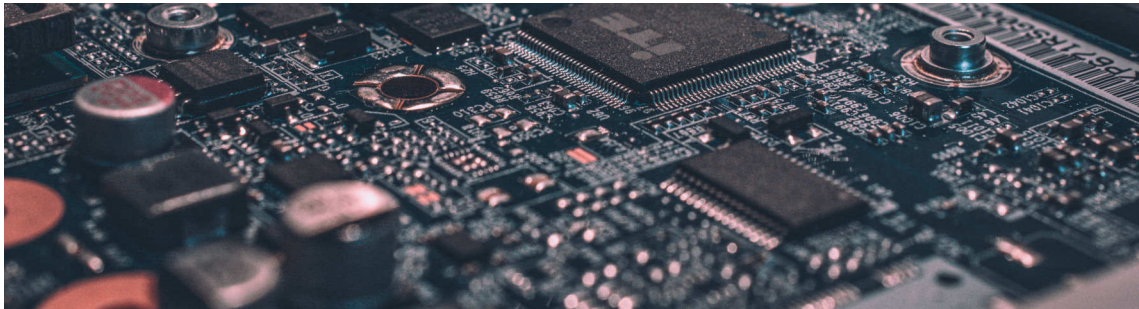




GPU ACCELERATORS AT JSC OF THREADS AND KERNELS

21 May 2019 | Andreas Herten | Forschungszentrum Jülich

Outline

GPUs at JSC

JUWELS

JURECA

JURON

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 & 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)



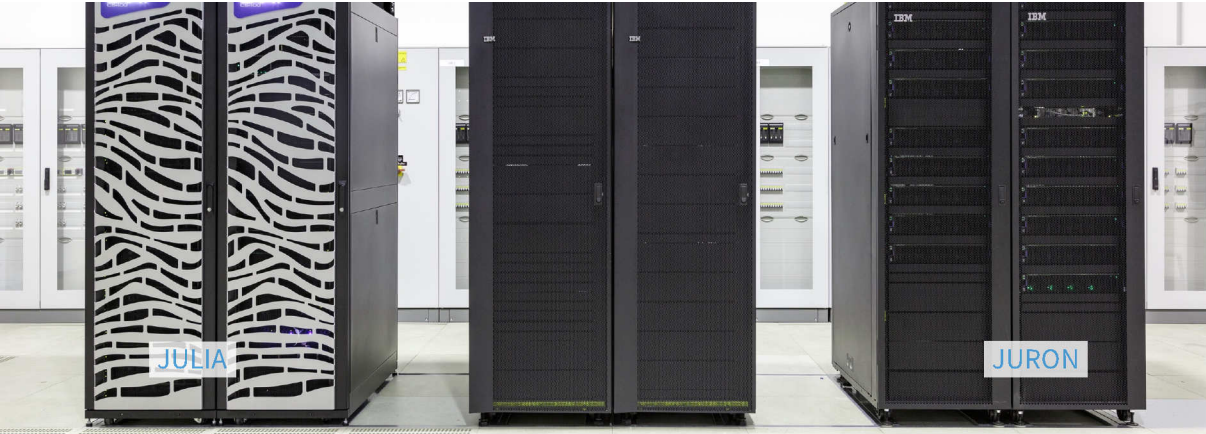
JUWELS – Jülich's New Large System

- 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)



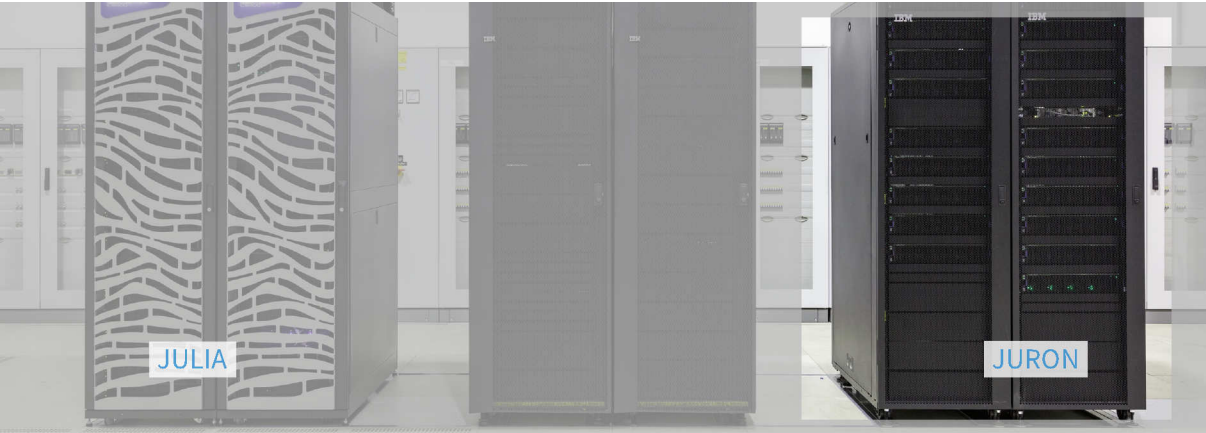
JURECA – Jülich's Multi-Purpose Supercomputer

- 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



JURON – A Human Brain Project *Pilot System*

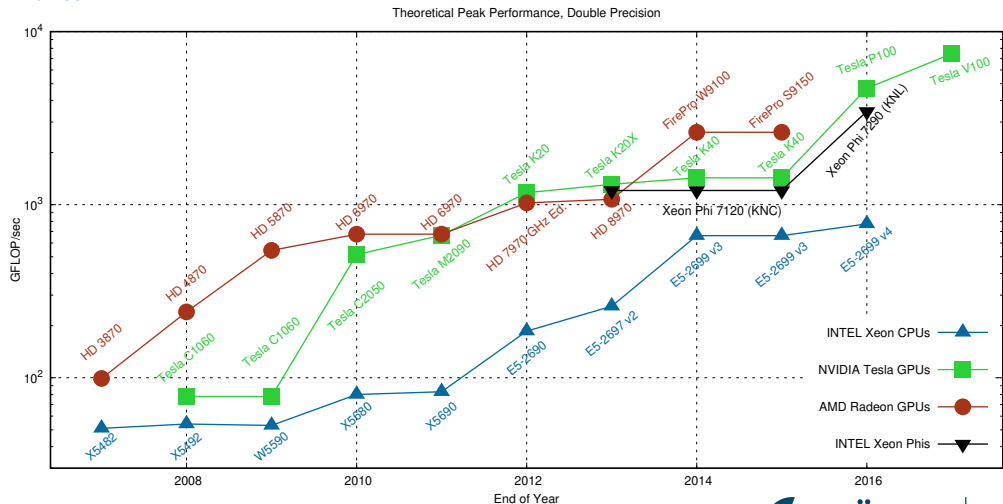
- 18 nodes with IBM POWER8NVL CPUs (2×10 cores)
- Per Node: 4 NVIDIA Tesla P100 cards (16 GB HBM2 memory), connected via NVLink
- GPU: 0.38 PFLOP/s peak performance

GPU Architecture

Why?

Status Quo Across Architectures

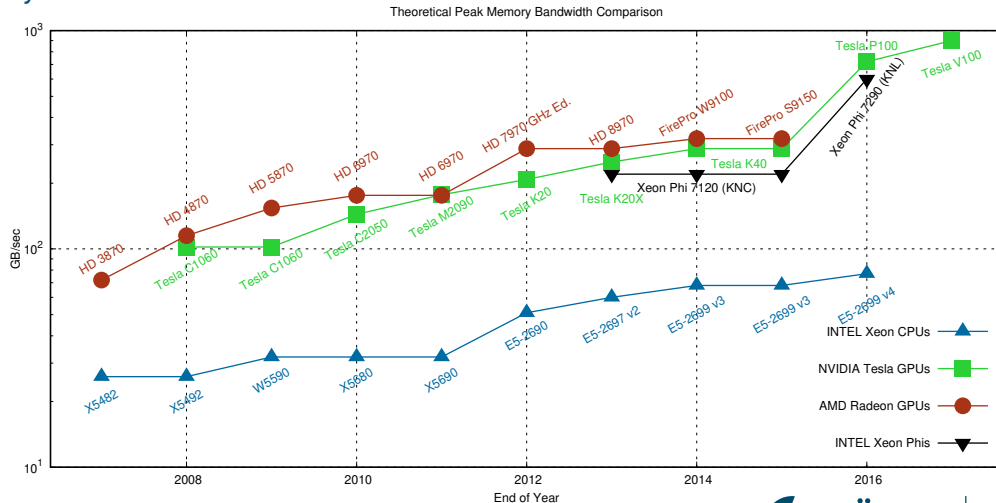
Performance



Graphic: Rupp [2]

Status Quo Across Architectures

Memory Bandwidth



Graphic: Rupp [2]

CPU vs. GPU

A matter of specialties



CPU vs. GPU

A matter of specialties



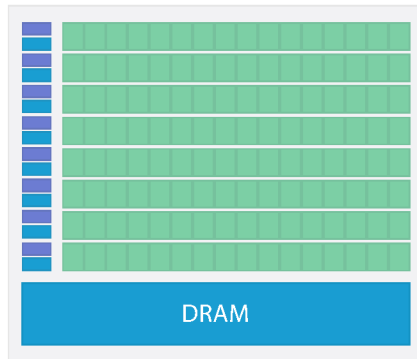
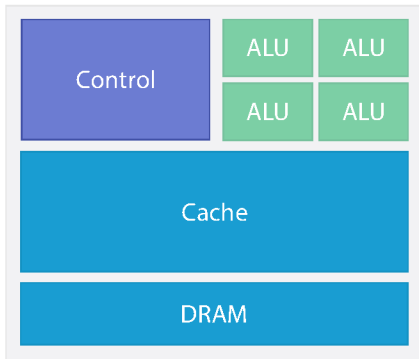
Transporting one



Transporting many

CPU vs. GPU

Chip



GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

Memory



GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

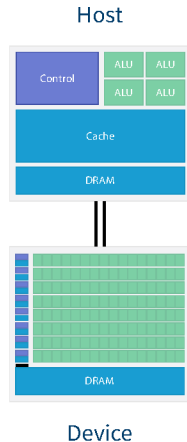
Asynchronicity

Memory

Memory

GPU memory ain't no CPU memory

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

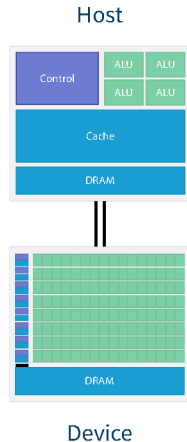


Memory

GPU memory ain't no CPU memory

Unified Virtual Addressing

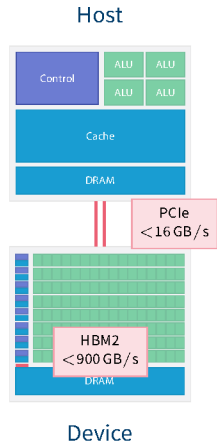
- GPU: accelerator / extension card
- Separate device from CPU
↓
Separate memory, but UVA



Memory

GPU memory ain't no CPU memory

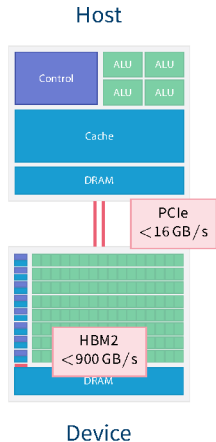
- GPU: accelerator / extension card
- Separate device from CPU
Separate memory, but UVA



Memory

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!

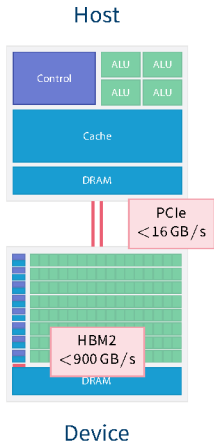


Memory

GPU memory ain't no CPU memory

Unified Memory

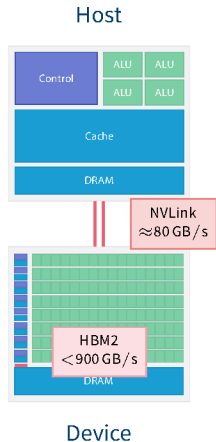
- GPU: accelerator / extension card
- Separate device from CPU
- **Separate memory, but UVA and UM**
- Memory transfers need special consideration!
Do as little as possible!
- Formerly: Explicitly copy data to/from GPU
Now: Done automatically (performance...?)



Memory

GPU memory ain't no CPU memory

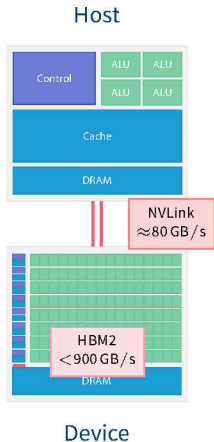
- GPU: accelerator / extension card
- Separate device from CPU
 - **Separate memory, but UVA and UM**
- Memory transfers need special consideration!
Do as little as possible!
- Formerly: Explicitly copy data to/from GPU
Now: Done automatically (performance...?)



Memory

GPU memory ain't no CPU memory

- 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



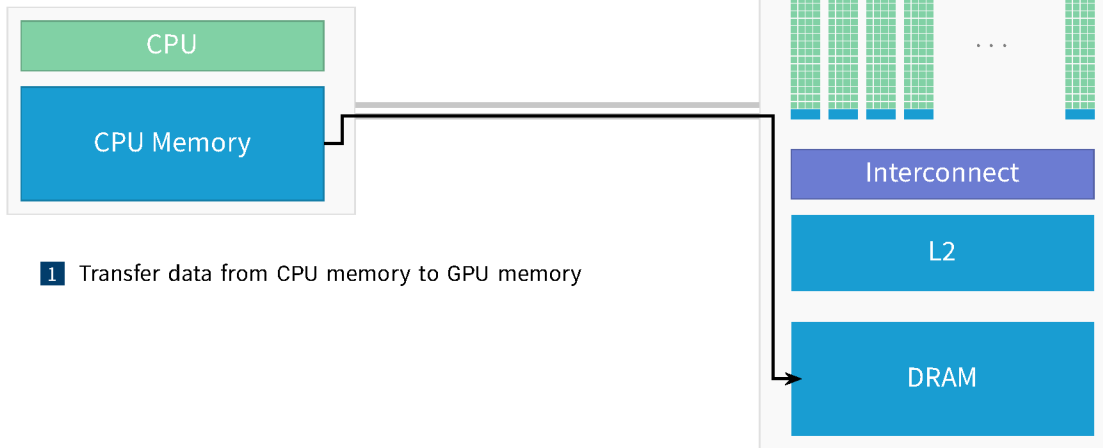
Processing Flow

CPU → GPU → CPU



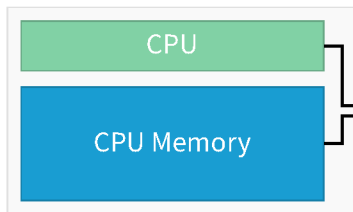
Processing Flow

CPU → GPU → CPU

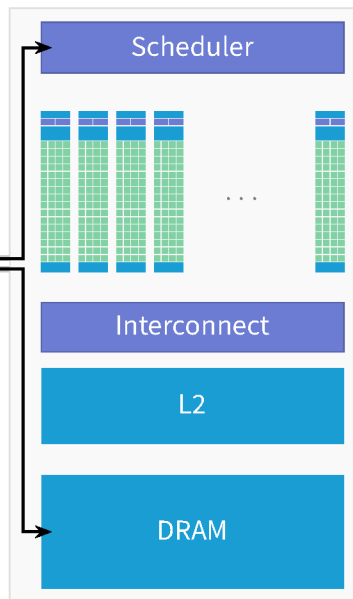


Processing Flow

CPU → GPU → CPU

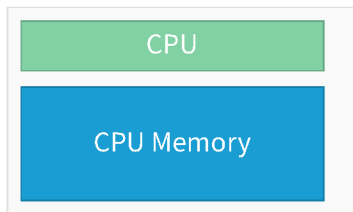


- 1 Transfer data from CPU memory to GPU memory, transfer program

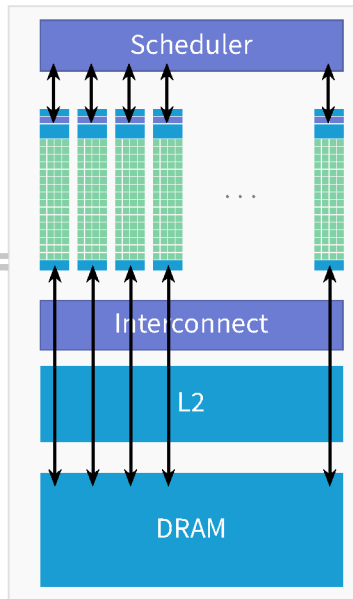


Processing Flow

CPU → GPU → CPU

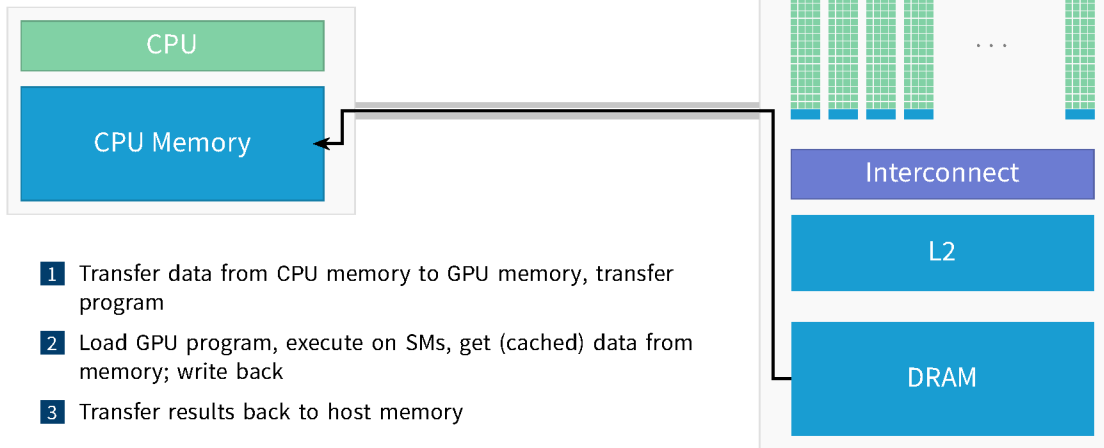


- 1 Transfer data from CPU memory to GPU memory, transfer program
- 2 Load GPU program, execute on SMs, get (cached) data from memory; write back



Processing Flow

CPU → GPU → CPU



GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

Memory

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

GPU Architecture

Overview

Aim: Hide Latency
Everything else follows

SIMT

Asynchronicity

Memory

SIMT

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

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

Scalar

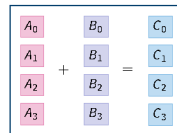
A_0	+	B_0	=	C_0
A_1	+	B_1	=	C_1
A_2	+	B_2	=	C_2
A_3	+	B_3	=	C_3

SIMT

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

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

Vector

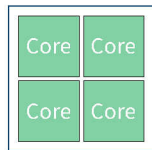
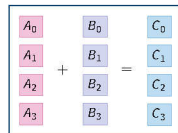


SIMT

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

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

Vector

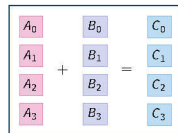


SIMT

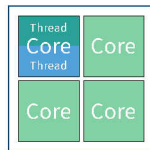
$$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$$

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

Vector



SMT

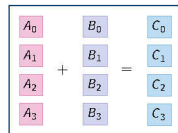


SIMT

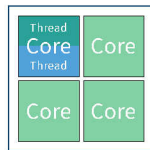
$$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$$

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

Vector



SMT

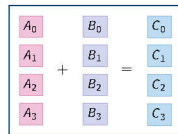


SIMT

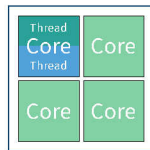
$$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$$

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

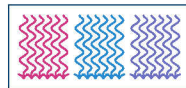
Vector



SMT



SIMT

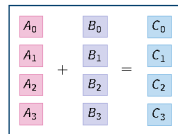


SIMT

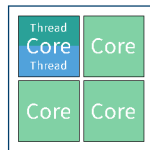
$$\text{SIMT} = \text{SIMD} \oplus \text{SMT}$$

- 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 

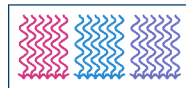
Vector



SMT



SIMT



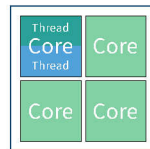
SIMT



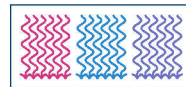
Vector

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

SMT



SIMT



Graphics: Nvidia Corporation [5]

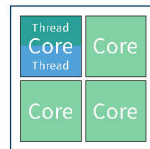
SIMT



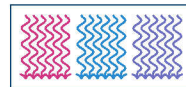
Vector

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

SMT



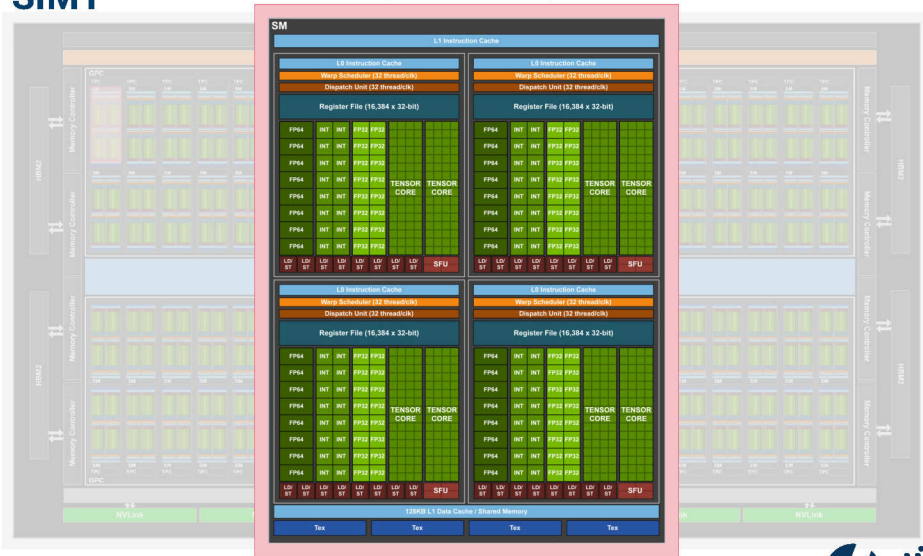
SIMT



Graphics: Nvidia Corporation [5]

SIMT

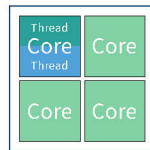
Multiprocessor



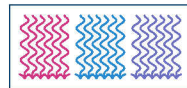
Vector

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

SMT



SIMT



Graphics: Nvidia Corporation [5]

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

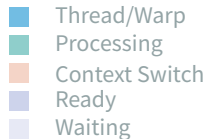
Low Latency vs. High Throughput

Maybe GPU's ultimate feature

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

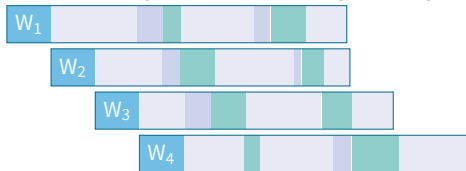
CPU Minimizes latency within each thread

GPU Hides latency with computations from other thread warps

CPU Core: Low Latency



GPU Streaming Multiprocessor: High Throughput



- Thread/Warp
- Processing
- Context Switch
- Ready
- Waiting

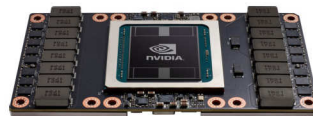
CPU vs. GPU

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++)  
        y[i] = a * x[i] + y[i];  
}
```

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

```
saxpy(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



Libraries

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

Use applications & libraries



cuBLAS



cuSPARSE



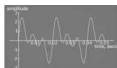
cuDNN



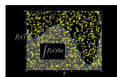
{A} ARRAYFIRE



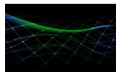
Numba



cuFFT



cuRAND



CUDA Math

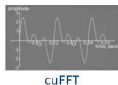


theano

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);
```

```
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

```
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);
```

```
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);
```

```
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);
```

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

Programming GPUs

OpenACC/OpenMP

GPU Programming with Directives

Keepin' you portable

- Annotate serial source code by directives

```
#pragma acc loop
```

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

GPU Programming with Directives

Keepin' you portable

- Annotate serial source code by directives

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

- **OpenACC**: Especially for GPUs; **OpenMP**: Has GPU support
- Compiler interprets directives, creates according instructions



GPU Programming with Directives

Keepin' you portable

- Annotate serial source code by directives

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

- **OpenACC**: Especially for GPUs; **OpenMP**: Has GPU support
- 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

- Compiler support only raising
- 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);
```

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];  
}
```

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

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



Programming GPUs

CUDA C/C++

Programming GPU Directly

Finally...

- Two solutions:

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



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)
`c\lang` has CUDA support, but CUDA needed for last step
- Also: CUDA Fortran

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**



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's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Thread




CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads



CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block



CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Block



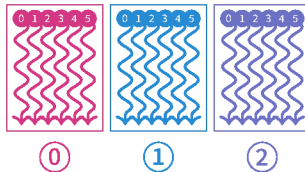
CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks



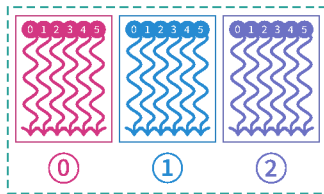
CUDA's Parallel Model

In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks → Grid



CUDA's Parallel Model

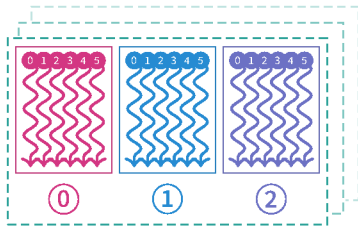
In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks → Grid

- Threads & blocks in 3D



CUDA's Parallel Model

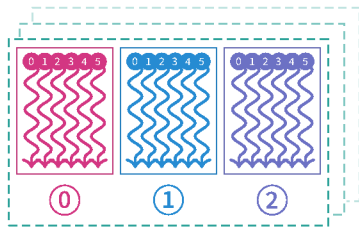
In software: Threads, Blocks

- Methods to exploit parallelism:

- Threads → Block

- Blocks → Grid

- Threads & blocks in 3D



- Parallel function: **kernel**

- `__global__ kernel(int a, float * b) { }`

- Access own ID by global variables `threadIdx.x`, `blockIdx.y`, ...

- Execution entity: **threads**

- Lightweight → fast switching!

- 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)  
        y[i] = a * x[i] + y[i];  
}
```

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y  
cudaMallocManaged(&x, n * sizeof(float));  
cudaMallocManaged(&y, n * sizeof(float));
```

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

```
cudaDeviceSynchronize();
```



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

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y  
cudaMallocManaged(&x, n * sizeof(float));  
cudaMallocManaged(&y, n * sizeof(float));  
  
saxpy_cuda<<<2, 5>>>(n, a, x, y);  
  
cudaDeviceSynchronize();
```

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

```
int a = 42;  
int n = 10;  
float x[n], y[n];  
// fill x, y  
cudaMallocManaged(&x, n * sizeof(float));  
cudaMallocManaged(&y, n * sizeof(float));  
  
saxpy_cuda<<<2, 5>>>(n, a, x, y);  
  
cudaDeviceSynchronize();
```


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

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));
```

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

```
cudaDeviceSynchronize();
```

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);
```

```
cudaDeviceSynchronize();
```

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

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.

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.

nvprof

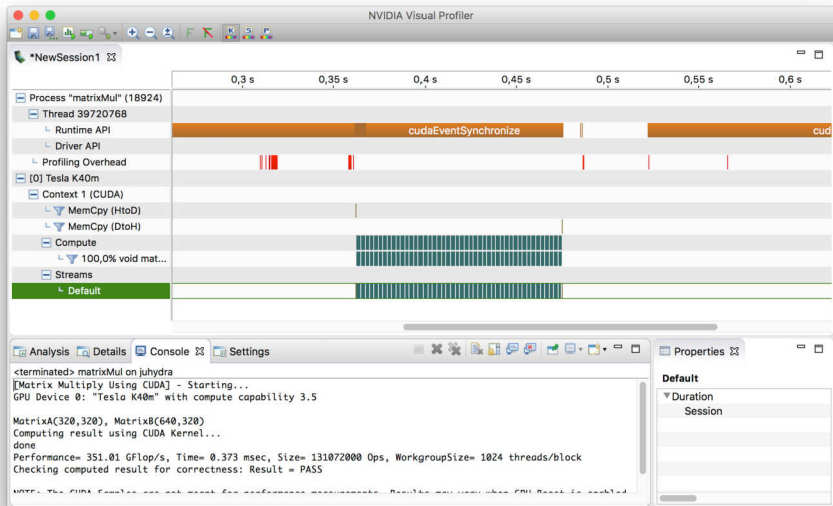
Command that line

```
$ 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
0.15%	612.20us	1505	406ns	361ns	1.1970us	cudaSetupArgument
0.12%	499.01us	3	166.34us	140.45us	216.16us	cudaFree

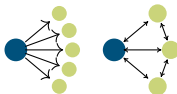
Visual Profiler



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
- Libraries, Abstractions: [Kokkos](#), [Alpaka](#), [Futhark](#), [HIP](#), [C++AMP](#), ...
- Use multiple GPUs
 - On one node
 - Across many nodes → MPI
- ...
- Some of that: Addressed at **dedicated training courses**



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!

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

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 in Jülich; [contact me!](#)

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 in Jülich; [contact me!](#)
- Interested in JURON? [Get access!](#)

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 in Jülich
- Interested in JURON? [Get access!](#)

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

APPENDIX

Appendix

Glossary

References

Glossary I

API A programmatic interface to software by well-defined functions. Short for application programming interface. [72](#), [73](#), [74](#), [75](#), [76](#)

CUDA Computing platform for [GPUs](#) from NVIDIA. Provides, among others, CUDA C/C++. [2](#), [71](#), [72](#), [73](#), [74](#), [75](#), [76](#), [77](#), [78](#), [79](#), [80](#), [81](#), [82](#), [83](#), [84](#), [85](#), [86](#), [87](#), [88](#), [89](#), [90](#), [91](#), [92](#), [100](#), [103](#), [104](#), [105](#), [106](#), [107](#), [111](#)

JSC Jülich Supercomputing Centre, the supercomputing institute of Forschungszentrum Jülich, Germany. [2](#), [103](#), [104](#), [105](#), [106](#), [107](#), [110](#)

JURECA A multi-purpose supercomputer with 1800 nodes at JSC. [2](#), [5](#), [99](#), [101](#)

JURON One of the two HBP pilot system in Jülich; name derived from Juelich and Neuron. [6](#), [7](#)

JUWELS Jülich's new supercomputer, the successor of JUQUEEN. [2](#), [3](#), [4](#), [99](#), [101](#)

Glossary II

MPI The Message Passing Interface, a API definition for multi-node computing. 98, 100

NVIDIA US technology company creating GPUs. 3, 4, 5, 6, 7, 72, 73, 74, 75, 76, 94, 95, 103, 104, 105, 106, 107, 110, 111, 112, 113

NVLink NVIDIA's communication protocol connecting CPU ↔ GPU and GPU ↔ GPU with high bandwidth. 6, 7, 112

OpenACC Directive-based programming, primarily for many-core machines. 2, 65, 66, 67, 68, 69, 70, 100, 103, 104, 105, 106, 107

OpenCL The *Open Computing Language*. Framework for writing code for heterogeneous architectures (CPU, GPU, DSP, FPGA). The alternative to CUDA. 72, 73, 74, 75, 76, 94, 95

Glossary III

OpenMP Directive-based programming, primarily for multi-threaded machines. 2, 65, 66, 67, 68

P100 A large GPU with the Pascal architecture from NVIDIA. It employs NVLink as its interconnect and has fast HBM2 memory. 6, 7

Pascal GPU architecture from NVIDIA (announced 2016). 112

POWER CPU architecture from IBM, earlier: PowerPC. See also POWER8. 112

POWER8 Version 8 of IBM's POWERprocessor, available also under the OpenPOWER Foundation. 6, 7, 112

SAXPY Single-precision $A \times X + Y$. A simple code example of scaling a vector and adding an offset. 50, 86, 87, 88, 89, 90, 91, 92

Glossary IV

Tesla The GPU product line for general purpose computing computing of NVIDIA. 3, 4, 5, 6, 7

CPU Central Processing Unit. 3, 4, 5, 6, 7, 12, 13, 14, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 50, 72, 73, 74, 75, 76, 111, 112

GPU Graphics Processing Unit. 2, 3, 4, 5, 6, 7, 8, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 33, 34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 49, 51, 52, 53, 54, 55, 56, 57, 65, 66, 67, 68, 71, 72, 73, 74, 75, 76, 90, 91, 92, 93, 94, 95, 98, 99, 101, 102, 103, 104, 105, 106, 107, 110, 111, 112, 113

HBP Human Brain Project. 110

SIMD Single Instruction, Multiple Data. 35, 36, 37, 38, 39, 40, 41, 42, 43, 44

Glossary V

SIMT Single Instruction, Multiple Threads. [15](#), [16](#), [17](#), [30](#), [31](#), [33](#), [34](#), [35](#), [36](#), [37](#), [38](#), [39](#), [40](#), [41](#), [42](#), [43](#), [44](#)

SM Streaming Multiprocessor. [35](#), [36](#), [37](#), [38](#), [39](#), [40](#), [41](#), [42](#), [43](#), [44](#)

SMT Simultaneous Multithreading. [35](#), [36](#), [37](#), [38](#), [39](#), [40](#), [41](#), [42](#), [43](#), [44](#)

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 10, 11).
- [6] Wes Breazell. *Picture: Wizard*. URL: <https://thenounproject.com/wes13/collection/its-a-wizards-world/> (pages 52–56).

References: Images, Graphics I

- [1] Alexandre Debiève. *Bowels of computer*. Freely available at Unsplash. URL: <https://unsplash.com/photos/F07JIlwj0tU>.
- [3] Mark Lee. *Picture: kawasaki ninja*. URL: <https://www.flickr.com/photos/pochacco20/39030210/>. License: Creative Commons BY-ND 2.0 (pages 12, 13).
- [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 (pages 12, 13).
- [5] Nvidia Corporation. *Pictures: Volta GPU*. Volta Architecture Whitepaper. URL: <https://images.nvidia.com/content/volta-architecture/pdf/Volta-Architecture-Whitepaper-v1.0.pdf> (pages 42–44).