



**CSCS**

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Swiss National Supercomputing Centre

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# Introduction to GPUs

**CSCS Summer School 2023**

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# Course Overview

Over these two days we will cover a range of topics:

- Learn about the GPU memory model;
- Implement parallel CUDA kernels for simple linear algebra;
- Learn how to scale our parallel kernels to utilize all resources on the GPU;
- Learn about thread cooperation and synchronization;
- Learn how to profile GPU applications;
- Port the miniapp to the GPU.

# Course Overview

We focus on HPC and GPU architectures, specifically:

- HPC development for P100 GPUs on Piz Daint;
- Using CUDA toolkit version 11 and above;
- Some are available on P100 and later GPUs.
  - e.g. double precision atomics.
- Likewise, we won't be covering some features available on the latest *Ampere* or *Hopper* GPUs.

# Course Overview

There aren't many prerequisites for the course:

- No GPU or graphics experience required.
- We assume C++11 knowledge.
- The generic GPU programming concepts from CUDA are useful for when:
  - Developing with OpenACC, OpenCL and GPU-ready libraries.
  - Using ML frameworks that use GPU for compute.

# Why GPUs?

# First, what do we really want?

- Scientific results, as fast as possible.

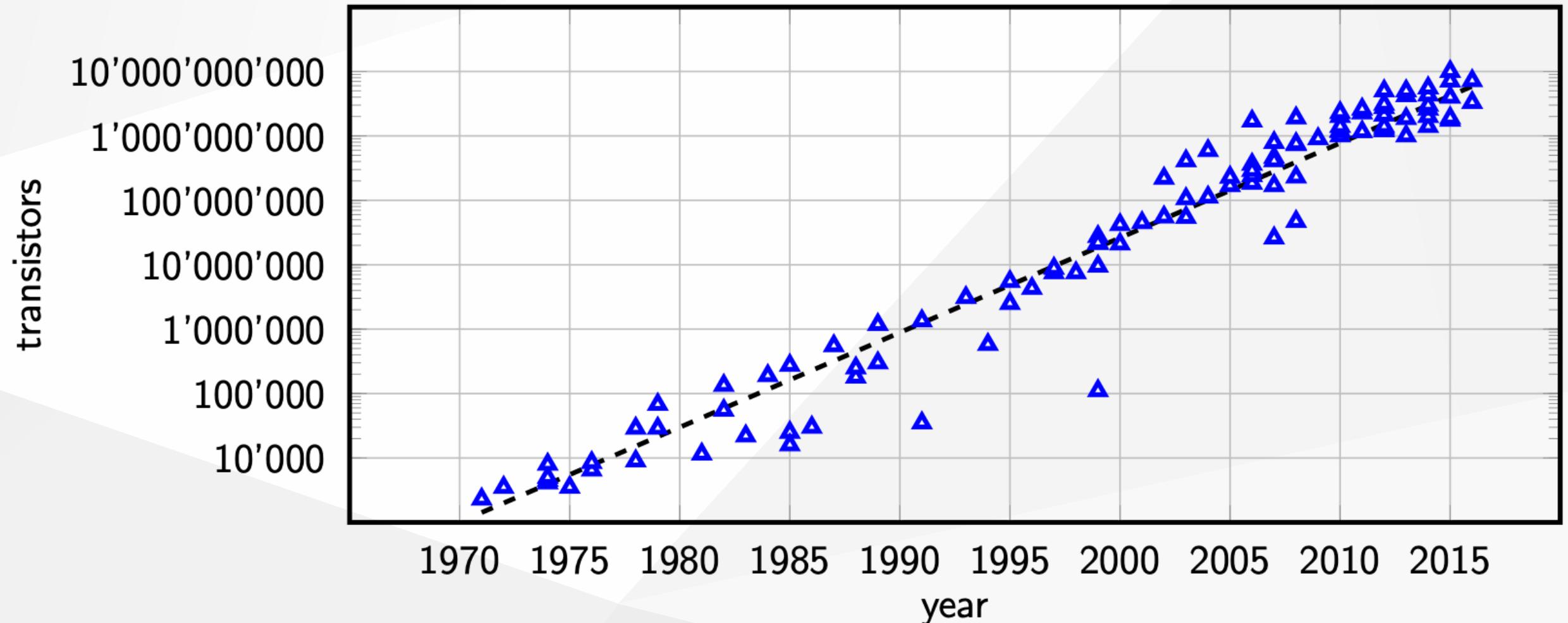
# What's stopping us?

- Processor compute speed
- Data movement
- Algorithmic efficiency

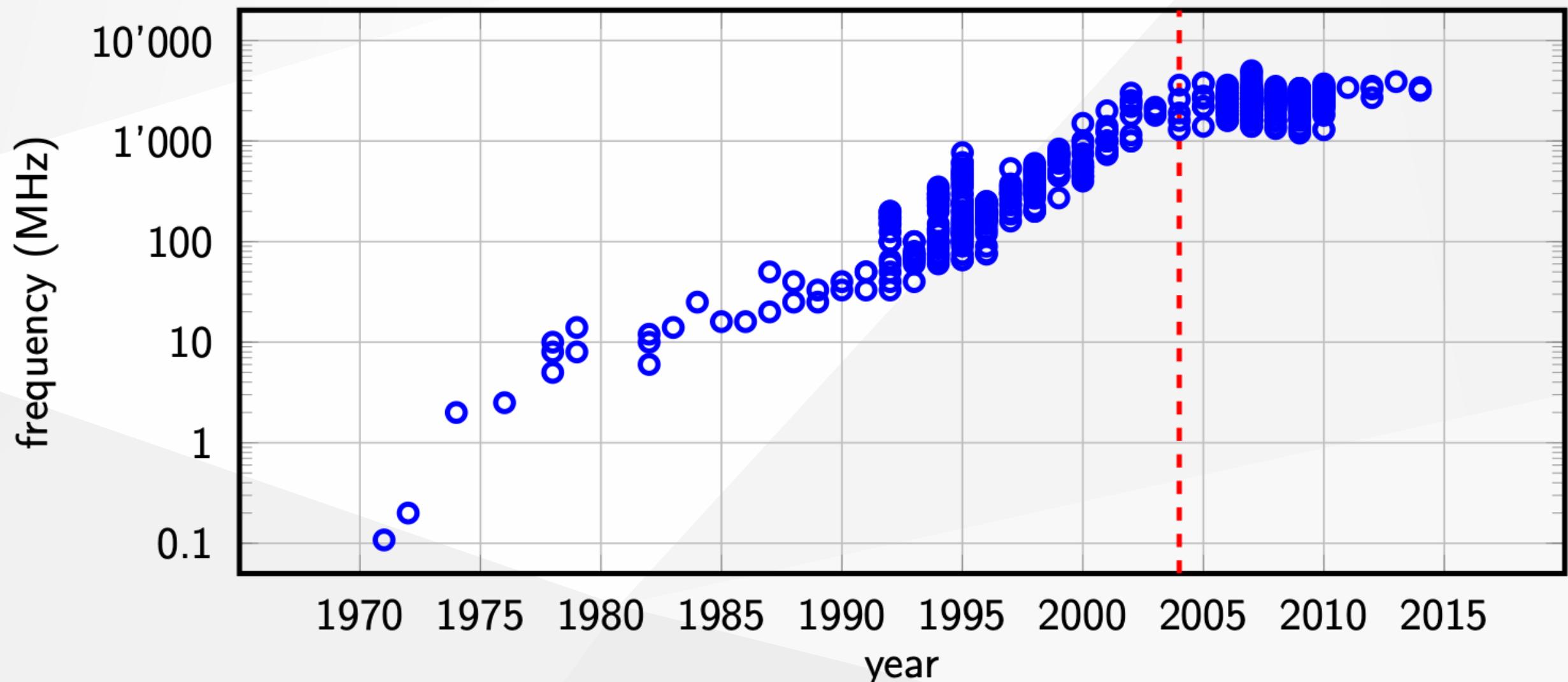
# Increasing CPU performance

There are 3 ways to increase performance on the CPU:

1. Increase the CPU clock speed (do every operation faster).
2. Increase the number of operations per clock cycle:
  - vectorization;
  - instruction level parallelism;
  - more cores / multiple machines.
3. Access/process data more efficiently:
  - Avoid stalling the processor while it waits for data to come from memory  
→ Better use of cache
  - Avoid stalling the processor pipeline  
→ Better use of branch prediction features.



**The number of transistors in processors has increased exponentially for 45 years.**



**And clock speeds were, for a time, also increasing.**

# MPI and the Free Lunch

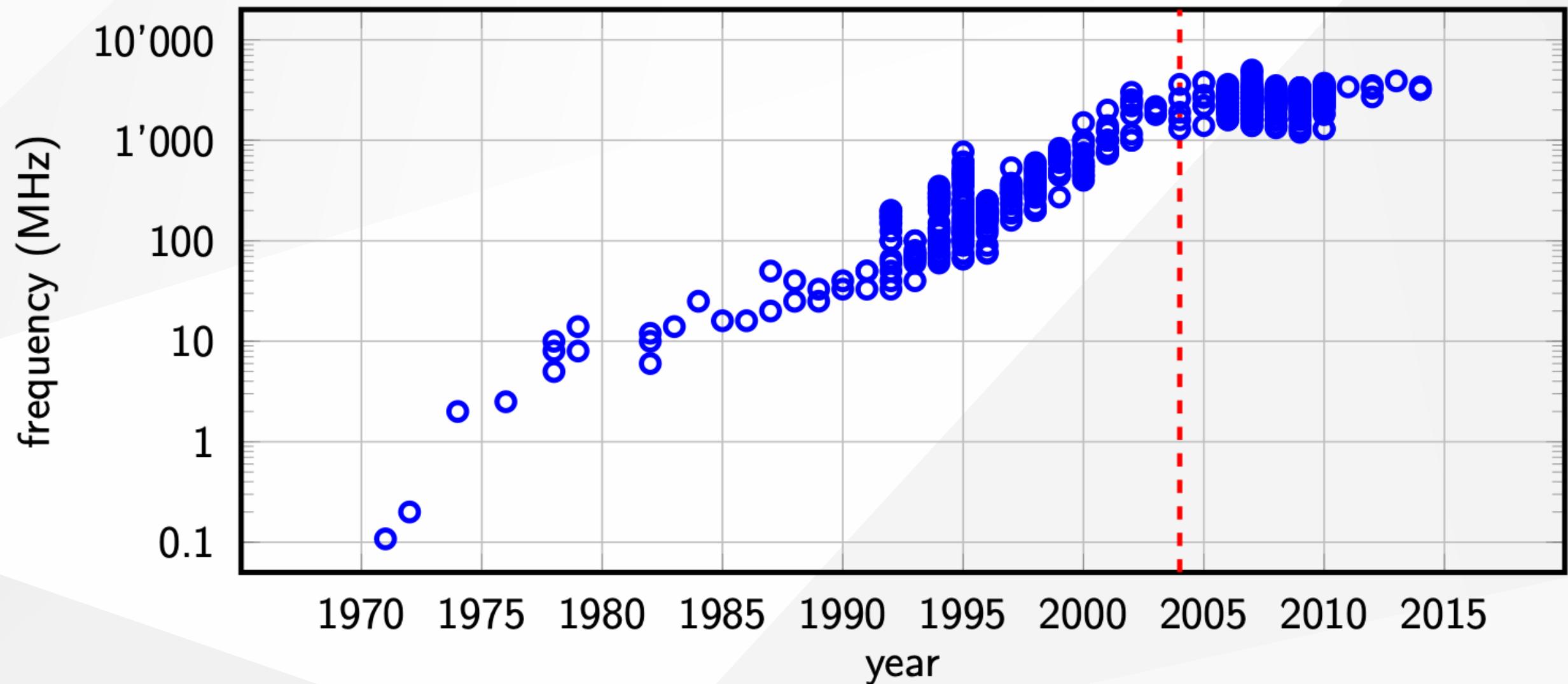
HPC applications were ported to use the message passing library MPI in the late 90s and early 2000s at great cost and effort

- Individual nodes with one or two CPUs
- Break problem into chunks/sub-domains
- Explicit message passing between sub-domains

The "free lunch" was the regular speedup in codes as CPU clock frequencies increased and as the number of nodes in systems increased

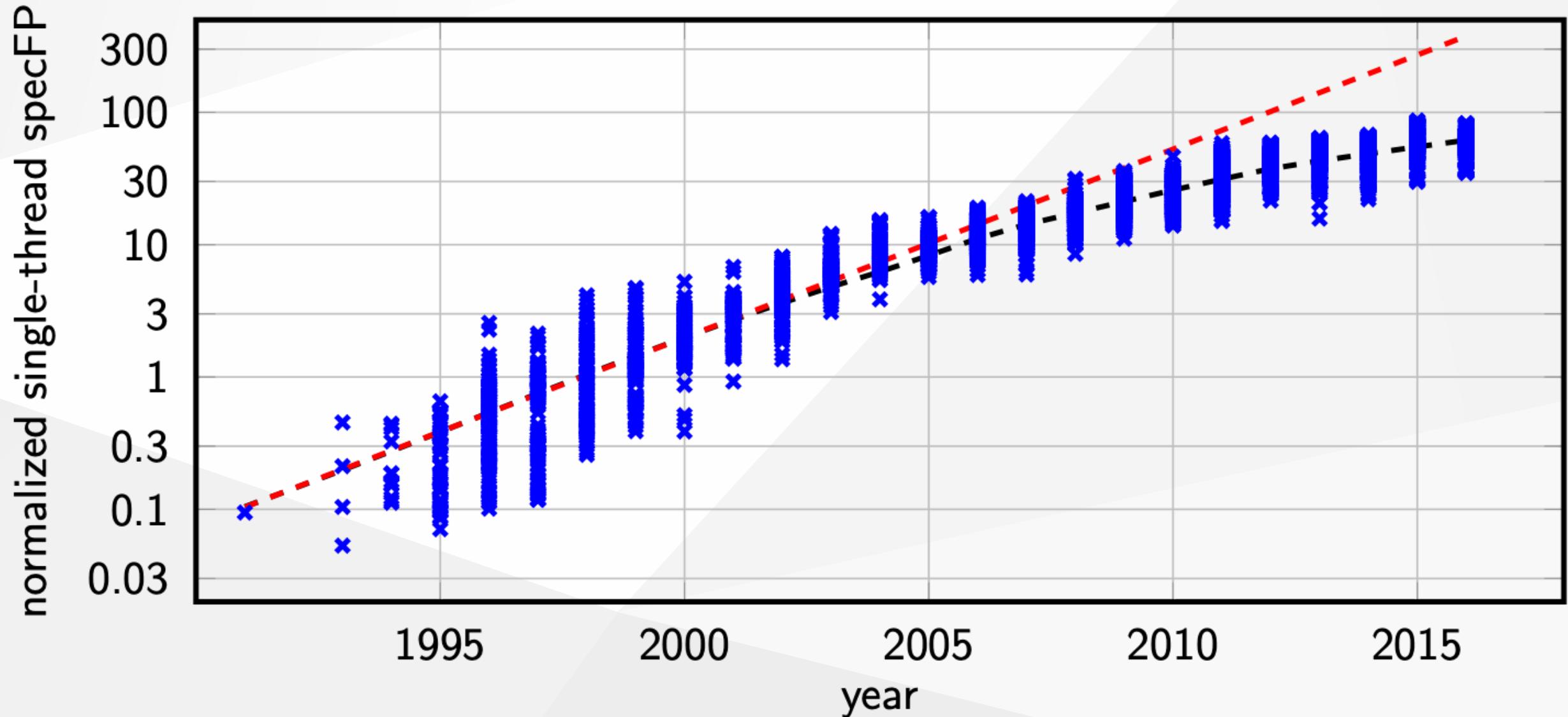
- With little/no effort, each new generation of processor bought significant speedups.

... but there is no such thing as a free lunch.



Clock speeds peaked around 2005.

- We can not build increasingly faster simple processors.
- $Power \sim Frequency^3$
- Higher frequency → much more power, more heat, more money, more difficult to engineer and build.



**As a result, floating point performance per core is not keeping up...**

# One solution: More parallelism

Instead of scaling some base frequency like this:

$$P_{\text{tot}} \sim (k \cdot \text{Frequency})^3,$$

we keep the base frequency fixed and increase the number of processors:

$$P_{\text{tot}} \sim N_{\text{cpu}} \times \text{Frequency}^3$$

In the best case, with  $N_{\text{cpu}}$  processors working in parallel, the job is done in  $1/N_{\text{cpu}}$  time.

**It takes the same power for a CPU to go 10x faster as it does for 1000 CPUs to run in parallel.**

# Clock Frequency WILL NOT Increase

In fact, clock frequencies have been going down as the number of cores increases:

- A 4-core Haswell processor at 3.5 GHz ( $4 \times 3.5 = 14$  Gops/second) has the same power consumption as a 12-core Haswell at 2.6 GHz ( $12 \times 2.6 = 31$  Gops/second);
- A P100 GPU with 3584 CUDA cores runs at 1.1 GHz.

## Caveat

It is not reasonable to compare a CUDA core and an X86 core.

# Parallelism WILL Increase

- The number of cores in both CPUs and accelerators will continue to increase
- The width of vector lanes in CPUs will increase
  - 8×SIMD double for AVX512 and SVE (Intel and ARM).
- The number of threads per core will increase
  - Intel SkyLake: 2 threads/core
  - Intel KNL: 4 threads/core
  - IBM Power-8: 8 threads/core

## There is a trend towards more parallelism "on node"

### **Multi-Core CPUs** get more cores and wider vector lanes:

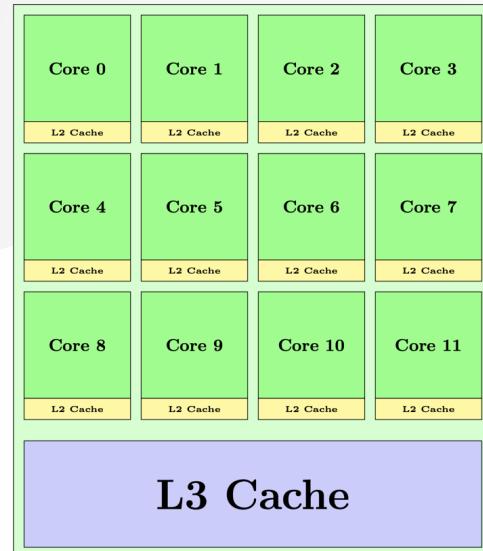
- 24-core  $\times$  SMT 4  $\times$  SIMD 128: IBM Power9 (2017);
- 28-core  $\times$  SMT 2  $\times$  SIMD 512: Intel Xeon (2020)
- 48-core  $\times$  SMT 1  $\times$  SIMD 512: Fujitsu ARM A64FX (2020).

### **Many-Core Accelerators** with many highly-specialized cores and high-bandwidth memory:

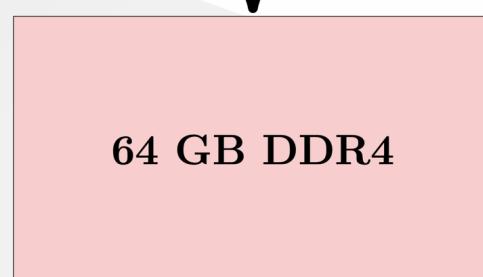
- NVIDIA P100 GPUs with 3,584 cores (2016);
- NVIDIA V100 GPUs with 5,120 cores (2017);
- NVIDIA A100 GPUs with 8,192 cores (2020);
- NVIDIA H100 GPUs with 18,432 cores (2023)

# A PiZ Daint Node

12 Core CPU



P100 GPU



... that's a lot of parallelism!

# Memory is Slow

However, memory is now *much* slower than processors

- For both CPU and GPU the latency of fetching a cache-line from memory is 100s of cycles...
- ... 100s of cycles that the processor is stalled
- Latency has to be hidden or reduced to minimise stalling

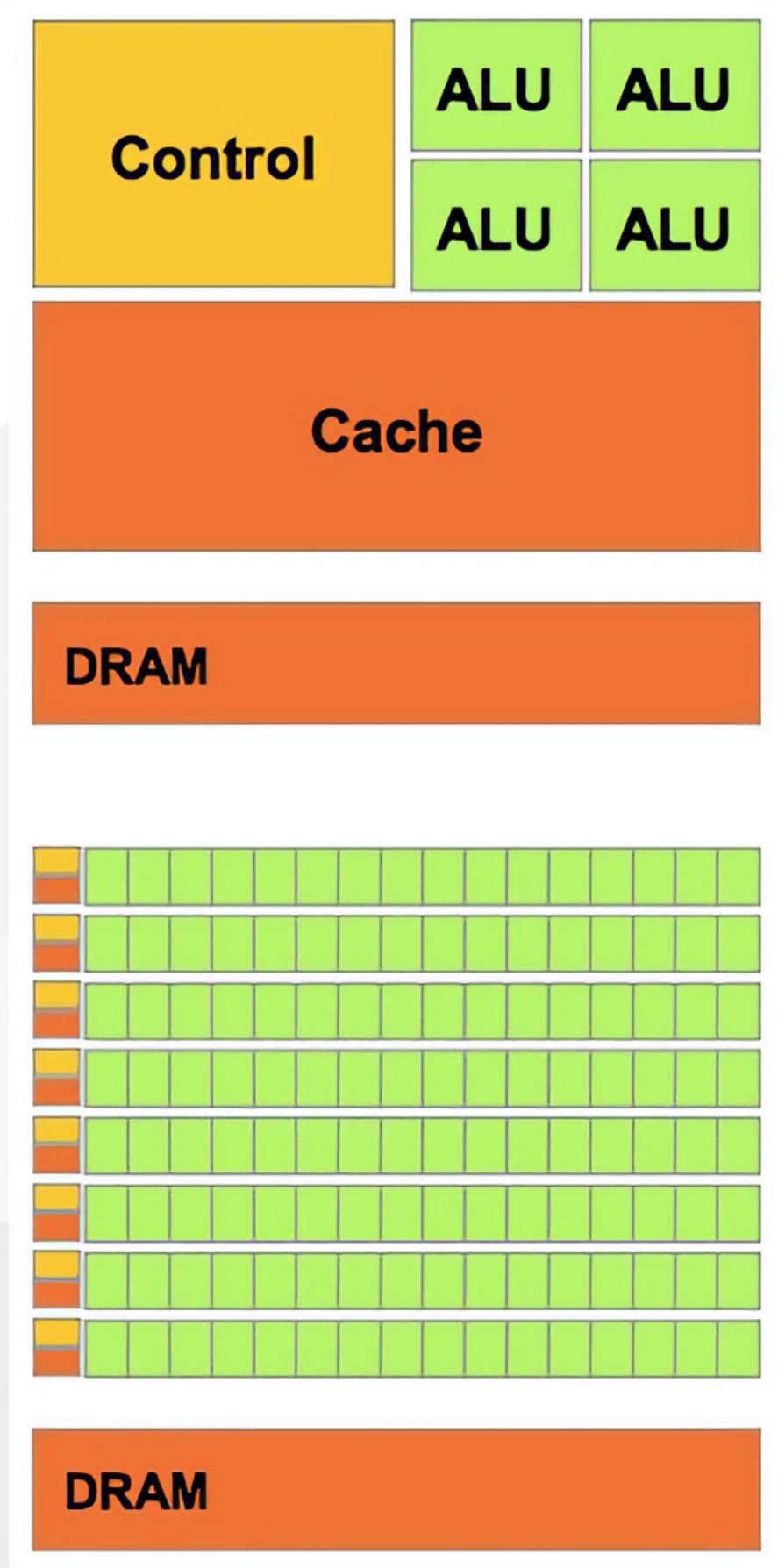
# Low-Latency or High-Throughput?

## CPU

- Optimized for low-latency access to cached data sets.
- Control logic for out-of-order and speculative execution.

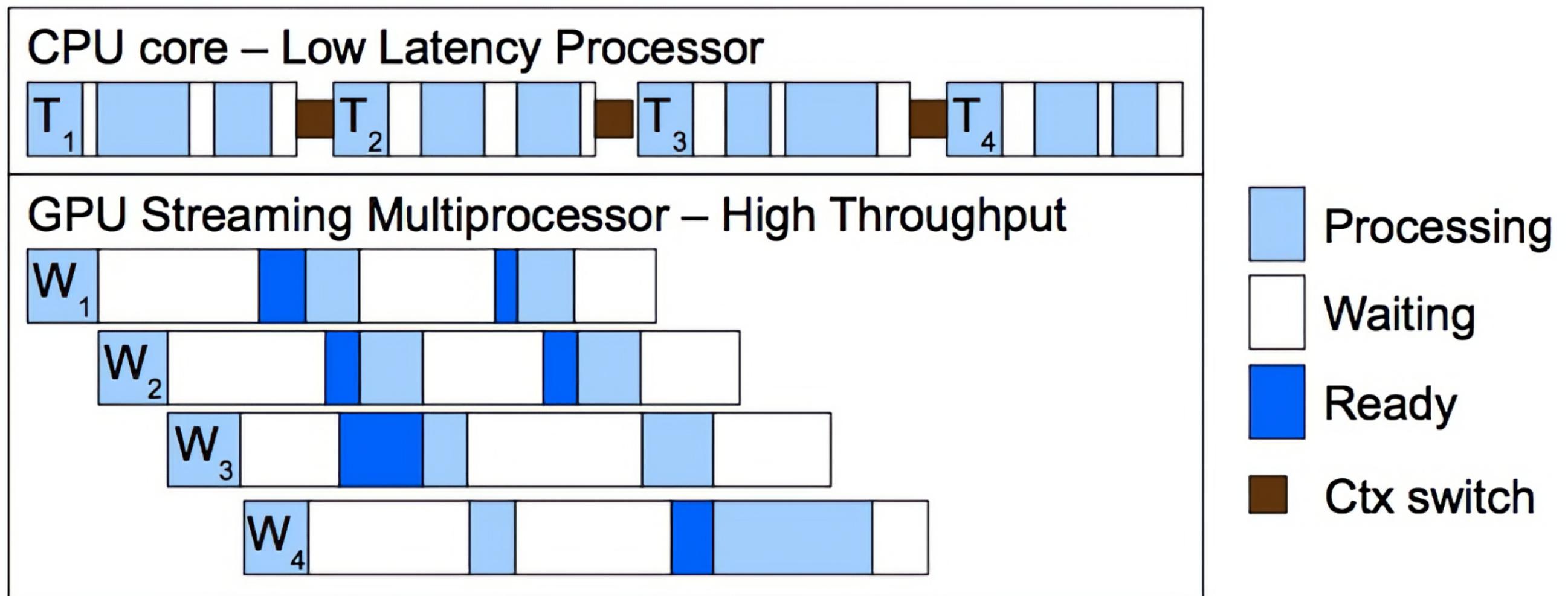
## GPU

- Optimized for data-parallel, throughput computation.
- Architecture tolerant of memory latency.
- More transistors dedicated to computation.



# GPUs are Throughput Devices

- CPU cores are optimized to minimize latency between operations
- GPUs aim to minimize latency between operations by scheduling multiple warps (thread bundles)



# Many Applications aren't Designed for Many-Core

- Exposing sufficient fine-grained parallelism for multi and many core processors is hard.
- New programming models are required.
- New algorithms are required.
- Existing code has to be rewritten or refactored

On-node parallelism will continue to increase:

- Piz Daint @ CSCS (2015): 1 GPU + 1 CPU
- Marconi100 @ CINECA (2020): 4 GPU + 2 CPU
- EUROHPC pre-exascale (2021): 4 GPU + 1 CPU
- US ECP exascale (2021-2023): 4 GPU + 1 CPU
- **ALPS @ CSCS (2024): 4 GPU + 4 CPU**

# TLDR: Change because power

Writing good concurrent code for many-core is difficult

- But the days of easy speed up each generation of CPU are over
  - Performance gains must not increase power consumption
- This course will be about one type of many-core architecture NVIDIA GPUs
  - CUDA is GPU-specific.
  - Conceptually very close to HIP, OpenCL and SYCL (AMD/NVIDIA/Intel)