ICME Fundamentals of Data Science

Introduction to High-Performance Computing

Eric Darve

What is high-performance computing?

- Standard computers perform tasks sequentially, that is transaction-by-transaction.
- This means that the next transaction, or job, happens only when the computer completes the previous one.
- In contrast, HPC uses a large number of resources such as processors to complete many jobs at once.

Supercomputers

- For the most part, HPC occurs on supercomputers.
- These powerful systems help companies solve problems that could otherwise be insurmountable.
- These problems, or tasks, require processors that can carry out instructions faster than standard computers.
- This is achieved by running many processors in parallel to obtain answers within a practical duration.

CPUs and GPUs

- HPC jobs require fast disks and high-speed memory.
- HPC systems include computing and data-intensive servers with powerful CPUs that can be vertically stacked.
- HPC systems often have powerful graphics processing units (GPUs) that can run general-purpose computations.

Clusters

- HPC systems can also scale by way of clusters.
- These clusters consist of networked computers, including scheduler, compute, and storage capabilities.
- Single HPC clusters are as large as 100 thousand or more compute cores, for example.
- Clusters can accommodate multiple applications and resources. They are managed by policy-based scheduling and can handle a dynamic workload consisting of large numbers of jobs.

HPC system designs

What is parallel computing?

Parallel computing HPC systems involve hundreds of processors, with each processor running calculation payloads simultaneously.

HPC system designs

What is cluster computing?

Cluster computing is a type of parallel HPC system consisting of a collection of computers working together as an integrated resource. It includes a scheduler and compute and storage capabilities.

HPC system designs

What is grid and distributed computing?

Grid and distributed computing HPC systems connect the processing power of multiple computers within a network. The network can be a grid at a single location or distributed across a wide area in different places, linking network, compute, data, and instrument resources.

Applications of HPC

Some of the key applications include:

- Big data: massive multi-dimensional datasets
- Data analytics
- Extreme performance database
- Machine learning

Applications!

Automotive and aerospace

- CFD-aerodynamic modeling
- FEA-impact and structural strength analysis
- CAD and CAM

Banking, financial services markets and insurance

- Monte Carlo simulations
- Risk analysis
- Fraud detection

Electronics design automation (EDA)

- Chip design and optimization
- Circuit simulation and verification
- Manufacturing optimization

Film, media and gaming

- Rendering
- Computer-aided graphics
- Computer-generated images (CGI)
- Transcoding and encoding
- Real-time image analysis and processing

Government and defense

- Intelligence agency
- Fraud analysis
- Climate modeling
- Weather forecasting
- Energy
- Nuclear stewardship
- Exploration

Life sciences

- Genomic processing and sequencing
- Pharmaceutical design
- Molecular modeling and biology simulation
- Protein docking

Oil and gas

- Seismic data processing
- Reservoir simulation and modeling
- Geospatial analytics
- Terrain and topology mapping
- CFD-aerodynamic modeling
- Wind simulation

Retail

- Inventory analysis
- Logistics and supply chain optimization
- Sentiment analysis
- Marketing offers

A short history of HPC

The beginnings:

- HPC market: scientific discoveries; Fortran (Formula Translation)
- Cray Research: supercomputers; focus: floating-point operations
- 1960's: specialized and expensive supercomputers; cold war, strategic necessity
- 1980's: number of processors goes up. Multiple processors (in some cases hundreds) are connected through a network

A short history of HPC

- Vendors turn to commodity markets where processors are sold in large quantities
  - Monolithic supercomputer systems splinter as many of the commodity components can be purchased from competing vendors
  - Economic barrier of entry is lowered by at least a factor of ten

Beowulf clusters

- Operating system: UNIX.
- 1981, Linus Torvalds released a freely available version of Linux
- Message Passing Interface (MPI) library

Beowulf clusters

- Performance of “Beowulf Clusters” (named for the NASA project that developed these systems) comes close to that of supercomputers of the day: commodity-grade computers + free and open source software + MPI
- High performance interconnects are developed; market settles on InfiniBand (Mellanox)
- Name “supercomputer” replaced by “HPC systems”

The multi and many core explosion

- Increase in clock speed limited by three issues:
  1. Memory Speed: gap between processor and memory speed continued to grow
  2. Instruction Level Parallelism: increasing difficulty of finding enough parallelism in a single instruction stream
  3. Power Wall: increased processor frequency causes an increase in operating temperature

The multi and many core explosion

- Era of multi-core: dual-core processors; more cores added to each new generation of processors
- Commodity Graphics Processing Units (GPUs) that contain large numbers (hundreds to thousands) of small efficient cores

Exascale computing and co-design

"On the Role of Co-design in High Performance Computing," R. F. Barrett et al.

The co-design strategy is based on developing partnerships with **computer vendors and application scientists** and engaging them in a highly **collaborative and iterative design process** well before a given system is available for commercial use. The process is built around identifying leading edge, high-impact scientific applications and providing concrete optimization targets rather than focusing on speeds and feeds (FLOPs and bandwidth) and percent of peak. **Rather than asking "what kind of scientific applications can run on an Exascale system" after it arrives, this application-driven design process instead asks "what kind of system should be built to meet the needs of the most important science problems."** This leverages eep understanding of specific application requirements and a broad-based computational science portfolio.

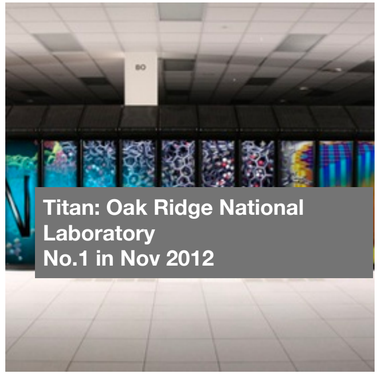
HPC history in pictures

CM-5: Los Alamos National Lab
No.1 in Jun 1993

ASCI Red: Sandia National Laboratory
No.1 from Jun 1997 until Jun 2000

BlueGene/L: Lawrence Livermore National Laboratory
No.1 from Nov 2004 until Nov 2007

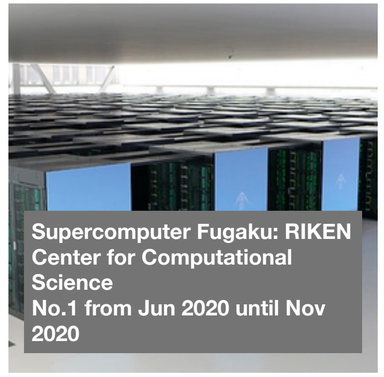
Tianhe-1A: National Supercomputing Center in Tianjin
No.1 in Nov 2010



Titan: Oak Ridge National Laboratory
No.1 in Nov 2012

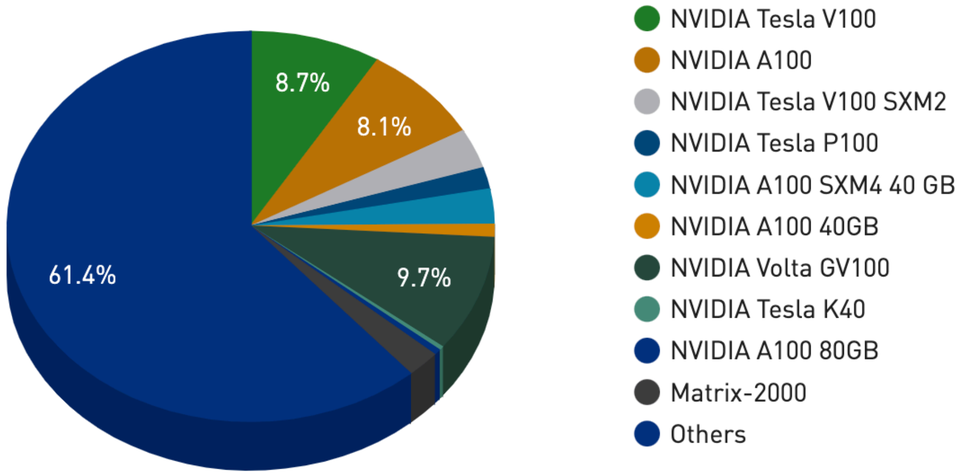
Sunway TaihuLight: National Supercomputing Center in Wuxi
No.1 from Jun 2016 until Nov 2017

Summit: DOE/SC/Oak Ridge National Laboratory
No.1 from Jun 2018 until Nov 2019



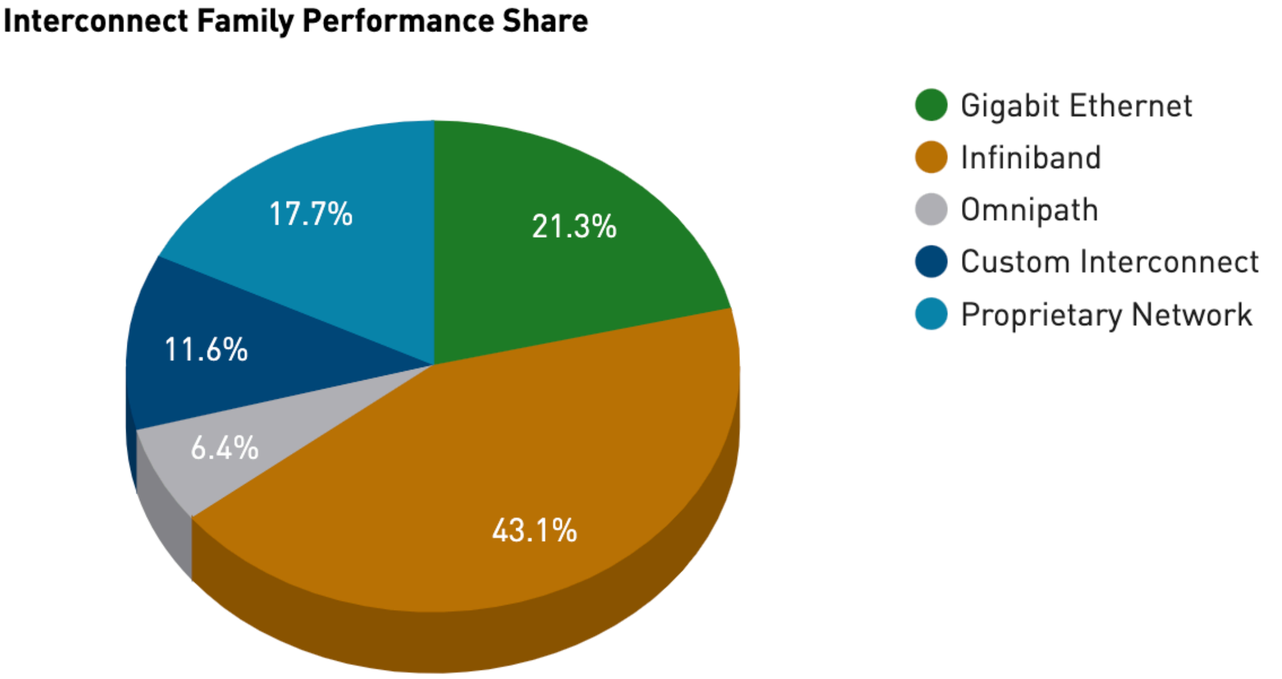
Supercomputer Fugaku: RIKEN Center for Computational Science
No.1 from Jun 2020 until Nov 2020

Accelerator/Co-Processor Performance Share



LINPACK achieved Theoretical peak

	Accelerator/Co-Processor	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
1	NVIDIA Tesla V100	80	16	243,448,930	475,572,809	5,059,976
2	NVIDIA A100	15	3	226,001,000	324,135,290	2,125,952
3	NVIDIA Tesla V100 SXM2	12	2.4	91,975,490	182,486,069	2,059,208
4	NVIDIA Tesla P100	8	1.6	49,751,640	73,680,456	1,005,472
5	NVIDIA A100 SXM4 40 GB	5	1	81,312,000	115,202,938	869,192
6	NVIDIA A100 40GB	4	0.8	30,133,600	47,814,630	315,812
7	NVIDIA Volta GV100	4	0.8	269,439,000	362,564,722	4,408,096
8	NVIDIA Tesla K40	3	0.6	8,824,090	14,612,320	201,328
9	NVIDIA A100 80GB	2	0.4	13,806,000	18,688,410	124,160
10	Matrix-2000	1	0.2	61,444,500	100,678,664	4,981,760
11	NVIDIA 2050	1	0.2	2,566,000	4,701,000	186,368
12	NVIDIA Tesla K40m	1	0.2	2,478,000	4,946,790	64,384
13	NVIDIA Tesla K40/Intel Xeon Phi 7120P	1	0.2	3,126,240	5,610,481	152,692
14	NVIDIA Tesla P100 NVLink	1	0.2	8,125,000	12,127,069	135,828

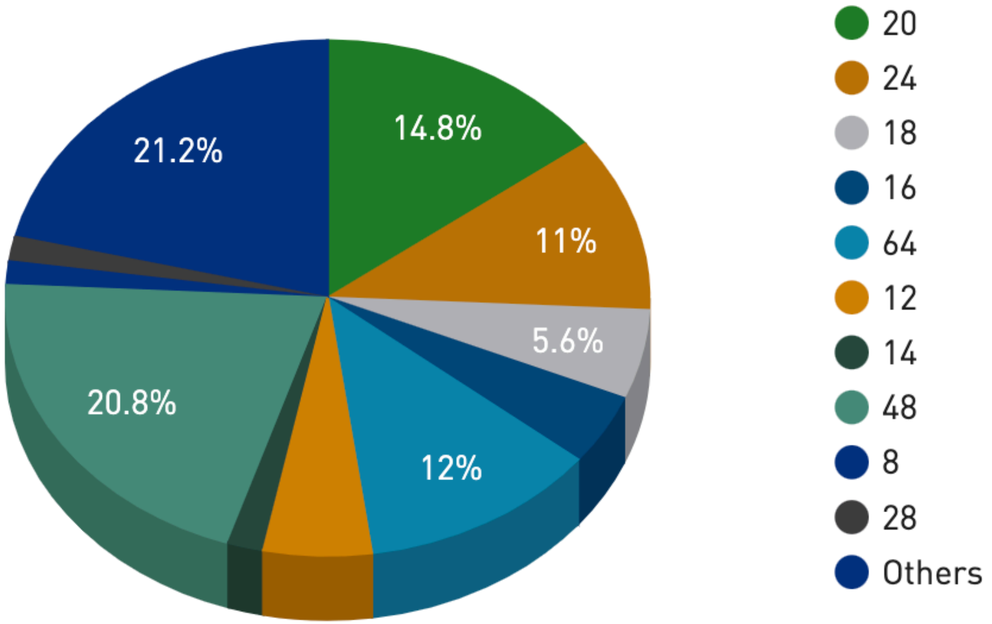


Mellanox

Intel

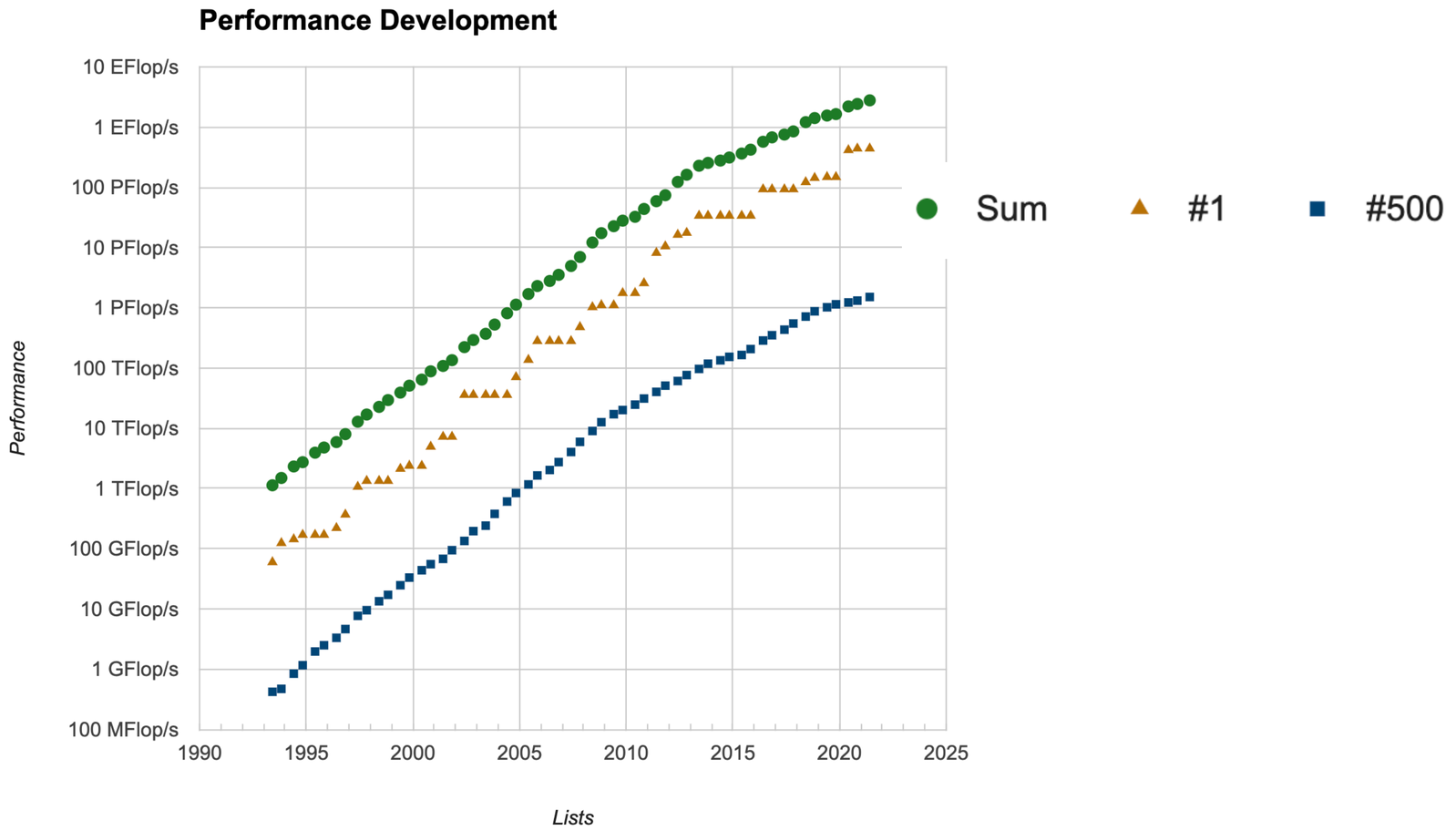
	Interconnect Family	Count	System Share (%)	Rmax (GFlops)	Rpeak (GFlops)	Cores
1	Gigabit Ethernet	247	49.4	592,043,220	1,210,167,243	19,827,104
2	Infiniband	168	33.6	1,200,636,818	1,832,049,310	22,511,764
3	Omnipath	42	8.4	178,516,898	281,314,234	4,361,016
4	Custom Interconnect	37	7.4	322,955,564	483,020,993	21,616,076
5	Proprietary Network	6	1.2	491,906,300	597,474,433	8,609,792

Cores per Socket Performance Share



- 20
- 24
- 18
- 16
- 64
- 12
- 14
- 48
- 8
- 28
- Others

Performance development



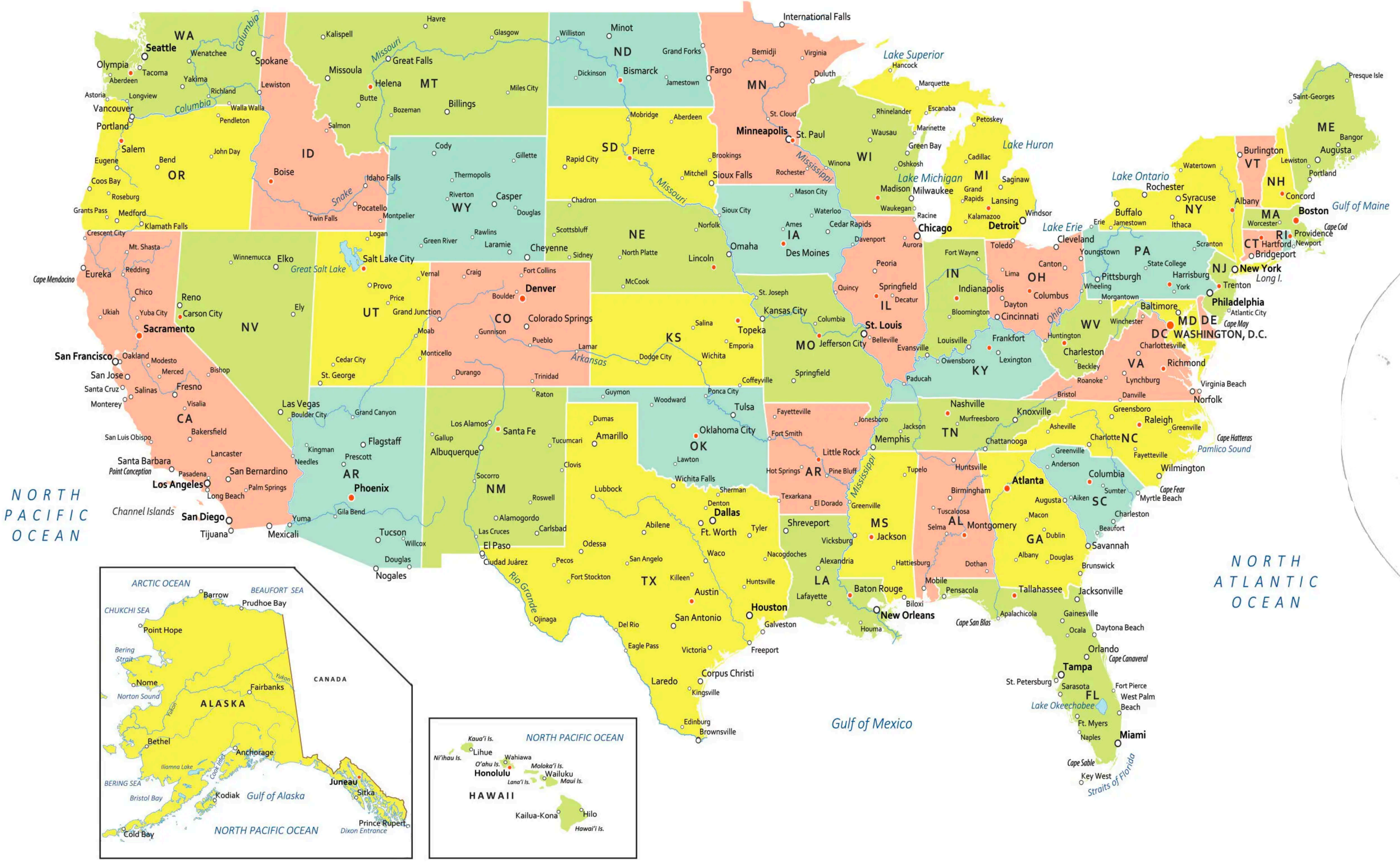
But before diving in further...
Let's get to know each other

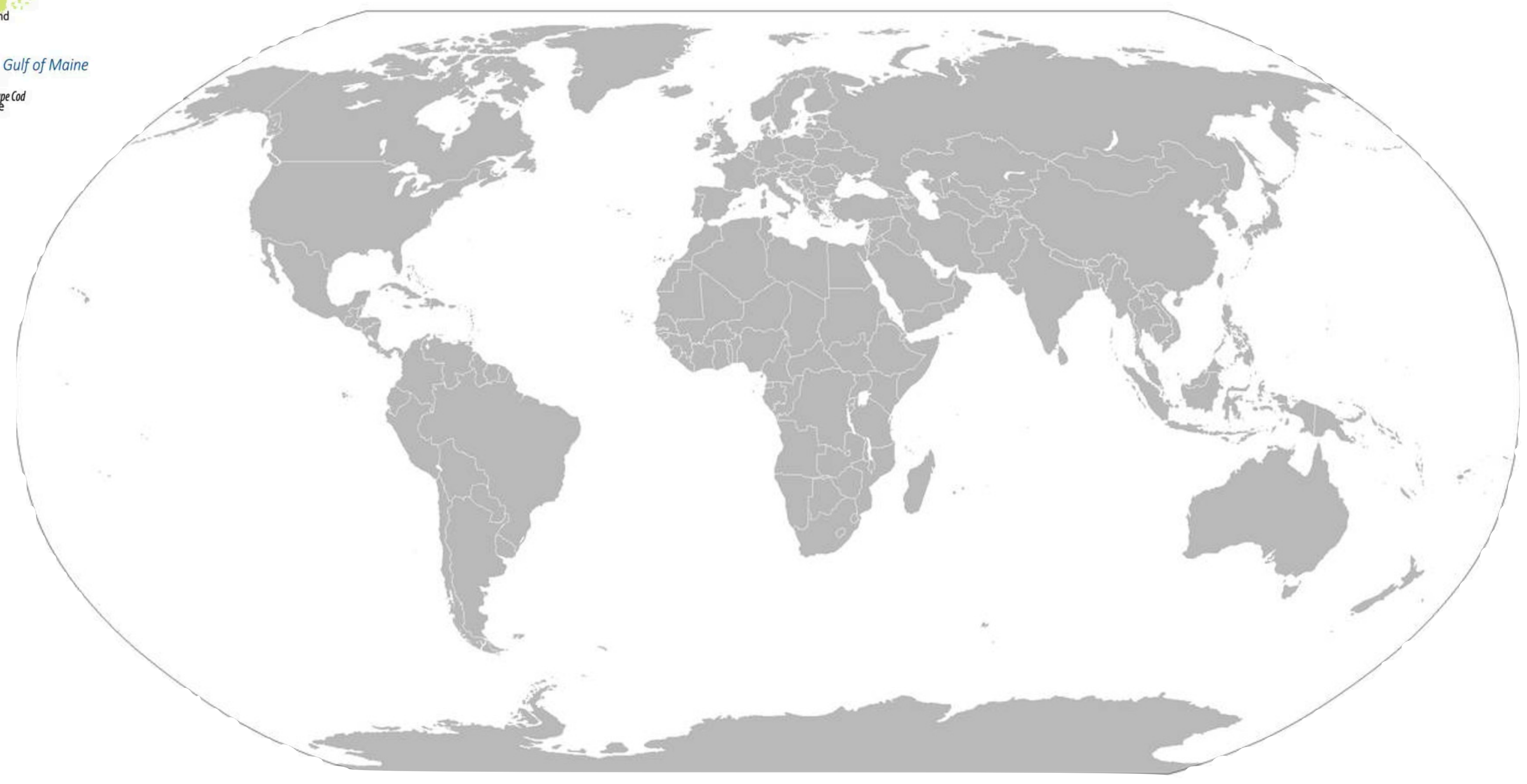
Instructor

- Eric Darve, ME, ICME, darve@stanford.edu
- Numerical linear algebra, machine learning for mechanics and engineering, parallel computing

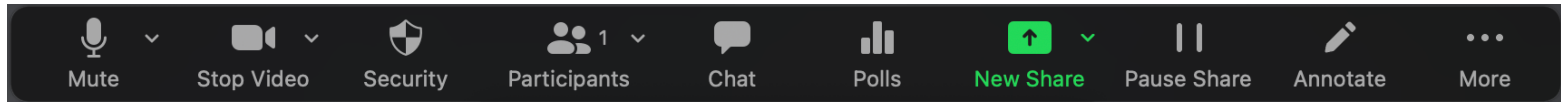
Teaching Assistant

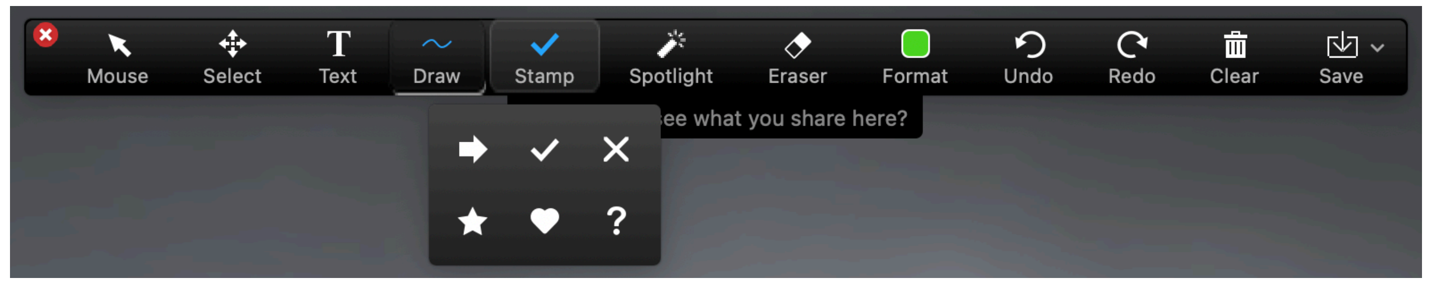
- Chenzhuo Zhu
- I am a graduating Ph.D. student at Stanford EE, advised by Prof. Bill Dally. I am interested in computer architecture and memory system design for data center applications.
- I grew up in Beijing, China. I received my B.S degree from Tsinghua University before coming to Stanford.
- I worked as a teaching assistant for CME courses on scientific and parallel programming.
- I am also a snowboarder and a private pilot.





Mark your current location using zoom “Annotate → Stamp”





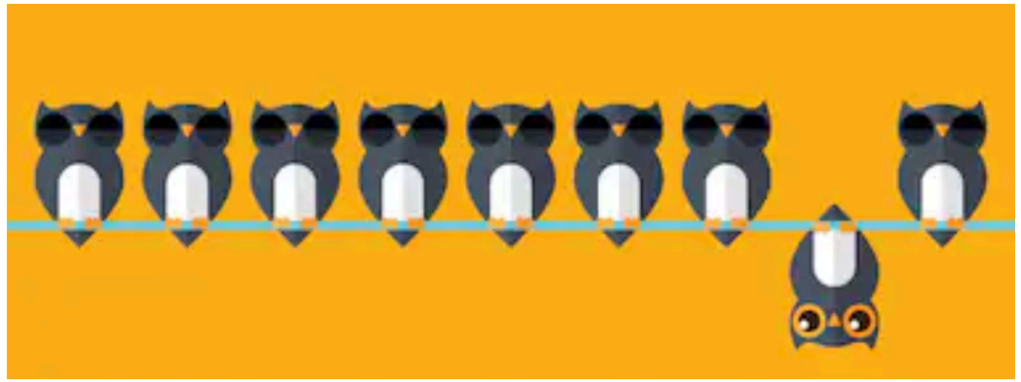
What this class is about

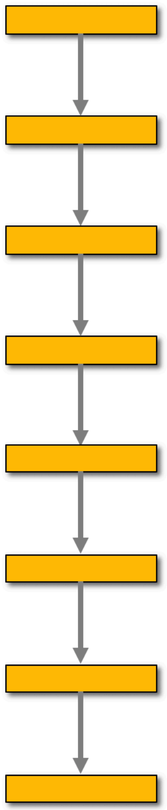
We will get an overview of parallel programming for the 3 main HPC approaches:

1. **Shared memory** multicore processors: C++ threads and openMP
2. **GPU** computing: NVIDIA CUDA (+ AMD)
3. **Distributed memory** computing with MPI

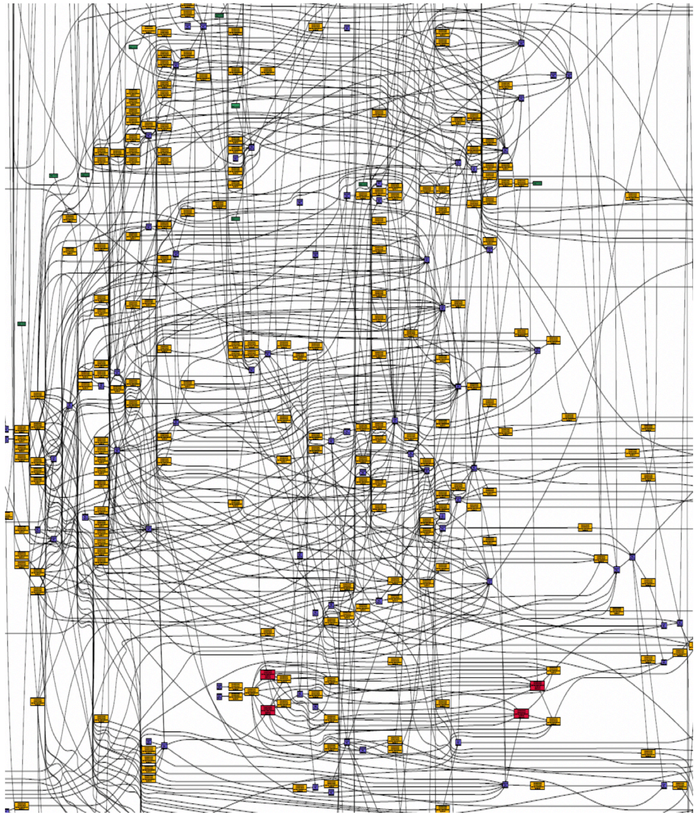
Thinking parallel

Parallel programs often look very different from sequential programs.



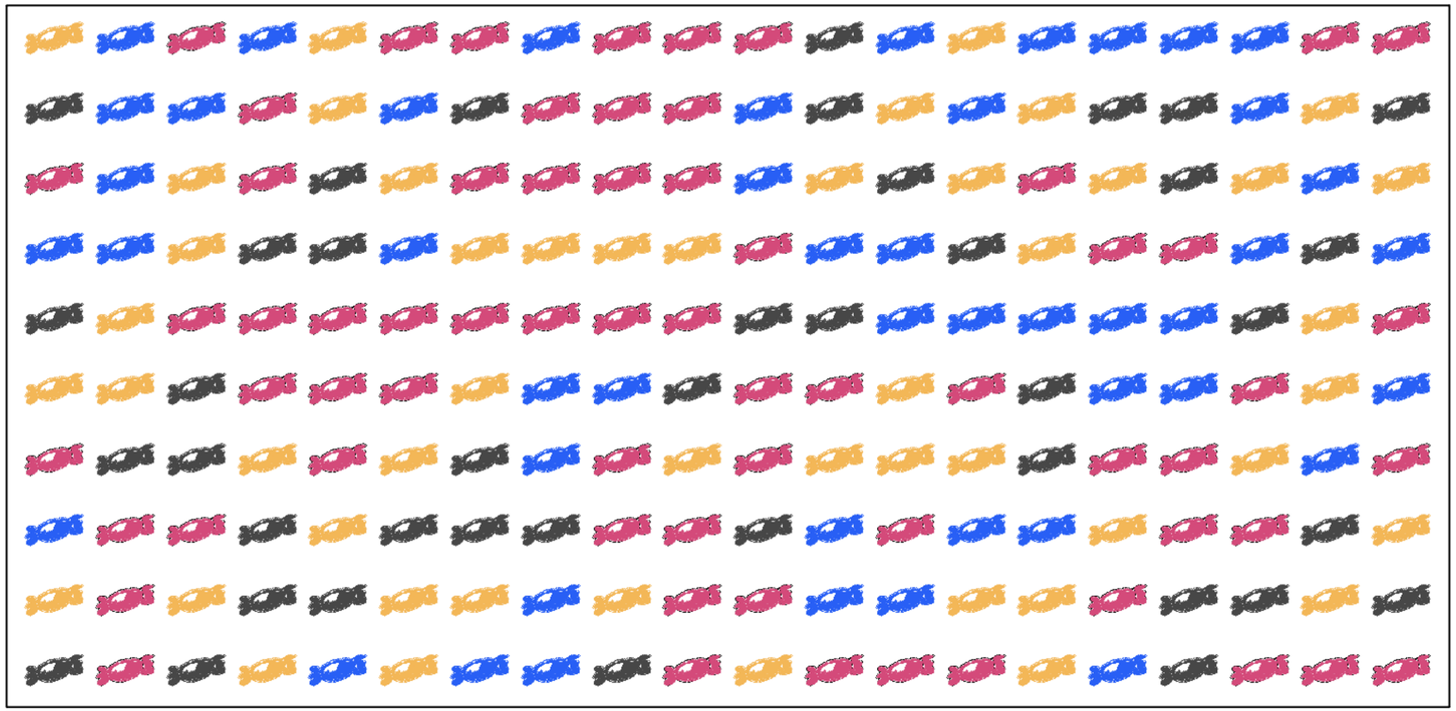


Sequential thinking

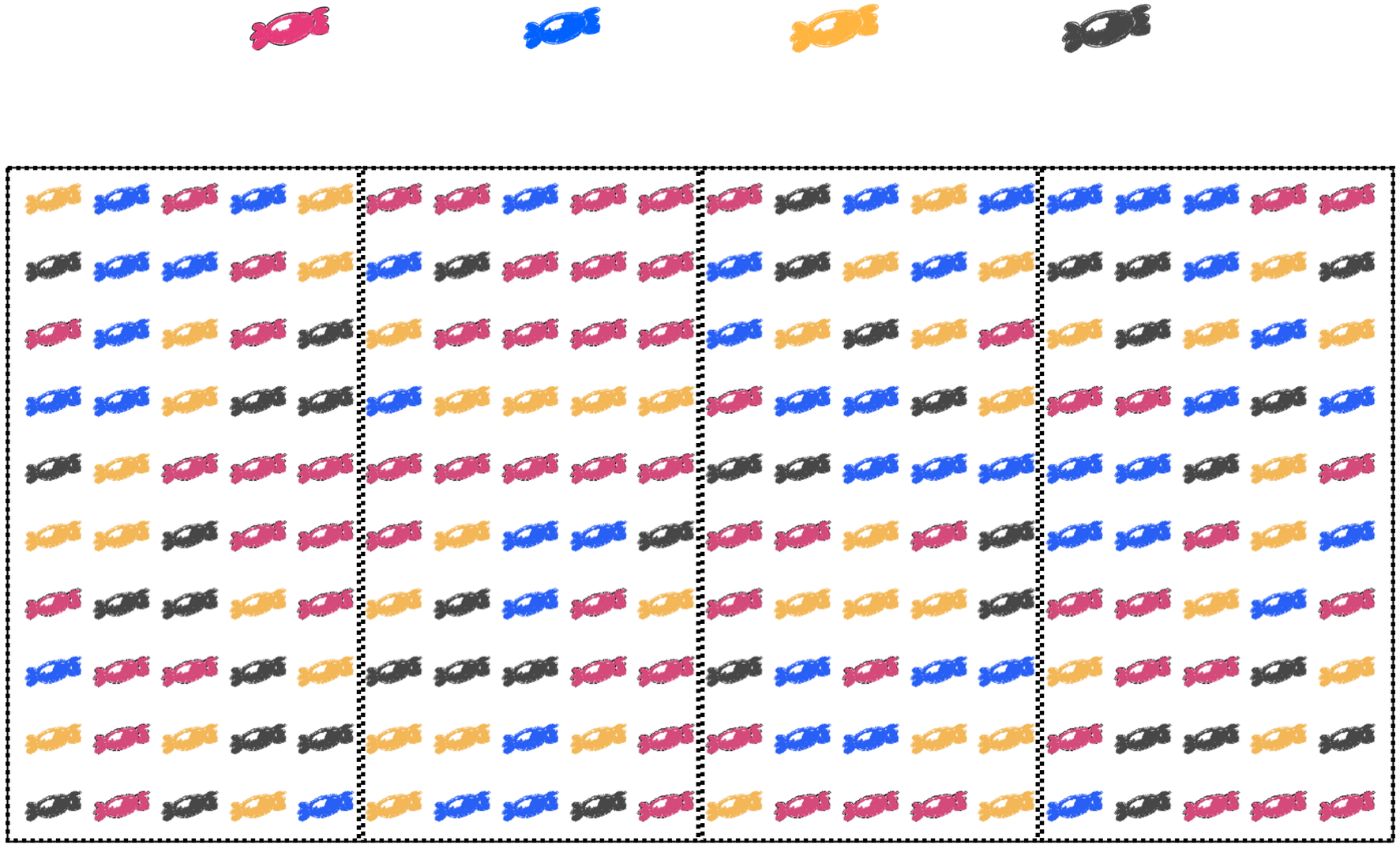


Parallel thinking

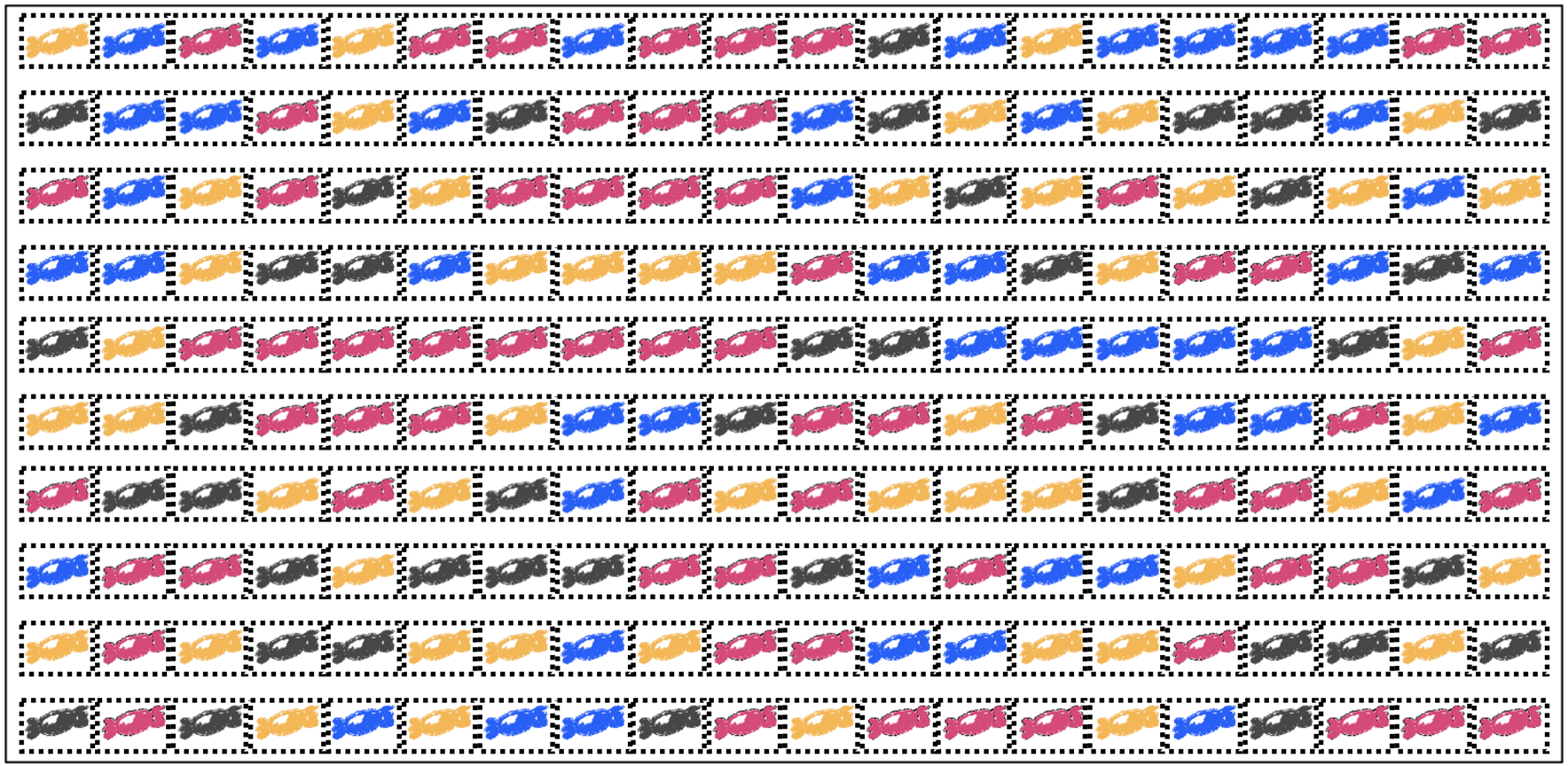
How would you count the number of candies of each color?



Using 2 cores



Using 4 cores



Using 200 cores

The initial step of counting candies goes fast.

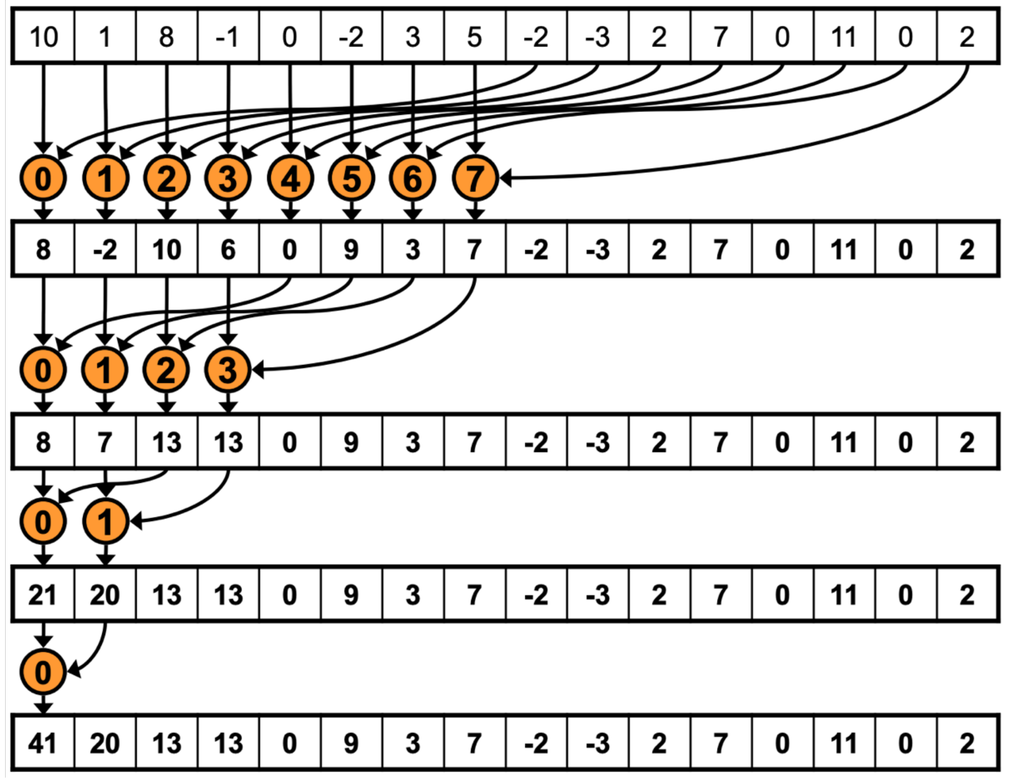
But after that, the next steps of reduction become problematic.

Can we use a single core to calculate the final sum for each candy?

- This is inefficient

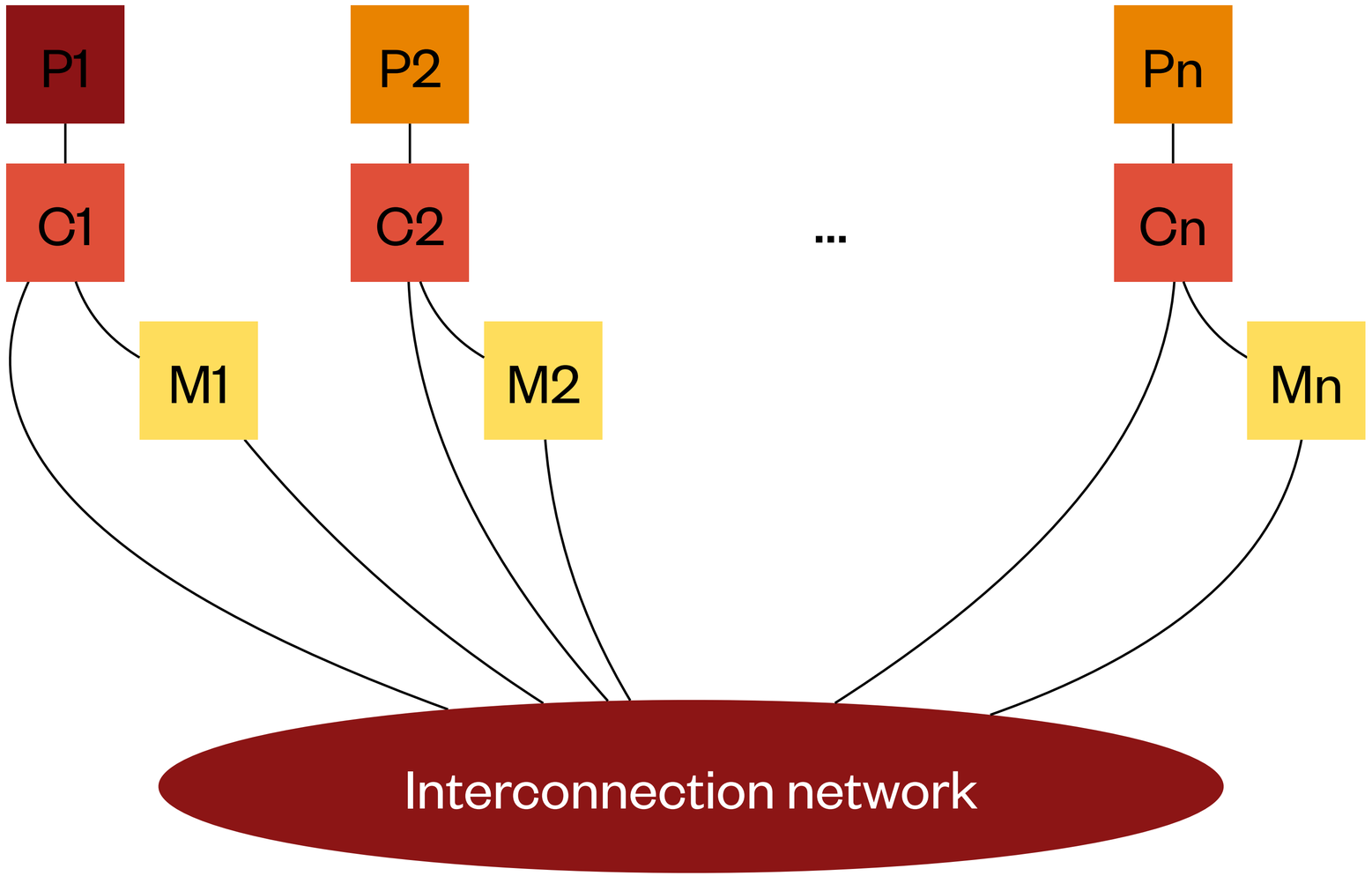
How can we compute the final reduction efficiently and in parallel?

Efficient algorithm requires a tree reduction



Counting candies in parallel is more complicated than we initially thought.

Shared memory processor architecture



Processing elements

Shared memory processor architecture

Schematic

- A number of processors or cores
- A shared physical memory (global memory)
- An interconnection network to connect the processors with the memory

Consequence: multicore performance

- Memory is key to developing high-performance multicore applications
- More cores does not necessarily mean faster execution
- **Memory traffic and time to access memory are often more important than flops**
- Memory is hierarchical and complex

Our teaching platform

- Google Colab
- Allows running CPU and GPU sample codes in the cloud with no setup required!
- Demo: colab_demo.ipynb

OpenMP and OpenACC

In this workshop, we will focus on two solutions:

- OpenMP to program multicore processors
- OpenACC to program GPUs

OpenMP makes scientific multithreaded programming very easy!

- OpenMP simplifies the programming significantly.
- In many cases, adding one line is sufficient to make it run in parallel.
- OpenMP is the standard approach in scientific computing for multicore processors.

Goals of OpenMP

Standardization:

- Provide a standard among a variety of shared memory architectures/platforms
- Jointly defined and endorsed by a group of major computer hardware and software vendors

Simple but powerful:

- Establish a simple and limited set of directives for programming shared memory machines.
- Significant parallelism can be implemented by using just 3 or 4 directives.
- This goal is becoming less true with each new release, unfortunately.

Goals of OpenMP

Ease of use:

- Provide the capability to incrementally parallelize a serial program
- Provide the capability to implement both coarse-grained and fine-grained parallelism

Portability:

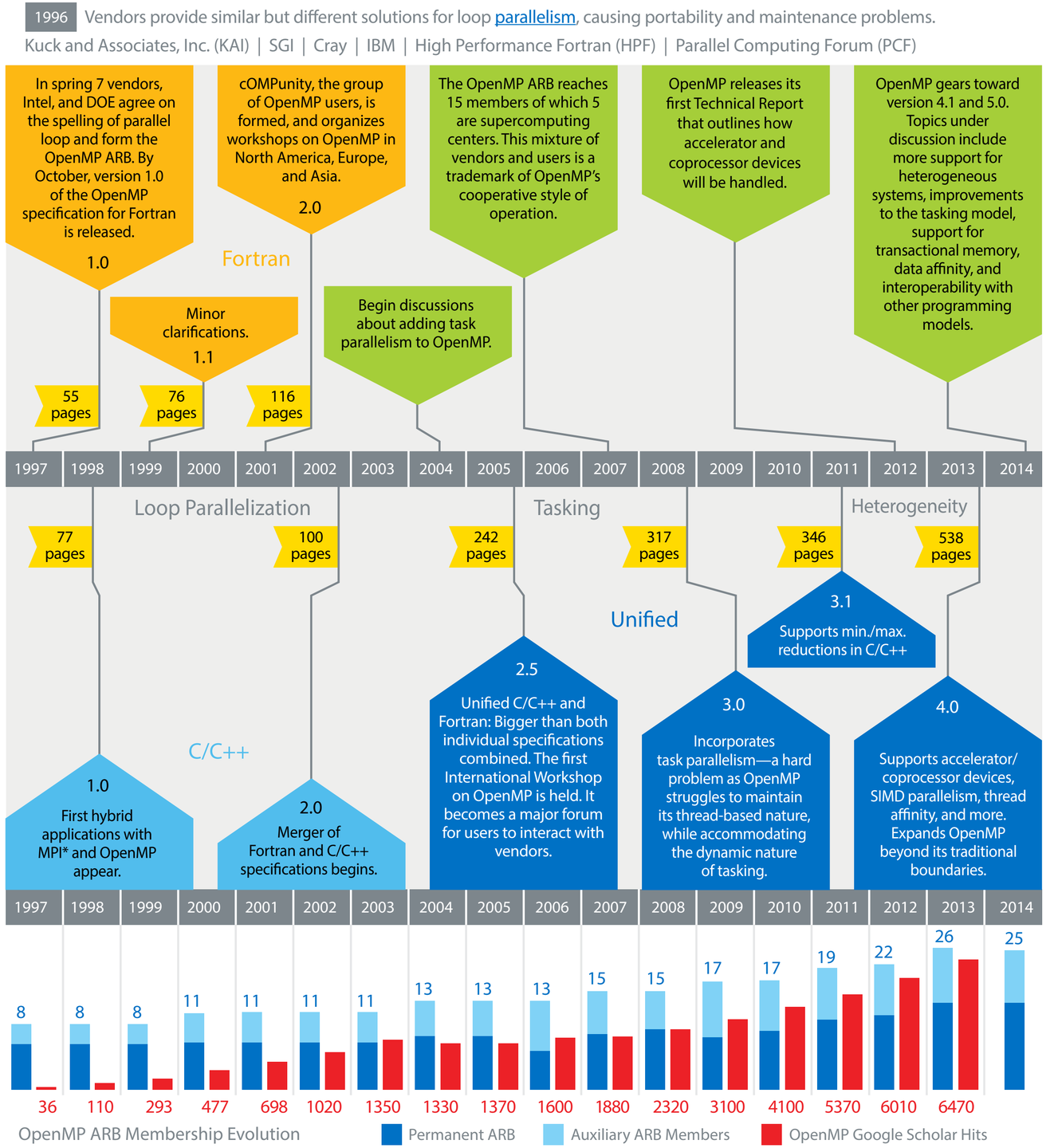
- The API is specified for C/C++ and Fortran
- Public forum for API and membership
- Most major platforms have been implemented, including Unix/Linux platforms and Windows

Reference material

- OpenMP website https://openmp.org
- Wikipedia https://en.wikipedia.org/wiki/OpenMP
- LLNL tutorial https://hpc-tutorials.llnl.gov/openmp
- Intel https://www.intel.com/content/dam/www/public/apac/xa/en/pdfs/ssg/Programming_with_OpenMP-Linux.pdf

History of OpenMP

https://www.openmp.org/uncategorized/openmp-timeline/



Hello World example

Let's take a simple piece of code to get started:

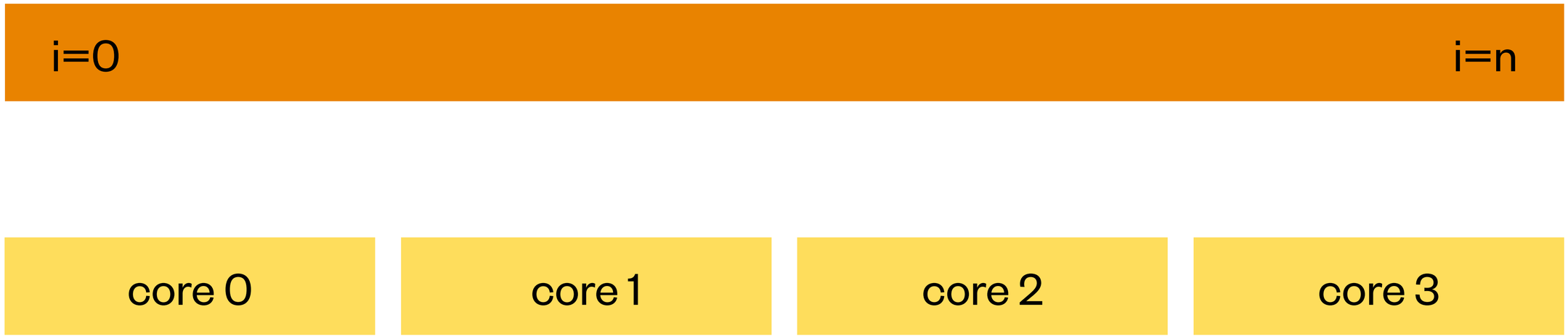
```
for (int i = 0; i < n; ++i) {
  x[i] = i;
  y[i] = std::sqrt(float(i));
}
for (int i = 0; i < n; ++i) z[i] = x[i] + 2. * y[i];
```

How can we parallelize this code?

- Assume you have multiple cores that can do computation in parallel.
- The for loop can be split across the cores and each core can compute a small chunk of the iterations

```
for (int i = 0; i < n; ++i) {
  x[i] = i;
  y[i] = std::sqrt(float(i));
}
```

How can we parallelize this code?



We can distribute the computation across the different cores using OpenMP.

OpenMP code

Let's parallelize the first loop that calculates x[i] and y[i].

```
  const int num_threads = 4;
  omp_set_num_threads(num_threads);
#pragma omp parallel for
  for (int i = 0; i < n; ++i) {
    x[i] = i;
    y[i] = std::sqrt(float(i));
    core[i] = omp_get_thread_num();
  }
  for (int i = 0; i < n; ++i)
    printf("Iteration %d was computed by thread %d\n", i, core[i]);
```

Output

```
Iteration 0 was computed by thread 0
Iteration 1 was computed by thread 0
Iteration 2 was computed by thread 1
Iteration 3 was computed by thread 1
Iteration 4 was computed by thread 2
Iteration 5 was computed by thread 2
Iteration 6 was computed by thread 3
Iteration 7 was computed by thread 3
```

Unit testing

Writing HPC code for scientific applications is not easy.

Thinking in parallel is much more complicated that thinking sequentially and is error-prone.

An important strategy to find errors is to use unit testing:

- Write a small piece of code in a function
- Immediately test that the function works as expected

Googletest

An excellent library for unit testing is Googletest.

It provides a simple infrastructure to write and manage tests.

Let's learn how it works and how to use it.

Example of test

Function to initialize a vector:

```
void init_i() {
  for (int i = 0; i < n; ++i) x[i] = i;
}
```

How to write a unit test

- Use the macro TEST
- Use testing macros like ASSERT_EQ.

```
TEST(demoTest, init) {
  init_i();
  for (int i = 0; i < n; ++i) ASSERT_EQ(x[i], float(i));
}
```

Beware of roundoff errors

- Calculations on a computer are not exact.
- A small roundoff error is generated by each operation.
- Approximate number of accurate digits depending on the precision of the floating point format:

Single precision	Double precision
~ 7.2	~ 15.9

“Exact” test

This test does not suffer from roundoff errors.

```
void init_1() {
  for (int i = 0; i < n; ++i) x[i] = 1;
}
void sum_x() {
  sum = 0;
  for (int i = 0; i < n; ++i) sum += x[i];
}
TEST(demoTest, sum) {
  init_1();
  sum_x();
  ASSERT_EQ(sum, float(n));
}
```

With larger numbers, roundoff errors start appearing

```
void init_i() {
  for (int i = 0; i < n; ++i) x[i] = i;
}
void sum_x() {
  sum = 0;
  for (int i = 0; i < n; ++i) sum += x[i];
}
TEST(demoTest, sum_i) {
  init_i();
  sum_x();
  const float expd = float(n * (n - 1) / 2.);
  ASSERT_NEAR(sum, expd, n * expd * mach_eps);
  printf("Roundoff errors are equal to: %g; tolerance threshold: %g.\n",
         abs((sum - expd) / expd), n * mach_eps);
}
```

```
Roundoff errors are equal to: 4.20842e-05; tolerance threshold:
0.00119209.
```

Is my calculation accurate?

In practice, determining whether a calculation is “correct” or not can be difficult.

Is the difference due to a coding error or is it a roundoff error?

```
TEST(ompTest, omp_loop) {
#pragma omp parallel for
  for (int i = 0; i < n; ++i) {
    x[i] = i;
    y[i] = i * i;
  }
  for (int i = 0; i < n; ++i) {
    ASSERT_EQ(x[i], i);
    ASSERT_EQ(y[i], i * i);
  }
#pragma omp parallel for
  for (int i = 0; i < n; ++i) {
    z[i] = x[i] + y[i];
  }
  for (int i = 0; i < n; ++i) {
    ASSERT_EQ(z[i], (float)(i + i * i));
  }
}
```

Let's test our OpenMP Hello World!

```
Running main() from googletest-main/googletest/src/gtest_main.cc
[==========] Running 4 tests from 1 test suite.
[----------] Global test environment set-up.
[----------] 4 tests from ompTest
[ RUN      ] ompTest.omp_loop
[       OK ] ompTest.omp_loop (0 ms)
[ RUN      ] ompTest.omp_reduction
[       OK ] ompTest.omp_reduction (0 ms)
[ RUN      ] ompTest.omp_schedule
[       OK ] ompTest.omp_schedule (0 ms)
[ RUN      ] ompTest.omp_collapse
[       OK ] ompTest.omp_collapse (0 ms)
[----------] 4 tests from ompTest (1 ms total)

[----------] Global test environment tear-down
[==========] 4 tests from 1 test suite ran. (1 ms total)
[  PASSED  ] 4 tests.
```

More on OpenMP

- OpenMP is a vast topic with a lot of additional functionalities.
- We will only review some of the main features.
- An important one is the reduction operator.

Reduction

Consider the following code:

```
float sum = 0;
for (int i = 0; i < n; ++i) {
  sum += x[i];
}
```

Race condition

```
    sum += x[i];
```

If multiple cores attempt to update the variable sum at the same time, the result becomes undetermined.

This will lead to an erroneous result. This is a bug!

OpenMP reduction

We need to tell the compiler that sum should be computed differently.

Adding numbers is called a reduction operation.

We have to use the OpenMP **reduction** clause to get a correct code.

Reduction clause

```
  float sum = 0;
#pragma omp parallel for reduction(+ : sum)
  for (int i = 0; i < n; ++i) {
    sum += x[i];
  }
```

- The final result will now be correct.
- Other reduction operators: -, *, max, min
- + logical and boolean operators

How should we schedule loops?

- Loop scheduling is critical for performance.
- OpenMP has extensive functionalities to improve performance of for loop executions.
- This can be achieved by specifying different loop scheduling policies.

Example of static policy

```
#pragma omp parallel for schedule(static, 32)
  for (int i = 0; i < n; ++i) {
    z[i] = x[i] + y[i];
  }
```

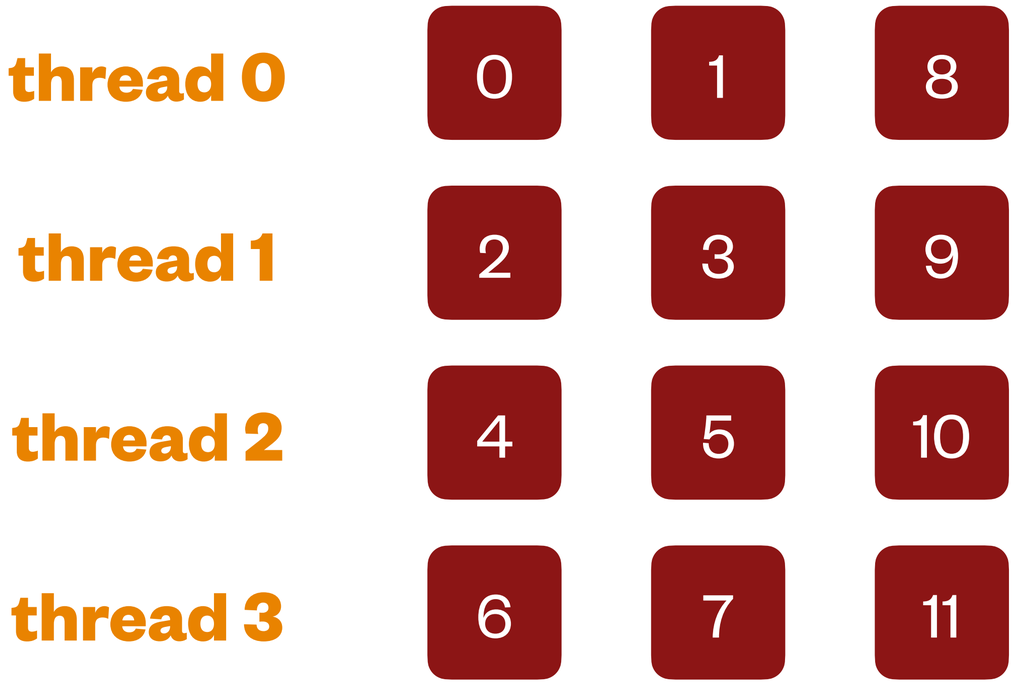
So what does this mean?

schedule(static, 1)

```
#pragma omp parallel for schedule(static, 1)
```

schedule(static, 2)

```
#pragma omp parallel for schedule(static, 2)
```



Example

```
#pragma omp parallel for
  for (int i = 0; i < n; ++i) {
    x[i] = i;
    y[i] = i * i;
  }
#pragma omp parallel for schedule(static, 32)
  for (int i = 0; i < n; ++i) z[i] = x[i] + y[i];

  for (int i = 0; i < n; ++i) ASSERT_EQ(z[i], (float)(i+i*i));
```

schedule(dynamic, 1)

```
#pragma omp parallel for schedule(dynamic, 1)
```

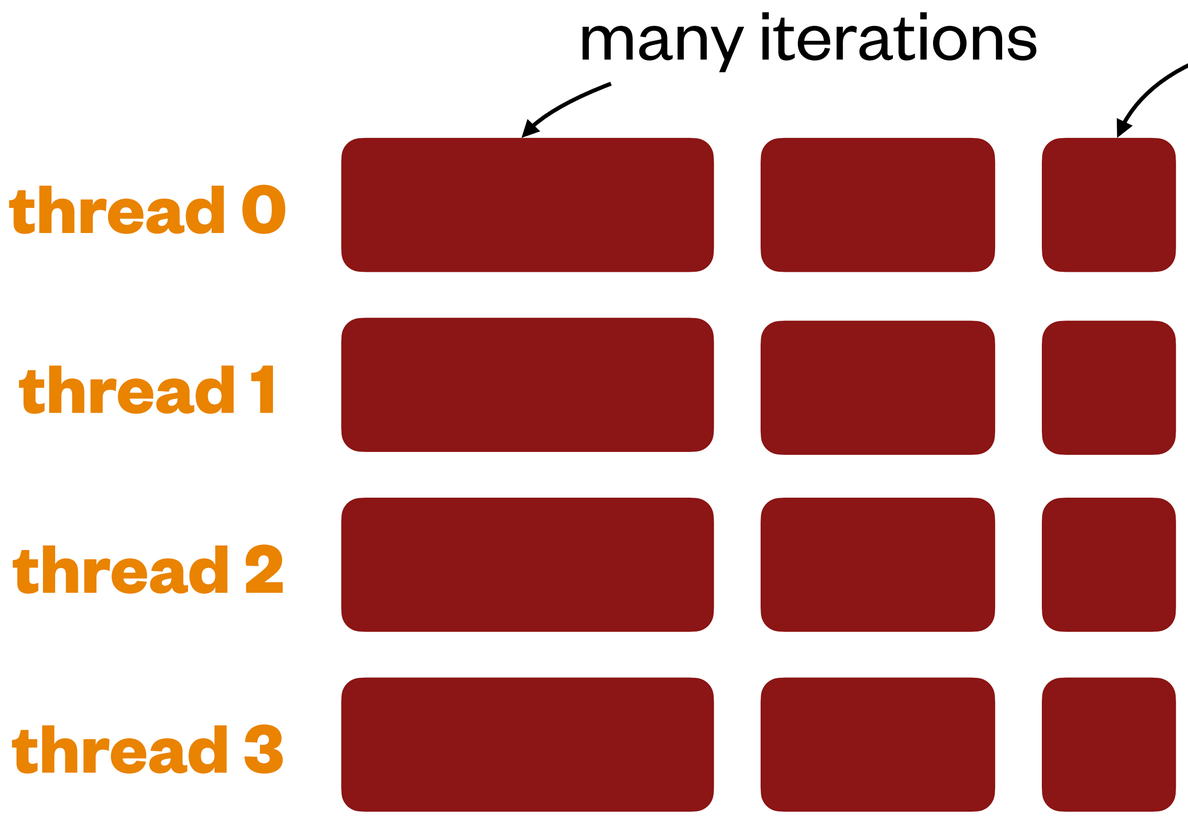
Example

```
#pragma omp parallel for schedule(dynamic, 32)
  for (int i = 0; i < n; ++i) z[i] = x[i] + y[i];

  for (int i = 0; i < n; ++i) ASSERT_EQ(z[i], (float)(i+i*i));
```

schedule(guided)

```
#pragma omp parallel for schedule(guided)
```



- Large iteration chunks are assigned initially.
- As the calculation progresses, smaller chunks are assigned.
- In most cases, this allows all cores to finish their computation at the same time, which is optimal.

Nested loops

- What happens if the number of iterations is small?
- Few iterations are assigned to each core.
- This may lead to a large load imbalance, i.e., one of the cores finishes much later than the others.

Balancing the workload

- In general, it is better to parallelize loops with a lot of iterations.
- This makes it easier for the scheduler to assign work to the cores such that they all finish at around the same time.
- If your loop does not have enough iteration, you have the option of “merging” it with the next nested loop.
- This is called loop collapse in OpenMP.

Example of loop collapse

```
#pragma omp parallel for collapse(2)
  for (int i = 0; i < n0; ++i) {
    for (int j = 0; j < n0; ++j) {
      x[i * n0 + j] = i * n0 + j;
      y[i * n0 + j] = i - j;
    }
  }
  for (int i = 0; i < n; ++i) ASSERT_EQ(x[i], float(i));
  for (int i = 0; i < n0; ++i)
    for (int j = 0; j < n0; ++j) ASSERT_EQ(y[i * n0 + j], float(i - j));
```

Example of loop collapse

```
#pragma omp parallel for collapse(2)
  for (int i = 0; i < n0; ++i)
    for (int j = 0; j < n0; ++j) z[i * n0 + j] = x[i * n0 + j] + y[i * n0 + j];

  for (int i = 0; i < n0; ++i)
    for (int j = 0; j < n0; ++j) ASSERT_EQ(z[i * n0 + j], float(i * (n0 + 1)));
```

Many other OpenMP concepts

- `atomic`
- `critical`
- `single`
- `task`
- `barrier, taskwait`
- …
- Reference guides


RTX 3090
GPUs!
NVIDIA
GEFORCE
RTX

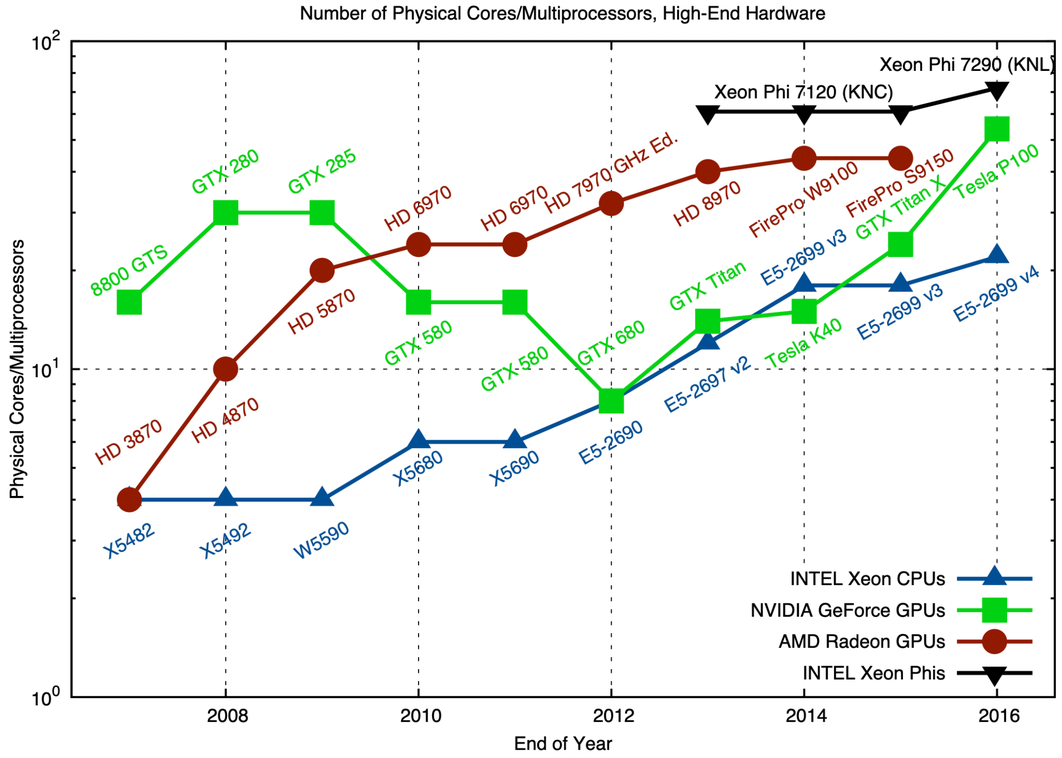
GPU for scientific computing

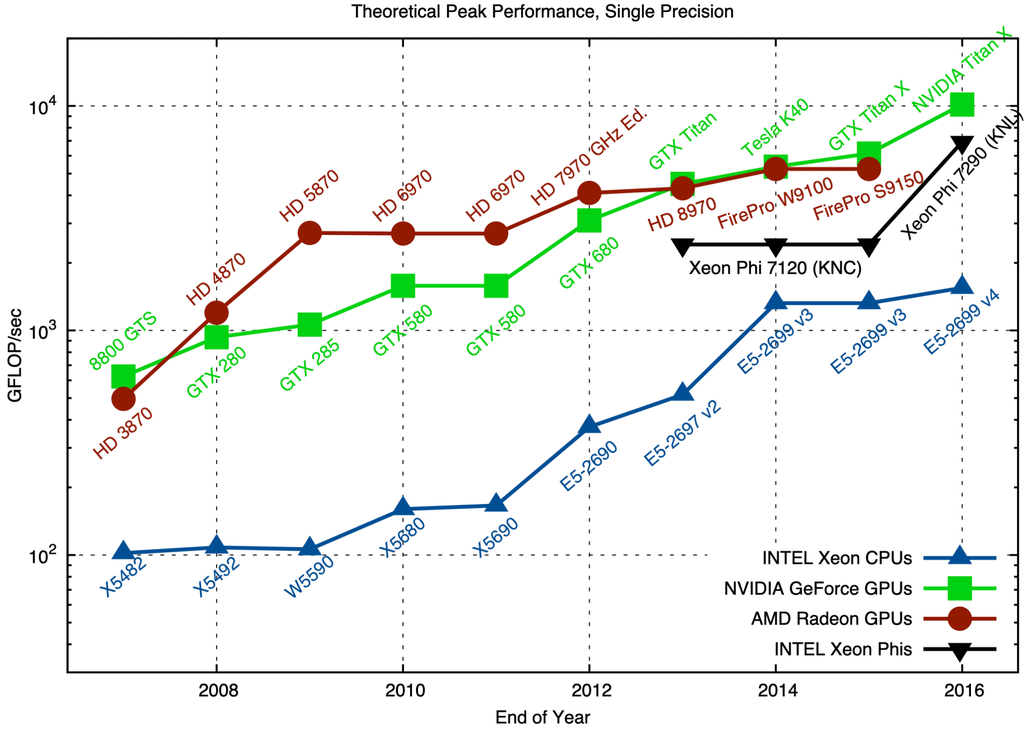
GPUs from NVIDIA and AMD boast significant single and double precision performance due to a very large number of cores.

These are specialized processors that can deliver high-performance but only on certain types of calculations:

- Massive amount of parallel operations
- Must be mostly data parallel
- Requires offloading large chunks of computations to the GPU to amortize the cost of transferring data to/from the GPU.

Performance trends





Karl Rupp

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

History

- GPUs were initially focused on 3D graphics = computing the color of each pixel on the screen based on a 3D model of a scene.
- Featured example: ray tracing global illumination (RTXGI)

GPGPU

General purpose GPU computing:

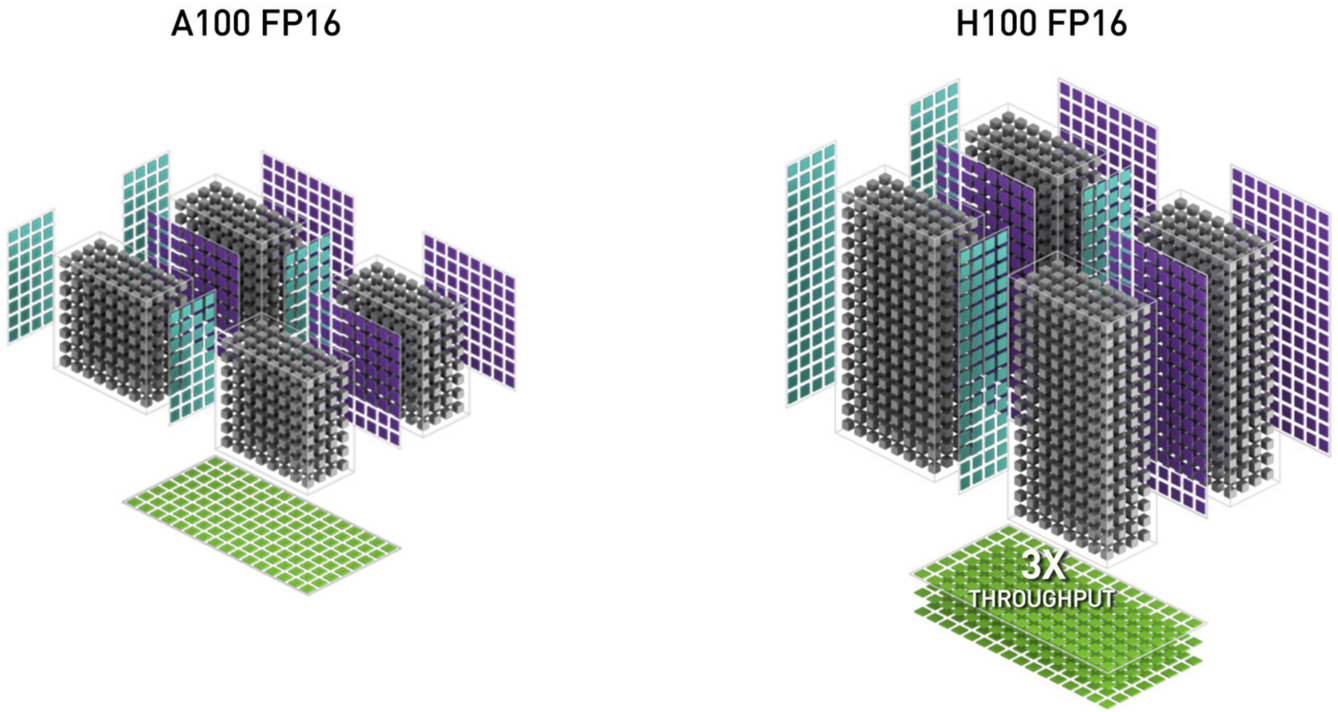
- Extension to general scientific computations.
- Solving equations on a grid is similar to rendering: perform the same regular calculations on a very large dataset.

Deep learning

Recent advances in GPU computing target deep learning.

1. Linear algebra: matrix-matrix multiplications.
2. Varying precision.

Tensor Cores



H100 FP16 Tensor Core has 3x throughput compared to A100 FP16 Tensor Core

GPUs are great for

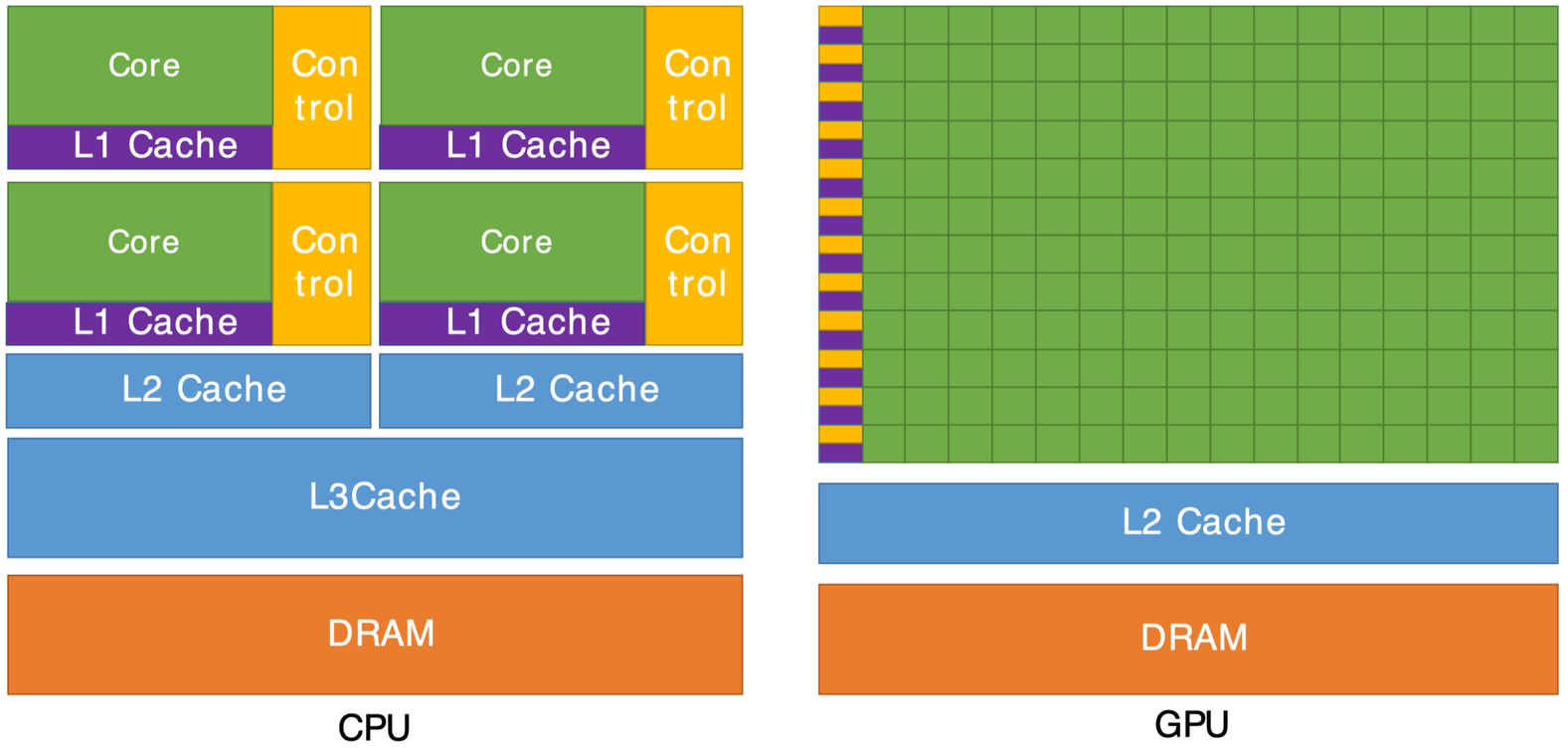
- Dense linear algebra with a massive amount of flops
- Finite-difference and regular grid calculations
- Deep neural networks.

Less suitable for:

- Irregular calculations with branching and irregular workloads
- Long series of sequential operations

What does a GPU processor look like?

Schematic organization



The GPU devotes more transistors to data processing

GH100 with 144 Streaming Multiprocessors (SM)

NVLink allows GPU processors to communicate without using the CPU

GH100 Streaming Multiprocessor (SM)

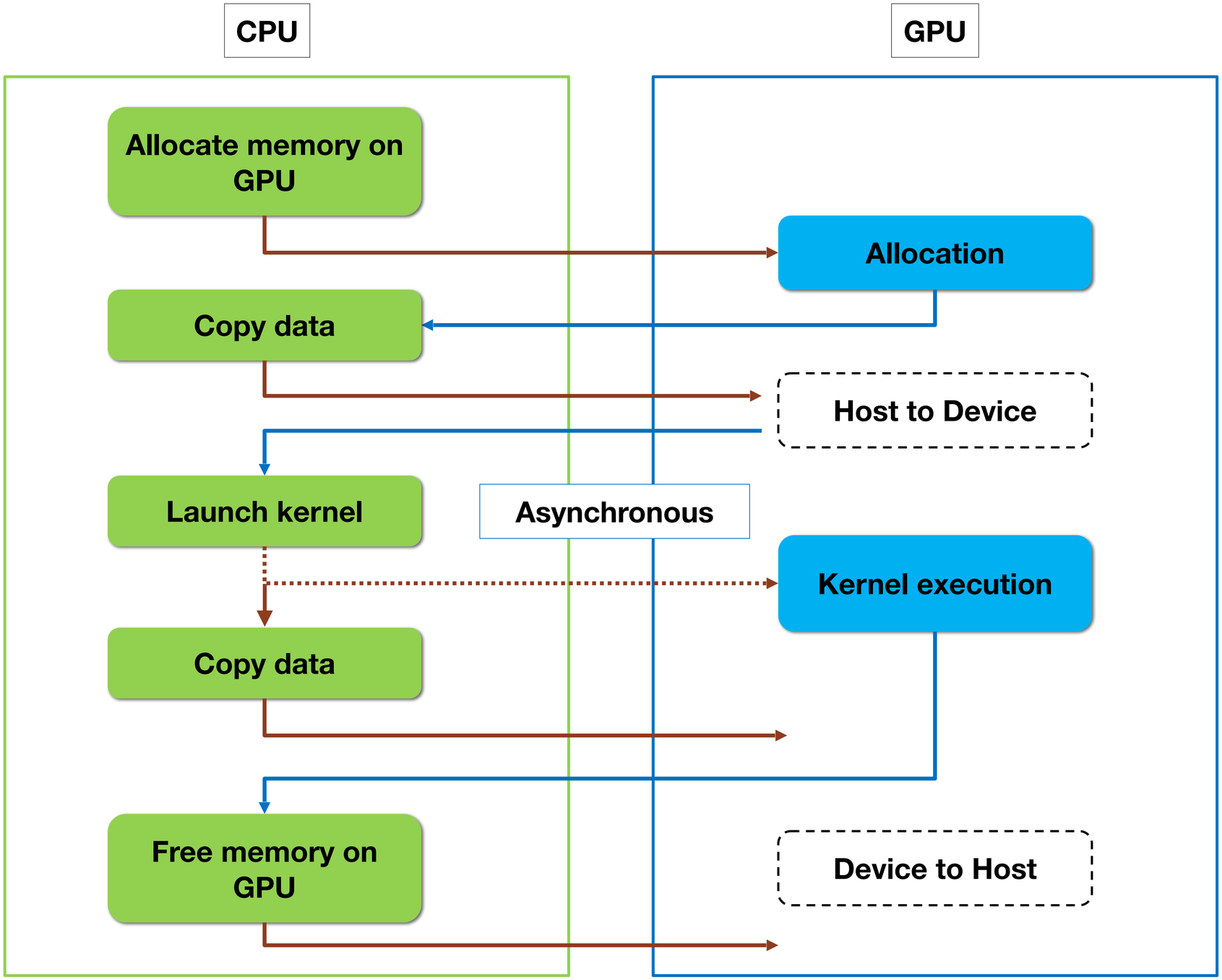
- Special Functions Units (SFUs): execute transcendental instructions such as sin, cosine, reciprocal, and square root.
- Dispatch Unit: instruction dispatch

How to program GPUs
Introduction

GPU processors are co-processors

- GPUs are different from conventional processors.
- They only work as co-processors.
- This means you need a host processor (e.g., Intel Xeon).

- Your program runs on the host and uses an API to move data back and forth to the GPU and run programs on the GPU.
- You cannot log on to the GPU directly or run an OS on the GPU.


CPU
GPU
Allocate memory on GPU
Allocation
Copy data
Host to Device
Launch kernel
Asynchronous
Kernel execution
Copy data
Free memory on GPU
Device to Host

OpenACC

- OpenMP can be used to program GPUs, but this is a recent, less robust addition to the language.
- Support is currently somewhat limited.
- We will cover instead OpenACC, which was designed from the beginning to program GPUs.
- OpenACC = OpenMP for **accelerator** processor.

Other programming solutions

Vendor agnostic:

- OpenCL
- Numba

Vendor specific:

- CUDA
- HIP

OpenCL

- OpenCL: Open Computing Language
- Framework for writing programs that execute across heterogeneous platforms, e.g., GPUs, digital signal processors (DSPs)
- OpenCL provides a standard interface for parallel computing using task- and data-based parallelism.
- OpenCL is an open standard maintained by the non-profit technology consortium Khronos Group.

Python

Python has extensions that allow generating GPU code.

Example: Numba

Numba

Many uses.

Just-in-time compilation of Python code for performance:

```
from numba import jit
import random

@jit(nopython=True)
def monte_carlo_pi(nsamples):
    acc = 0
    for i in range(nsamples):
        x = random.random()
        y = random.random()
        if (x ** 2 + y ** 2) < 1.0:
            acc += 1
    return 4.0 * acc / nsamples
```

Numba multi-threaded programming

Example of **parallel** for loop in Numba:

```
@jit(nopython=True, parallel=True)
def simulator(out):
    # iterate loop in parallel
    for i in prange(out.shape[0]):
        out[i] = run_sim()
```

Numba for NVIDIA GPUs (CUDA)

```
from numba import cuda, float32

@cuda.jit
def matmul(A, B, C):
    i, j = cuda.grid(2)
    if i < C.shape[0] and j < C.shape[1]:
        tmp = 0.
        for k in range(A.shape[1]):
            tmp += A[i, k] * B[k, j]
        C[i, j] = tmp
```

Numba for AMD ROC GPUs

```
from numba import roc, float32

@roc.jit
def matmul(A, B, C):
    i = roc.get_global_id(0)
    j = roc.get_global_id(1)
    if i < C.shape[0] and j < C.shape[1]:
        tmp = 0.
        for k in range(A.shape[1]):
            tmp += A[i, k] * B[k, j]
        C[i, j] = tmp
```

Vendor specific solutions

NVIDIA CUDA

- Currently the standard with writing GPU code.
- Only targets NVIDIA GPU.
- Very mature and robust.
- But complex to use and requires major code changes
- Initial release: June 23, 2007 (14 years ago)

AMD GPUs

- AMD has a proprietary language for programming its GPUs called **HIP**.
- HIP can generate code for AMD and NVIDIA GPUs.
- HIP is close to CUDA.
- HIP is designed to allow developers to easily convert CUDA code.
- Part of the open-source **ROCm** stack

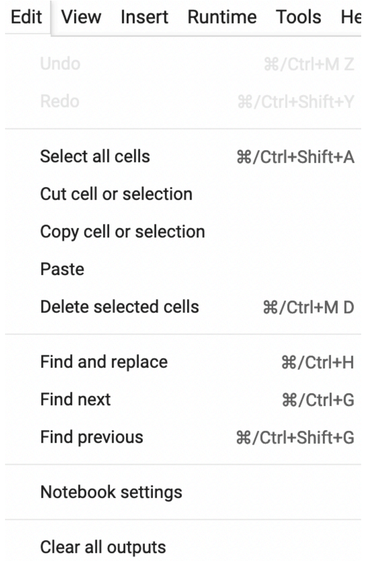
Let’s get started with OpenACC

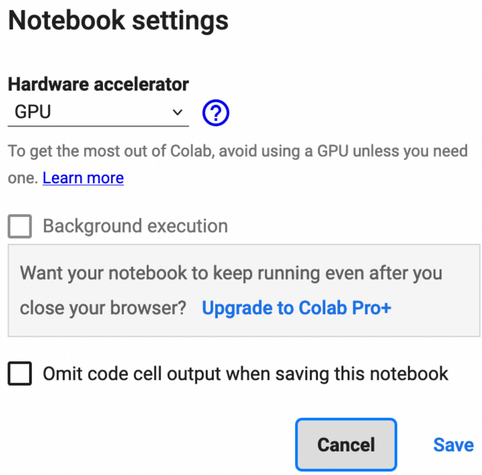
GPU access

First, you will need a GPU!

Go to: Notebook settings

Then select GPU under Hardware accelerator





Hardware

You should be able to test which GPU you have access to:

```
[2]   1 !nvidia-smi --query-gpu=gpu_name,gpu_bus_id,vbios_version --format=csv
```

```
name, pci.bus_id, vbios_version
Tesla T4, 00000000:00:04.0, 90.04.A7.00.01
```

Installation

You will need to install the NVIDIA HPC SDK, which contains the OpenACC compiler and can generate code for NVIDIA GPUs.

Run the cells at the beginning of the notebook to install:

1. install_hpc.sh: installs the NVIDIA HPC SDK
2. install_gtest.sh: installs Google Test

The installation will take a few minutes.

Our first GPU parallel loop

Very similar to OpenMP (at least in appearance)

```
  const int n = 32000000;
  float* x = new float[n];

#pragma acc parallel loop
  for (int i = 0; i < n; ++i) x[i] = i;

  for (int i = 0; i < n; ++i) ASSERT_EQ(x[i], float(i));
```

Let's see what the compiler says

```
acc_lab.cpp:
accTest_loop_Test::TestBody():
      7, Generating NVIDIA GPU code
         10, #pragma acc loop gang, vector(128) /* blockIdx.x threadIdx.x */
      7, Generating implicit copyout(x[:32000000]) [if not already present]
```

What are these messages saying?

Let's focus on gang/vector first.

Gang, worker, vector

This is less important for us.

These variables were added because they reflect the way the hardware is organized.

Thread: smallest execution unit in the program.

Gang, worker, vector

Vector: a group of threads that can coordinate and execute "together"

Worker: a group of vectors that can coordinate and execute "together;" this is a less important concept

Gang: a group of workers

Gang, worker, vector

For optimization purposes, the sizes of a vector, worker, or gang can be specified.

This is a more advanced optimization.

```
#pragma acc parallel loop num_gangs(40) num_workers(32) vector_length(32)
  for (int i = 0; i < n; ++i) x[i] = i;
```

```
accTest_vector_loop_Test::TestBody():
     37, Generating NVIDIA GPU code
         40, #pragma acc loop gang(40), worker(32), vector(32) /* blockIdx.x threadIdx.y threadIdx.x */
     37, Generating implicit copyout(x[:32000000]) [if not already present]
```

CPU and GPU memories

The memory of the CPU and the GPU are physically separate.

So data needs to be transferred between the two memories before a calculation can be run on the GPU.

In this case, the compiler detected that x was initialized on the GPU.

So it automatically generated instructions to copy the result back from the GPU to the CPU memory.

Data transfer options

```
#pragma acc parallel loop copyout(x[:n])
  for (int i = 0; i < n; ++i) x[i] = i;
```

Clause	Description
`copy`	create space, initialize by copying to the device, copy back to host at the end, release device memory
`copyin`	same but without copy back to host
`copyout`	same but without initial copy to the device
`create`	create space at the beginning, release at the end
`present`	no action taken

Array shaping

```
#pragma acc parallel loop copyout(x[:n])
```

`x[:n]`

- `copy(array[starting_index:length])`
- The first number is the start index of the array
- The second number is how much data is to be transferred.

Data locality

- (x,y) initialization
- Vector z computation

```
for (int i = 0; i < n; ++i) {
  x[i] = i;
  y[i] = i * i;
}
for (int i = 0; i < n; ++i) {
  ASSERT_EQ(x[i], float(i));
  ASSERT_EQ(y[i], float(i * i));
}
for (int i = 0; i < n; ++i) z[i] = x[i] + y[i];
for (int i = 0; i < n; ++i) ASSERT_EQ(z[i], float(i * (i + 1)));
```

Data transfer

By default, the code would:

- Copy (x,y) to the device.
- Copy them back to the host for testing.
- Copy (x,y) again to the device.
- Copy z to the host.

The copies of (x,y) can be optimized.

acc enter data

```
#pragma acc enter data create(x[:n], y[:n])
#pragma acc parallel loop
  for (int i = 0; i < n; ++i) {
    x[i] = i;
    y[i] = i * i;
  }
```

`enter data create`

- create the data on the GPU and leave it there until instructed to delete the data

acc update self

```
#pragma acc update self(x[:n], y[:n])
  for (int i = 0; i < n; ++i) {
    ASSERT_EQ(x[i], float(i));
    ASSERT_EQ(y[i], float(i * i));
  }
```

- Because we used `enter data` create, the data is not automatically copied back to the host.
- We need to add `update self` to copy the data from device to host.
- Also
  - `#pragma acc update device()`

acc exit data

```
#pragma acc exit data delete(x[:n], y[:n])
```

- Because we used `enter data` create, the data is not automatically copied back to the host.
- We need to add `update self` to copy the data from device to host.

Full code

```
#pragma acc enter data create(x[:n], y[:n])
#pragma acc parallel loop
  for (int i = 0; i < n; ++i) {
    x[i] = i;
    y[i] = i * i;
  }

#pragma acc update self(x[:n], y[:n])
  for (int i = 0; i < n; ++i) {
    ASSERT_EQ(x[i], float(i));
    ASSERT_EQ(y[i], float(i * i));
  }

#pragma acc parallel loop copyout(z[:n])
  for (int i = 0; i < n; ++i) z[i] = x[i] + y[i];

#pragma acc exit data delete (x[:n], y[:n])

  for (int i = 0; i < n; ++i) ASSERT_EQ(z[i], float(i * (i + 1)));
```

Reduction

As in OpenMP, we need to use a special construct when we have a reduction.

```
sum += x[i];
```

Otherwise, the different cores will attempt to access and modify `sum` at the same time, which is a bug.

Reduction example

```
  float sum = 0;
#pragma acc data create(x[:n])
  {
#pragma acc parallel loop
    for (int i = 0; i < n; ++i) x[i] = 1;
#pragma acc parallel loop reduction(+ : sum)
    for (int i = 0; i < n; ++i) sum += x[i];
  }
  for (int i = 0; i < n; ++i) ASSERT_EQ(sum, float(n));
```

Note the `data create` to avoid unnecessary copies.

collapse

- GPU are massively parallel processors.
- They can contain thousands of cores.
- Example: GeForce RTX 3090 Ti: 10,752 cores.
- So we need to generate as much concurrency (parallelism) in our code.
- Loop fusion is critical for performance when the number of iterations is not large enough.

for loop with collapse

```
#pragma acc parallel loop collapse(2)
  for (int i = 0; i < n; ++i) {
    for (int j = 0; j < n; ++j) {
      z[i * n + j] = x[i * n + j] + y[i * n + j];
    }
  }
```

- i and j loops will be merged and executed in parallel.
- Without collapse, only the i loop is parallelized while the j loop is executed sequentially.
- collapse allows generating n*n parallel threads instead of just n.
- This can potential improve performance significantly.

Complete example with collapse

```
#pragma acc enter data create(x[:n * n], y[:n * n])
#pragma acc parallel loop collapse(2)
  for (int i = 0; i < n; ++i)
    for (int j = 0; j < n; ++j) {
      x[i * n + j] = i * n + j;
      y[i * n + j] = i - j;
    }

#pragma acc update self(x[:n * n], y[:n * n])
  for (int i = 0; i < n * n; ++i) ASSERT_EQ(x[i], float(i));
  for (int i = 0; i < n; ++i)
    for (int j = 0; j < n; ++j) ASSERT_EQ(y[i * n + j], float(i - j));

#pragma acc parallel loop collapse(2) copyout(z[:n * n])
  for (int i = 0; i < n; ++i)
    for (int j = 0; j < n; ++j) z[i * n + j] = x[i * n + j] + y[i * n + j];

#pragma acc exit data delete(x[:n * n], y[:n * n])
  for (int i = 0; i < n; ++i)
    for (int j = 0; j < n; ++j) ASSERT_EQ(z[i * n + j], float(i * (n + 1)));
```

n body problem

Let's look at a more complex real-life application.

We want to model the gravitational interactions between n bodies with mass.

This is similar to modeling the motions of the planets around the sun in the solar system.

Gravitational force

We start from: $F_i = m_i a_i$.

The acceleration is given by the gravitational force:

$$F_i = m_i \sum_j m_j \frac{r_j - r_i}{\|r_j - r_i\|_2^3}$$

Equations of motion

$$F_i = m_i \sum_j m_j \frac{r_j - r_i}{\|r_j - r_i\|_2^3}$$

Equations of motion:

$$\frac{d^2 r_i}{dt^2} = \sum_j m_j \frac{r_j - r_i}{\|r_j - r_i\|_2^3}$$

Time integrator

We numerically solve these equations using the velocity Verlet time integrator.

It's not very accurate, but it is very stable over many time steps.

This is a two-step method.

Velocity Verlet

- Step 1: advance the velocity
- $$v_i^{n+1} = v_i^n + \Delta t \sum_j m_j \frac{r_j - r_i}{\|r_j - r_i\|_2^3}\Bigg|_n$$
- Step 2: advance the position
- $$r_i^{n+1} = r_i^n + \Delta t\, v_i^{n+1}$$
- Repeat

Force computation

```
for (int i = 0; i < n; i++) {
  real fx, fy, fz; fx = fy = fz = 0;
  for (int j = 0; j < n; j++) {
    real3 ff = forceComputation(pos[i].x, pos[i].y, pos[i].z,
                                pos[j].x, pos[j].y, pos[j].z, pos[j].w);
    fx += ff.x;
    fy += ff.y;
    fz += ff.z;
  }
  force[i].x = fx;
  force[i].y = fy;
  force[i].z = fz;
}
```

Time step

```
  for (int i = 0; i < n; i++) {
    // acceleration = force / mass;
    // new velocity = old velocity + acceleration * deltaTime
    vel[i].x += force[i].x * dt;
    vel[i].y += force[i].y * dt;
    vel[i].z += force[i].z * dt;

    // new position = old position + velocity * deltaTime
    pos[i].x += vel[i].x * dt;
    pos[i].y += vel[i].y * dt;
    pos[i].z += vel[i].z * dt;
  }
```

Time integration

```
for (int i = 0; i < iterations; i++) {
  seqIntegrate(pos, vel, force, dt, n);
}
```

Parallel time stepping loop

```
#pragma acc data copy(pos[:n], vel[:n]) copyout(force[:n])
  for (int i = 0; i < iterations; i++) {
    integrate(pos, vel, force, dt, n);
  }
```

- Optimize the movement of data by reducing memory copies between host and device.
- Only done before the iterations start and after they complete.

Nested parallel loops with reduction

```
#pragma acc parallel loop
  for (int i = 0; i < n; i++) {
    real fx, fy, fz;
    fx = fy = fz = 0;
#pragma acc loop reduction(+ : fx, fy, fz)
    for (int j = 0; j < n; j++) {
      real3 ff = forceComputation(pos[i].x, pos[i].y, pos[i].z, pos[j].x,
                                  pos[j].y, pos[j].z, pos[j].w);
      fx += ff.x;
      fy += ff.y;
      fz += ff.z;
    }
    force[i].x = fx;
    force[i].y = fy;
    force[i].z = fz;
  }
```

Parallel time stepping

```
#pragma acc parallel loop
  for (int i = 0; i < n; i++) {
    vel[i].x += force[i].x * dt;
    vel[i].y += force[i].y * dt;
    vel[i].z += force[i].z * dt;
    pos[i].x += vel[i].x * dt;
    pos[i].y += vel[i].y * dt;
    pos[i].z += vel[i].z * dt;
  }
```

Performance results

```
!name=nbody; nvc++ -I. -acc=host -O -o $name $name.cpp && ./$name 4096 20
!name=nbody; nvc++ -I. -acc=multicore -O -o $name $name.cpp && ./$name 4096 20
!name=nbody; nvc++ -I. -acc=gpu -O -o $name $name.cpp && ./$name 4096 20
!name=nbody; nvc++ -I. -mp=multicore -O -o $name $name.cpp && ./$name 4096 20
!name=nbody; g++ -std=c++17 -I. -O -o $name $name.cpp && ./$name 4096 20
```

```
n = 4096 bodies for 20 iterations
OpenACC:        2185.000000 ms: 3.071344 GFLOP/s
Sequential:     2206.000000 ms: 3.042106 GFLOP/s
n = 4096 bodies for 20 iterations
OpenACC:        1959.000000 ms: 3.425669 GFLOP/s
Sequential:     2197.000000 ms: 3.054568 GFLOP/s
n = 4096 bodies for 20 iterations
OpenACC:        380.000000 ms: 17.660228 GFLOP/s
Sequential:     2155.000000 ms: 3.114100 GFLOP/s
n = 4096 bodies for 20 iterations
OpenMP:         2197.000000 ms: 3.054568 GFLOP/s
Sequential:     2169.000000 ms: 3.094000 GFLOP/s
n = 4096 bodies for 20 iterations
c++:            4257.000000 ms: 1.576436 GFLOP/s
Sequential:     4257.000000 ms: 1.576436 GFLOP/s
```

We only use a single CPU thread on Google compute.

```
1 !name=test_nbody; nvc++ -I. -acc=gpu -o $name $name.cpp gtest_main.a && ./$name
```

```
test_nbody.cpp:
Running main() from googletest-main/googletest/src/gtest_main.cc
[==========] Running 5 tests from 1 test suite.
[----------] Global test environment set-up.
[----------] 5 tests from nbodyTest
[ RUN      ] nbodyTest.iterations_small_0
8 tests PASSED. Maximum error = 0.
6 tests PASSED. Maximum error = 0.
6 tests PASSED. Maximum error = 0.
[       OK ] nbodyTest.iterations_small_0 (259 ms)
[ RUN      ] nbodyTest.iterations_small_1
128 tests PASSED. Maximum error = 1.13687e-13.
96 tests PASSED. Maximum error = 9.31323e-10.
96 tests PASSED. Maximum error = 7.45058e-09.
[       OK ] nbodyTest.iterations_small_1 (0 ms)
[ RUN      ] nbodyTest.iterations_medium_0
4096 tests PASSED. Maximum error = 2.27374e-13.
3072 tests PASSED. Maximum error = 1.49012e-08.
3072 tests PASSED. Maximum error = 1.49012e-07.
[       OK ] nbodyTest.iterations_medium_0 (14 ms)
[ RUN      ] nbodyTest.iterations_medium_1
4096 tests PASSED. Maximum error = 4.76837e-07.
3072 tests PASSED. Maximum error = 3.8147e-06.
3072 tests PASSED. Maximum error = 1.22935e-07.
[       OK ] nbodyTest.iterations_medium_1 (32 ms)
[ RUN      ] nbodyTest.iterations_large
16384 tests PASSED. Maximum error = 5.96046e-07.
12288 tests PASSED. Maximum error = 3.8147e-06.
12288 tests PASSED. Maximum error = 4.02331e-07.
[       OK ] nbodyTest.iterations_large (457 ms)
[----------] 5 tests from nbodyTest (764 ms total)

[----------] Global test environment tear-down
[==========] 5 tests from 1 test suite ran. (764 ms total)
[  PASSED  ] 5 tests.
```

Accuracy

Roundoff errors between CPU and GPU in single precision

We hope you enjoyed this class!