Parallel Programming Overview

Introduction to High Performance Computing 2021

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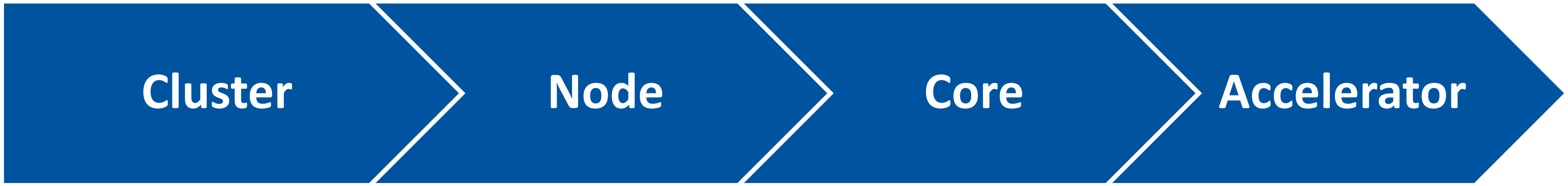
Agenda

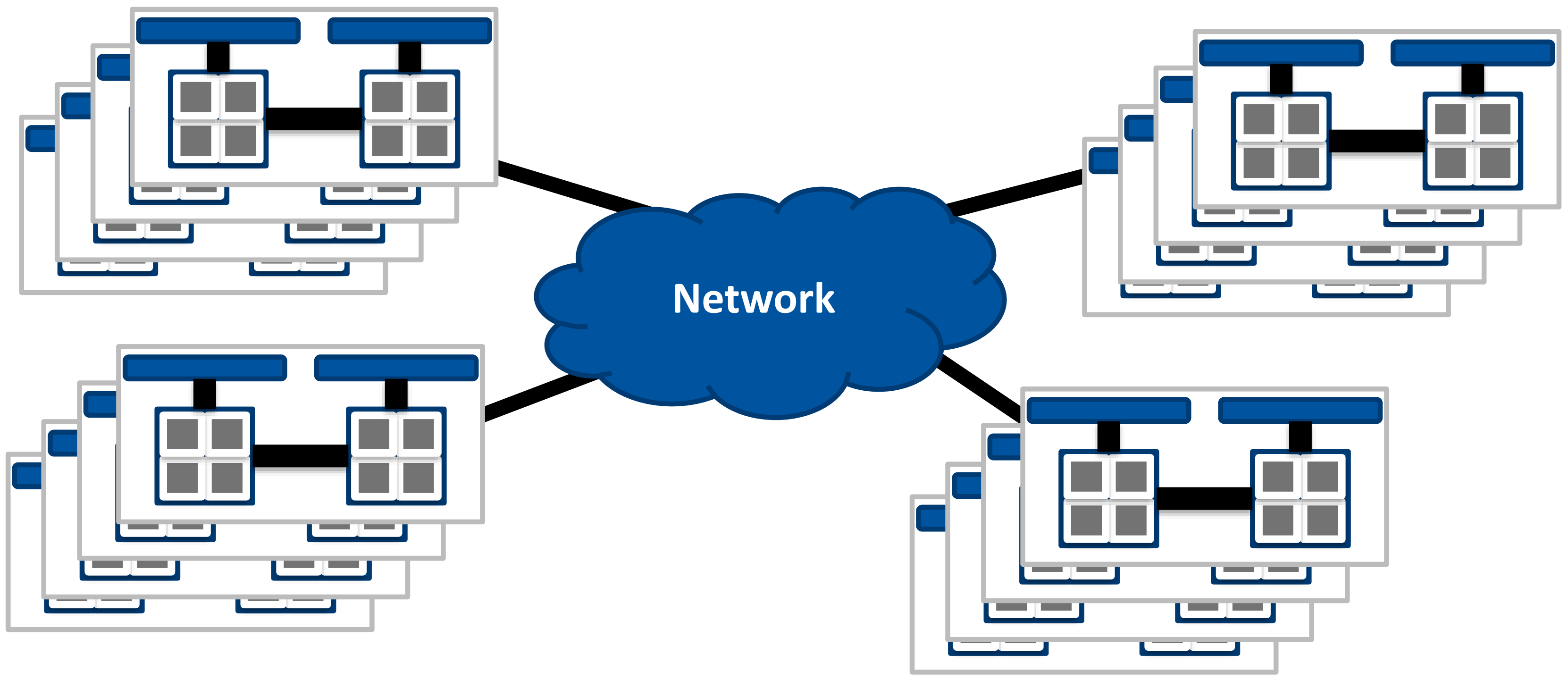
- Programming concepts and models for



Programming for Clusters

Motivation

- **Clusters**
  - → HPC market is dominated by distributed memory multicomputers (clusters)
  - → Many nodes with no direct access to other nodes’ memory



SPMD – Identity

- **How to do useful work in parallel if source code is the same?**
  - → Each process receives a unique identifier
  - → Multiple code paths based on the ID

```
int my_id = get_my_id();

if (my_id == id_1) {
   // Code for process id_1
}
else if (my_id == id_2) {
   // Code for process id_2
}
else {
   // Code for other processes
}
```

SPMD – Data Exchange

- **Serial program**

```
a[0..9] = a[100..109];
```

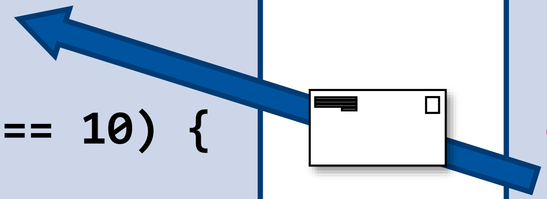
- **SPMD program**

→ process 0: **aa** holds **a[0..9]**

process 10: **aa** holds **a[100..109]**

```
array aa[10];

if (my_id == 0) {
  recv(aa, 10);
}
else if (my_id == 10) {
  send(aa, 0);
}
```



```
array aa[10];

if (my_id == 0) {
  recv(aa, 10);
}
else if (my_id == 10) {
  send(aa, 0);
}
```

Hello, MPI!

- **C**

```
  #include <stdio.h>
1 #include <mpi.h>
  int main(int argc, char **argv) {
    int rank, nprocs;

2   MPI_Init(&argc, &argv);

3   MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &nprocs);

4   printf(“Hello, MPI! I am %d of %d\n”,
           rank, nprocs);

5   MPI_Finalize();
    return 0;
  }
```

1 Header file inclusion – makes available prototypes of all MPI functions

2 MPI library initialisation – must be called before other MPI operations are called

3 MPI operations – more on that later

4 Text output – MPI programs also can print to the standard output

5 MPI library clean-up – no other MPI calls after this one allowed

Query operations on communicators

- **How many processes are there in a given communicator?**

```
MPI_Comm_size (MPI_Comm comm, int *size)
```

→ Returns the total number of MPI processes when called on **`MPI_COMM_WORLD`**

→ Returns 1 when called on **`MPI_COMM_SELF`**

- **What is the rank of the calling process in a given communicator?**

```
MPI_Comm_rank (MPI_Comm comm, int *rank)
```

→ Returned rank will differ in each calling process given the same communicator

→ Ranks values are in **`[0, size-1]`** (always **`0`** for **`MPI_COMM_SELF`**)

Messages

- MPI passes data around in the form of messages
- Two components
  - → Message content (user data)
  - → Envelope

Field	Meaning
Sender rank	Who sent the message
Receiver rank	To whom the message is addressed to
Tag	Additional message identifier
Communicator	Communication context

- MPI retains the logical order in which messages between any two ranks are sent (FIFO)
  - → But the receiver have the option to peek further down the queue

Sending messages

- Messages are sent using the MPI_Send family of operations

$$\texttt{MPI\_Send (}\underbrace{\texttt{buf, count, datatype,}}_{\text{message content}}\ \underbrace{\texttt{dest, tag, comm}}_{\text{envelope}}\texttt{)}$$

Parameter	Meaning
buf	Location of data in memory
count	Number of consecutive data elements to send
datatype	MPI data type handle
dest	Rank of the receiver
tag	Message tag
comm	Communicator handle

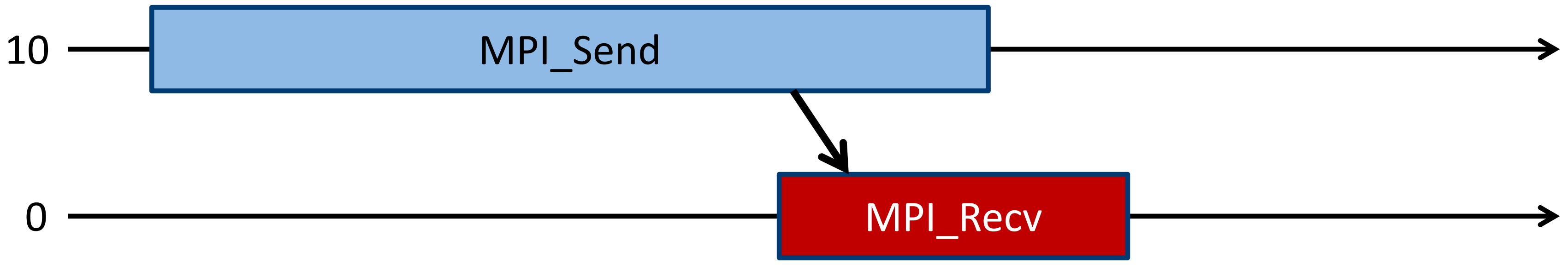
- The MPI API is built on the idea that data structures are array-like
  - → No fancy C++ objects supported

Example

- Our earlier SPMD example written in MPI

```
int aa[10];
MPI_Status status;

if (rank == 0) {
  MPI_Recv(aa, 10, MPI_INT, 10, 0, MPI_COMM_WORLD, &status);
}
else if (rank == 10) {
  MPI_Send(aa, 10, MPI_INT, 0, 0, MPI_COMM_WORLD);
}
```



Develop with MPI @ CLAIX

- **Two MPI implementations**
  - → Intel MPI (default)
  - → Open MPI

```
$ module switch intelmpi openmpi
```

- **Universal environment variables**
  - → **`$MPICC`** – C compiler wrapper
  - → **`$MPICXX`** – C++ compiler wrapper
  - → **`$MPIF77`** – Fortran 77 compiler wrapper
  - → **`$MPIFC`** – Fortran 90+ compiler wrapper
  - → **`$MPIEXEC`** – MPI launcher
  - → **`$FLAGS_MPI_BATCH`** – Recommended launcher flags in batch mode

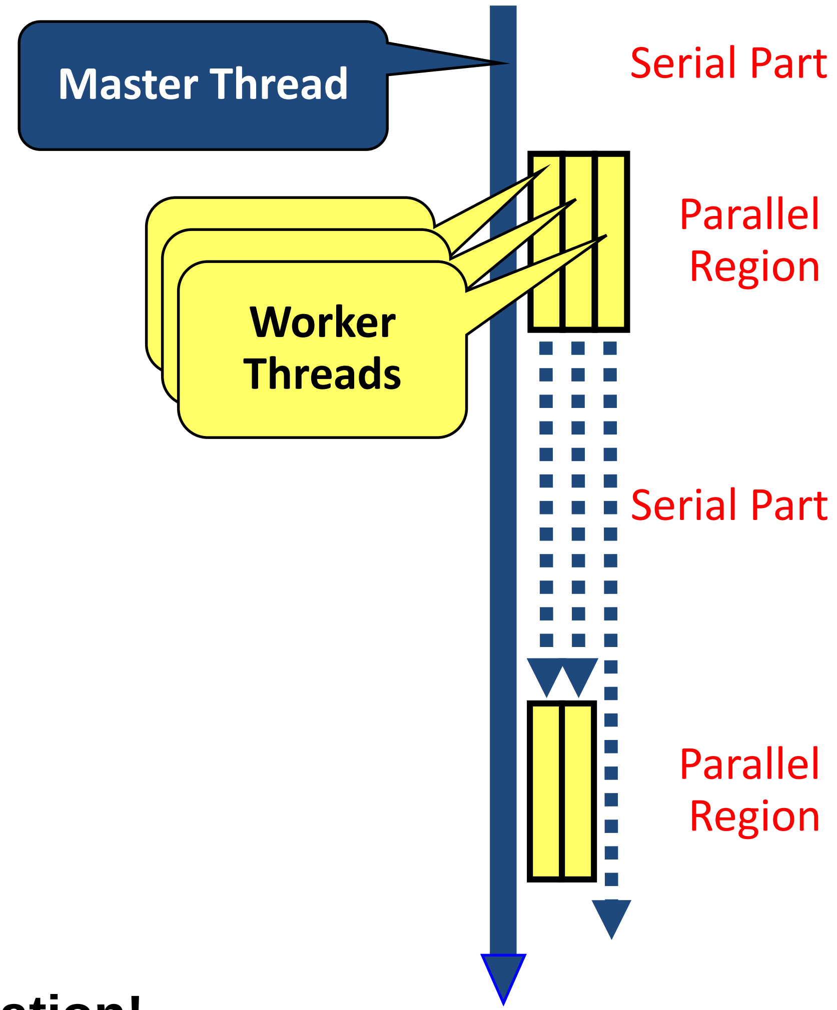
Hello, world!

- 1. Type the code on slide 7 into a text file named hello.c
- 2. Compile:
  - → C: `mpicc -o hello.exe hello.c`
  - → Fortran: `mpif90 -o hello.exe hello.f90`
- 3. Run:
  - → `mpiexec -n 4 hello.exe`
- On CLAIX we recommend the RWTH specific environment variables:
  - → `$MPICC -o hello.exe hello.c`
  - → `$MPIEXEC $FLAGS_MPI_BATCH hello.exe`

Programming for Multi-Core Nodes

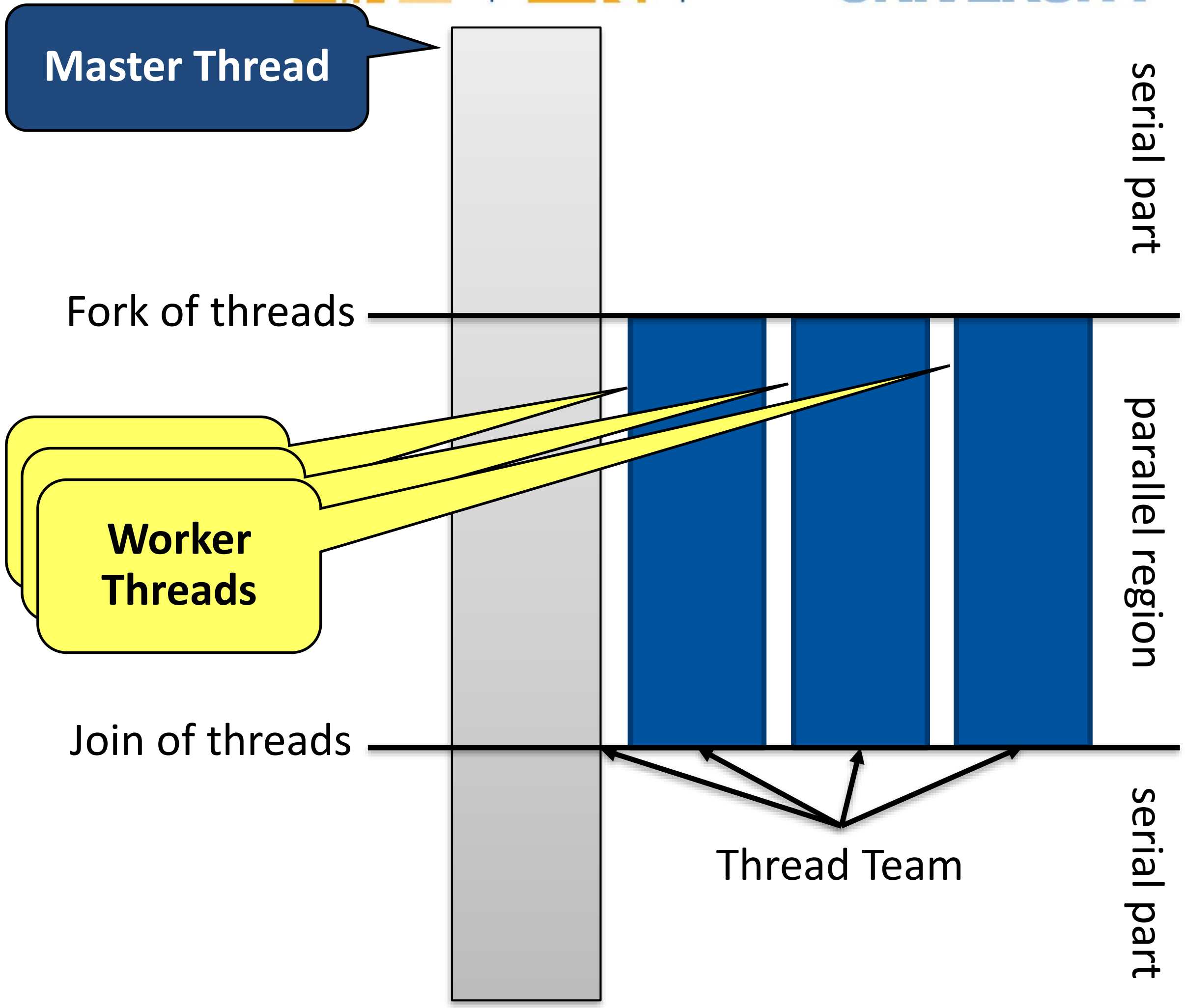
OpenMP Execution Model

- OpenMP programs start with just one thread: The *Master*.
- *Worker* threads are spawned at *Parallel Regions*, together with the Master they form the *Team* of threads.
- In between Parallel Regions the Worker threads are put to sleep. The OpenMP *Runtime* takes care of all thread management work.
- Concept: *Fork-Join*.
- Allows for an incremental parallelization!



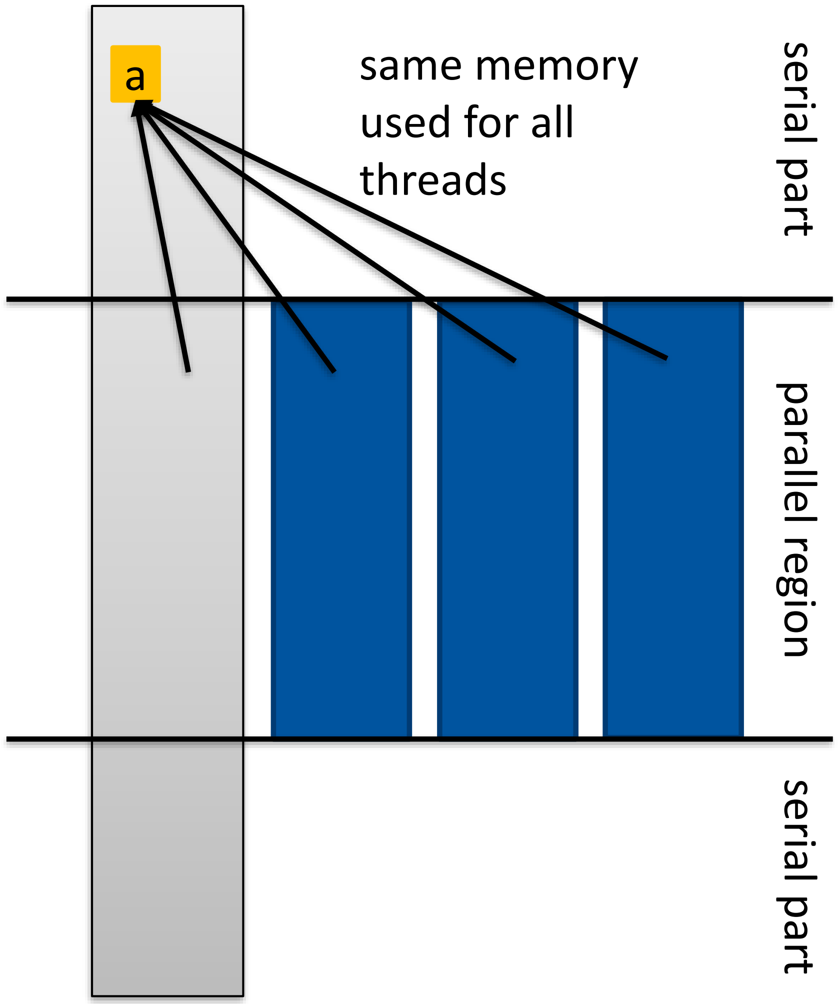
Fork-Join Execution Model

```
.
.
.
#pragma omp parallel
{
.
.
.
}
.
.
.
```



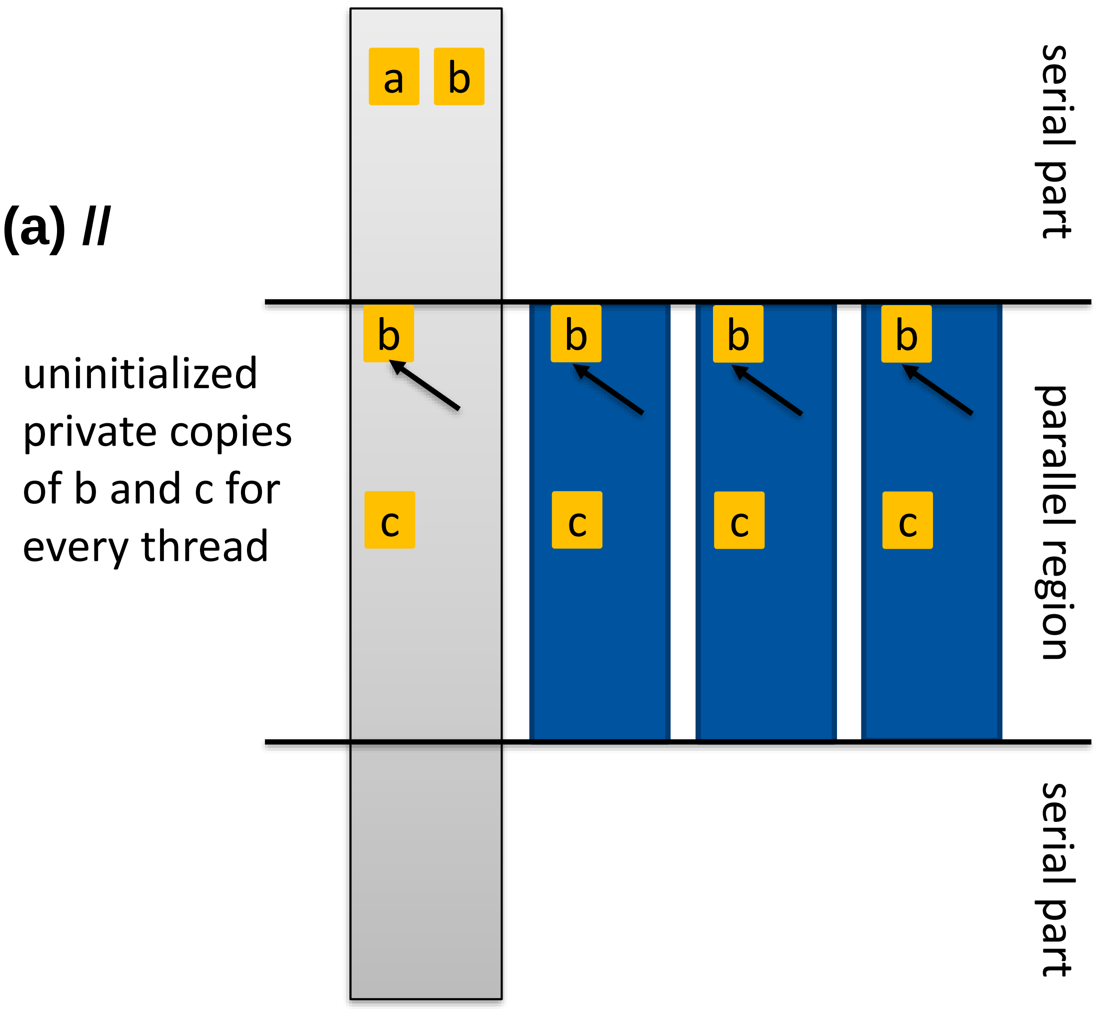
Data Sharing Attributes (1/3)

```
int a;
.
.
#pragma omp parallel shared(a)
{
.
.
.
}
.
.
.
```



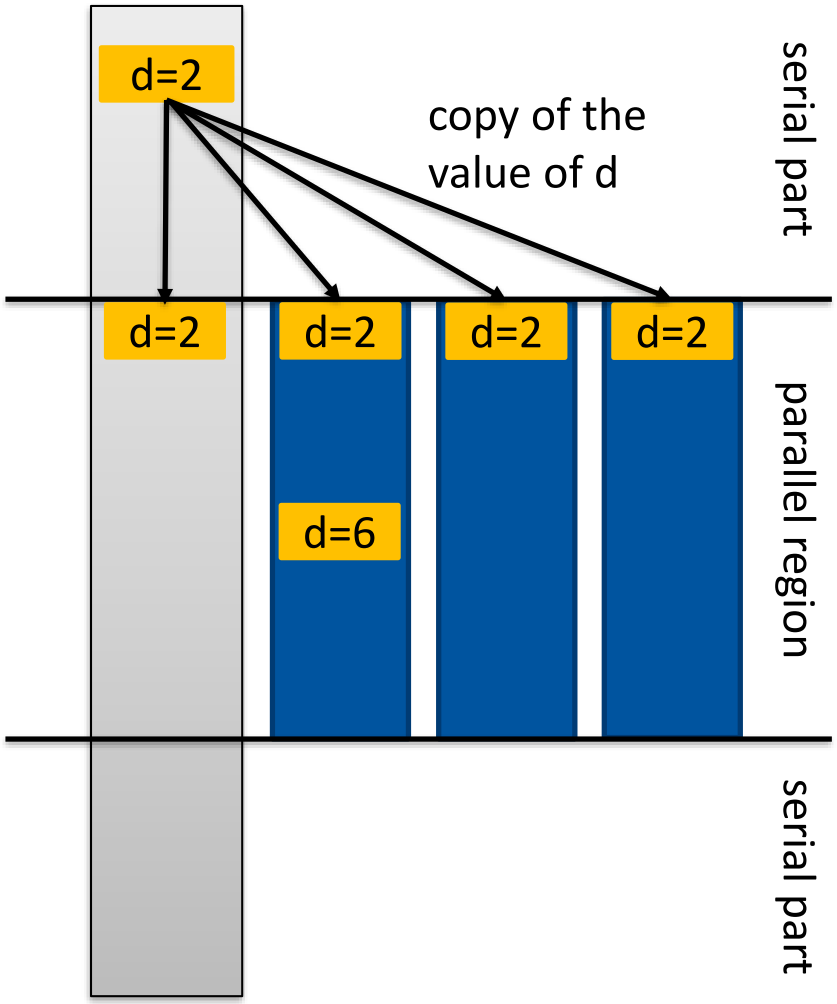
Data Sharing Attributes (2/3)

```
int a,b;
.
#pragma omp parallel shared(a) //
  private(b)
{
.
int c;
.
}
.
.
.
```



Data Sharing Attributes (3/3)

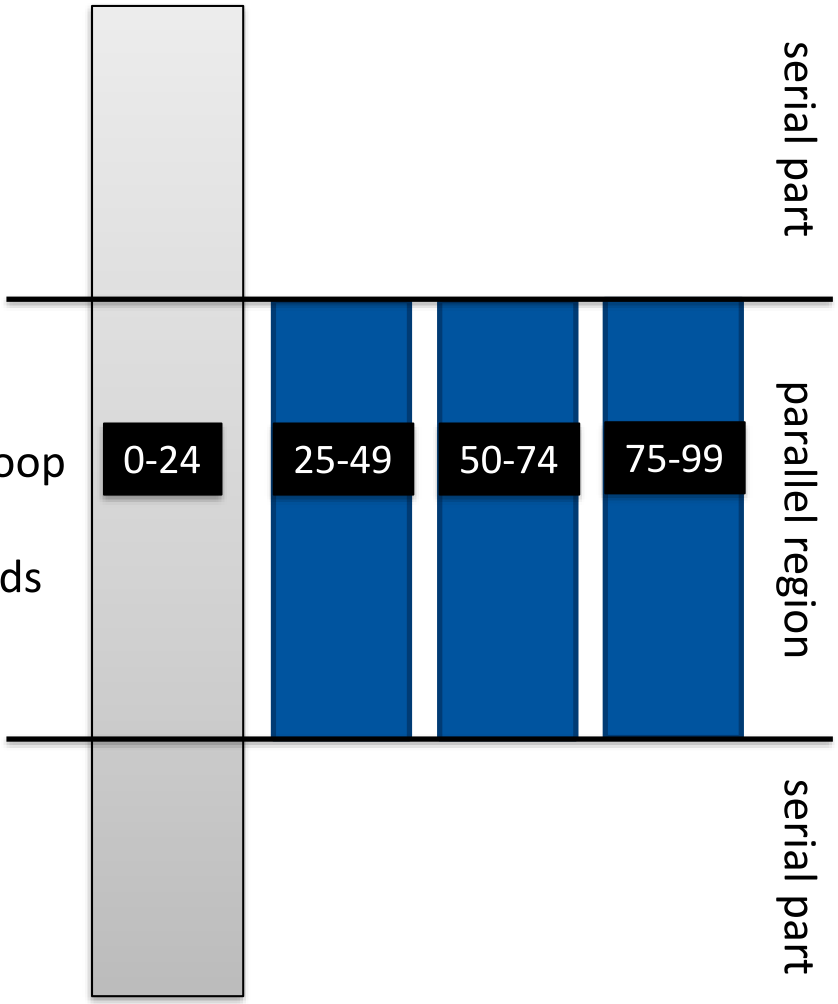
```
int d=2;
.
.
#pragma omp parallel firstprivate(d)
{
#pragma omp single
{d=6;}
.
}
.
.
.
```



For Worksharing

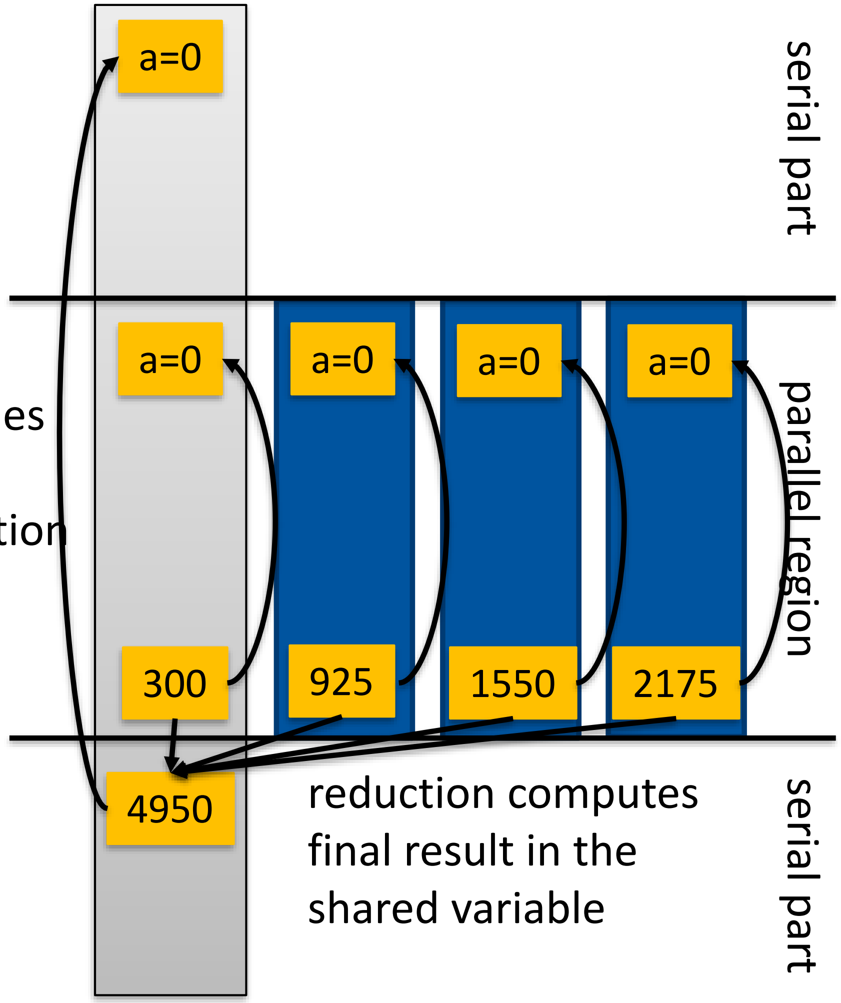
```
.
.
.
#pragma omp parallel
#pragma omp for
for (int i=0; i<100; i++){
.
.
.
}
.
.
.
```

distributes loop iterations across threads



Reduction Operations

```
int a=0;
.
.
#pragma omp parallel
#pragma omp for reduction(+:a)
for (int i=0; i<100; i++)
{
        a+=i;
}
.
.
.
```



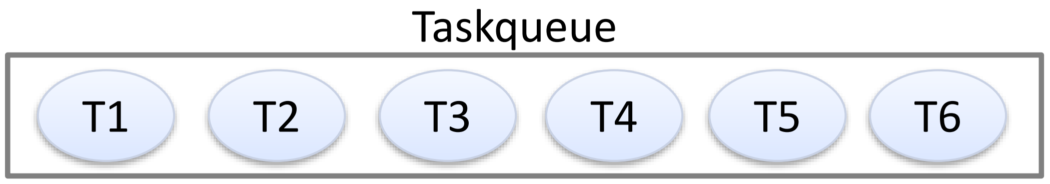
local copies for computation

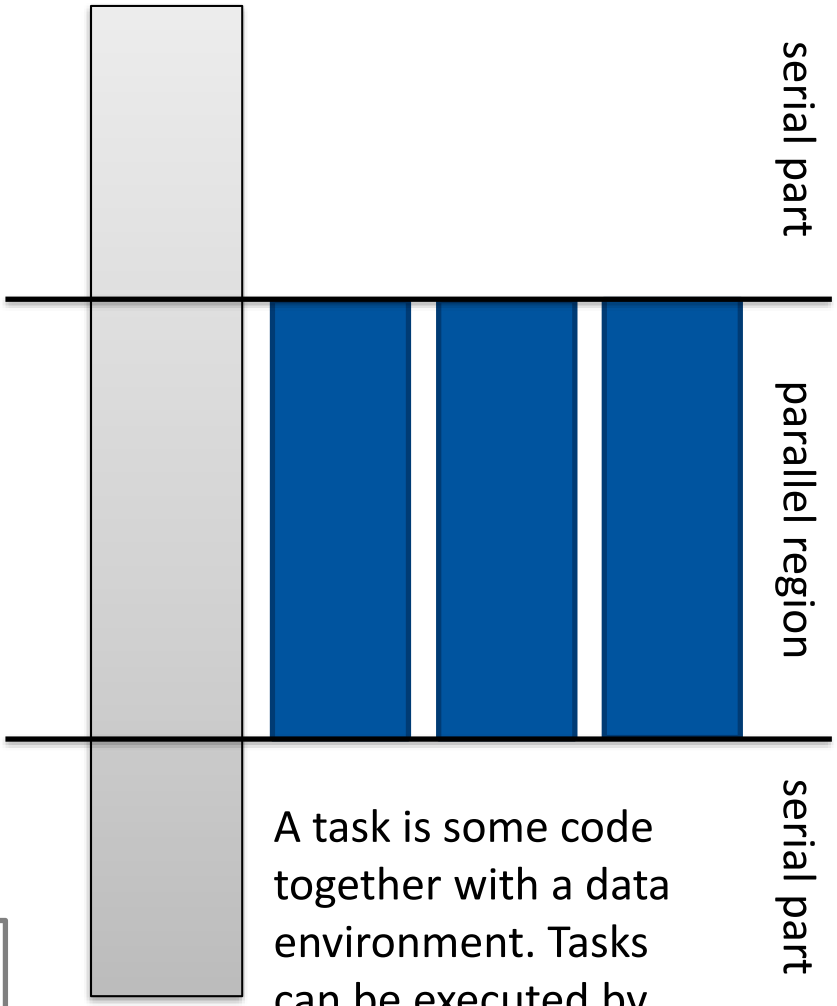
update is written to the shared variable

reduction computes final result in the shared variable

Tasks

```
#pragma omp parallel
#pragma omp single
while (work()){
          #pragma omp task
          {
          …
          }
}// implicit barrier here
.
.
```





A task is some code together with a data environment. Tasks can be executed by any thread in any order.

OpenMP Programs on CLAIX

- **Compilation: add `–fopenmp` flag to compiler (and linker)**
  - → In our environment better use **`$FLAGS_OPENMP`**

- **From within a shell, global setting of the number of threads:**

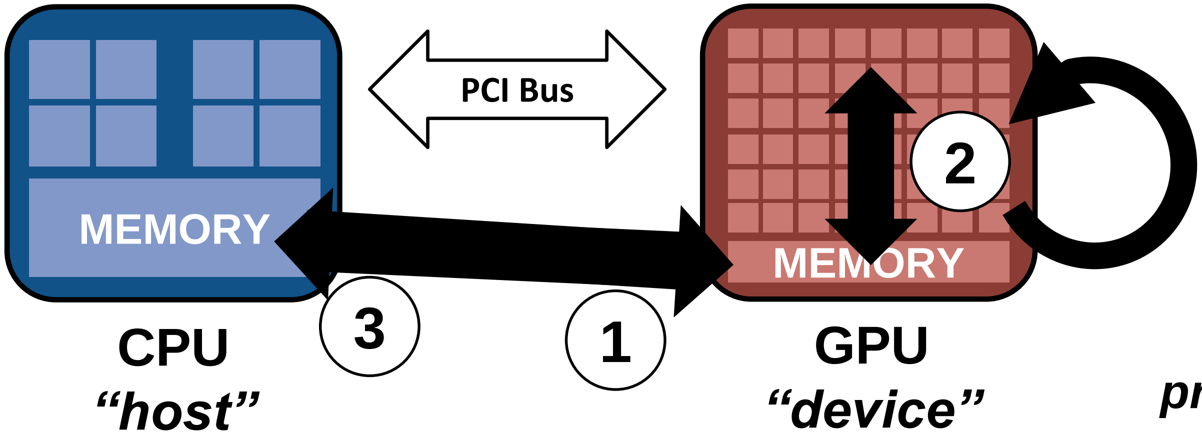
```
export OMP_NUM_THREADS=4
./program
```

- **From within a shell, one-time setting of the number of threads:**

```
OMP_NUM_THREADS=4   ./program
```

Programming for Accelerators

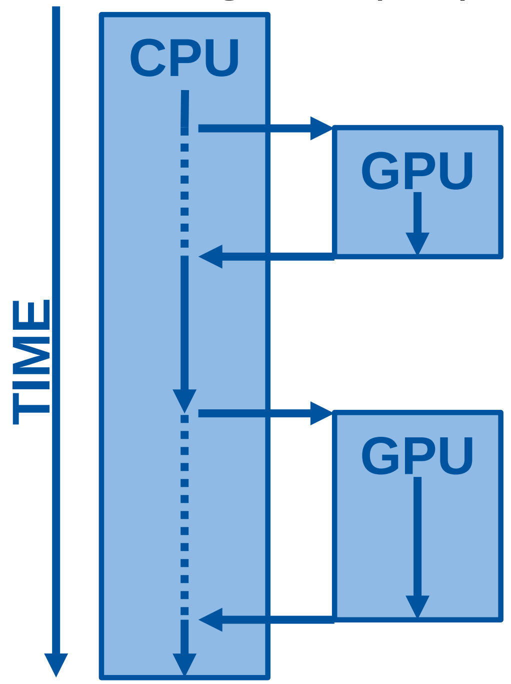
Offloading



We refer to "discrete GPUs" here.

- **Weak memory model**
  - → Host + device memory = separate entities
  - → No coherence between host + device
    - → Data transfers needed
- **Host-directed execution model**
  - → Copy input data from CPU mem. to device mem.
  - → Execute the device program
  - → Copy results from device mem. to CPU mem.

processing flow *(simplified)*



GPGPU programming

- **CUDA (Compute Unified Device Architecture)**
  - → C/C++ (NVIDIA): architecture + programming language, NVIDIA GPUs
  - → Fortran (PGI): NVIDIA‘s CUDA for Fortran, NVIDIA GPUs
- **OpenCL**
  - → C (Khronos Group): open standard, portable, CPU/GPU/…
- **OpenACC**
  - → C/Fortran (PGI): Directive-based accelerator programming, industry standard published in Nov. 2011 (NVIDIA GPUs)
- **OpenMP**
  - → C/C++, Fortran: Directive-based programming for hosts and accelerators, standard, portable, published in July 2013
- **…**

Example SAXPY – CPU

```
void saxpyCPU(int n, float a, float *x, float *y) {
    for (int i = 0; i < n; ++i)
        y[i] = a*x[i] + y[i];
}


int main(int argc, const char* argv[]) {
  int n = 10240; float a = 2.0f;
  float *x = (float*) malloc(n * sizeof(float));
  float *y = (float*) malloc(n * sizeof(float));

  // Initialize x, y
  for(int i=0; i<n; ++i){
    x[i]=i;
    y[i]=5.0*i-1.0;
  }

  // Invoke serial SAXPY kernel
  saxpyCPU(n, a, x, y);

  free(x); free(y);
  return 0;
}
```

SAXPY = Single-precision real Alpha X Plus Y

$$\vec{y} = \alpha \cdot \vec{x} + \vec{y}$$

Example SAXPY – OpenACC

```
void saxpyOpenACC(int n, float a, float *x, float *y) {
#pragma acc parallel loop copy(y[0:n]) copyin(x[0:n])
    for (int i = 0; i < n; ++i)
        y[i] = a*x[i] + y[i];
}

int main(int argc, const char* argv[]) {
  int n = 10240; float a = 2.0f;
  float *x = (float*) malloc(n * sizeof(float));
  float *y = (float*) malloc(n * sizeof(float));

  // Initialize x, y
  for(int i=0; i<n; ++i){
    x[i]=i;
    y[i]=5.0*i-1.0;
  }

  // Invoke serial SAXPY kernel
  saxpyOpenACC(n, a, x, y);

  free(x); free(y);
  return 0;
}
```

Example SAXPY – CUDA

```
__global__ void saxpy_parallel(int n,
   float a, float *x, float *y) {
    int i = blockIdx.x * blockDim.x +
    threadIdx.x;
    if (i < n){
        y[i] = a*x[i] + y[i];
    }
}

int main(int argc, char* argv[]) {
 int n = 10240; float a = 2.0f;
 float* h_x,*h_y; // Pointer to CPU memory
 h_x = (float*) malloc(n* sizeof(float));
 h_y = (float*) malloc(n* sizeof(float));
 // Initialize h_x, h_y
 for(int i=0; i<n; ++i){
   h_x[i]=i;
   h_y[i]=5.0*i-1.0;
 }
 float *d_x,*d_y; // Pointer to GPU memory
 cudaM
 cudaM
```

1. Allocate data on GPU + transfer data

```
cudaMemcpy(d_x, h_x, n * sizeof(float),
  cudaMemcpyHostToDevice);
cudaMemcpy(d_y, h_y, n * sizeof(float),
  cudaMemcpyHostToDevice);
// Invoke parallel SAXPY kernel
dim3 threadsPerBlock(128);
dim3 b                                   .x);
saxpy_parallel<<<blocksPerGrid,
  threadsPerBlock>>>(n, 2.0, d_x, d_y);
```

2. Launch kernel

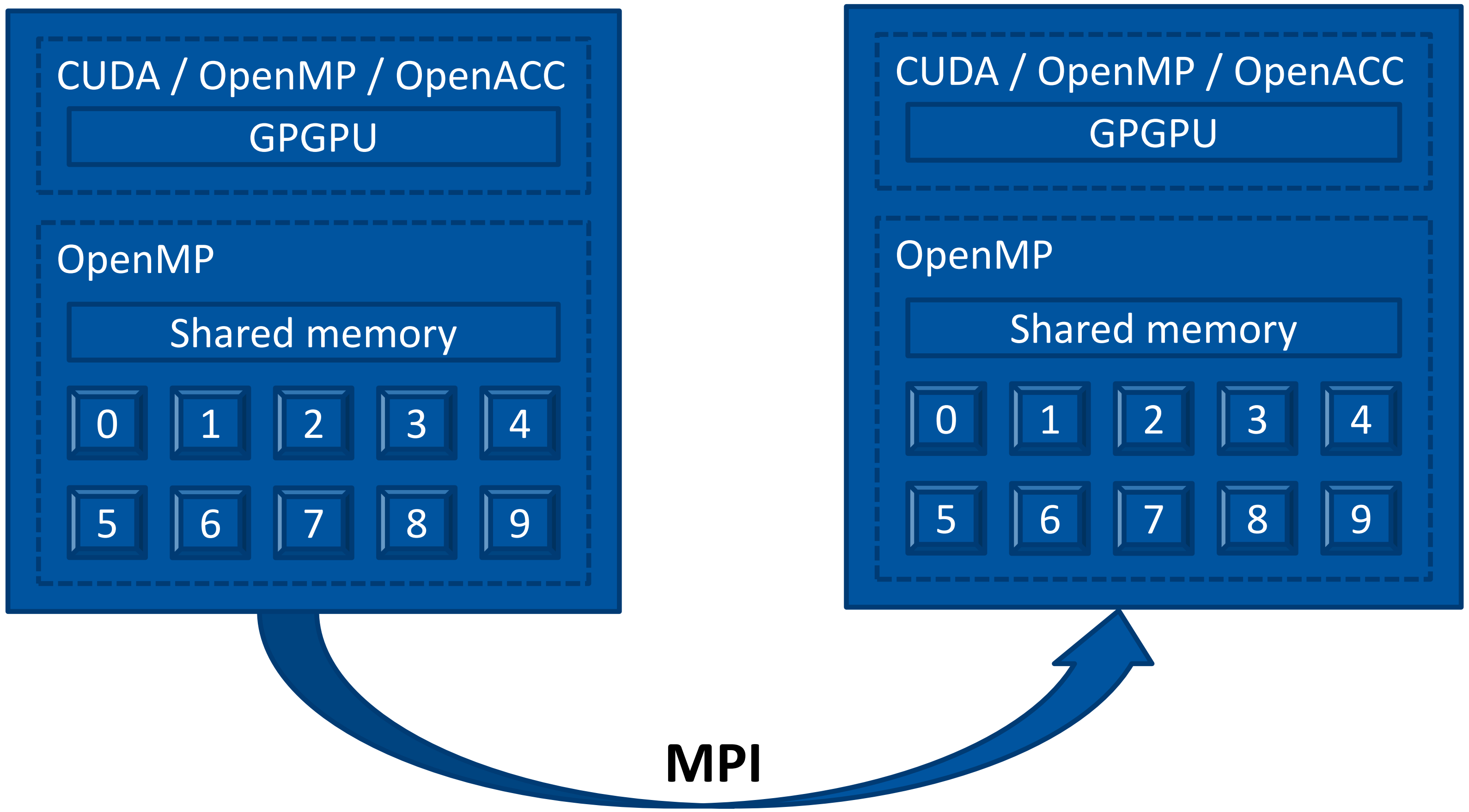
```
cudaMemcpy(h_y, d_y, n * sizeof(float),
  cuda
cudaFree(d_x); cudaFree(d_y);
free(h_x); free(h_y);
return 0;
}
```

3. Transfer data to CPU + free data on GPU

Putting it all together

Hybrid programming

- (Hierarchical) mixing of different programming paradigms


CUDA / OpenMP / OpenACC
GPGPU
OpenMP
Shared memory
0
1
2
3
4
5
6
7
8
9
CUDA / OpenMP / OpenACC
GPGPU
OpenMP
Shared memory
0
1
2
3
4
5
6
7
8
9
MPI