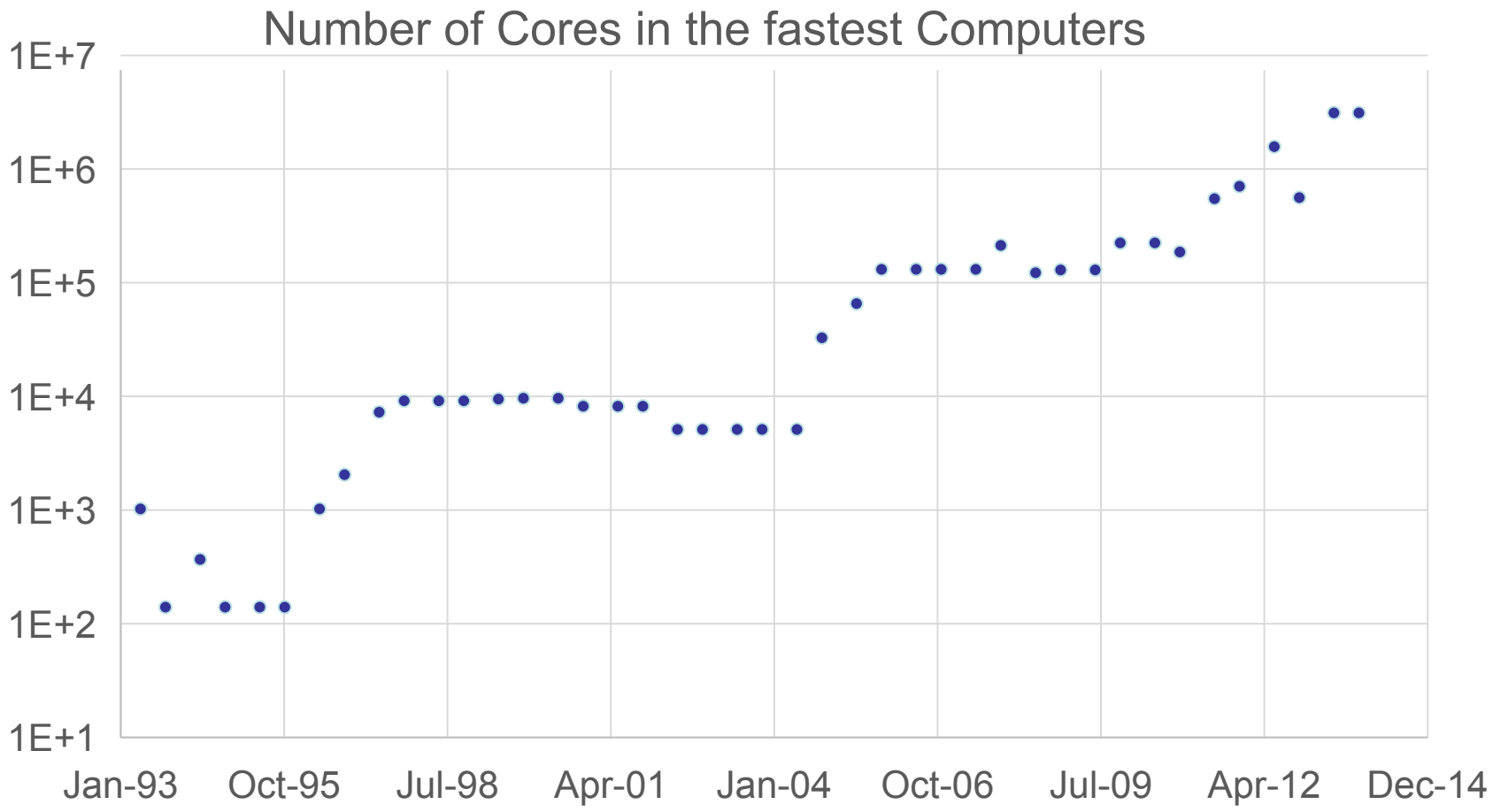
Introduction to High-Performance Computing

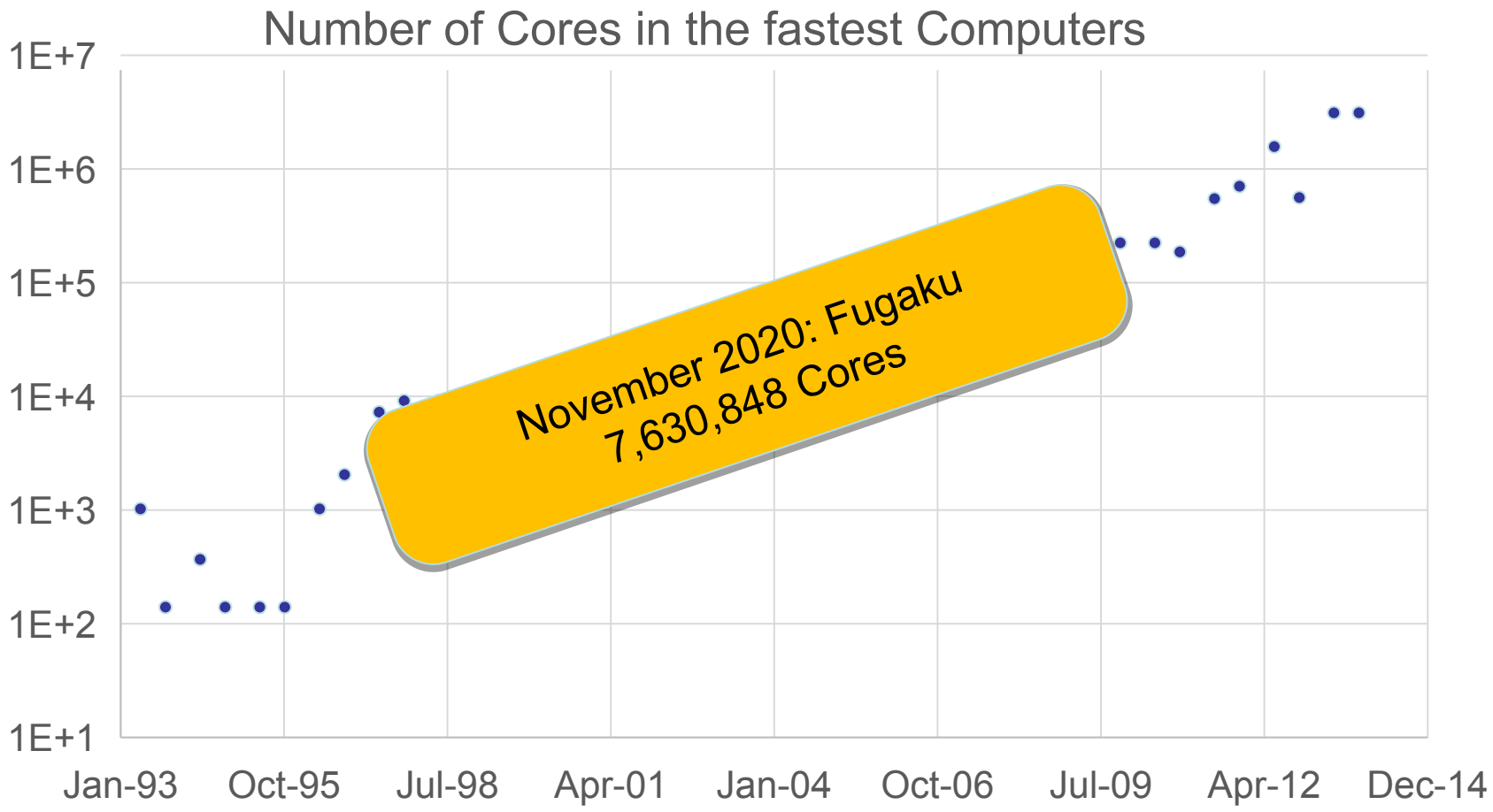
Session 04

Introduction to Parallel Computing

Why Parallel Computing?

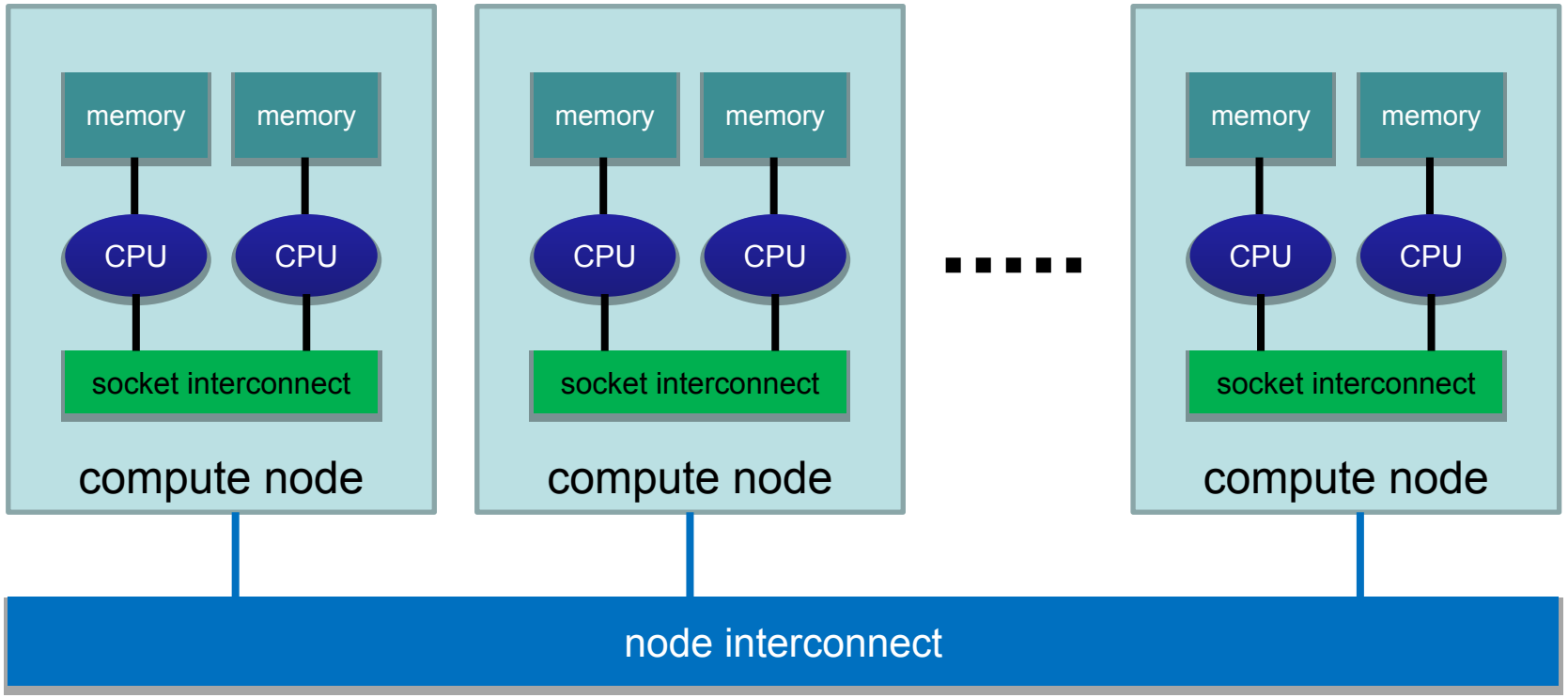


Why Parallel Computing?



Parallel Hardware Architectures

- most modern HPC systems (e.g. CARL and EDDY) are clusters of SMP/ccNUMA nodes

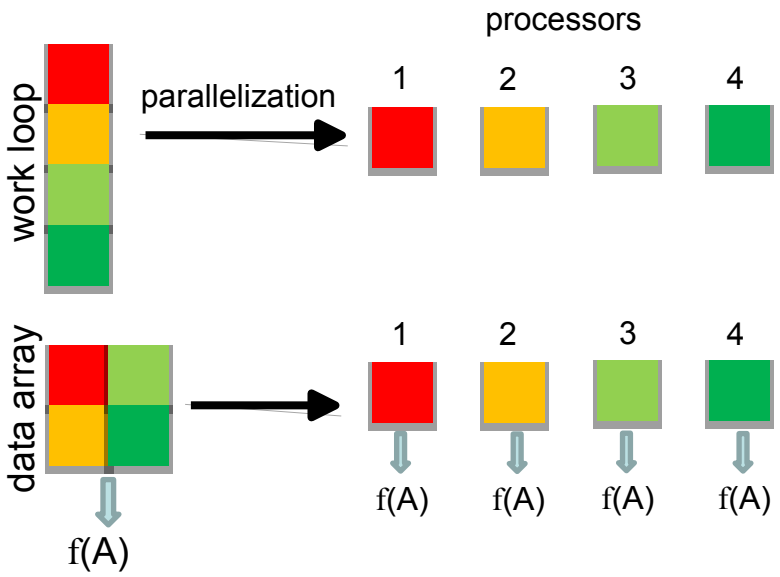


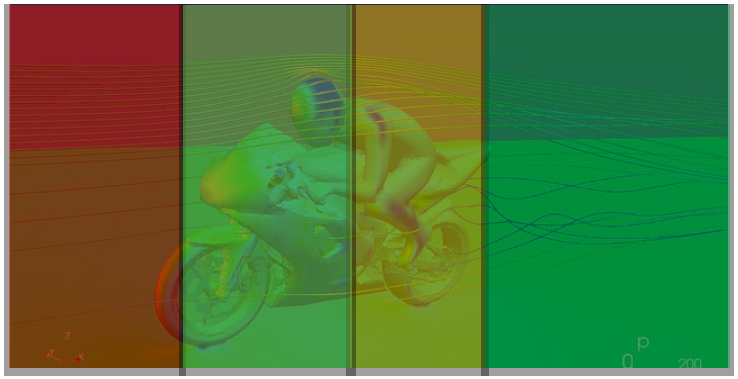
Parallelization Strategies

- major resources for computations
  - processor
  - memory
  - I/O
- parallelization means
  - distributing the work
  - distributing the data (on distributed memory machines)
  - synchronization of work
  - communication of data (on distributed memory machines)
- parallel programming models provide the methods to achieve the above goals

Distributing Work and Data

- Work decomposition
  - based on loop decomposition
- Data decomposition
  - all the work for a local chunk of the data is done by the local processor
- Domain decomposition
  - work and data are distributed according to a higher model, e.g. reality





Parallel Programming Models

- two dominating programming models:
  - OpenMP: uses directives to define work decomposition
  - MPI: standardized message-passing interface
- other programming models
  - HPF (high-performance Fortran)
  - PGAS (Partitioned Global Address Space), e.g. Co-Array Fortran UPC (Unified Parallel C)
- programming models for compute devices
  - CUDA
  - OpenCL
  - OpenACC

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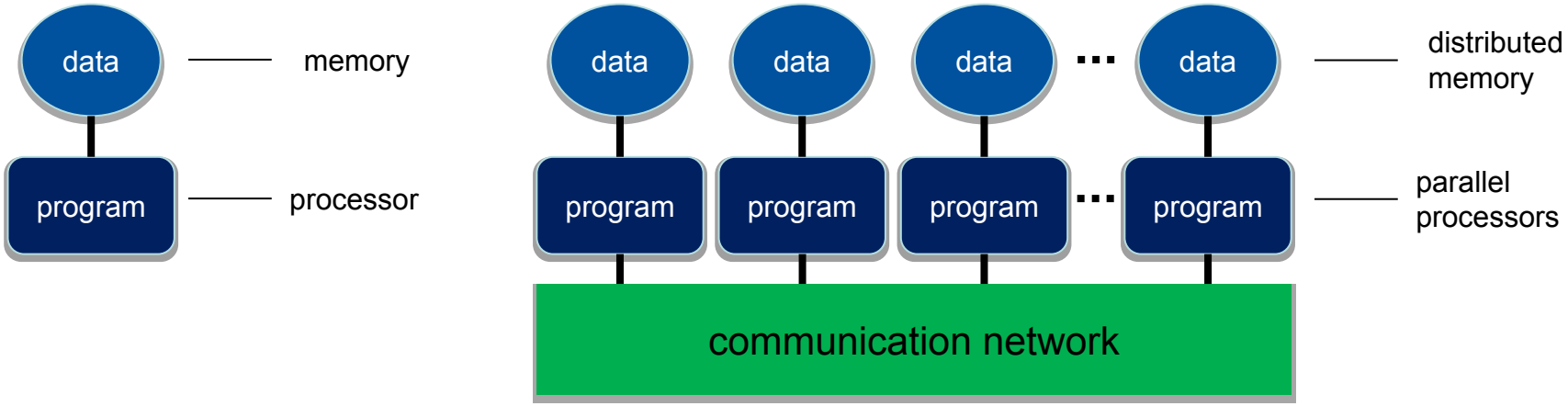
History of MPI

- MPI is a standard with the prime goals
  - to provide a message-passing interface
  - to provide source-code portability
  - to allow efficient implementations
- MPI exists for more than 20 years
  - MPI-1.0 was released in June, 1994
  - MPI-2.0 was released in July, 1997 and provided additional functionality
  - MPI-3.0 (current standard MPI-3.1) was released in October, 2012 and was developed for better platform and application support (in particular clusters of SMP nodes)

http://mpi-forum.org/docs/

A Message-Passing Interface

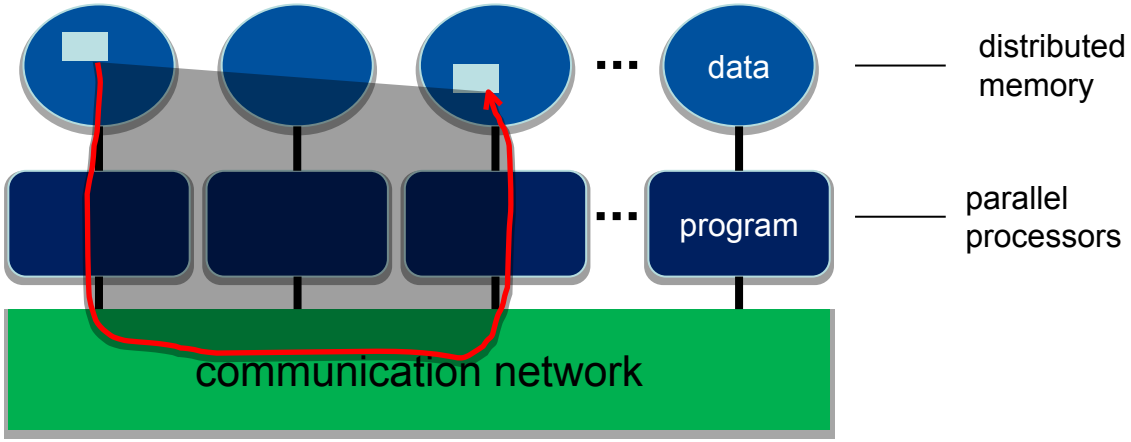
- sequential program vs. message-passing program



- message-passing programming paradigm:
  - each processor runs a (sub)program, typically the same (SPMD)
  - variables of subprograms have the same name but different (distributed) data
  - communication by special library routines Ⓟ message passing

Message Passing

- messages are passed through the communication network
- messages require the following information:
  - sending and receiving process
  - data location
  - data type
  - data size



- in order to use the message-passing interface the program must be
  - connected to the MPI library (at compile time)
  - started with the MPI startup tool (mpirun or mpiexec)
  - at runtime MPI is initialized with special library calls (MPI_Init())

Example MPI Program in C/C++

```
#include <mpi.h>

using namespace std;

int main(int argc, char *argv[]) {
   // initialization of MPI
   MPI_Init(&argc, &argv);

   // do some computation in parallel
   int partial_result = some_computation();
   int global_result = 0;

   // collect the result by an all-to-one communication
   MPI_Reduce(&partial_result, &global_result, 1,
              MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);

   // finalization of MPI
   MPI_Finalize();
}
```

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GPUs in HPC

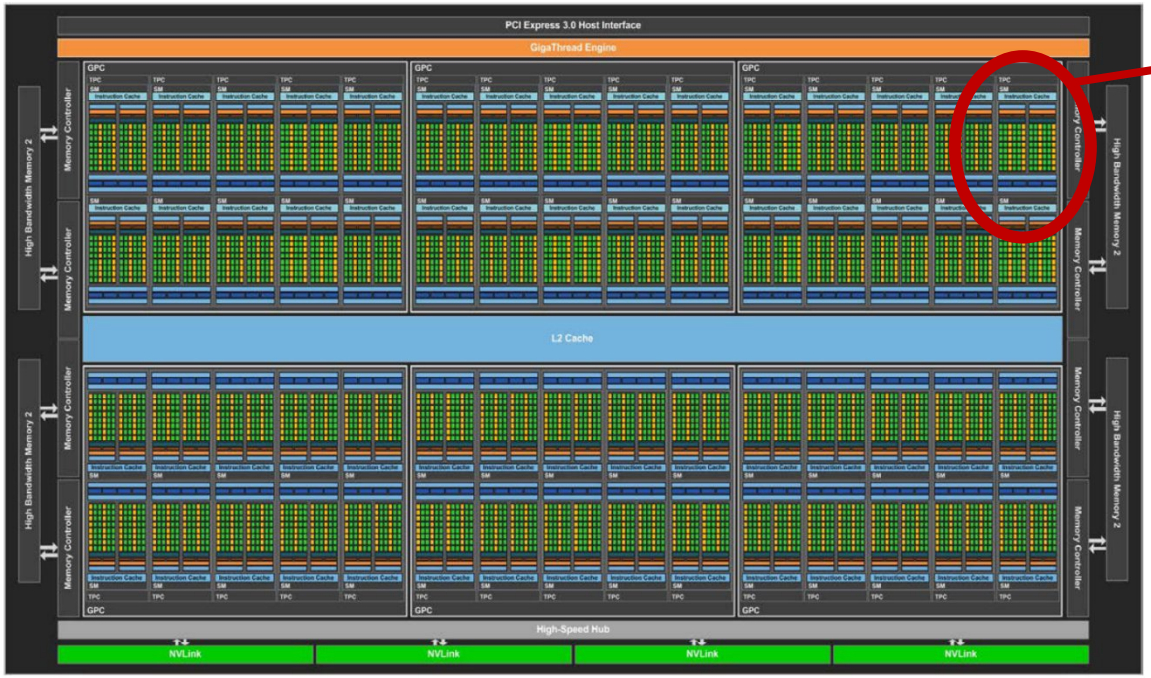
- GPUs appeared in the early 2000s in HPC
  - good cost/performance ratio due to mass production for gaming
- initially consumer-grade graphic cards were used
  - limited general-purpose computing
  - algorithms have to mimic graphics display
- today special GPUs are used in HPC
  - no display port
  - run real algorithms

old Geforce 8800 GTX

recent Tesla P100

Design of GPUs

- Example NVIDIA P100

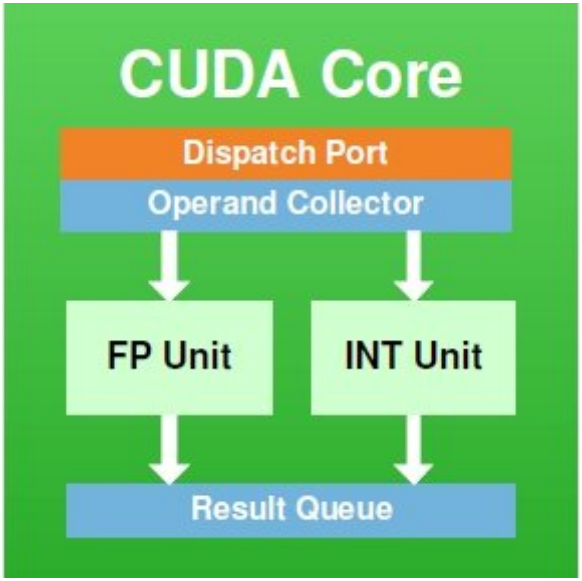


- organized in Graphics (GPCs) and Texture (TPCs) Processing Clusters
- 60 streaming multi-processor (SM)
  - basic compute resource
  - each SM has 64 CUDA cores
- 4 MB L2 Cache
  - accessed by 8 memory controllers

Design of GPUs

- the SM is divided into two blocks
  - each has 32 SP core and 16 DP cores
  - 8 Special Function Units (SFUs)
- 64kB of shared memory

CUDA Core vs. CPU core



- CUDA cores have no control logic
  - control logic is in SM only
  - all cores (in a SM) must perform same instruction - except for an activity mask
  - SM is SIMD unit

Hybrid Parallel Programming Models

- parallel programming models can be combined in a hybrid approach for better performance or special needs
- common approach is MPI + OpenMP to reduce the number of MPI process (communication overhead)
  - example: use MPI to start a parallel program on multiple dual-socket nodes, one MPI process per socket and OpenMP to utilize the available cores per socket
- MPI + CUDA/OpenACC to use GPUs across multiple nodes or OpenMP + CUDA for multiple GPUs in a single node
  - NVLink (or similar) may allow you to address multiple GPUs within a node as a single device

SLURM OPTIONS FOR PARALLEL COMPUTING

Slurm Options for Parallel Computing

- a Slurm job can request to run multiple tasks
  - the option **`--ntasks`** or a combination of **`--nodes`** and **`--tasks-per-node`** can be used to set the number of tasks
  - tasks can be executed using with **`srun`** (but this is not a typical use case)
  - a process in a parallel MPI programs corresponds to a task and **`mpirun`** is aware of the requested number of tasks

- a Slurm job can also request multiple (logical) cores per task
  - the option **`--cpus-per-task`** can be used for that
  - a Slurm **`cpu`** can be a physical core or a logical (hyper)thread

Variables in Job Scripts

- if you have a parallel application and you have requested multiple tasks and/or CPUs you can use corresponding variables in your job script
  - **`SLURM_JOB_NODELIST`**: List of nodes allocated to the job
  - **`SLURM_JOB_NUM_NODES`**: Total number of nodes in the job's resource allocation
  - **`SLURM_NTASKS`**: Number of tasks requested
  - **`SLURM_NTASKS_PER_NODE`**: Number of tasks requested per node
  - **`SLURM_CPUS_PER_TASK`**: Number of cpus requested per task

Slurm Options for GPU Computing

- to use the GPU nodes your job script should include
  - selection of an appropriate partition

```
#SBATCH --partition mpcg.p    # or mpcb.p or cfdg.p
```

  - request for one or two gpus (Generic RESource in Slurm)

```
#SBATCH –gres=gpu:1           # 1 or 2 gpus
```

  - you also need to load the CUDA Toolkit

```
module load CUDA              # add version if needed
```

  - note that the driver is only available on the GPU nodes