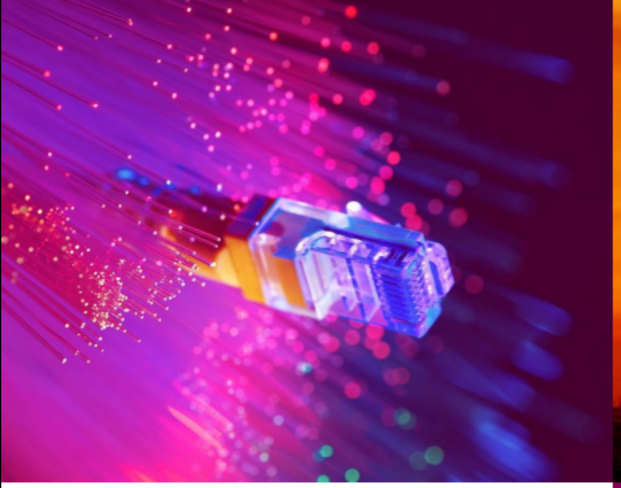


Parallel programming

Towards exascale solutions in Green function methods and advanced DFT

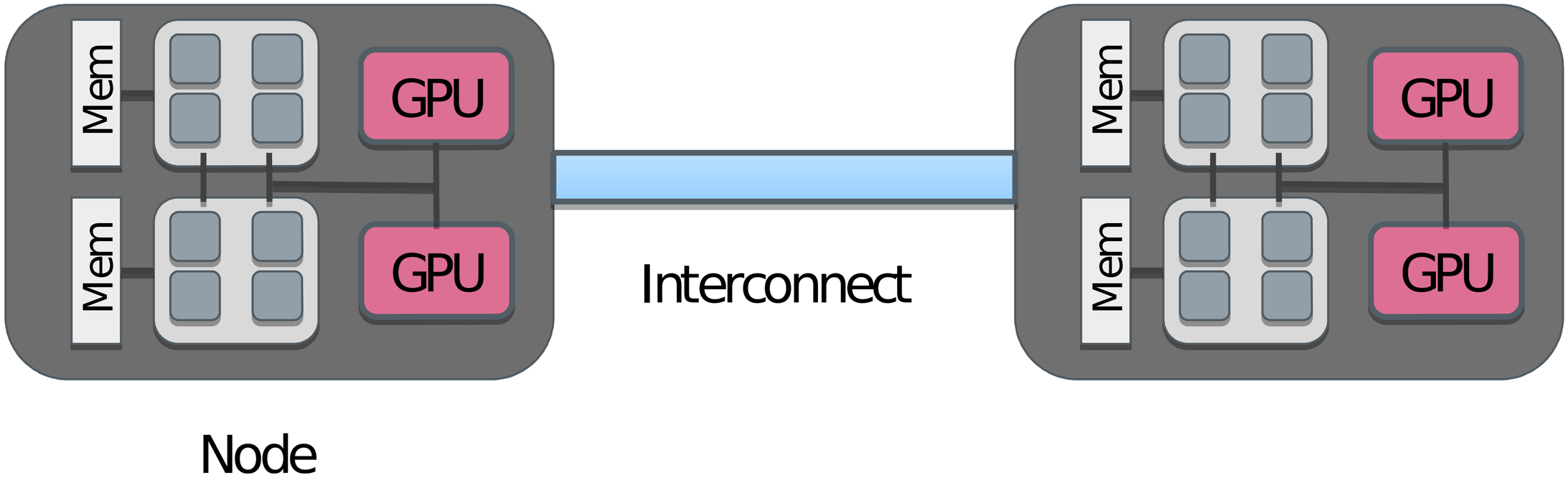

CSC – Finnish expertise in ICT for research, education and public administration

Parallel programming

Programming languages

- The de-facto standard programming languages in HPC are (still!) C/C++ and Fortran
- Higher level languages like Python and Julia are gaining popularity
  - Often computationally intensive parts are still written in C/C++ or Fortran
- Low level GPU programming with CUDA or HIP
- Performance portability frameworks
  - SYCL, Kokkos
- High-level frameworks for special tasks
  - PETSc, Trilinos, TensorFlow, PyTorch

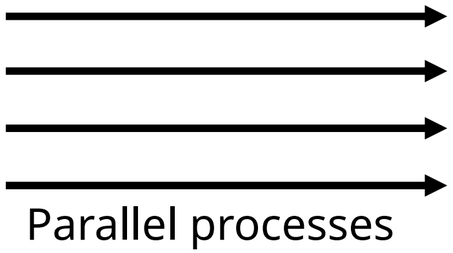
Parallel programming models

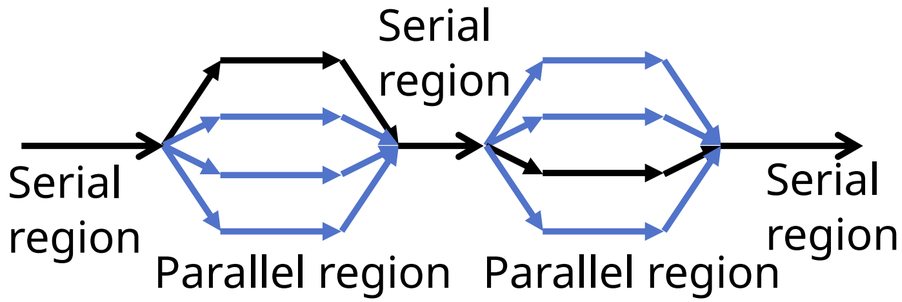


Parallel programming models

- Parallel execution is based on threads or processes (or both) which run at the same time on different CPU cores
- Processes
  - Have their own state information and *own memory* address space
  - Interaction is based on exchanging messages between processes
  - MPI (Message passing interface)
- Threads
  - Share the memory address space
  - Interaction is based on shared memory, i.e. each thread can access directly other threads data
  - OpenMP, pthreads

Parallel programming models





MPI: Processes

- Independent execution units
- MPI launches N processes at application startup
- Works over multiple nodes

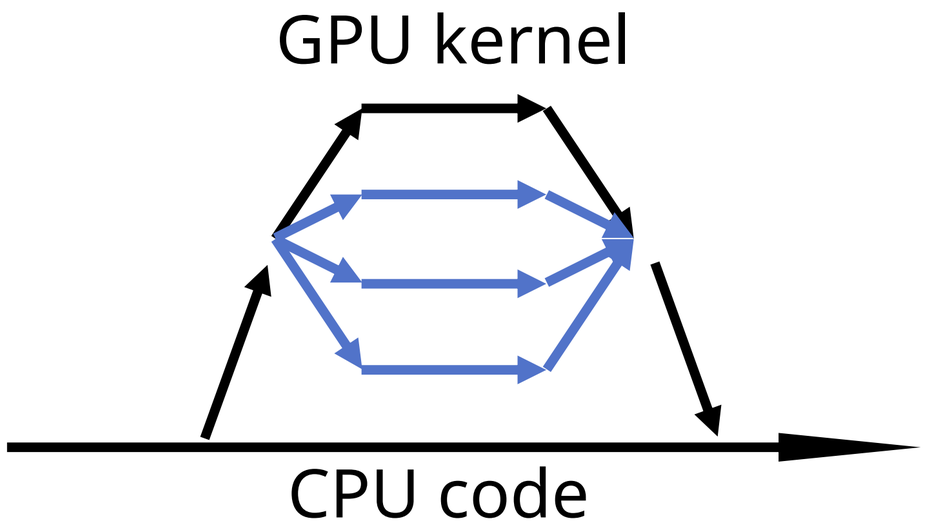
OpenMP: Threads

- Threads share memory space
- Threads are created and destroyed (parallel regions)
- Limited to a single node

GPU programming models

- GPUs are co-processors to the CPU
- CPU controls the work flow:
  - *offloads* computations to GPU by launching *kernels*
  - allocates and deallocates the memory on GPUs
  - handles the data transfers between CPU and GPUs
- GPU kernels run multiple threads
  - Typically much more threads than “GPU cores”
- When using multiple GPUs, CPU runs typically multiple processes (MPI) or multiple threads (OpenMP)

GPU programming models



- CPU launches kernel on GPU
- Kernel execution is normally asynchronous
  - CPU remains active
- Multiple kernels may run concurrently on same GPU

Brief introduction to MPI

Message-passing interface

- MPI is an application programming interface (API) for distributed parallel computing
- MPI programs are portable and scalable
  - the same program can run on different types of computers, from laptops to supercomputers
- MPI is flexible and comprehensive
  - large (hundreds of procedures)
  - concise (only 10-20 procedures are typically needed)
- First version of standard (1.0) published in 1994, latest (4.0) in June 2021
  - https://www.mpi-forum.org/docs/

Execution model in MPI

- Normally, parallel program is launched as a set of *independent*, *identical processes*
  - execute the *same program code* and instructions
  - processes can reside in different nodes (or even in different computers)
- The way to launch parallel program depends on the computing system
  - **`mpiexec`**, **`mpirun`**, **`srun`**, **`aprun`**, ...
  - **`srun`** on LUMI (and generally when using Slurm batch job system)
- MPI supports also dynamic spawning of processes and launching *different* programs communicating with each other
  - rarely used especially with DFT codes

MPI ranks

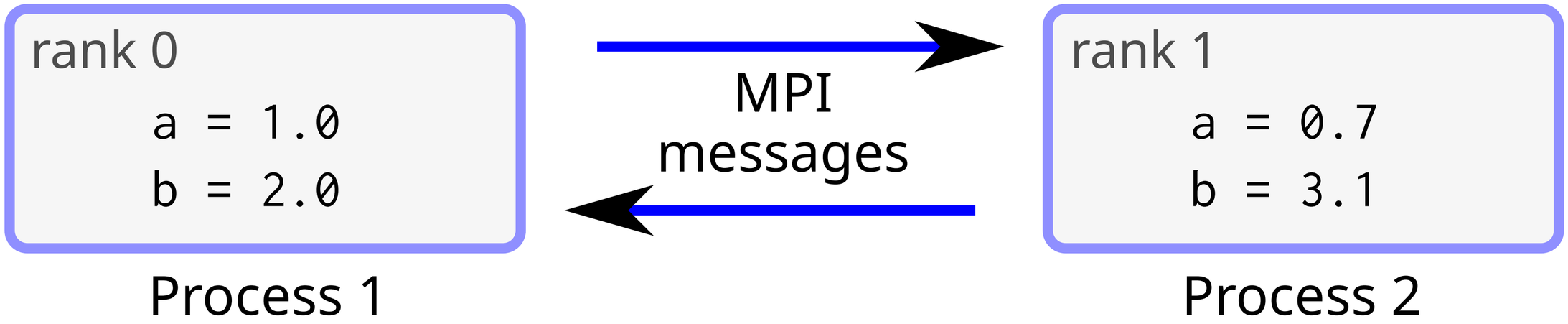
- MPI runtime assigns each process a unique rank (index)
  - identification of the processes
  - ranks range from 0 to N-1
- Processes can perform different tasks and handle different data based on their rank

```
integer :: a

if (rank == 0) then
   a = 1.0
   ...
else if (rank == 1) then
   a = 0.7
   ...
end if
...
```

Data model

- All variables and data structures are local to the process
- Processes can exchange data by sending and receiving messages



MPI library

- Information about the communication framework
  - the number of processes
  - the rank of the process
- Communication between processes
  - sending and receiving messages between two or several processes
- Synchronization between processes
- Advanced features
  - Communicator manipulation, user defined datatypes, one-sided communication, ...

Look and feel of a MPI program

```
program mpi_example
  use mpi_f08
  ...
  call mpi_init(ierr)  ! Initialize MPI
  ! Query number of MPI tasks and rank
  call mpi_comm_size(MPI_COMM_WORLD, ntasks, ierr)
  call mpi_comm_rank(MPI_COMM_WORLD, rank, ierr)
  ...
  ! Send messages between two neighboring processes
  left = rank - 1
  right = rank + 1
  call mpi_sendrecv(sendbuf, 100, MPI_DOUBLE, left, tag,  &
    &               recvbuf, 100, MPI_DOUBLE, right, tag, &
    &               MPI_COMM_WORLD, status, ierr)
   ...
  ! Perform element-wise reduction over all MPI tasks
  call mpi_reduce(sendbuf, recvbuf, 100, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD, ierr)
   ...
```

MPI summary

- In parallel programming with MPI, the key concept is a set of independent processes
- Data is always local to the process
- Processes can exchange data by sending and receiving messages
- The MPI library contains functions for communication and synchronization between processes

Brief introduction to OpenMP

What is OpenMP?

- A collection of *compiler directives* and *library routines* , together with a *runtime system*, for **multi-threaded**, **shared-memory parallelization**
- Fortran 77/9X/0X and C/C++ are supported
- Latest version of the standard is 5.2 (November 2021)
  - Full support for accelerators (GPUs)
  - Support latest versions of C, C++ and Fortran
  - Support for a fully descriptive loop construct
  - and more
- Compiler support for 5.0 is still incomplete

What is OpenMP

- OpenMP parallelized program can be run on your many-core workstation or on a node of a cluster
- Enables one to parallelize one part of the program at a time
  - Get some speedup with a limited investment in time
  - Efficient and well scaling code still requires effort
- Serial and OpenMP versions can easily coexist
- GPU programming with OpenMP offloading
- Pure OpenMP program is always limited to a single node
  - Combining with MPI allows to run hybrid MPI/OpenMP programs on multiple nodes

Three components of OpenMP

- Compiler directives, i.e. language extensions
  - Expresses shared memory parallelization
  - Preceded by sentinel, can compile serial version
- Runtime library routines
  - Small number of library functions
  - Can be discarded in serial version via conditional compiling
- Environment variables
  - Specify the number of threads, thread affinity etc.

OpenMP directives

- OpenMP directives consist of a *sentinel*, followed by the directive name and optional clauses

	sentinel	directive	clauses
C/C++	`#pragma omp`	`parallel`	`private(x,y)`
Fortran	`!$omp`	`parallel`	`private(x,y)`

- Directives are ignored when code is compiled without OpenMP support

OpenMP directives

- In C/C++, a directive applies to the following structured block

```
#pragma omp parallel
{
  // calculate in parallel
    printf("Hello world!\n");
}
```

- In Fortran, an `end` directive specifies the end of the construct

```
!$omp parallel
  ! calculate in parallel
    write(*,*) "Hello world!"
!$omp end parallel
```

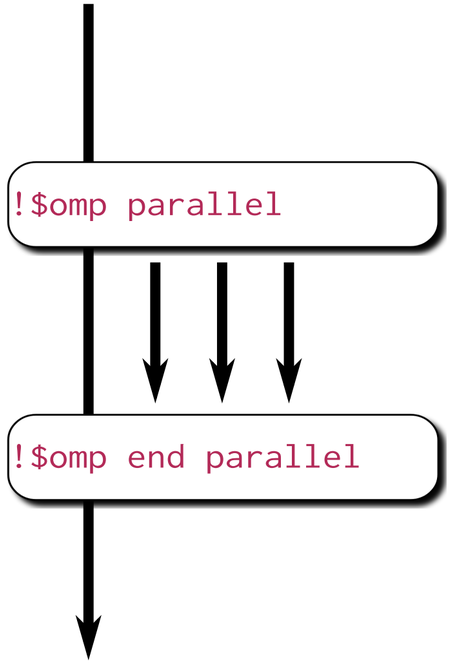
Fork-join model

- Threads are launched (forked) at the start of a *parallel region*

```
!$omp parallel [clauses]
   structured block
 !$omp end parallel
```

- Prior to it only one thread (main)
- Multiple threads execute the structured block
- After end only main thread continues executiona (join)

- Single Program Multiple Data



Look and feel of an OpenMP program

```
program openmp_example
  ...
! Calculate dot product of x and y in parallel
!$omp parallel do shared(x,y,n) private(i) reduction(+:asum)
  do i = 1, n
     asum = asum + x(i)*y(i)
  end do
!$omp end parallel do
```

OpenMP summary

- OpenMP is an API for thread-based parallelisation in shared memory architectures
- Compiler directives, runtime API, environment variables
- Relatively easy to get started but specially efficient and/or real-world parallelisation non-trivial

Process and thread affinity

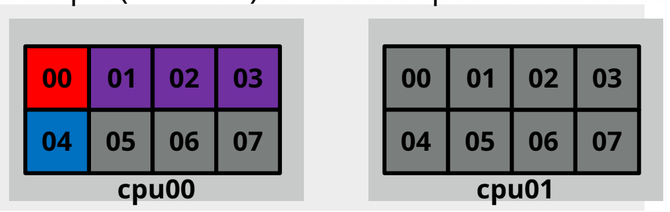
Process and thread affinity

- For obtaining parallel speedup, multiple CPU cores need to be executing concurrently
- Process and thread are software constructs which operating systems maps to the physical CPU cores
  - Operating system can even move a process/thread from one core to another
- Running more than single process/thread per core may cause significant performance penalty

Controlling affinity

- MPI and OpenMP must be aware of each other for proper mapping of processes and threads to CPU cores
- Batch job schedulers may also affect mapping
- Heavily system dependent
  - At best, everything works out of the box
  - At worts, complex settings for MPI and OpenMP
- See LUMI User Documentation for examples:
  - https://docs.lumi-supercomputer.eu/runjobs/scheduled-jobs/distribution-binding/

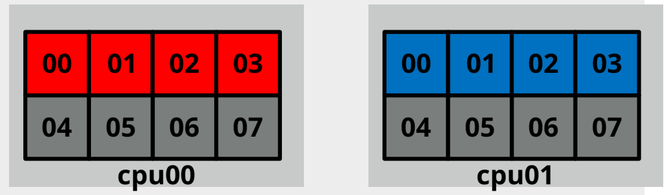
Example (incorrect): oversubscription of resources



MPI task 0: cpu00:00, cpu00:01, cpu00:02, cpu00:03

MPI task 1: cpu00:01, cpu00:02, cpu00:03, cpu00:04

Example (correct): better use of resources



MPI task 0: cpu00:00, cpu00:01, cpu00:02, cpu00:03

MPI task 1: cpu01:00, cpu01:01, cpu01:02, cpu01:03

Simultaneous multithreading

- Many Intel and AMD CPUs support simultaneous multithreading (SMT)
- When SMT is enabled, each physical core is seen as two logical cores by the operating system (256 cores per node in LUMI)
- The two logical cores share most of the resources (arithmetic units, caches, memory bus)
  - Typically, performance benefit up to 30 % at best
- Well optimized HPC applications do not typically benefit from SMT
- Many HPC systems (including LUMI) have SMT turned off by default
  - Trying SMT is easy performance tuning opportunity

GPU programming

Introduction to GPUs

- GPUs have become ubiquitous in high-performance computing
- Better FLOPS / W than CPUs
  - LUMI CPU nodes: ~9 GLOPS / W
  - LUMI GPU nodes: ~85 GLOPS / W
- Single GPU provides high performance
  - Whole LUMI GPU partition = 20 000 GPUs
  - Whole LUMI CPU partition = 200 000 CPU cores
  - GPU partition has ~50 times more performance
- Currently, two players in the market: NVIDIA and AMD

When to use GPUs ?

- Even though theoretical peak performance of GPUs is very high, many applications can reach only small proportion of it
- Programming effort might be considerable if application does not yet support GPUs
  - Still, GPUs are here to stay
- One should always measure how much GPUs speed up the time to solution
  - For fair comparison one should measure full GPU nodes vs. full CPU nodes
  - If application supports only single GPU, GPU vs. single multicore CPU is ok
- In LUMI, GPU node is more energy efficient when speedup is 4-5

CPU vs GPU

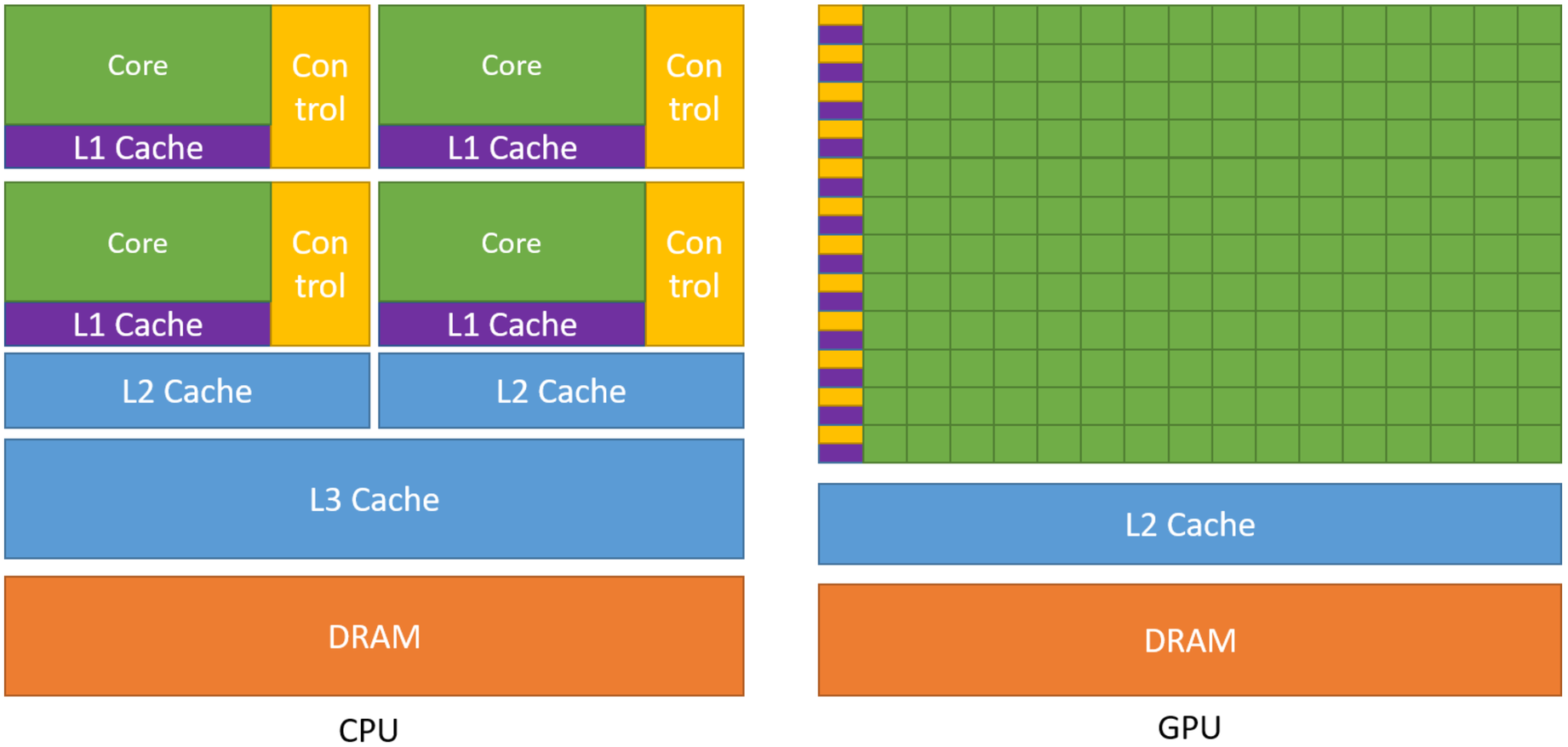
CPU

- More complex and oriented towards general purpose usage.
- Can run operating systems and very different types of applications
- Better control logic, caches and cache coherence

GPU

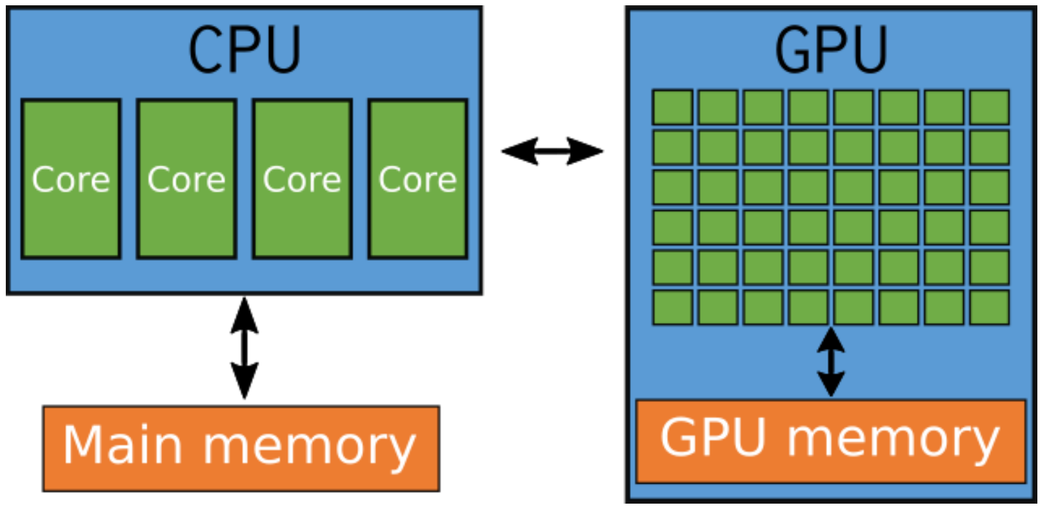
- Large fraction of transistors dedicated to the mathematical operations and less to contorl and caching
- Individual core is less powerful, but there can be thousands of them

CPU vs GPU


Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
Core
Con trol
L1 Cache
L2 Cache
L2 Cache
L3 Cache
DRAM
CPU
L2 Cache
DRAM
GPU

GPU as co-processor

- CPU and GPU have physically separate memories
  - Data needs to be copied via (slow) bus
- CPU controls the work flow:
  - *offloads* computations to GPU by launching *kernels*
  - allocates and deallocates the memory on GPUs
  - handles the data transfers between CPU and GPUs



Programming for GPUs

- Porting application to GPUs is non-trivial
- Algorithms and data structures may need to be adapted (massive amount of parallelism required)
- The physical memory in current GPUs is distinct from CPUs
  - Memory copies between CPU and GPU can easily become bottlenect
- If only part of the application is ported, performance improvement may be modest

GPU programming approaches

- Directive based approaches: OpenACC and OpenMP
  - “standard” and “portable”
- Native low level languages: CUDA (NVIDIA) and HIP (AMD)
  - HIP supports in principle also NVIDIA devices
  - Fortran needs wrappers via C-bindings
- Performance portability frameworks: SYCL, Kokkos
  - Support only C++
- Standard language features: parallel C++, `do concurrent`
  - Rely on implicit data movements
  - Compiler support incomplete

OpenMP offloading

- OpenMP programming for GPUs is similar to normal OpenMP threading
- Directives specify which parts of the program are executed on GPUs and how they can be parallelized
- Additional directives and clauses for controlling data movement between CPU and GPU
- In principle offload target can be also multicore CPU
  - Same program can be run both on GPUs and CPUs
- Relatively simple programming, compiler and runtime take care of the details (in theory)

Look and feel for OpenMP offloading

```
program offload_example
  ...
! Calculate dot product of x and y in GPU
!$omp target  ! Offload following block to GPU with implicit data movements
!$omp teams distribute parallel do reduction(+:asum)
  do i = 1, n
     asum = asum + x(i)*y(i)
  end do
!$omp end teams distribute parallel do
!$omp end target
```

CUDA/HIP programming

- CUDA/HIP add few additional constructs to standard C/C++
- Programming model: single instructions multiple threads (SIMT)
  - Programmer writes kernels that all the threads execute
- Threads are combined into groups (warps / wavefronts) which execute in lockstep
  - If statements in the kernels may be vary bad for performance

Look and feel for CUDA/HIP

```
// Calculates y = y + a*x
__global__ void axpy_kernel(int n, float a, float *x, float *y)
{
    int tid = threadIdx.x + blockIdx.x * blockDim.x;

    if (tid < n) y[tid] += a * x[tid];
}

// x and y need to be "GPU" arrays
void axpy(int n, float a, float *x, float *y)
{
    dim3 blocks(32);
    dim3 threads(256);

    axpy_kernel<<<blocks, threads>>>(n, a, x, y);
}
```

Look and feel for CUDA/HIP

```
// Memory management
hipMalloc((void **) &x_gpu, sizeof(float) * n);
hipMemcpy(x_gpu, x, sizeof(float) * n, hipMemcpyHostToDevice);
...
hipMemcpy(y, y_gpu, sizeof(float) * n, hipMemcpyDeviceToHost);
```

```
interface
  subroutine axpy_gpu(n, a, x, y) bind(C, name='axpy')
    use, intrinsic :: iso_c_binding
    type(c_ptr), value :: x, y
    real(c_float), value :: a
    integer(c_int), value :: n
  end subroutine
end interface
```

Best practices for GPU programming (personal thoughts)

- Landscape for GPU programming is far from clear
- CUDA is in many ways a good approach
  - However, vendor lock in to NVIDIA
  - Automatic tools for “hipifying” CUDA core work quite well
- HIP supports in principle both AMD and NVIDIA devices
  - HIP environment is not necessarily available in NVIDIA based systems
  - No “cudafy” tool for going back to CUDA
- Header only portability approach
  - Write generic CUDA/HIP-like GPU code, the backend is chosen at compile time

Best practices for GPU programming (personal thoughts)

- Directive based approaches promise good portability and performance
  - In principle, a key subroutines can be implemented in CUDA/HIP for better performance
  - Fortran is supported in the same level as C/C++
  - In practice, currently compilers have lot of room for improvement
- Kokkos and SYCL look promising
  - SYCL still largely driven by Intel
  - Require typical major rewriting of the program
  - Support only C++

Best practices for porting to AMD GPUs (personal thoughts)

- Existing CUDA code
  - Use “hipify” or try header-only porting library
- Existing OpenACC/OpenMP offload code
  - Cross your fingers and hope for the best

- CPU-only C/C++ code
  - Write generic GPU code and use header-only porting library
  - Try SYCL or Kokkos
- CPU-only Fortran code
  - Write generic GPU code with C together with header-only library and use C-bindings for interfacing to Fortran
  - Try OpenMP offloading

Summary on GPU programming

- GPUs offer in theory a significant performance boost
- Programming can be more complicated
  - Memory copies between CPU and GPU
  - Large amount of parallelism needed
- Programming approaches:
  - OpenACC, OpenMP
  - HIP/CUDA
  - SYCL, Kokkos (C++ only)

Web resources: MPI

- List of MPI functions with detailed descriptions
  - https://rookiehpc.org/mpi/index.html
  - http://mpi.deino.net/mpi_functions/
- Good online MPI tutorials
  - https://hpc-tutorials.llnl.gov/mpi/
  - http://mpitutorial.com/tutorials/
  - https://www.youtube.com/watch?v=BPSgXQ9aUXY
- MPI coding game in C
  - https://www.codingame.com/playgrounds/47058/have-fun-with-mpi-in-c/lets-start-to-have-fun-with-mpi

Web resources: MPI

- MPI 4.0 standard http://www.mpi-forum.org/docs/
- MPI implementations
  - OpenMPI http://www.open-mpi.org/
  - MPICH https://www.mpich.org/
  - Intel MPI https://software.intel.com/content/www/us/en/develop/tools/oneapi/components/m library.html

Web resources: OpenMP

- OpenMP homepage: http://openmp.org/
- Good online reference: https://rookiehpc.org/openmp/index.html
- Online tutorials: http://openmp.org/wp/resources/#Tutorials

Web resources: GPUs

- NVIDIA Training material: https://developer.nvidia.com/cuda-education
- AMD Training material: https://rocm.docs.amd.com/en/latest/examples/all.html
- HOP (HIP/CUDA portability library): https://github.com/mlouhivu/hop