix Glossary References



Glossary I

- API A programmatic interface to software by well-defined functions. Short for application programming interface. 71, 72, 73, 74, 75
- CUDA Computing platform for GPUs from NVIDIA. Provides, among others, CUDA C/C++. 2, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 93, 96, 97, 98, 99, 100, 103
 - JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. 2, 96, 97, 98, 99, 100, 103
- JURECA A multi-purpose supercomputer with 1800 nodes at JSC. 2, 3, 92, 93, 94
- JURON One of the two HBP pilot system in Jülich; name derived from Juelich and Neuron. 4



Glossary II

- JUWELS Jülich's new supercomputer, the successor of JUQUEEN. 5
 - MPI The Message Passing Interface, a API definition for multi-node computing. 91, 93
 - NVIDIA US technology company creating GPUs. 3, 4, 5, 71, 72, 73, 74, 75, 87, 88, 96, 97, 98, 99, 100, 103
 - NVLink NVIDIA's communication protocol connecting CPU \leftrightarrow GPU and GPU \leftrightarrow GPU with high bandwidth. 4, 103
- OpenACC Directive-based programming, primarily for many-core machines. 2, 64, 65, 66, 67, 68, 69, 93, 96, 97, 98, 99, 100
 - OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 71, 72, 73, 74, 75, 87, 88



Glossary III

- OpenMP Directive-based programming, primarily for multi-threaded machines. 2, 64, 65, 66, 67
 - P100 A large GPU with the Pascal architecture from NVIDIA. It employs NVLink as its interconnect and has fast *HBM2* memory. 4
 - Pascal GPU architecture from NVIDIA (announced 2016). 103
 - POWER CPU architecture from IBM, earlier: PowerPC. See also POWER8. 103
- POWER8 Version 8 of IBM's POWERprocessor, available also under the OpenPOWER Foundation. 4, 103
 - SAXPY Single-precision $A \times X + Y$. A simple code example of scaling a vector and adding an offset. 49, 85



Glossary IV

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

CPU Central Processing Unit. 3, 4, 5, 11, 12, 13, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 49, 71, 72, 73, 74, 75, 103

GPU Graphics Processing Unit. 2, 3, 4, 5, 6, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 48, 50, 51, 52, 53, 54, 55, 56, 64, 65, 66, 67, 70, 71, 72, 73, 74, 75, 86, 87, 88, 91, 92, 94, 95, 96, 97, 98, 99, 100, 103

HBP Human Brain Project. 103

SIMD Single Instruction, Multiple Data. 34, 35, 36, 37, 38, 39, 40, 41, 42, 43



Glossary V

SIMT Single Instruction, Multiple Threads. 14, 15, 16, 29, 30, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43

SM Streaming Multiprocessor. 34, 35, 36, 37, 38, 39, 40, 41, 42, 43

SMT Simultaneous Multithreading. 34, 35, 36, 37, 38, 39, 40, 41, 42, 43



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Clide 010

