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Introduction to GPUs in HPC

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Using GPUs in Your Application

Rule #1: **don't** develop your own GPU code!

Libraries

There are many open libraries for GPUs.

- cuBLAS: Dense linear algebra primitives.
- Thrust: C++ STL-like algorithms and containers.
- cuRAND and Random123: Random numbers.
- cuFFT: FFT
- Kokkos: Generic performance portable parallel motifs.

. . . And many more!

Take some time to investigate what is available before starting.

You are going to write your own code?

Directives

- OpenACC and OpenMP define **directives** that can be used to instruct the compiler how to generate GPU code.
- In theory the easiest path for porting.

GPU-specific Languages

- Languages designed for GPU programming.
- Maximum flexibility and performance.
- For example: CUDA, OpenCL and Sycl.

Things to consider

Before starting on a GPU implementation, it pays to ask some questions and do some preliminary exploration:

1. Is my program computationally or bandwidth intensive?
2. Does it have enough parallel work to utilize the GPU?
3. Must I change algorithms to expose enough parallelelism?
4. Are there serial bottlenecks that will limit scaling?
5. Is the pain worth the gain?

- Questions 1, 2 and 3 will be discussed in this course.
- Question 4 will be considered briefly here.
- Questions 5 requires answers for 1–4.

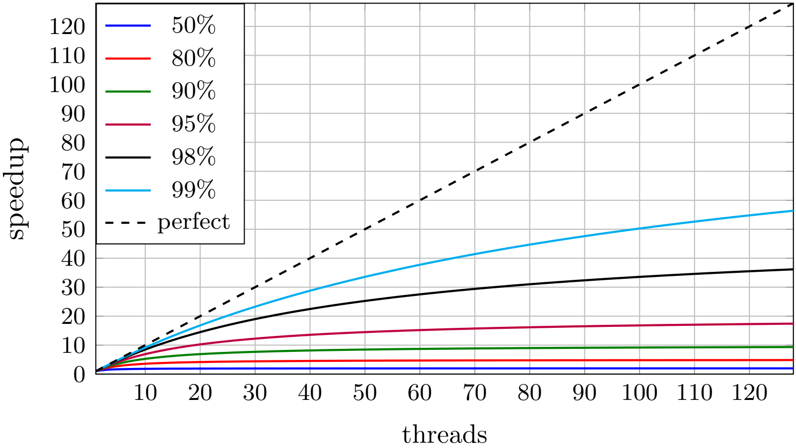
Limitations to parallel speedup

- Parallel speedup is limited by **the proportion of serial work** in your code.
- **Amdahl's law** defines the **maximum possible speedup** when only parts of the code can be parallelised

  $$t_n = t_1 \left(p + \frac{(1-p)}{n} \right),$$

  where t_n is time to solution for n threads and $p \in [0,1]$ is the proportion of sequential code.
- The limit on time to solution is $\lim_{n\to\infty} = pt_1$
  - e.g. 1% of serial code gives a maximum 100× speedup.

Amdahl illustrated



CUDA

CUDA is a **parallel computing platform and API**

- For CUDA-enabled Nvidia GPUs.

We use CUDA as short hand for CUDA C/C++ and API

- CUDA C++ is a **superset** of C++
- Adds keywords for writing kernels to run on the GPU.
- Adds syntax for launching kernels on the GPU.

The CUDA toolkit is more than a programming language:

- Runtime API for managing GPU resources and execution.
- Tools including profilers and debuggers.

Compiling CUDA

CUDA code is compiled with the **nvcc** compiler driver

- source files have `.cu` extension
- headers have `.h`, `.hpp`, `.hcu` extension.

CUDA compilation involves multiple splitting, compilation, preprocessing and merging steps

- nvcc hides this complexity from the user.
- It closely mimics the interface of the GNU compiler.
- Behind the scenes it:
  - uses GCC to compile the code that runs on CPU;
  - and compiles the GPU code separately.

Compiling CUDA

Example CUDA compilation

```
> nvcc -arch=sm_60 -lineinfo -O2 -std=c++11 -g -o foo foo.cu
```

Some flags are for **device** code generation:

- `-arch=sm_60` target GPU architecture (Pascal)
- `-lineinfo` debug information for device code.

Some are for **host**:

- `-g` debug information for host code.

And some are for both **host and device**:

- `-O2` optimization level
- `-std=c++11` target language
- `-o foo` name of executable.

Exercise: Getting Started on Piz Daint

In this exercise we will get introduced to Daint and make sure that everybody is set up.

```
# log on to daint with your course username & password
> ssh -X <your account name>@daint

# get one node on the course reservation for 60 minutes
> salloc -Cgpu --reservation=course -t60

# go to scratch and get the course material
> cd $SCRATCH/SummerSchool2019
> git pull

# compile and test the demo
> cd topics/cuda/practicals/demos
> cat hello.cu
> module load gcc cudatoolkit
> nvcc -arch=sm_60 hello.cu -o hello
> srun ./hello
```