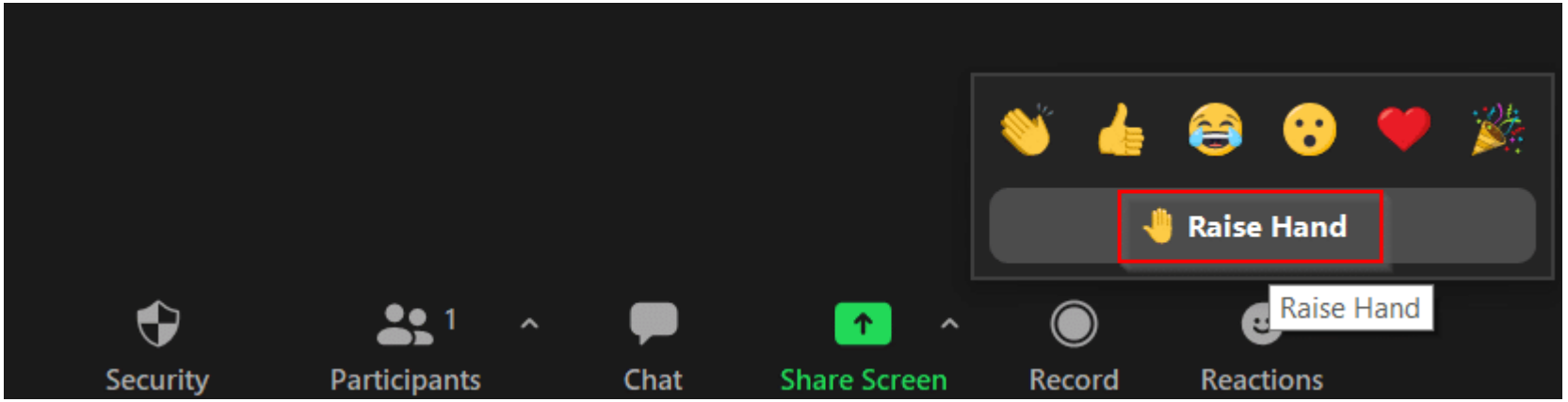
Intro to High-Performance Computing with GPUs

CERN openlab Summer Student Programme 2021

Ahmad Hesam

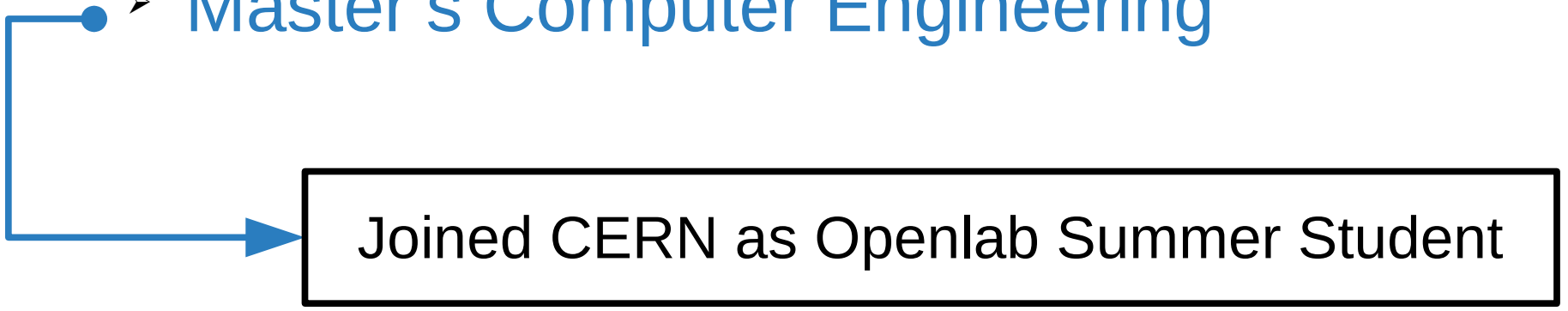
19/07/2021

Questions during the lecture?



About Me

- Bachelor's Applied Physics
- Master's Computer Engineering

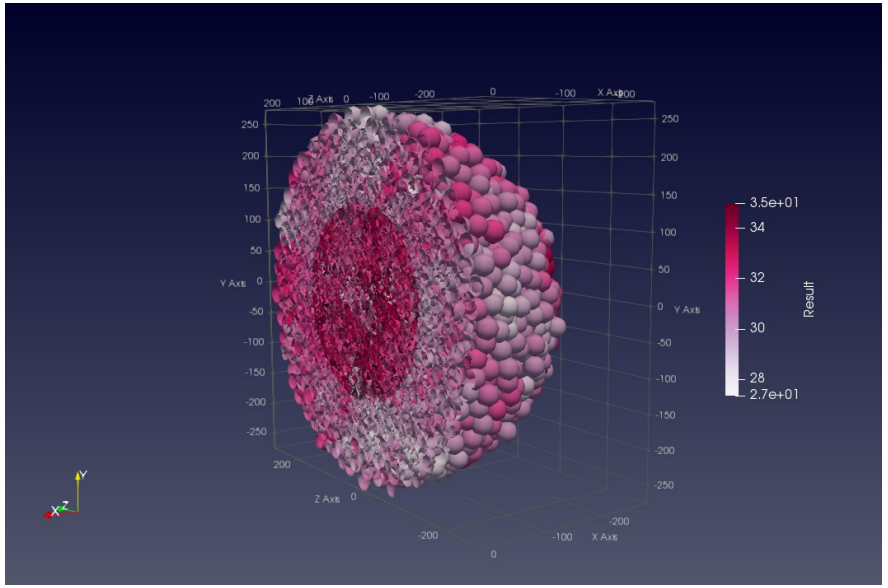


- Research Fellow (currently)

Openlab Summer Programme 2016

Summer Student Project

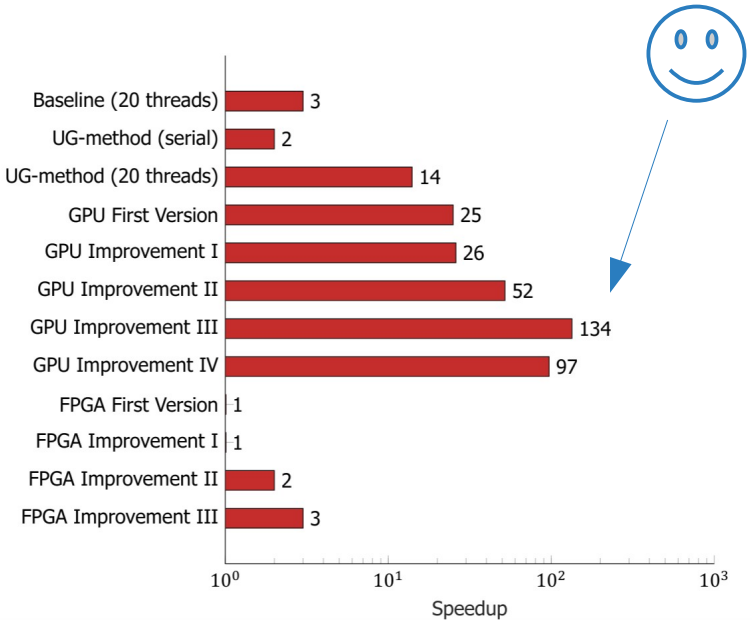
- Agent-based simulation platform (BioDynaMo)
- Integrated ROOT I/O for back-up & restore



Lightning talk winner :-D

Technical Studentship → Fellow

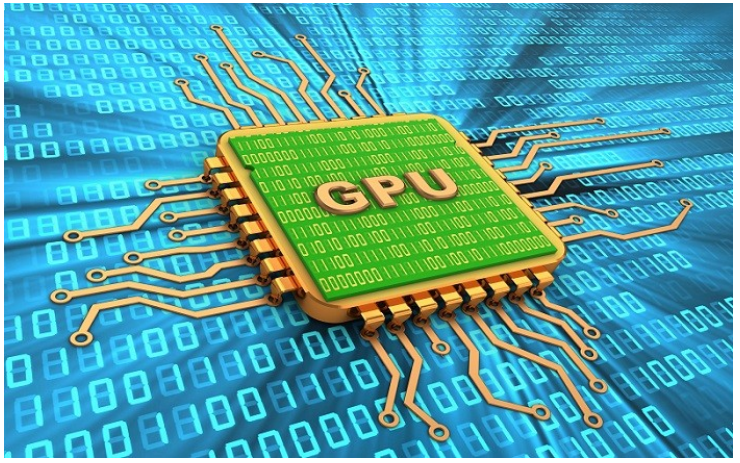
- Continued on the same project as a Technical Student
  - Implemented visualization
  - More ROOT
  - **Mainly: GPU & FPGA acceleration**
- Continued as a Fellow
  - Even more ROOT
  - (**Heterogeneous**) distributed runtime



– More on BioDynaMo coming Friday! –

Today's Talk

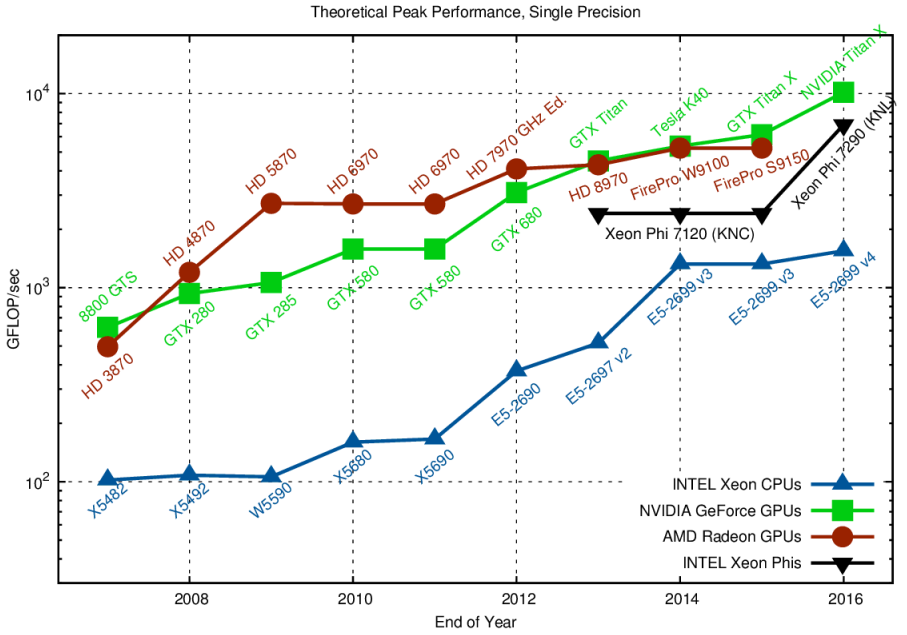
- What are GPUs?
- Why do we need them (at CERN)?
- How do we program them?
- **Hands-on session**



https://www.hpcwire.com/2018/03/27/nvidia-riding-high-as-gpu-workloads-and-capabilities-soar/

What are GPUs?

- **G**raphics **P**rocessing **U**nits
- Name from the ‘old days’ when only used for graphics processing
- Increasingly more powerful
  - → **General-purpose** use cases were coming up
- Offloading computational intensive workloads to GPUs



https://www.karlrupp.net/2013/06/cpu-gpu-and-mic-hardware-characteristics-over-time/

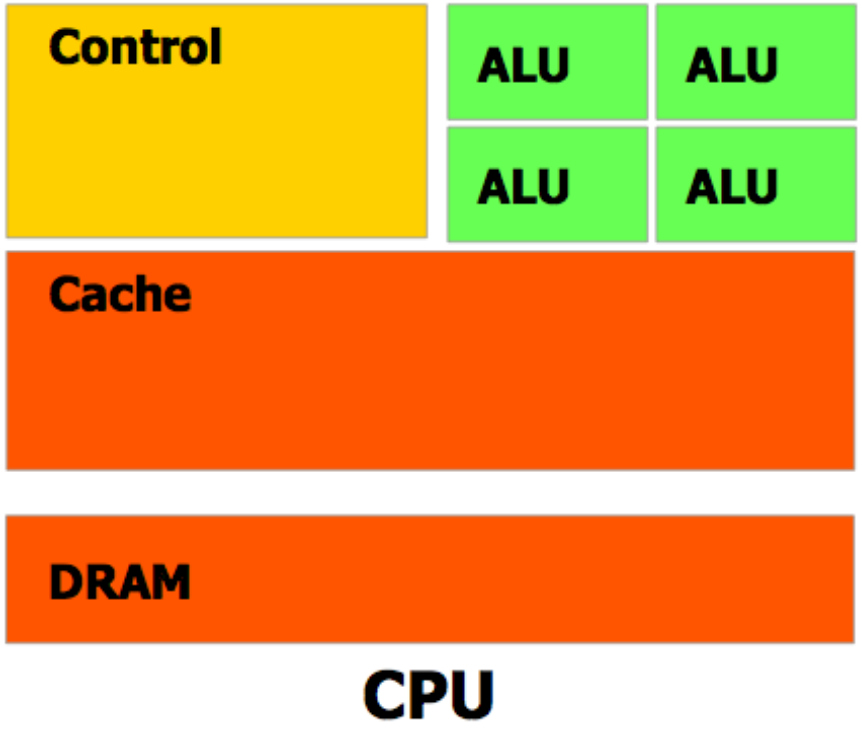
How do GPUs compare against CPUs?

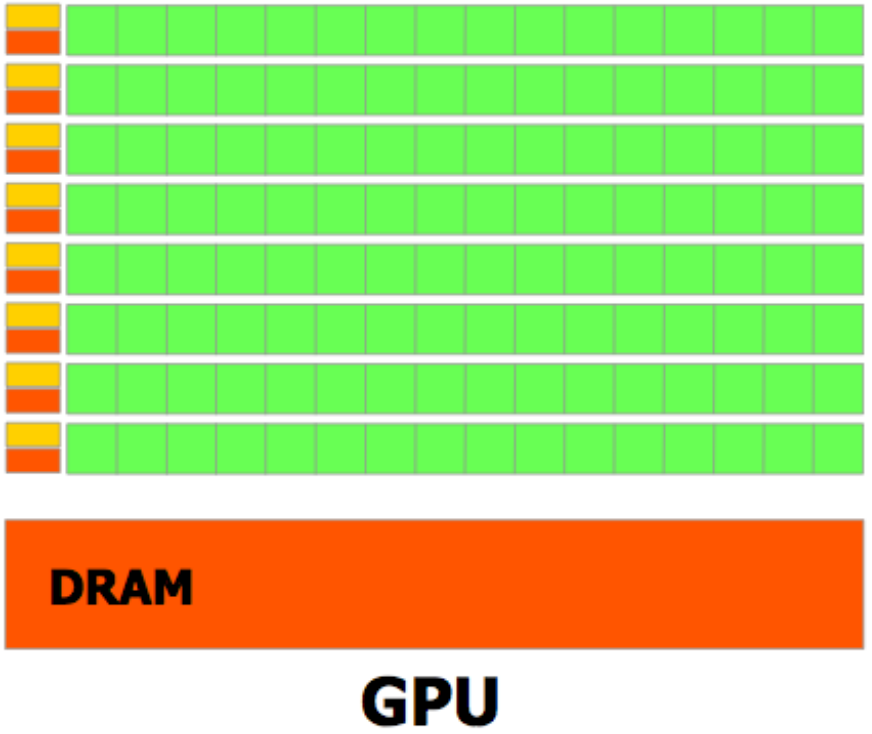
GPU vs CPU

A short, but convincing, demonstration...

https://www.youtube.com/watch?v=-P28LKWTzrI

GPU vs CPU





- Out of order execution
- Few fast cores (~3 GHz)

- In order execution
- Many slower cores (~1 GHz)

For certain workloads, GPUs can outperform a small CPU-only cluster!

GPU vs CPU: Deep Learning

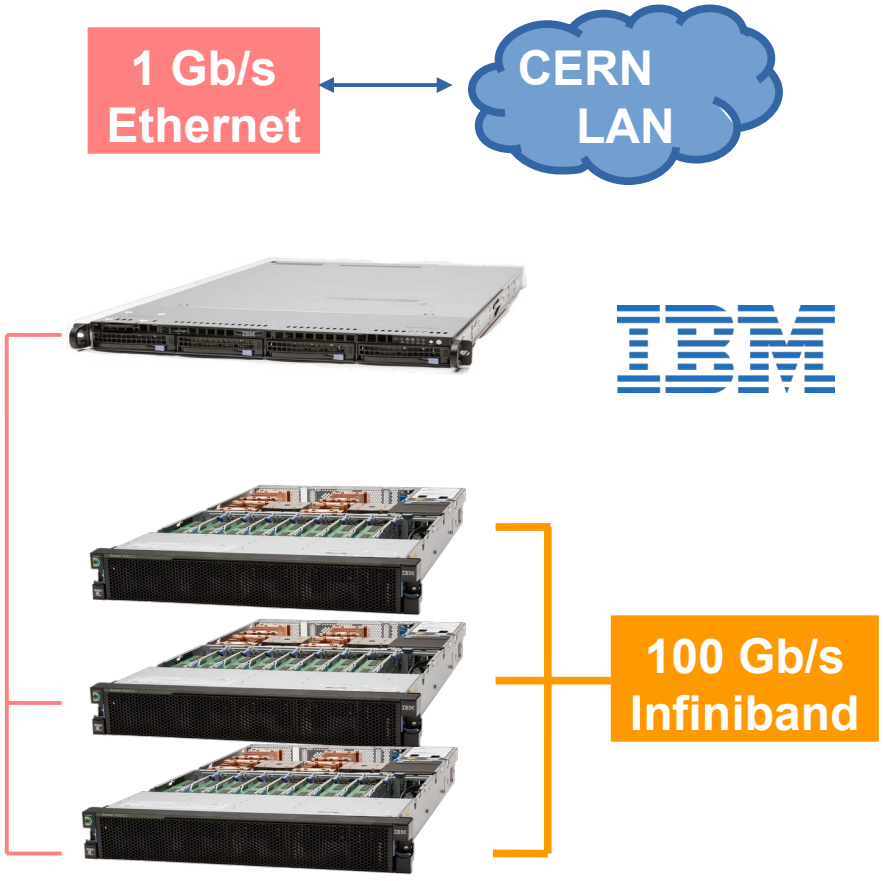
1x IBM SC821LC (login node)

- 1x POWER8 socket (=8 cores)
- 64 GB DDR4

3x IBM SC822LC (worker nodes)

- 2x POWER8 sockets (=16 cores)
- **4x NVIDIA P100 GPUs**
- CPU ↔ GPU NVLink
- 256GB DDR4

Delivered roughly the same performance as a 256-CPU cluster!
+
~10X more energy-efficient



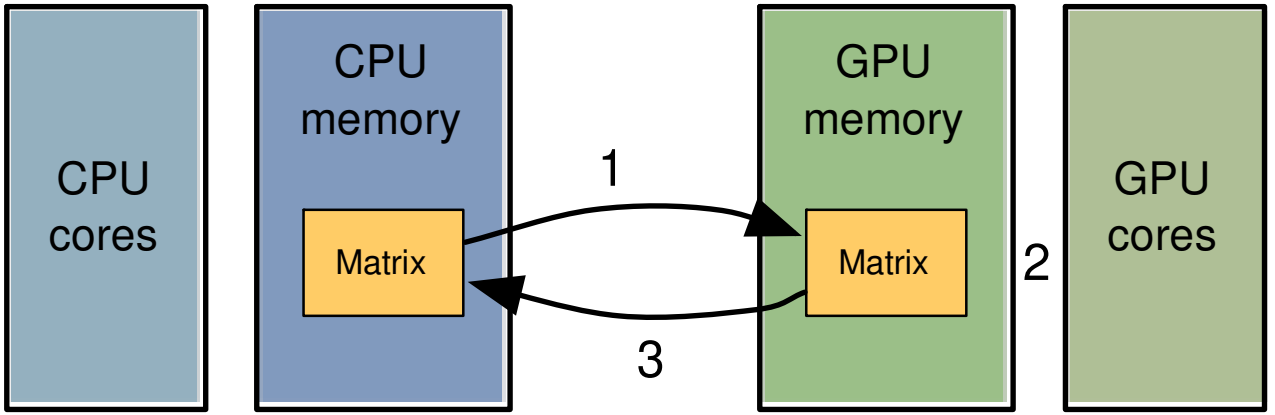
Use case: distributed training in deep learning

GPU Computing Basics

Computation is offloaded to the GPU in three steps:

1. CPU → GPU data transfer
2. GPU kernel execution
3. GPU → CPU data transfer

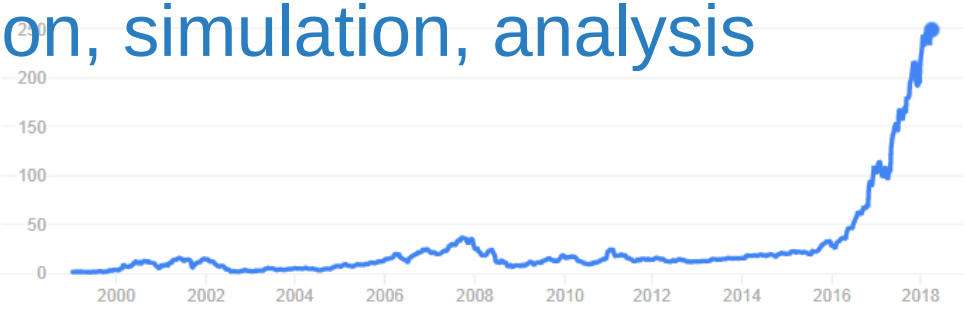
- Overhead
- Potential bottleneck
  - Why?



Credits: https://safari.ethz.ch/architecture/fall2017/lib/exe/fetch.php?media=onur-comparch-fall2017-lecture14-afterlecture.pdf

Why do we need GPUs?

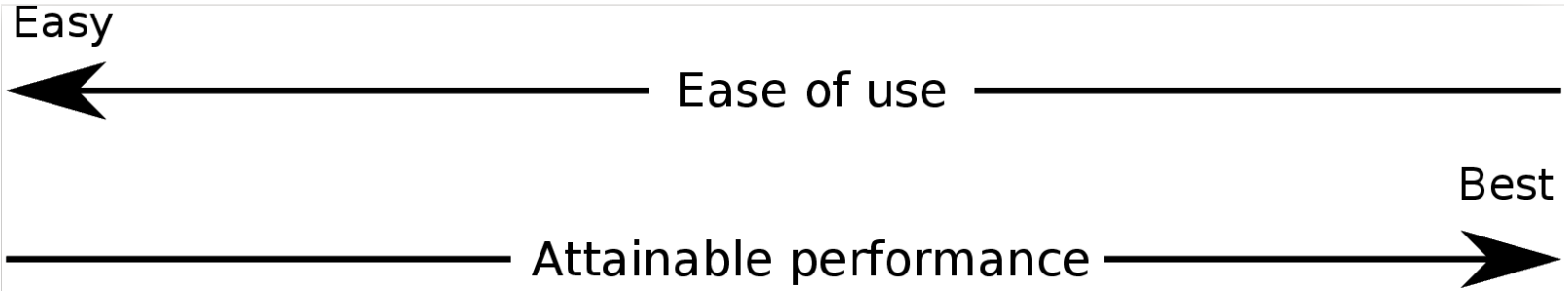
- Reaching physics limits for CPUs
  - Multi-core era started nearly 2 decades ago
- Massively many-core era is the now (stock prices don't lie)
- Heterogeneous computing
- At CERN
  - Trigger, reconstruction, simulation, analysis
  - High Lumi



Nvidia's stock price has risen 1,900% over the past 5 years (data from 2018)

https://www.hpcwire.com/2018/03/27/nvidia-riding-high-as-gpu-workloads-and-capabilities-soar/

How do we program GPUs?



Libraries	**Compiler directives**	**Low-level APIs**
• NVIDA Libraries • cuBlas, cuSolver, etc • ESSL / PESSL	• OpenACC • OpenMP	• CUDA • OpenCL
+ Easy to implement + Well-tested and community support - Limited functionality	+ Modification of existing programs with directives - Requires knowledge on data structures	+ Achieves highest performance results - Most time intensive - Requires expertise

SAXPY

Single-Precision A*X Plus Y

$$z = ax + y$$

x,y,z: vector
a : scalar

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

// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
```

Regular C implementation of saxpy

https://devblogs.nvidia.com/six-ways-saxpy/

Using Libraries

Many popular frameworks with a GPU back-end rely on CUDA libraries:

- Deep Learning: Tensorflow, Keras, PyTorch
- Molecular Dynamics: NAMD, LAMMPS
- General Scientific Libraries: MATLAB, R

```
int N = 1<<20;
cublasInit();
cublasSetVector(N, sizeof(x[0]), x, 1, d_x, 1);
cublasSetVector(N, sizeof(y[0]), y, 1, d_y, 1);

// Perform SAXPY on 1M elements
cublasSaxpy(N, 2.0, d_x, 1, d_y, 1);

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

Saxpy with CUBLAS library

https://devblogs.nvidia.com/six-ways-saxpy/

Using Compiler Directives

Goal: insert directives into existing code base, without changing the code

+ Very simple in use
- Increasingly more difficult to use in more complex (or messier) codebases

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

...
// Perform SAXPY on 1M elements
saxpy(1<<20, 2.0, x, y);
```

Saxpy with OpenACC

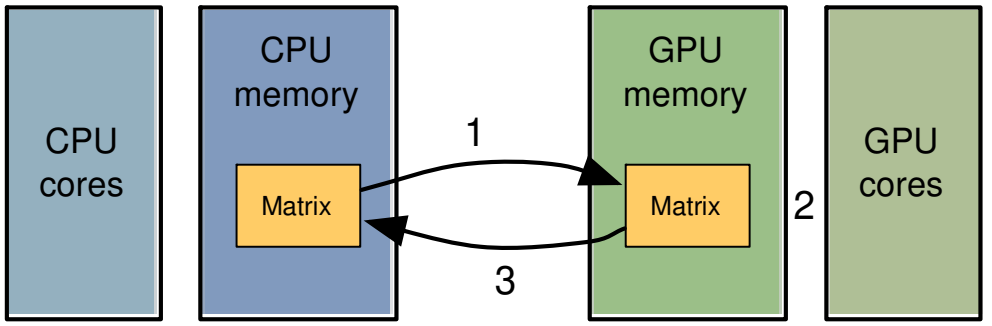
https://devblogs.nvidia.com/six-ways-saxpy/

Using Low-Level APIs

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

...
int N = 1<<20;
cudaMemcpy(d_x, x, N, cudaMemcpyHostToDevice);
cudaMemcpy(d_y, y, N, cudaMemcpyHostToDevice);

// Perform SAXPY on 1M elements
saxpy<<<4096,256>>>(N, 2.0, d_x, d_y);

cudaMemcpy(y, d_y, N, cudaMemcpyDeviceToHost);
```

Saxpy with CUDA

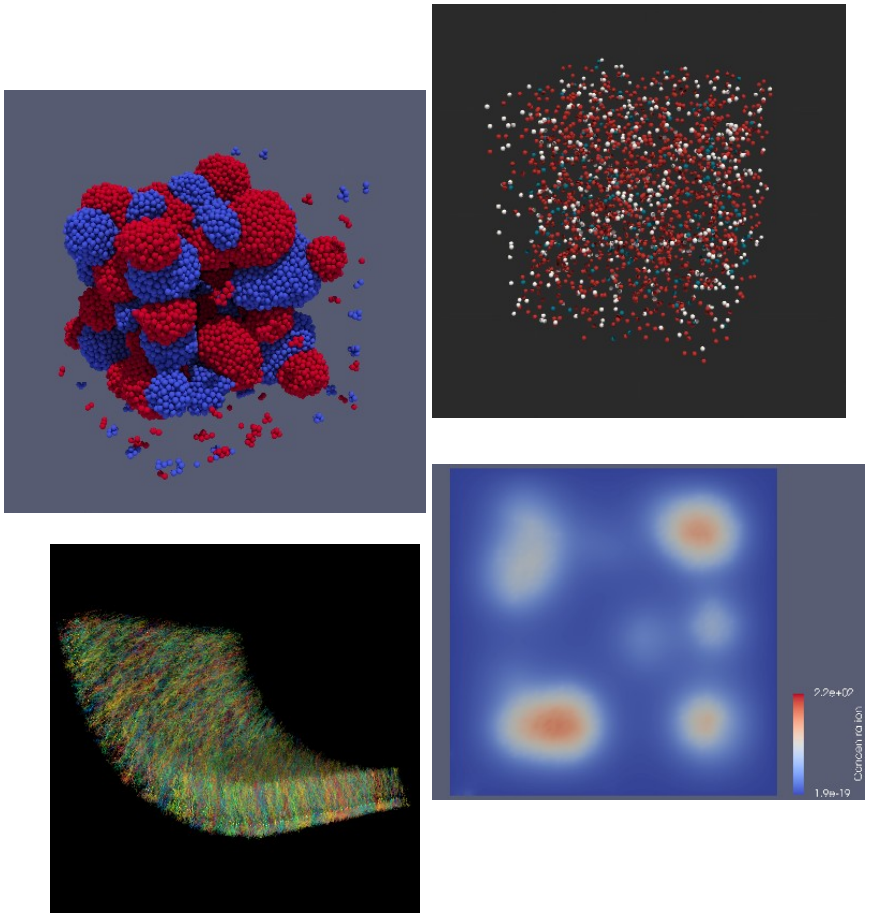
- Steepest learning curve of all methods
- Often most rewarding



https://devblogs.nvidia.com/six-ways-saxpy/

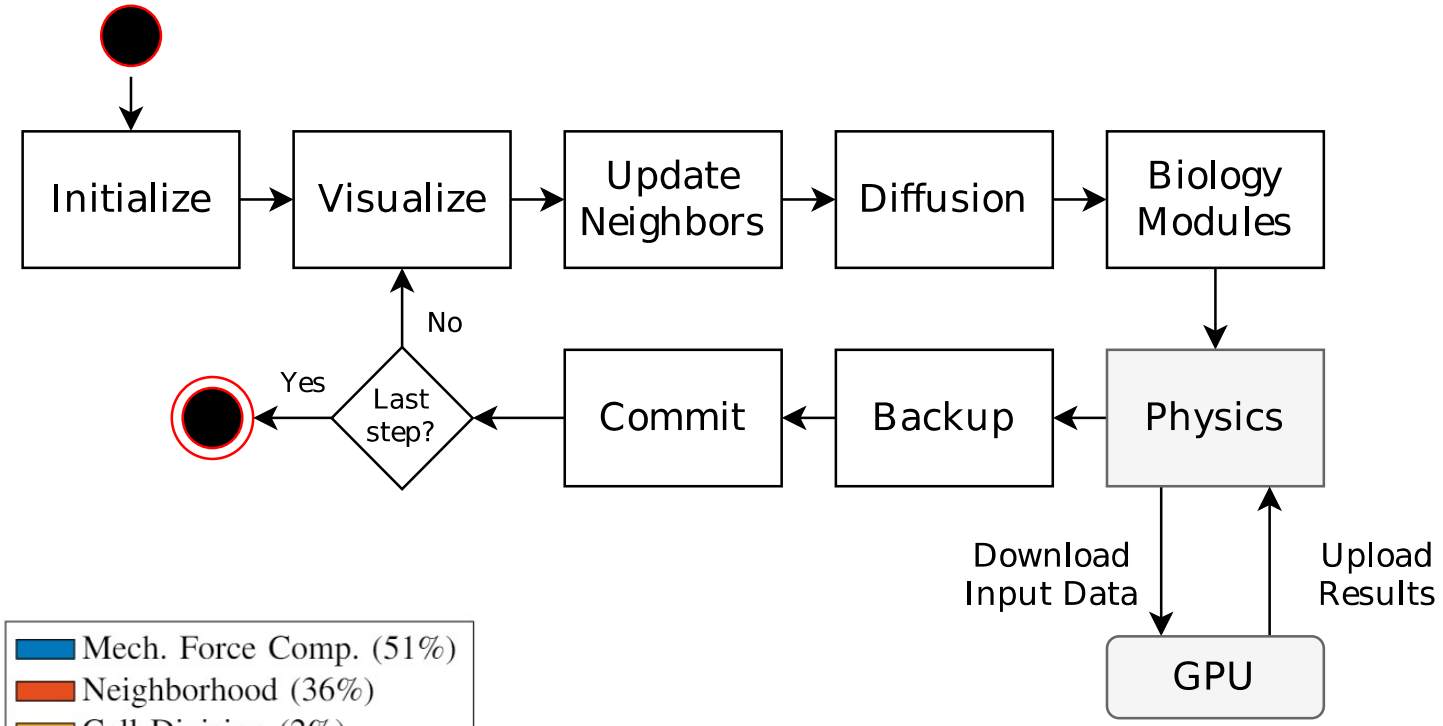
BioDynaMo

- High-performance open-source ABS platform
- Written in C++
- Multi-threading with OpenMP
- Modular architecture
- Collaboration project at CERN
- https://biodynamo.org

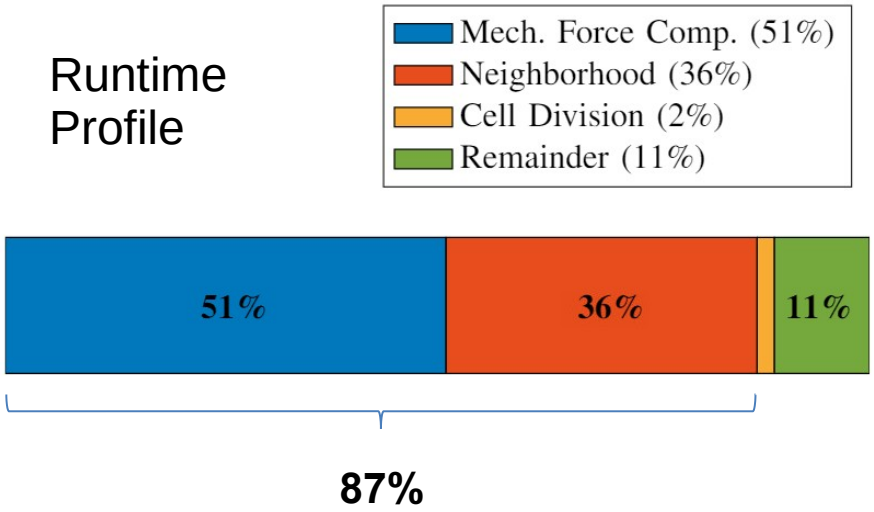


https://doi.org/10.1101/2020.06.08.139949

Accelerating BioDynaMo with GPUs



Runtime Profile



- CUDA
- OpenCL

Accelerating BioDynaMo with GPUs

GPU: Nvidia GTX1080 Ti

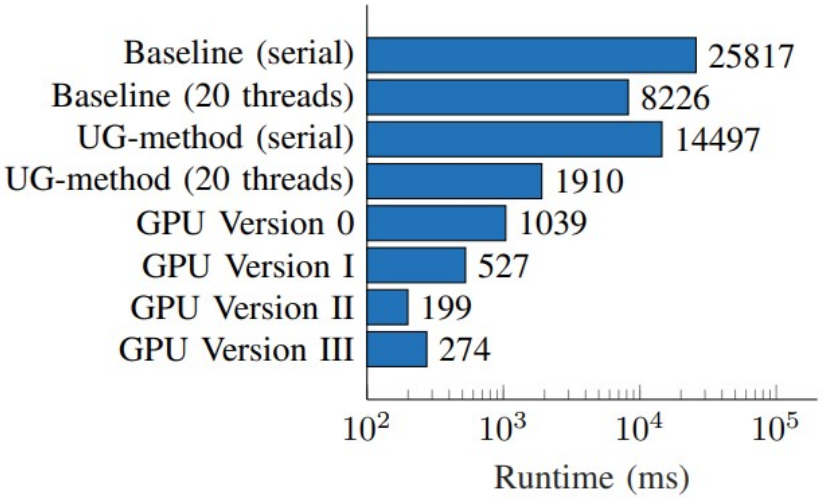


Fig. 8: The runtime for various implementations of the mechanical interaction operation running benchmark A. The GPU results are obtained from the CUDA runtime on system A.

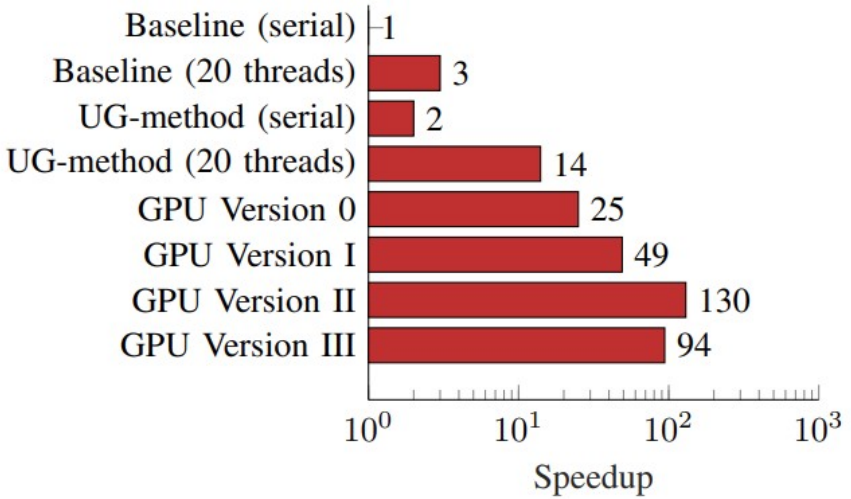
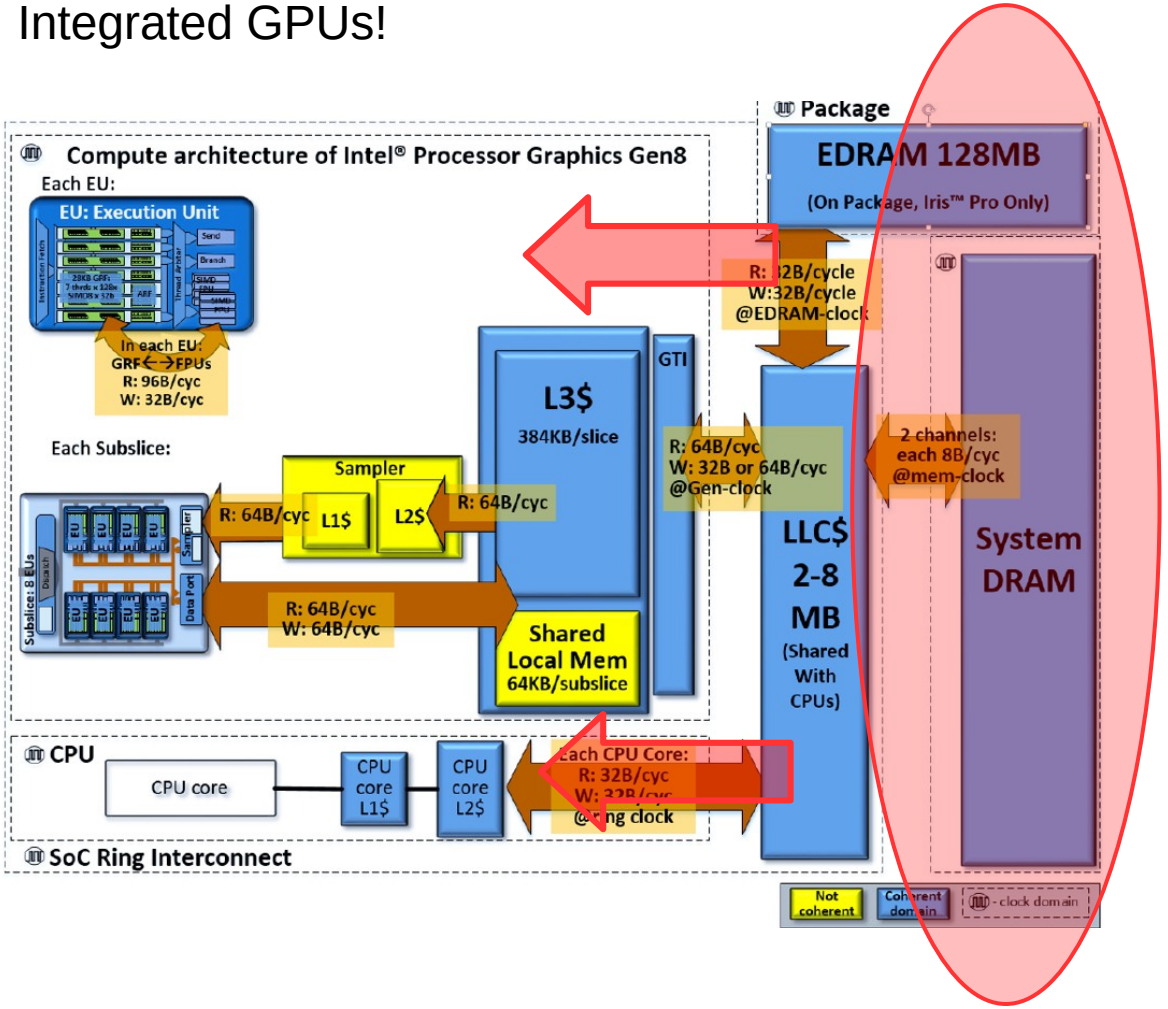


Fig. 9: The speedup with respect to the serial baseline version as obtained with benchmark A. The GPU results are obtained from the CUDA runtime on system A.

Intel Integrated GPU

Intel Graphics Technology (GT) : Integrated GPUs!

- CPU and GPU on same die
- Share same DRAM
- Often less powerful than dedicated GPUs
- Supports OpenCL for programming the GPU

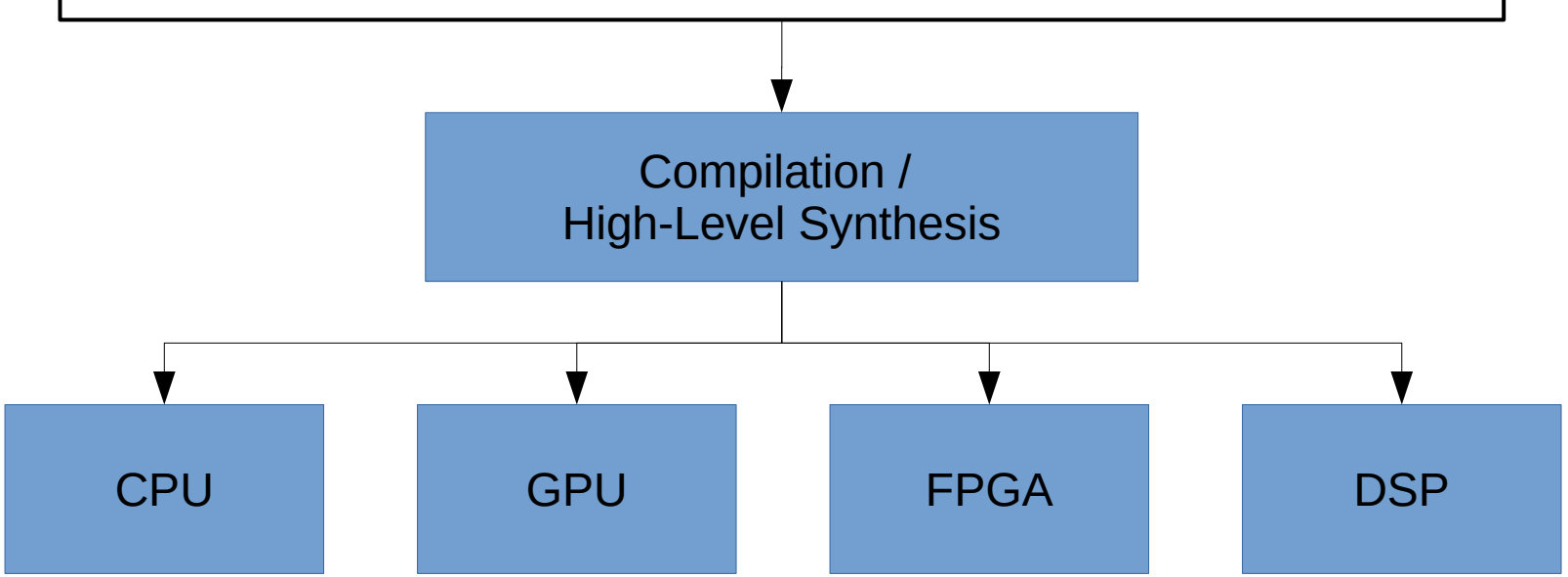


https://software.intel.com/en-us/forums/opencl/topic/541290

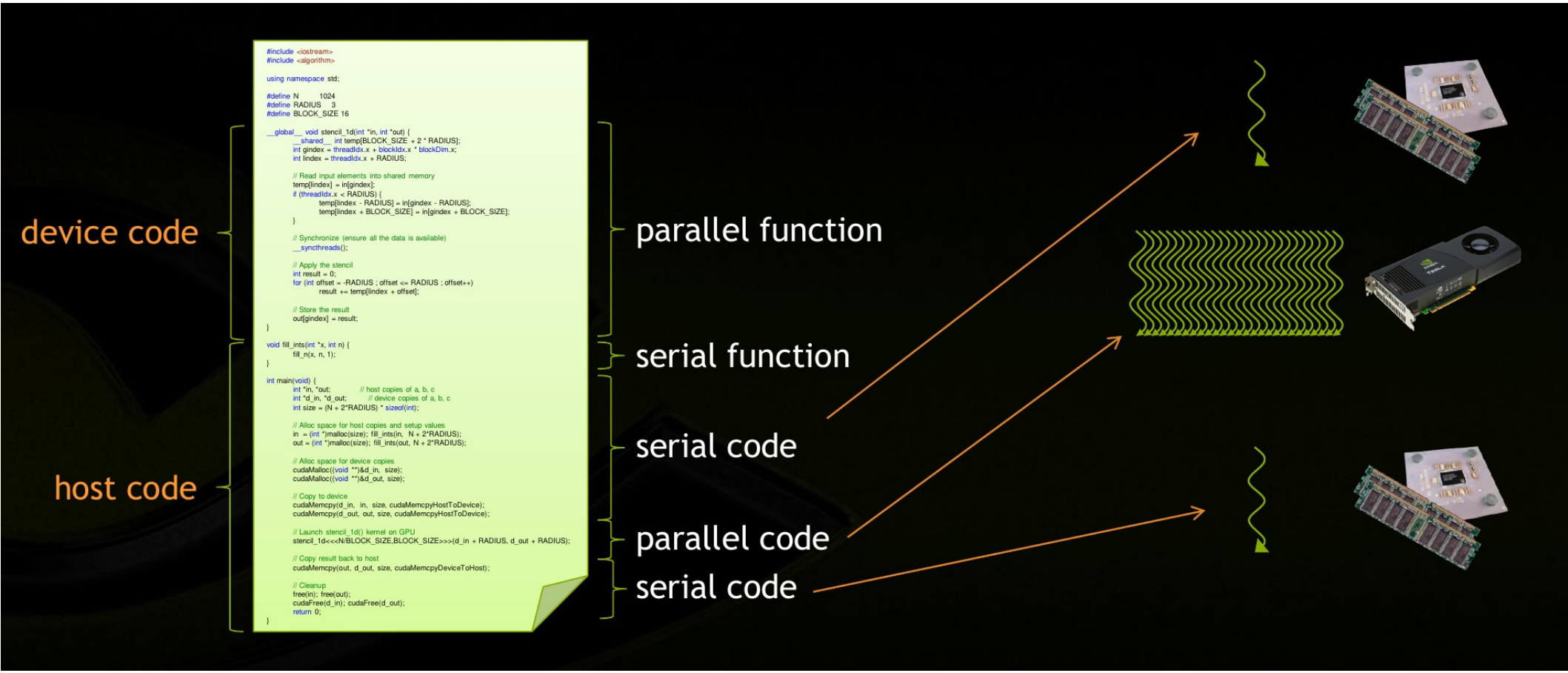
OpenCL: Open Computing Language

- Framework to program on heterogeneous platform (CPU, GPU, DSP, FPGA…)

```
__kernel void saxpy(float a, __global float* X,
                    __global float* Y) {
    const int i = get_global_id(0);
    Y[i] += a * X[i];
}
```



OpenCL: Open Computing Language



Source: https://www.nvidia.com/docs/IO/116711/sc11-cuda-c-basics.pdf

If you look closely this is CUDA, but it's conceptually the same as OpenCL

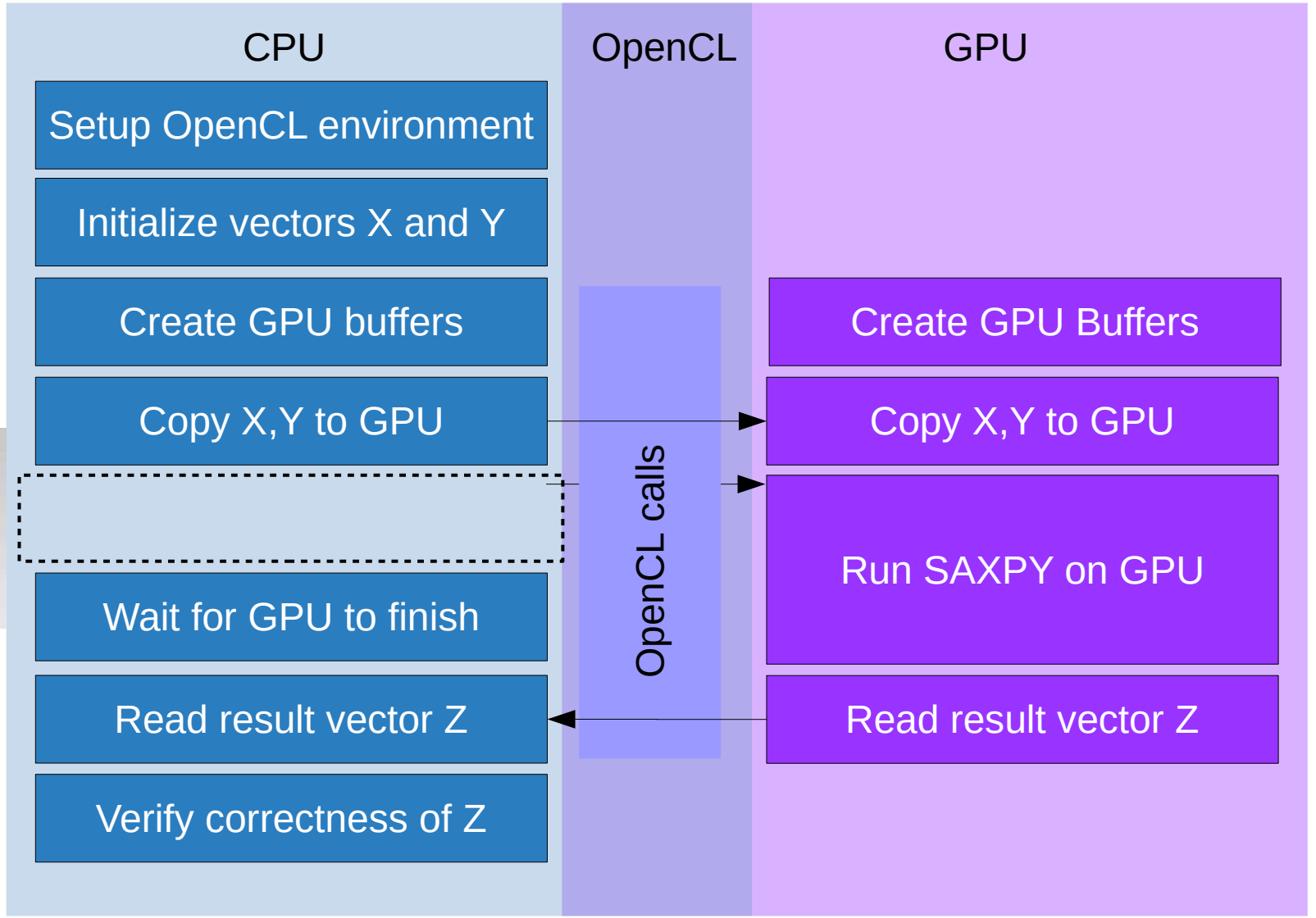
Saxpy on GPU

...with OpenCL

$z = ax + y$

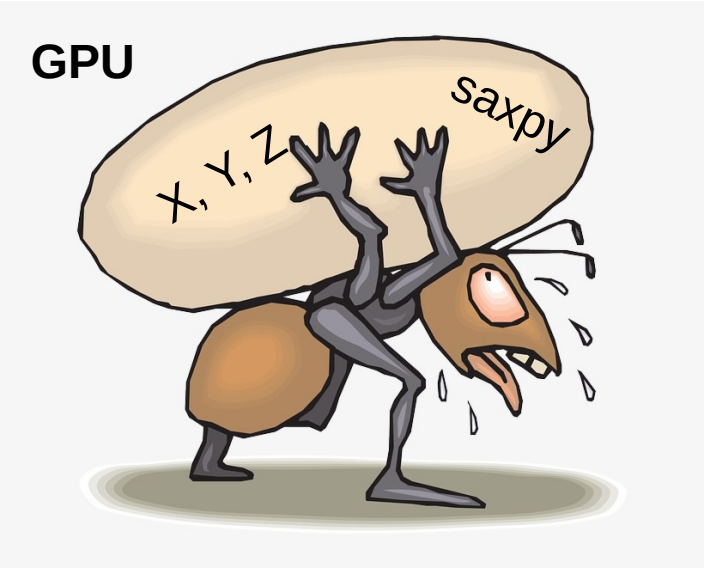
x,y,z: vector
a : scalar

How to capitalize on that?



How to improve?


```
__kernel void saxpy(float a, __global float* X,
                    __global float* Y) {
    const int i = get_global_id(0);
    Y[i] += a * X[i];
}
```



On My Machine

```
ahmad@ahmad:~/saxpy-benchmark/src$ ./saxpy_ocl1
Platform "Intel(R) OpenCL". Devices:
 - [gpu ] Intel(R) Corporation: Intel(R) HD Graphics
   (Max compute units: 23, max work group size: 256)
 - [cpu ] Intel(R) Corporation: Intel(R) Core(TM) i7-7
   (Max compute units: 4, max work group size: 8192)

Using Intel(R) Corporation Intel(R) HD Graphics
GPU execution time is: 61.759 ms
Errors: 0
```

```
ahmad@ahmad:~/saxpy-benchmark/src$ ./saxpy_cpu
N: 67108864
CPU execution time = 57.8496 ms
Errors: 0
```

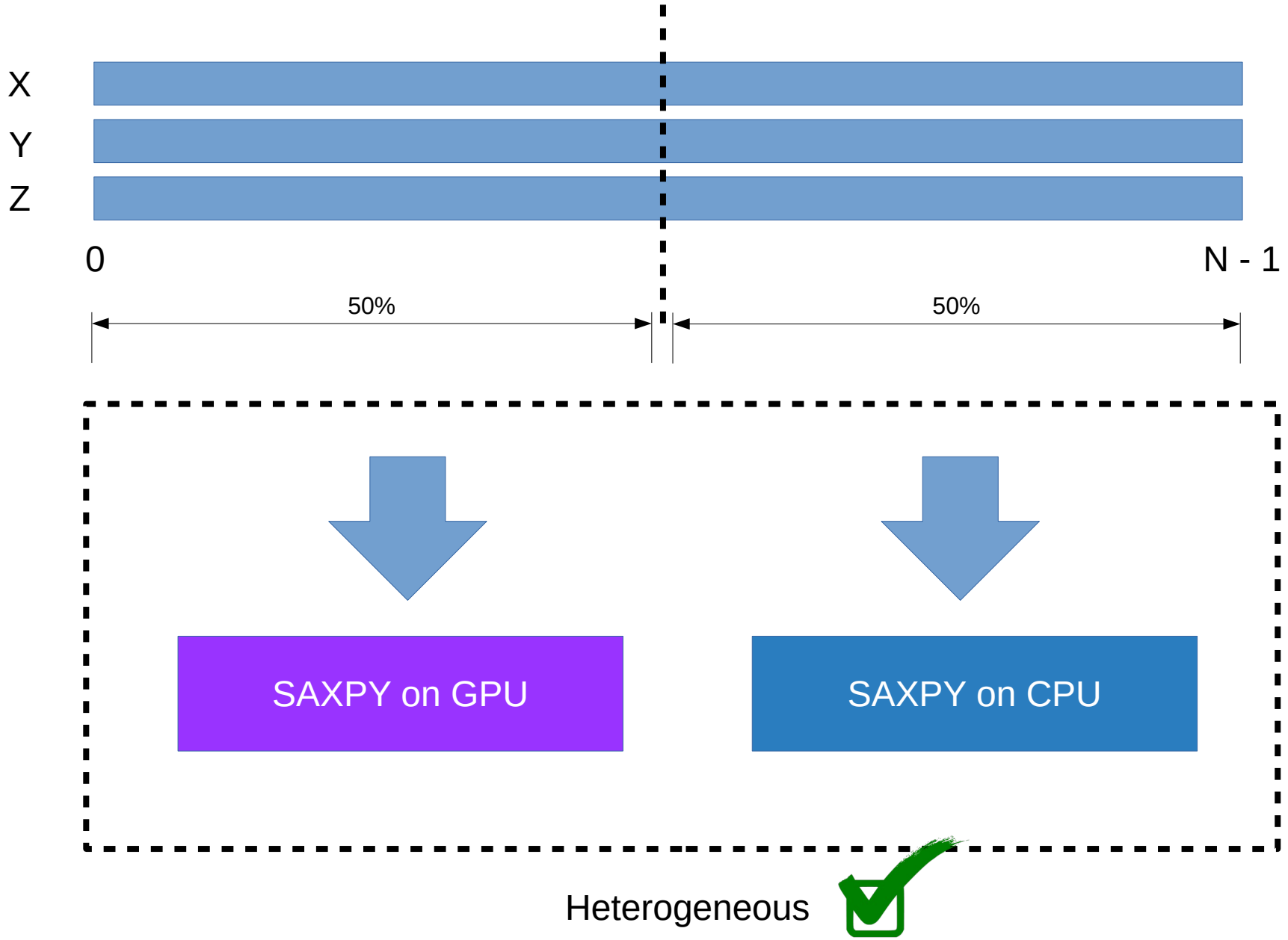
On my machine GPU is about as fast as my CPU for saxpy

On Another Machine

```
ahhesam@tlab-gpu-gtx1080ti-09:~/saxpy-benchmark/src$ ./saxpy_ocl1
Platform "NVIDIA CUDA". Devices:
 - [gpu ] NVIDIA Corporation: GeForce GTX 1080 Ti
   (Max compute units: 28, max work group size: 1024)

Using NVIDIA Corporation GeForce GTX 1080 Ti
GPU execution time = 2.238 ms
Errors: 0
ahhesam@tlab-gpu-gtx1080ti-09:~/saxpy-benchmark/src$ ./saxpy_cpu
N: 67108864
CPU execution time = 56.7027 ms
Errors: 0
```

On another machine the GPU is much faster than the CPU for saxpy

Heterogeneous Execution



I want you to observe:

```
ahmad@ahmad:~/saxpy-benchmark/src$ ./saxpy_ocl1
Platform "Intel(R) OpenCL". Devices:
 - [gpu ] Intel(R) Corporation: Intel(R) HD Graphics
   (Max compute units: 23, max work group size: 256)
 - [cpu ] Intel(R) Corporation: Intel(R) Core(TM) i7-7600U CPU @ 2.80GHz
   (Max compute units: 4, max work group size: 8192)

Using Intel(R) Corporation Intel(R) HD Graphics
GPU execution time = 121.896 ms
Errors: 0
ahmad@ahmad:~/saxpy-benchmark/src$ ./saxpy_ocl1_hg
Platform "Intel(R) OpenCL". Devices:
 - [gpu ] Intel(R) Corporation: Intel(R) HD Graphics
   (Max compute units: 23, max work group size: 256)
 - [cpu ] Intel(R) Corporation: Intel(R) Core(TM) i7-7600U CPU @ 2.80GHz
   (Max compute units: 4, max work group size: 8192)

Using Intel(R) Corporation Intel(R) HD Graphics
CPU execution time = 59.187 ms
GPU execution time = 63.403 ms
Errors: 0
```

GPU-only runtime

heterogeneous runtime

And no, this is not a valid solution:

```
cout << "CPU execution time = 59.187 ms" << endl;
cout << "GPU execution time = 63.403 ms" << endl;
```

Operating System Survey

Quite a spread usage of operating systems

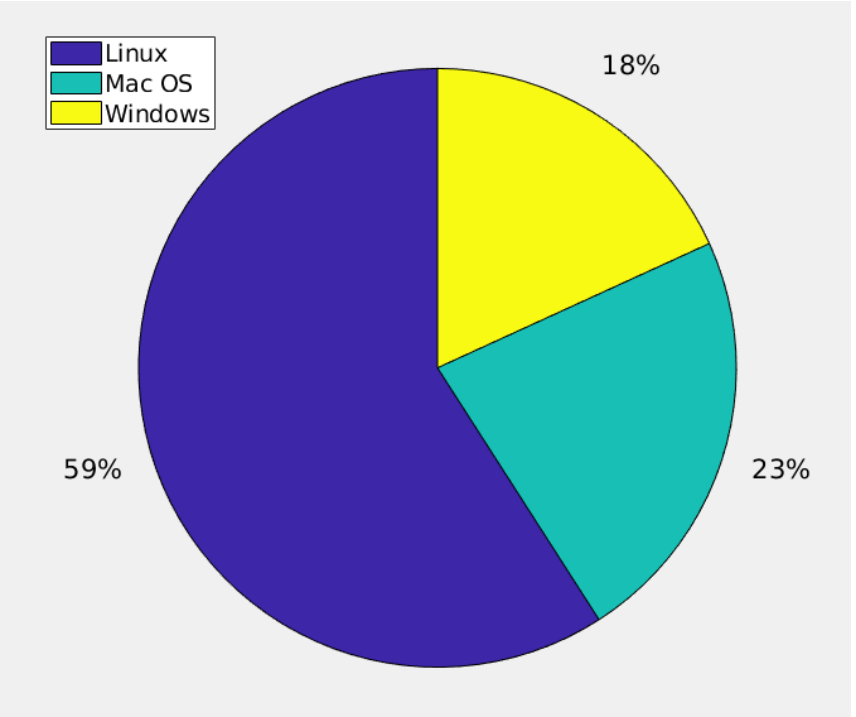
~75% managed to get it to work

Why does the OS even matter?

Mac OS: the only OS that comes with OpenCL pre-installed

Linux: does not come with OCL pre-installed

Windows: - Virtual environment cuts off access to (integrated) GPU
- Upcoming support for native Linux subsystem
- Possible to run natively, but not tested!



OSs of Summer Students 2019

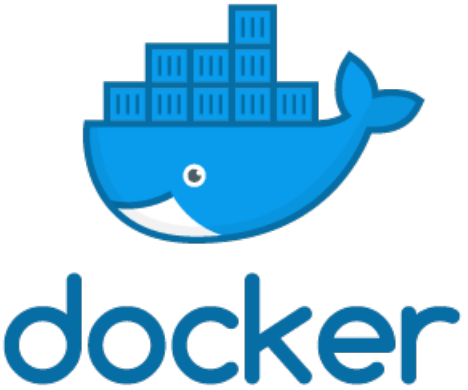
Hands-On Session

Current setup

OS X: run natively

Linux: run in Docker container (useful commands in the course materials!)

Windows: look for someone with Linux / OSX or run natively if you dare...



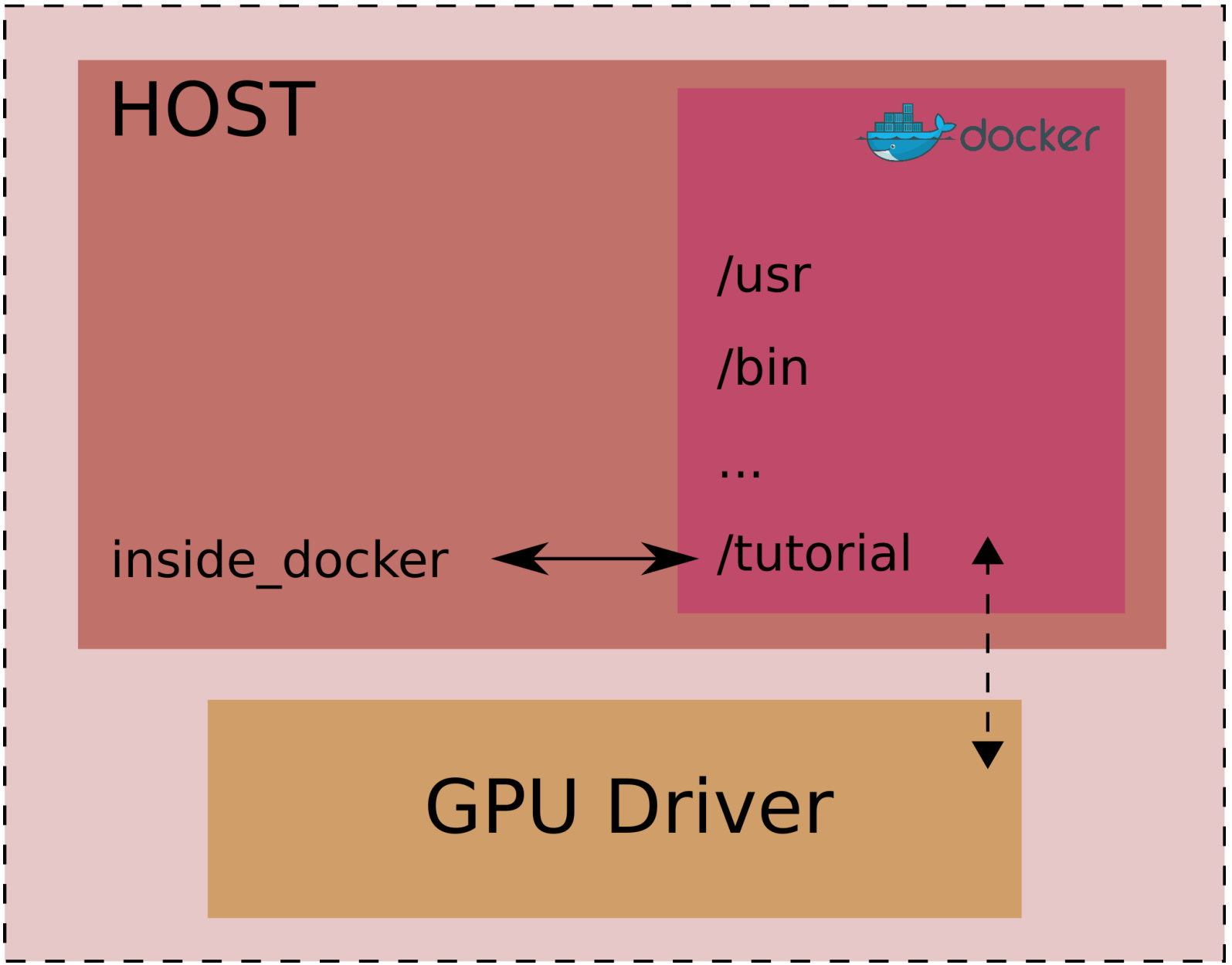
NB: Make sure the source files are up to date!

Linux: docker pull ahesam/intro-gpu
OS X : git pull

Code available at (already in docker container):

https://github.com/Senui/saxpy-benchmark/

(forked repo)


HOST
docker
/usr
/bin
...
inside_docker
/tutorial
GPU Driver

Demo Docker setup

Hands-On Session

Go through the code and understand it by reading the comments:

`saxpy-benchmark/src/saxpy_ocl1_hg.cpp`

`OpenCL API: https://github.khronos.org/OpenCL-CLHPP/`

Exercise: Heterogeneous Runtime
Edit the file such that:

- Half of the computation on GPU
- Other half on CPU
- Add timer for CPU execution (GPU timer already there)
- Error stays 0

Follow-up exercise (if time permits):
Profile the time it takes for data transfers (CPU → GPU, and GPU → CPU),
And compare them against the execution times

Q: Are they what you expect? Why (not)?
Q: How could you effectively ‘hide’ the data transfers?
Q: How would your observations differ with a dedicated GPU?

Useful Commands

- The source files can be found in:

  `saxpy-benchmark/src`

- You will only need to edit: `saxpy_ocl1_hg.cpp`
- To compile your program simply run `make`
- To run your program run:

  `./saxpy_ocl1_hg`

  in the src directory

QUESTIONS?

Problems

- ERROR: clGetPlatformIDs(code: -1001)
  - Most likely because you have an older Intel CPU that is not supported with OpenCL

Is development for Ivy Bridge architecture going to start soon? #128

Closed **ivanmlerner** opened this issue on Feb 9 · 2 comments

ivanmlerner commented on Feb 9

Hello, according to intel's page, this driver stack will substitute both closed source drivers and beignet, when is support for Ivy Bridge going to get in?

bfliflet commented on Feb 9 Contributor

There are no plans that I am aware of to internally back port this library for Gen7 class (ie. Ivybridge and Haswell) hardware. There is a fair amount of runtime work but the bigger effort would be related to the compiler itself which was completely rearchitected in the Gen8/9 timeframe. That said, there's nothing prohibiting the underlying compute-runtime SW architecture from supporting it through community provided submissions.

Assi
No o
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