

MPI and OpenMP in Scientific Software Development

Day 3

Maxim Masterov
SURF, Amsterdam, The Netherlands
09-11.06.2021

Agenda

Day 3

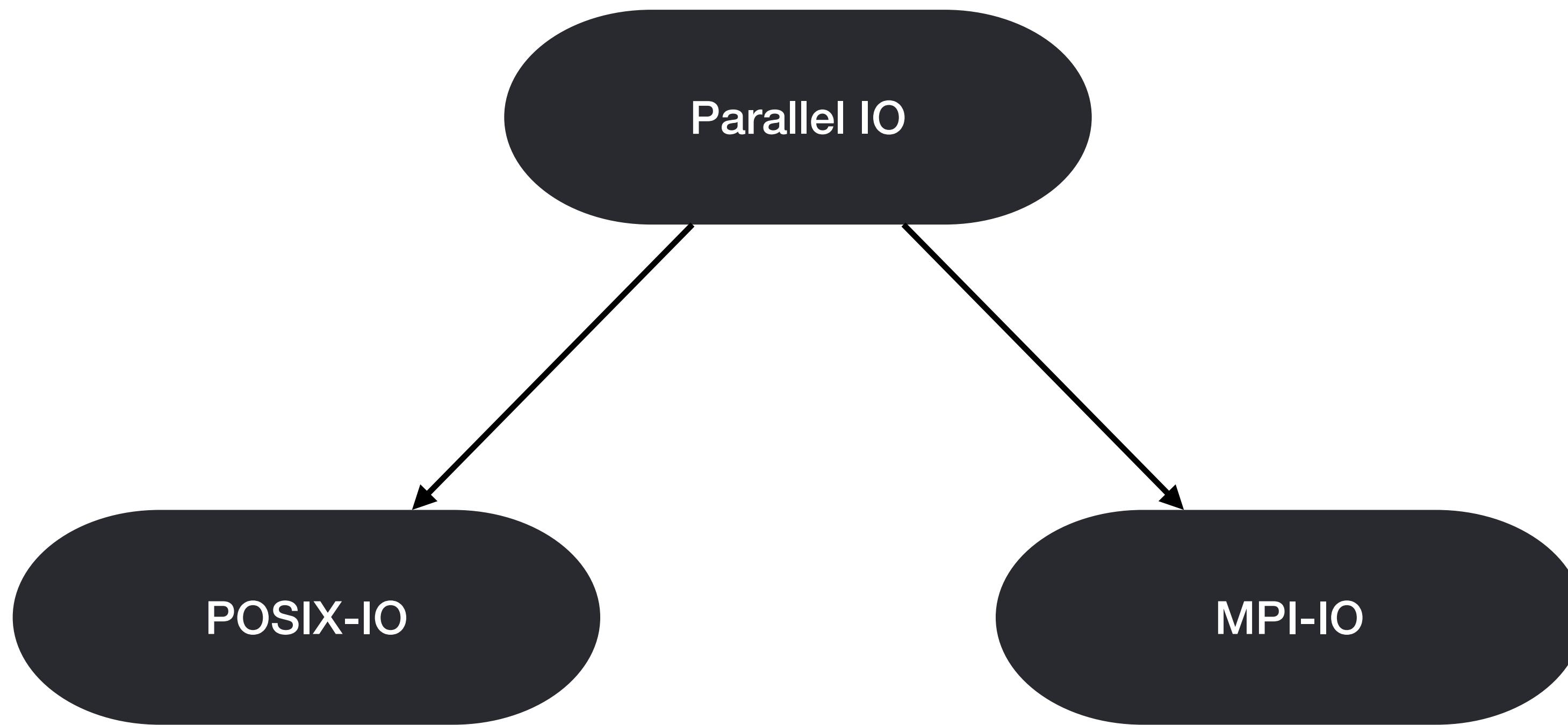
- Invited talk: **Dr. Satish Kamath (SURF)**
- MPI IO
- Hands-on
- Advanced OpenMP
- Hands-on
- Hybrid programming
- Hands-on

Invited talk

MPI IO

MPI IO

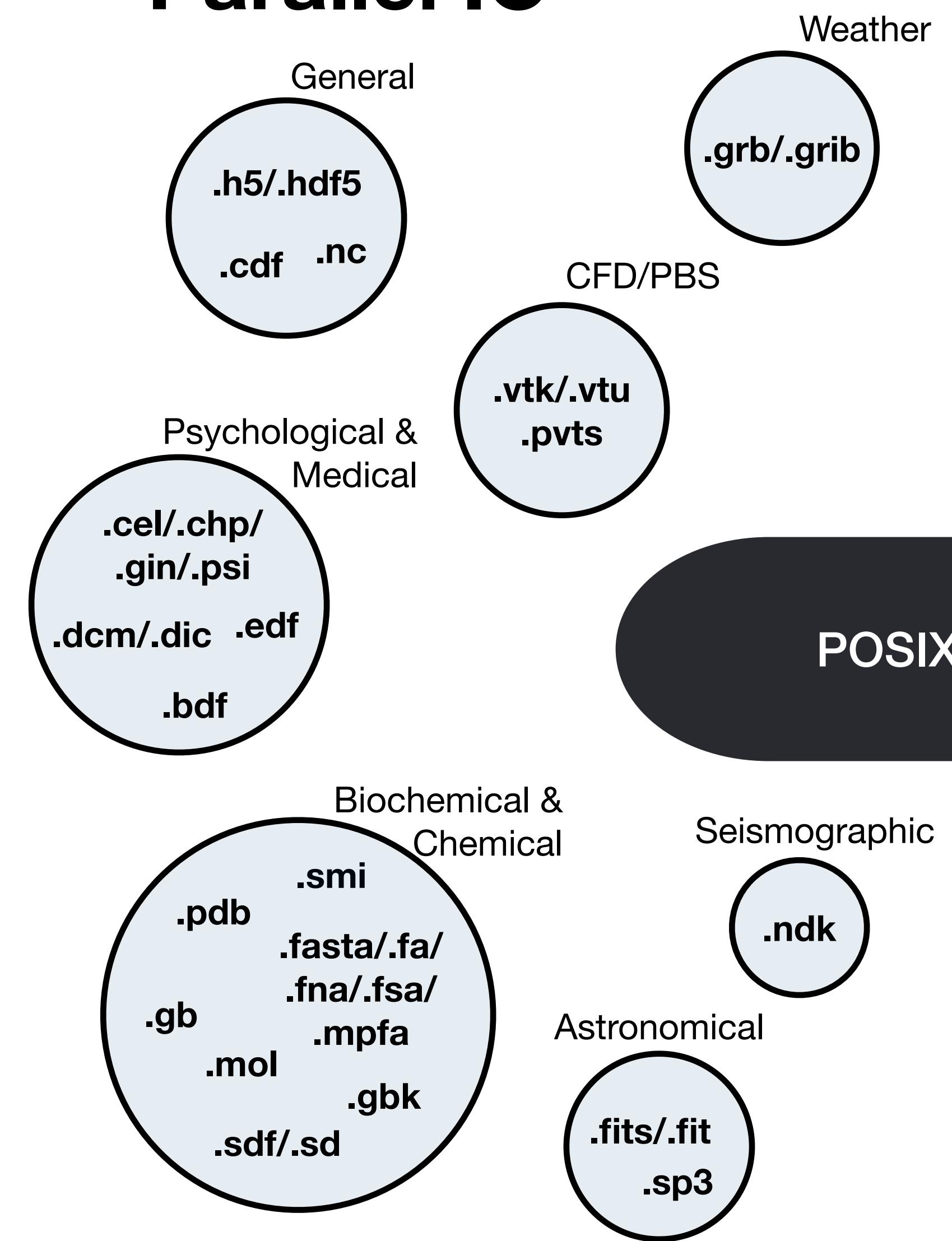
Parallel IO



- The root process writes all data
- Each process writes a single independent file
- Each process writes into the same single file

MPI IO

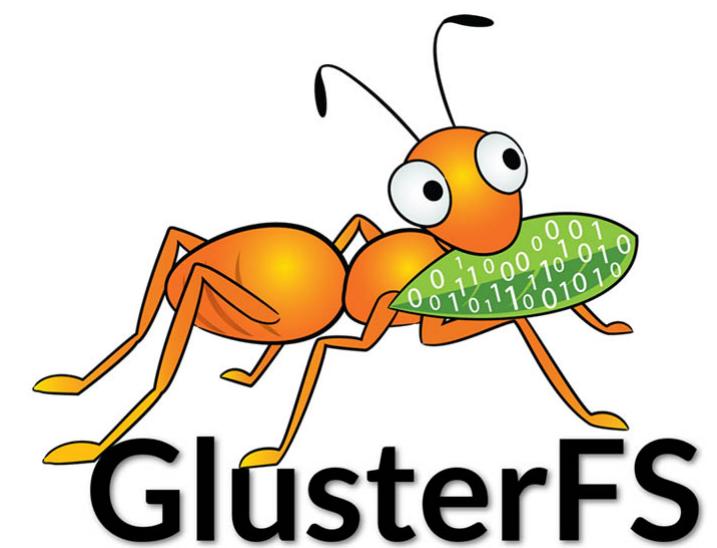
Parallel IO



- Performance
- Scalability
- Robustness

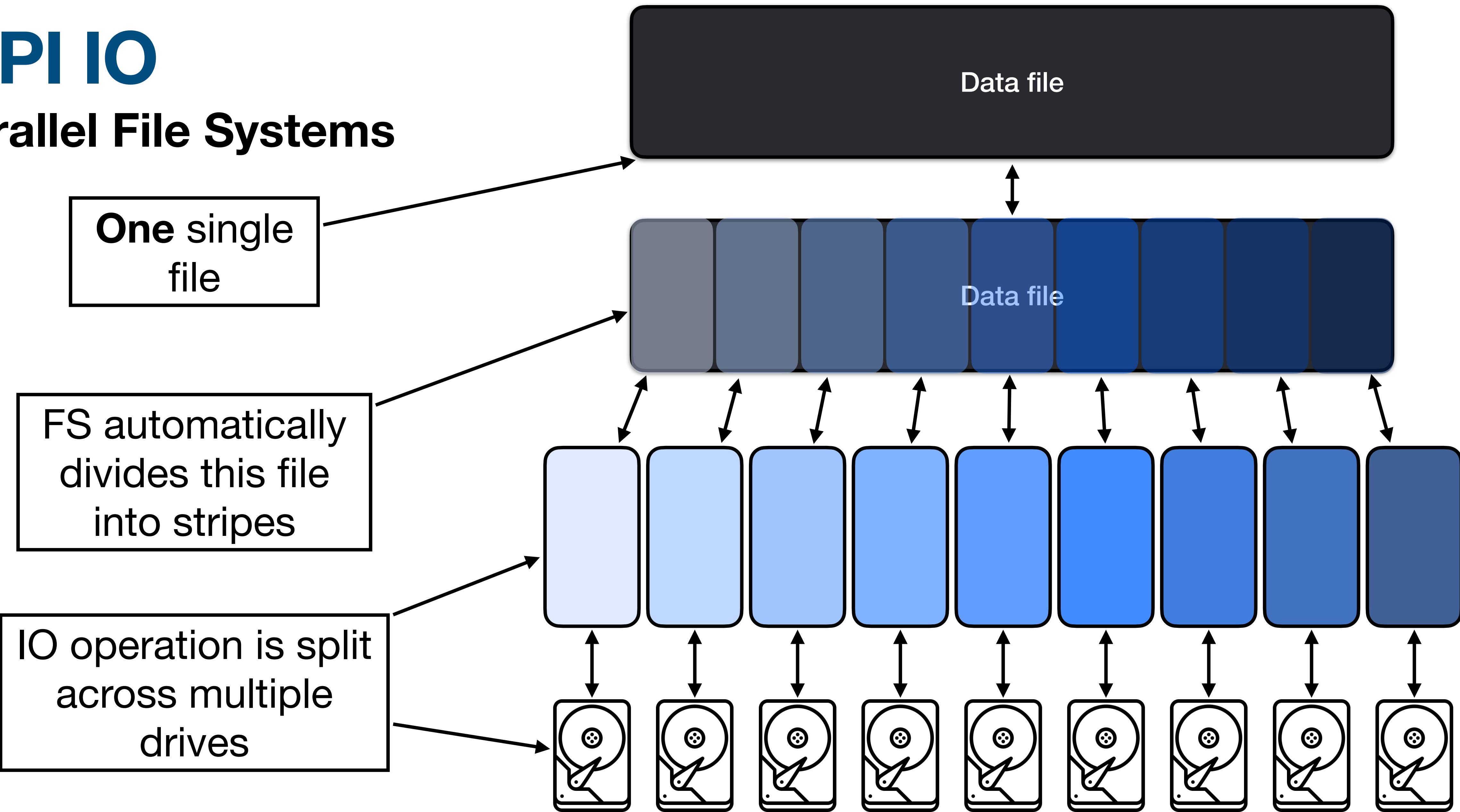


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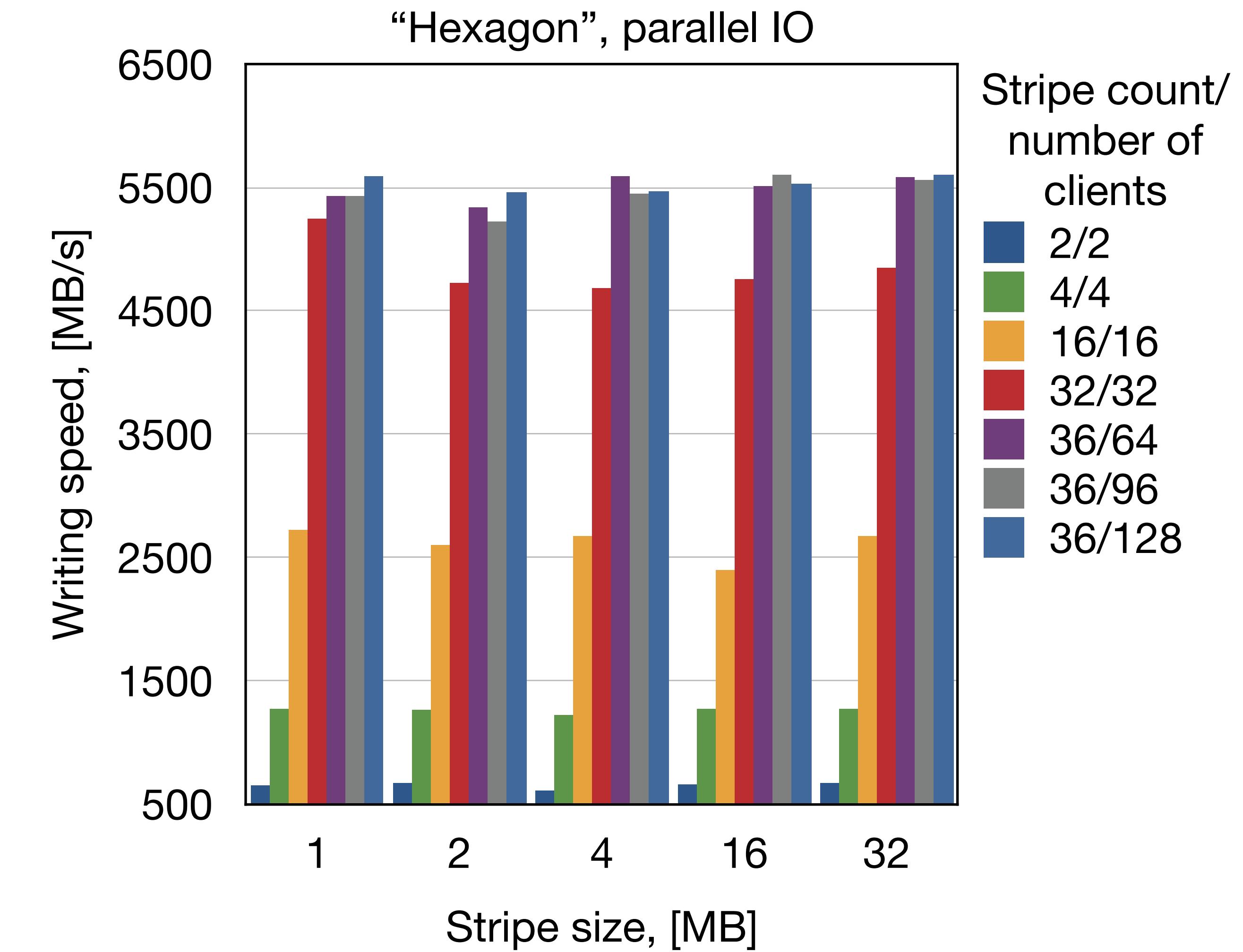
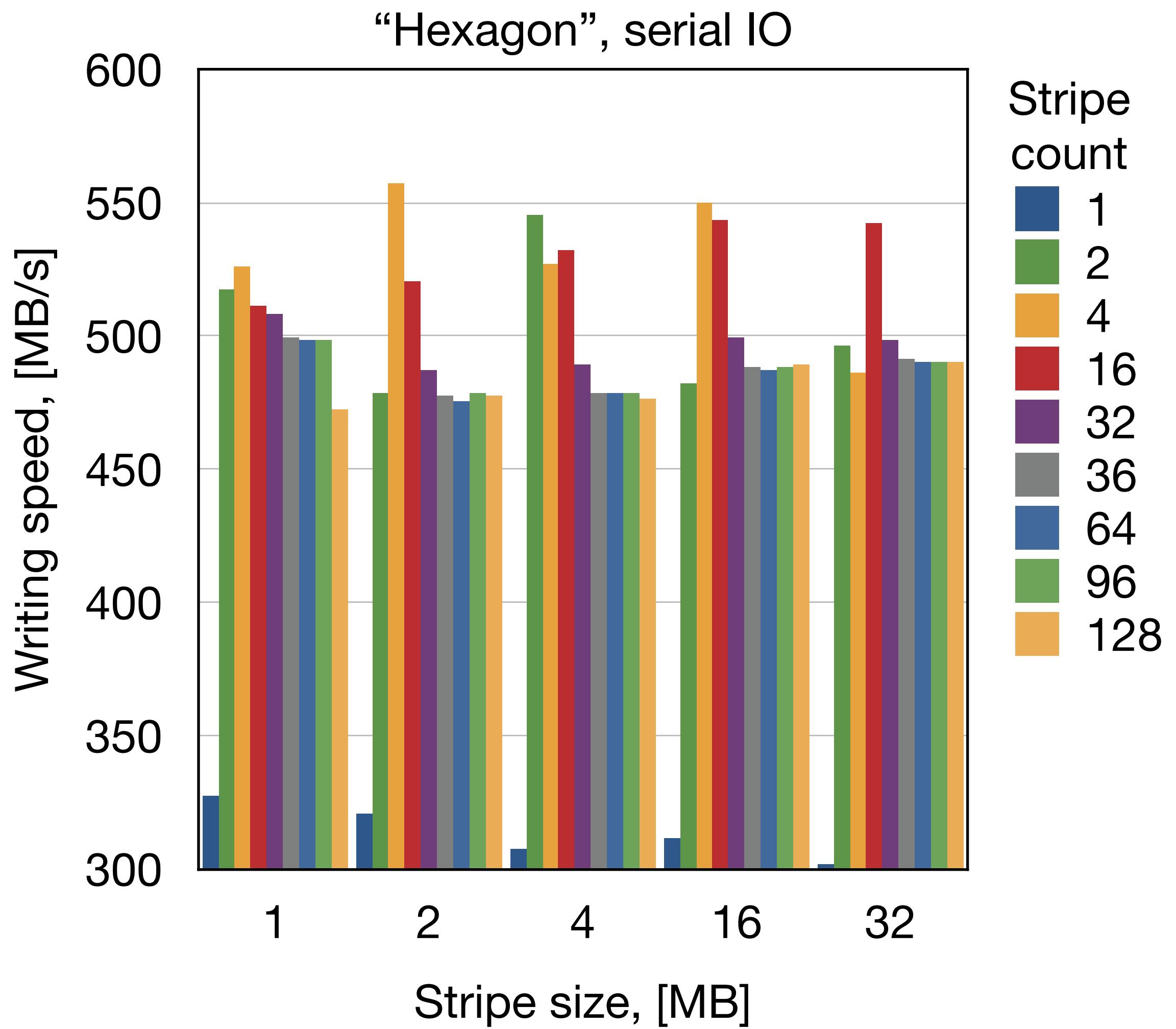
MPI IO

Parallel File Systems



MPI IO

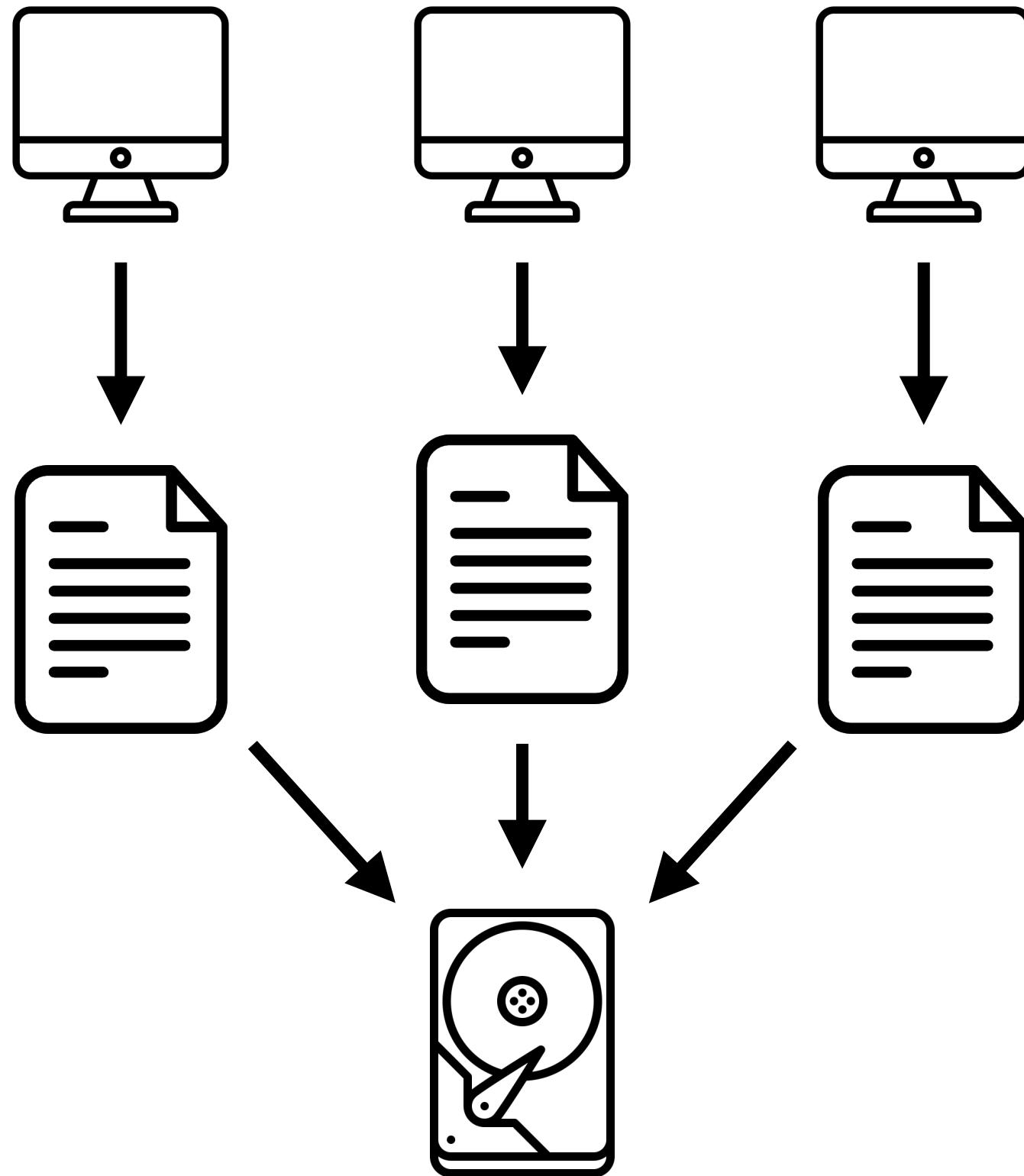
File Systems Performance



MPI IO

Independent files

- Each process performs IO operations on independent files concurrently
- Very simple implementation
- **Limited by the FS**
- **Does not scale (see previous point)**



```
std::ofstream out;  
out.open(file_name);  
  
for(...) { out << ... << "\n"; }  
  
out.close();
```

C++

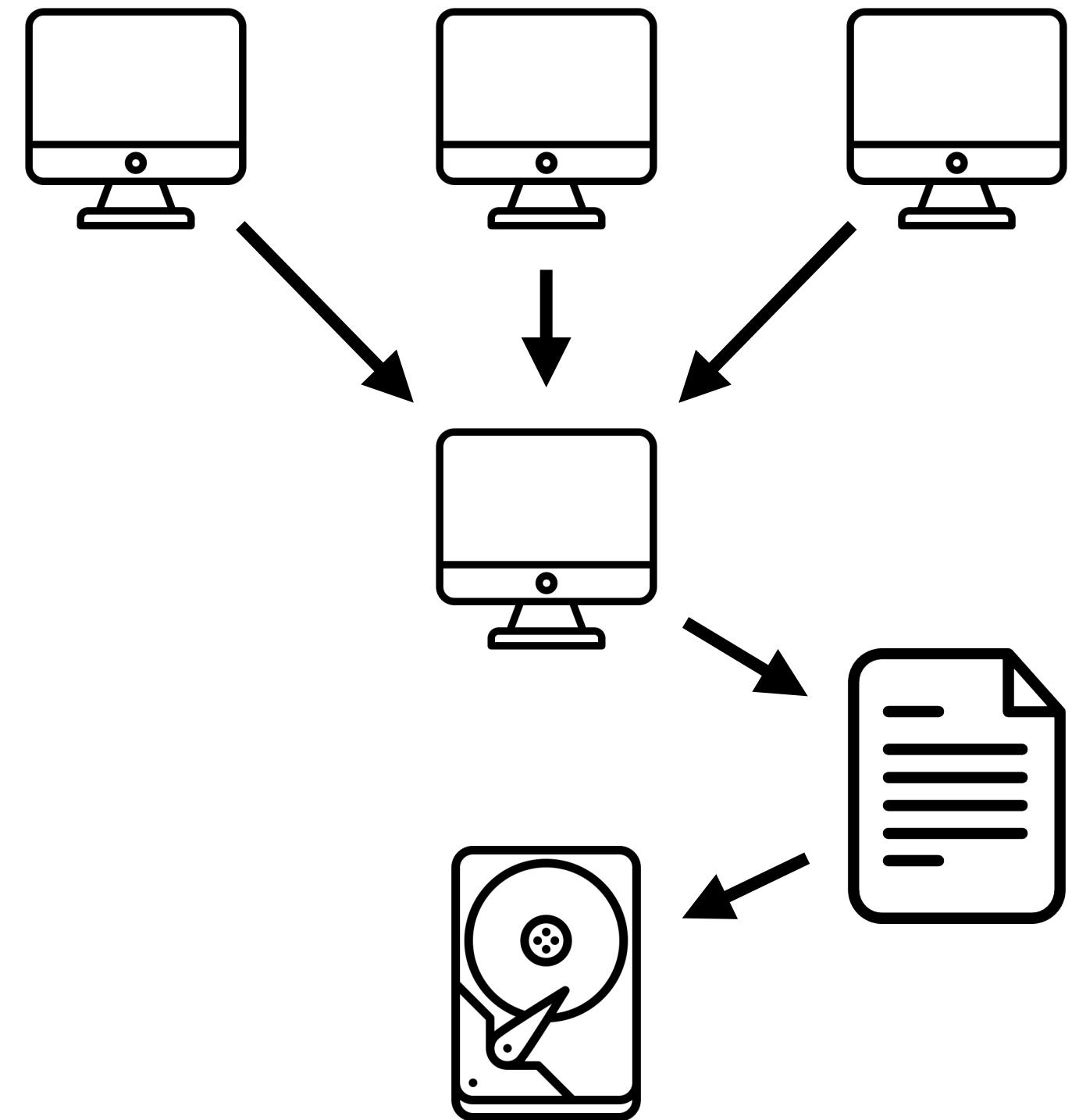
```
open(fh, file = file_name, status = 'new')  
  
do i=1,100  
    write(fh,*) ...  
end do  
  
close(fh)
```

FORTRAN

MPI IO

Master-process approach

- All IO operations are performed by the “root” process using POSIX or MPI library
- Data gathering is required (**MPI_Gather()**, **MPI_Gatherv()**)
- Relatively simple implementation
- **Does not scale (serial)**



```
int MPI_File_open(MPI_Comm comm,           // communicator
                  const char *filename,    // name of file to open
                  int amode,               // file access mode
                  MPI_Info info,           // info object
                  MPI_File *fh);          // file handle

int MPI_File_close(MPI_File *fh);           // file handle
```

- MPI_MODE_RDONLY – read only
- MPI_MODE_RDWR – reading and writing
- MPI_MODE_WRONLY – write only
- MPI_MODE_CREATE – create the file if it does not exist
- MPI_MODE_EXCL – error if creating file that already exists
- MPI_MODE_DELETE_ON_CLOSE – delete file on close
- MPI_MODE_UNIQUE_OPEN – file will not be concurrently opened elsewhere
- MPI_MODE_SEQUENTIAL – file will only be accessed sequentially
- MPI_MODE_APPEND – set initial position of all file pointers to end of file

MPI IO

Shared file

```
int MPI_Gatherv(const void *sendbuf,  
                 int sendcount,  
                 MPI_Datatype sendtype,  
                 void *recvbuf,  
                 const int recvcounts[],  
                 const int displs[],  
                 MPI_Datatype recvtype,  
                 int root,  
                 MPI_Comm comm);  
  
int MPI_Gather(const void *sendbuf,  
               int sendcount,  
               MPI_Datatype sendtype,  
               void *recvbuf,  
               int recvcount,  
               MPI_Datatype recvtype,  
               int root,  
               MPI_Comm comm);
```

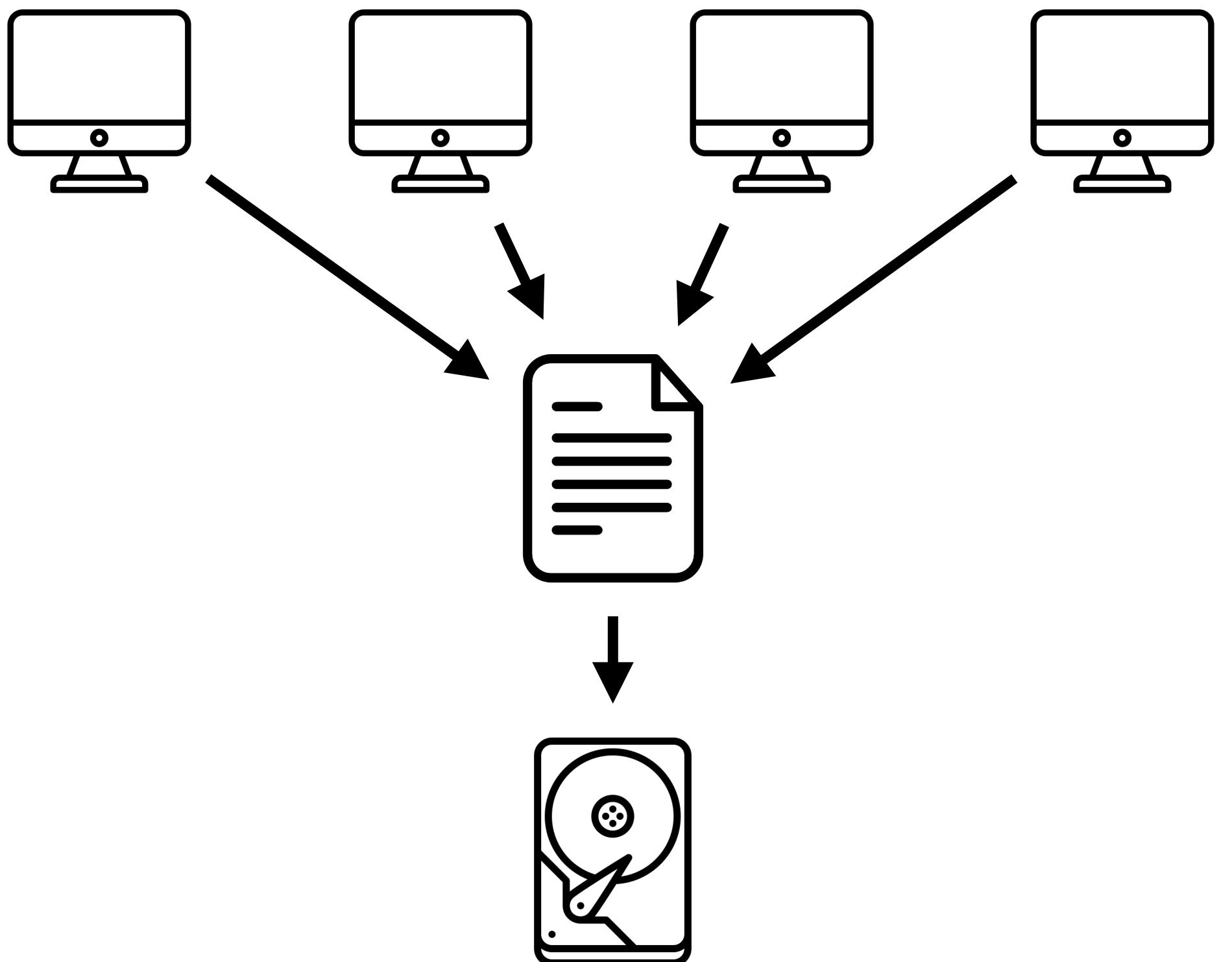
// starting address of send buffer
// number of elements in send buffer
// data type of send buffer elements
// address of receive buffer
// integer array (of length group size) containing the number of
// elements that are received from each process (significant only
// at root)
// integer array (of length group size). Entry i specifies the
// displacement relative to recvbuf at which to place the incoming
// data
// from process i (significant only at root)
// data type of recv buffer elements (significant only at root)
// rank of receiving process
// communicator

// starting address of send buffer
// number of elements in send buffer
// data type of send buffer elements
// number of elements for any single receive (integer, significant
// only at root)
// data type of recv buffer elements (significant only at root)
// data type of recv buffer elements (significant only at root)
// rank of receiving process
// communicator

MPI IO

Shared file

- Each process performs IO operations with one **shared file**
- Implementation complexity depends on the data structure
- **Scalability depends on**
 - **implementation**
 - **file system**



MPI IO

Definitions

file

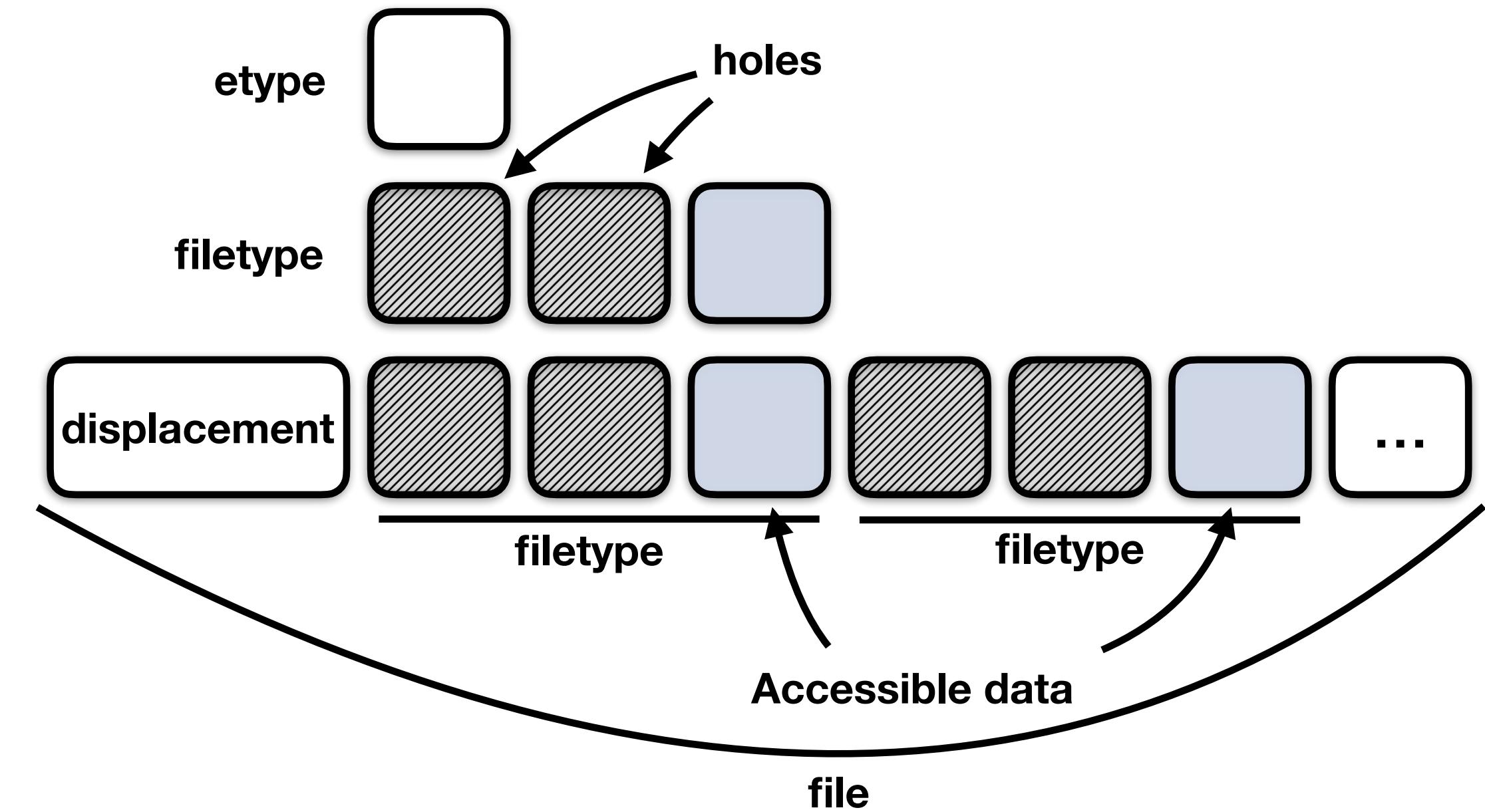
- (MPI file) is an ordered collection of typed data items

displacement

- An absolute byte position relative to the beginning of a file

etype (elementary datatype)

- is the unit of data access and positioning / offsets
- can be any MPI predefined or derived datatype
- typically the same at all processes



filetype

- the basis for partitioning a file among processes
- defines a template for accessing the file
- either a single **etype** or a derived MPI datatype constructed from multiple instances of the same **etype**
- different at each process

MPI IO

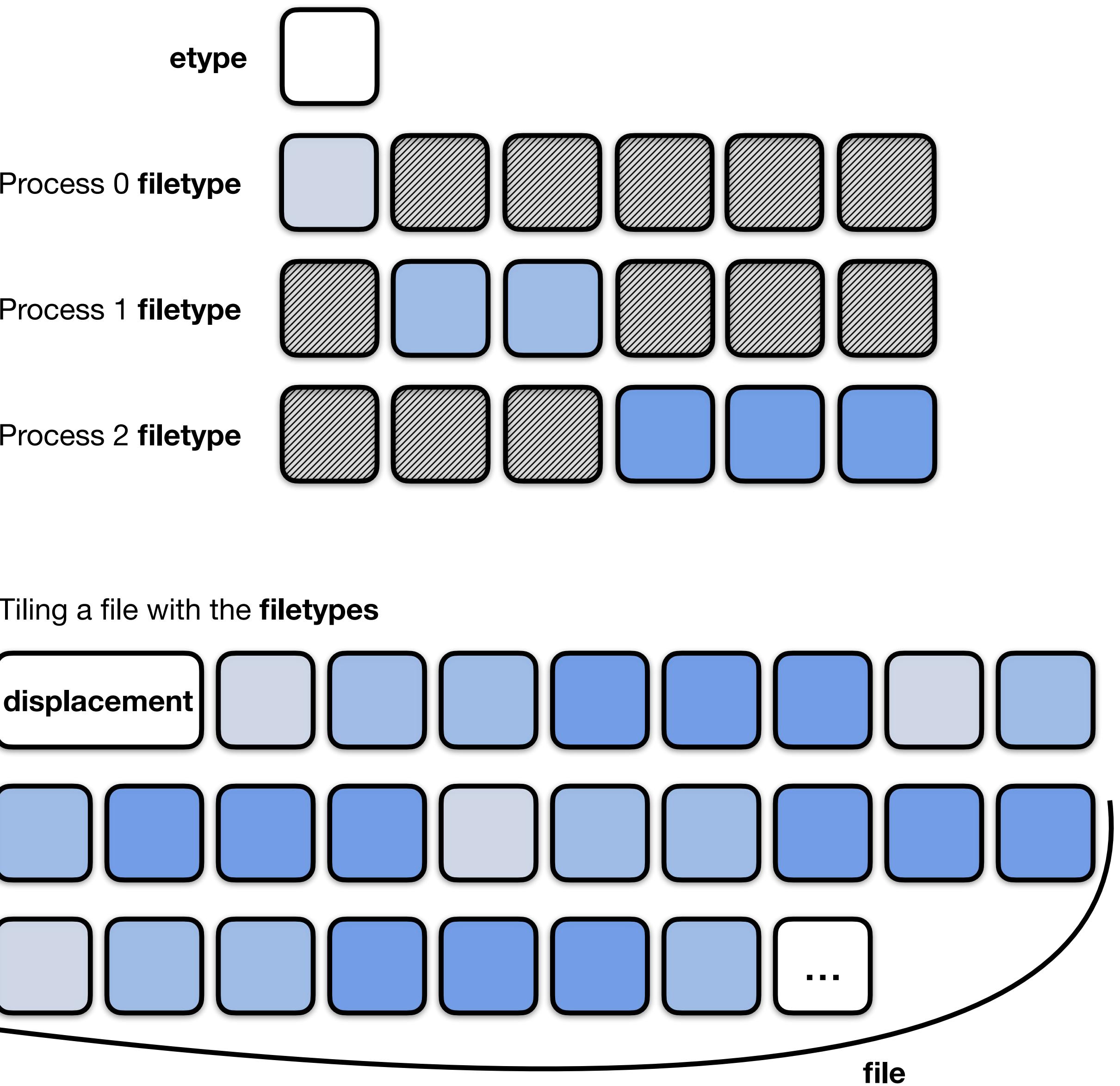
Definitions

view

- defines the current set of data visible and accessible from an open file as an ordered set of **etypes**
- each process has its own view, defined by a **displacement**, an **etype**, and a **filetype**
- the pattern described by a **filetype** is repeated, beginning at the **displacement**

offset

- a position in the file relative to the current view, expressed as a count of **etype**
- holes are skipped when calculating this position



MPI IO

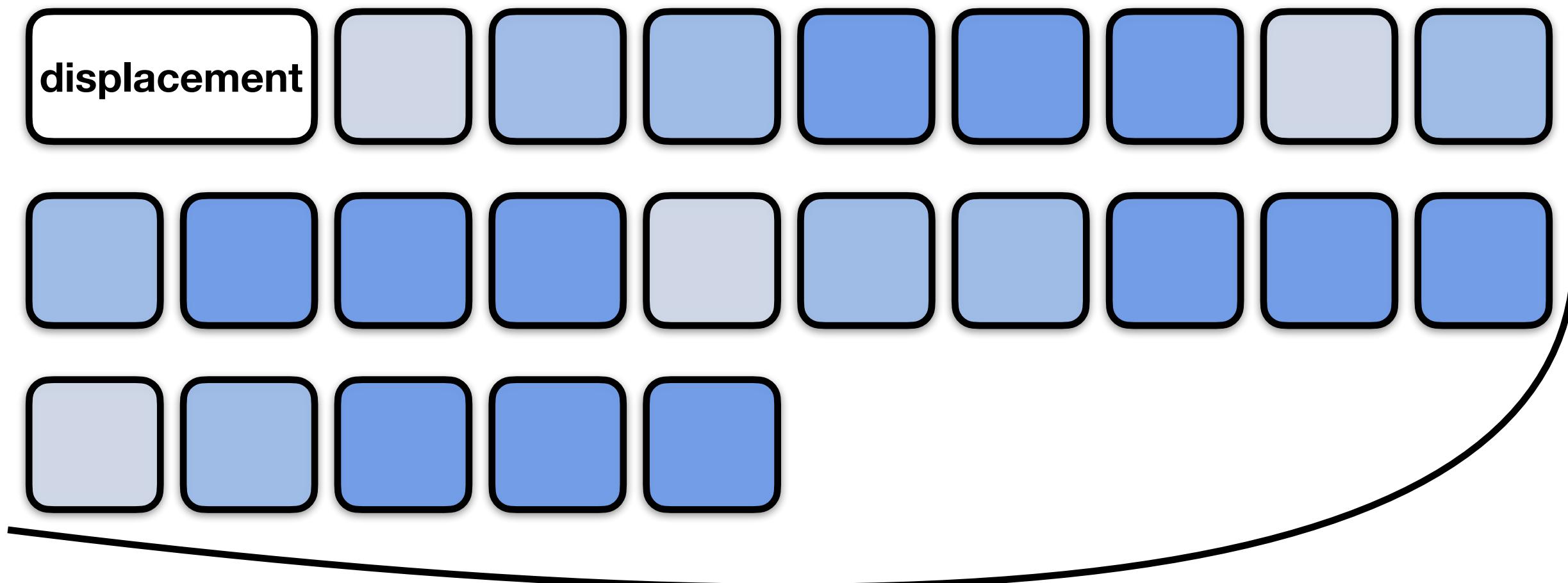
Definitions

file size and end of file

- the size of an MPI file, measured in bytes from the beginning of the file
- for any given **view**, the **end of file** is the offset of the first **etype** accessible in the current **view** starting after the last byte in the file

file pointer

- an implicit offset maintained by MPI
- individual **file pointers** are local to each process
- shared **file pointers** are shared by the group of processes



file size = `sizeof(displacement) + sizeof(etype)`, [B]

file handle

- an opaque object
- created by `MPI_FILE_OPEN`
- freed by `MPI_FILE_CLOSE`

MPI IO

Write to file

```
/* Sets the file view */
int MPI_File_set_view(MPI_File fh,
                      MPI_Offset disp,
                      MPI_Datatype etype,
                      MPI_Datatype filetype,
                      const char *datarep,
                      MPI_Info info);
```

```
// file handle
// displacement
// elementary data type
// file type
// data representation
// info object
```

- Changes the process's view of the data in the file

```
/* Write using individual file pointer */
int MPI_File_write(MPI_File fh,
                   const void *buf,
                   int count,
                   MPI_Datatype datatype,
                   MPI_Status *status);
```

```
// file handle
// initial address of buffer
// number of elements in buffer
// datatype of each buffer element
// status object
```

- Will invoke multiple write/seeks
- May lock the file for other processes

```
/* Collective write using individual file pointer */
int MPI_File_write_all(MPI_File fh,
                       const void *buf,
                       int count,
                       MPI_Datatype datatype,
                       MPI_Status *status);
```

```
// file handle
// initial address of buffer
// number of elements in buffer
// datatype of each buffer element
// status object
```

- MPI library has a “global view” of the file
- Each process knows in advance where to write (collective I/O)

MPI IO

Read from file

```
/* Updates the individual file pointer */
int MPI_File_seek(MPI_File fh,
                  MPI_Offset offset,
                  int whence);                                // file handle
                                                // file offset
                                                // update mode

/* Read using individual file pointer */
int MPI_File_read(MPI_File fh,
                   void *buf,
                   int count,
                   MPI_Datatype datatype,
                   MPI_Status *status);                      // file handle
                                                // initial address of buffer
                                                // number of elements in buffer
                                                // datatype of each buffer element
                                                // status object

/* Collective read using individual file pointer */
int MPI_File_read_all(MPI_File fh,
                      void *buf,
                      int count,
                      MPI_Datatype datatype,
                      MPI_Status *status);                     // file handle
                                                // initial address of buffer
                                                // number of elements in buffer
                                                // datatype of each buffer element
                                                // status object
```

- MPI_SEEK_SET – the pointer is set to offset
- MPI_SEEK_CUR – the pointer is set to the current pointer position plus offset
- MPI_SEEK_END – the pointer is set to the end of the file plus offset



MPI IO

Complex data types

- One can create a **derived data types** and use collective operations in order to **simplify IO** operations.

For an arbitrary 2D array:

```
int arr[nx_glob][ny_glob];                                // declare a 2D array
// use the array...
int dims = 2;                                              // dimensions of the array
int glob_sizes[dims] = {nx_glob, ny_glob};                  // global sizes of the array
int loc_sizes[dims] = {nx_loc, ny_loc};                     // local sizes of the array
int start_inds[dims] = {beg_glob_ind_x, beg_glob_ind_y};  // starting indices in the global view
MPI_Datatype subarray_type;                                // the name of the new data type

MPI_Type_create_subarray(2,                                     // number of dimensions
                       glob_sizes,                         // number of elements of type oldtype in each dimension of the full array
                       loc_sizes,                          // number of elements of type oldtype in each dimension of the subarray
                       start_inds,                         // starting coordinates of the subarray in each dimension
                       MPI_ORDER_C,                        // array storage order flag
                       MPI_INT,                            // array element datatype
                       &subarray_type); // new datatype

MPI_Type_commit(&subarray_type);

MPI_Send(arr, 1, subarray_type, ...);
```

MPI IO

Complex data types

```
/* Create a datatype for a subarray of a regular, multidimensional array */
int MPI_Type_create_subarray(int ndims,                                // number of array dimensions
                            const int size_array[],           // number of elements of type oldtype in each dimension
                            const int subsize_array[],       // number of elements of type oldtype in each dimension
                            const int start_array[],        // of the full array
                            int order,                      // of the subarray
                            MPI_Datatype oldtype,          // starting coordinates of the subarray in each dimension
                            MPI_Datatype *newtype);         // array storage order flag
                                                // array element datatype
                                                // new datatype

/* Commits the datatype */
int MPI_Type_commit(MPI_Datatype *type);                                // datatype
```

Hands-on

Hands-on

MPI-IO

- Implement in the Jacobi code:
 - MPI-write using all-to-one communication in ***IO/io.cpp:writeByRoot()***
 - Use **MPI_Gather()** and **MPI_Gatherv()** to assemble the data on the root process
 - MPI-write using shared file ***IO/io.cpp:writeByAll()***
 - Create a new data type for the temperature field using **MPI_Type_create_subarray()**
 - Use **MPI_File_write_all()** and **MPI_File_write()** (compare the performance)
 - Visualise the output using the following commands in *gnuplot* (change the **array** size accordingly):

```
gnuplot> set pm3d map
gnuplot> splot "output.dat" bin array=10x10 format='%lf' w image
```

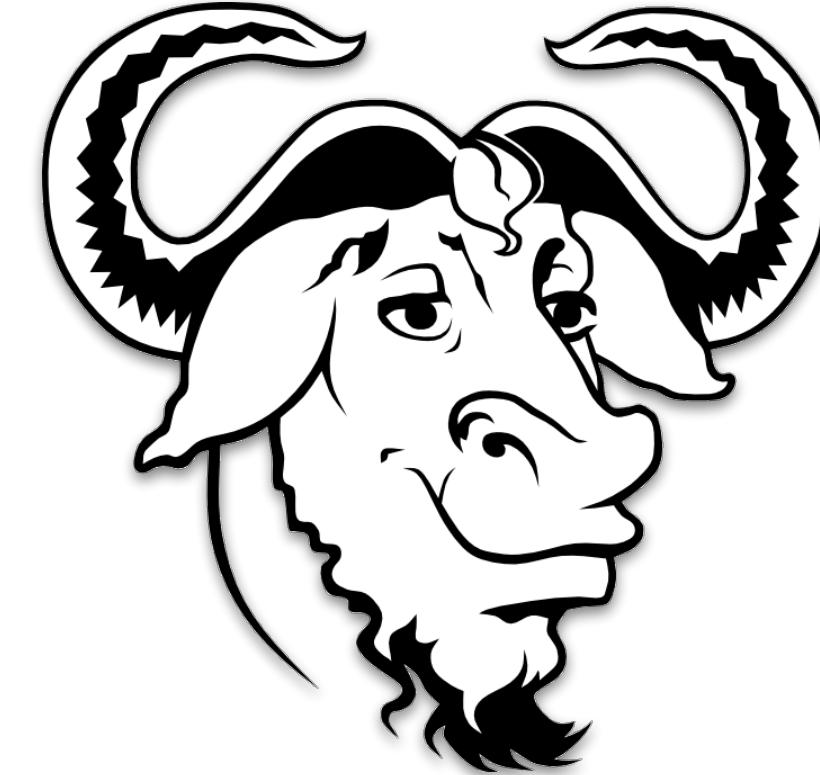
OpenMP-1

OpenMP

Basics

- Different implementations/vendors provide different level of support
- Officially, 19 compilers implement the OpenMP API¹
- The most popular: **GNU, LLVM, Intel**

```
#pragma omp parallel for
for (int n = 0; n < N; ++n) {
    compute(...);
}
```



 Lawrence Livermore
National Laboratory

 **BSC**
Barcelona
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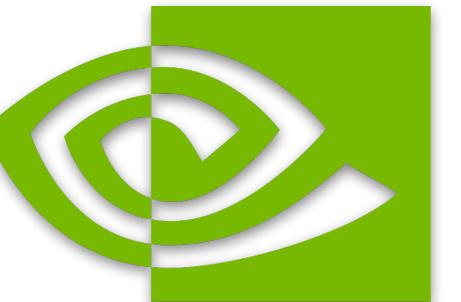
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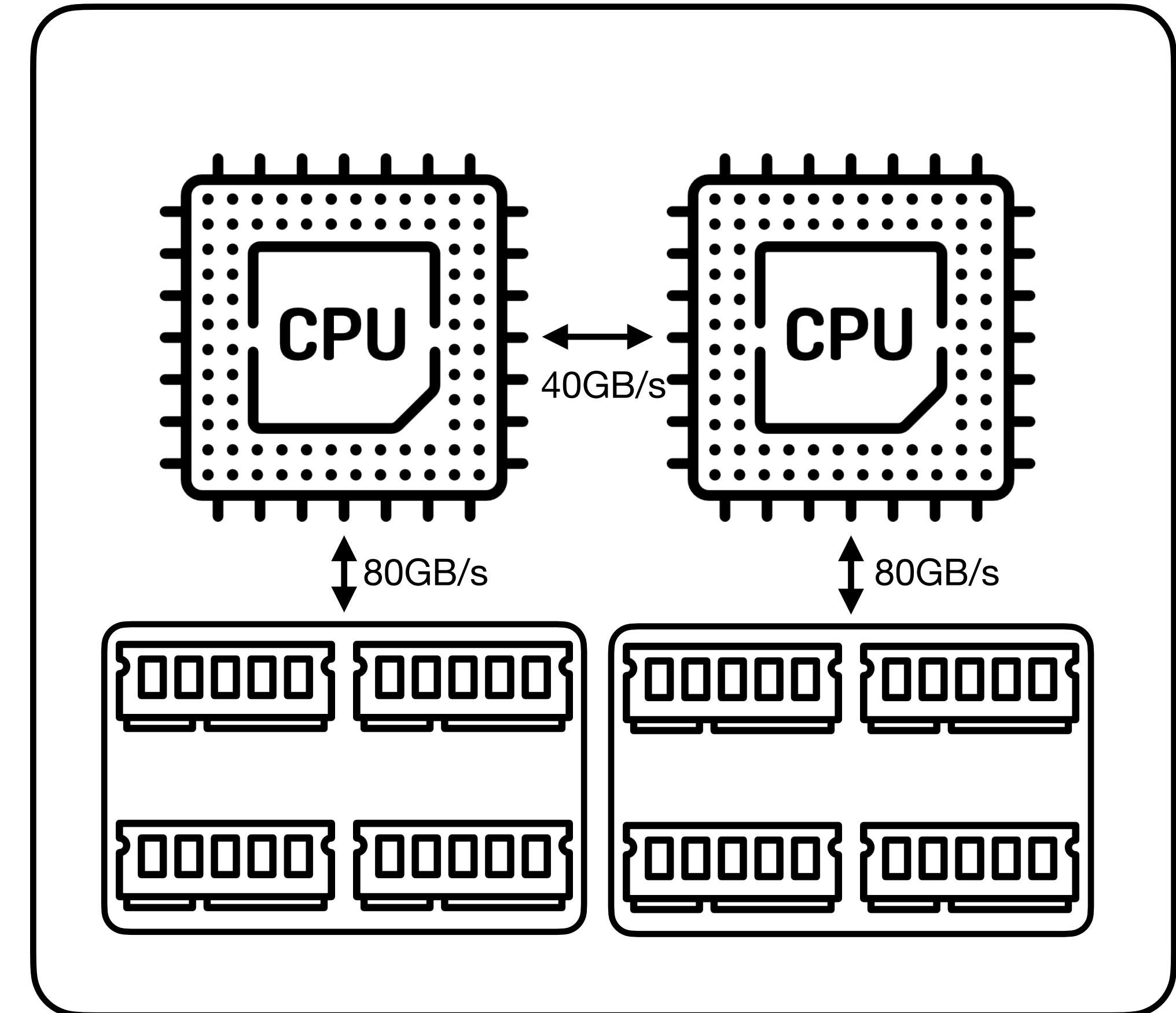
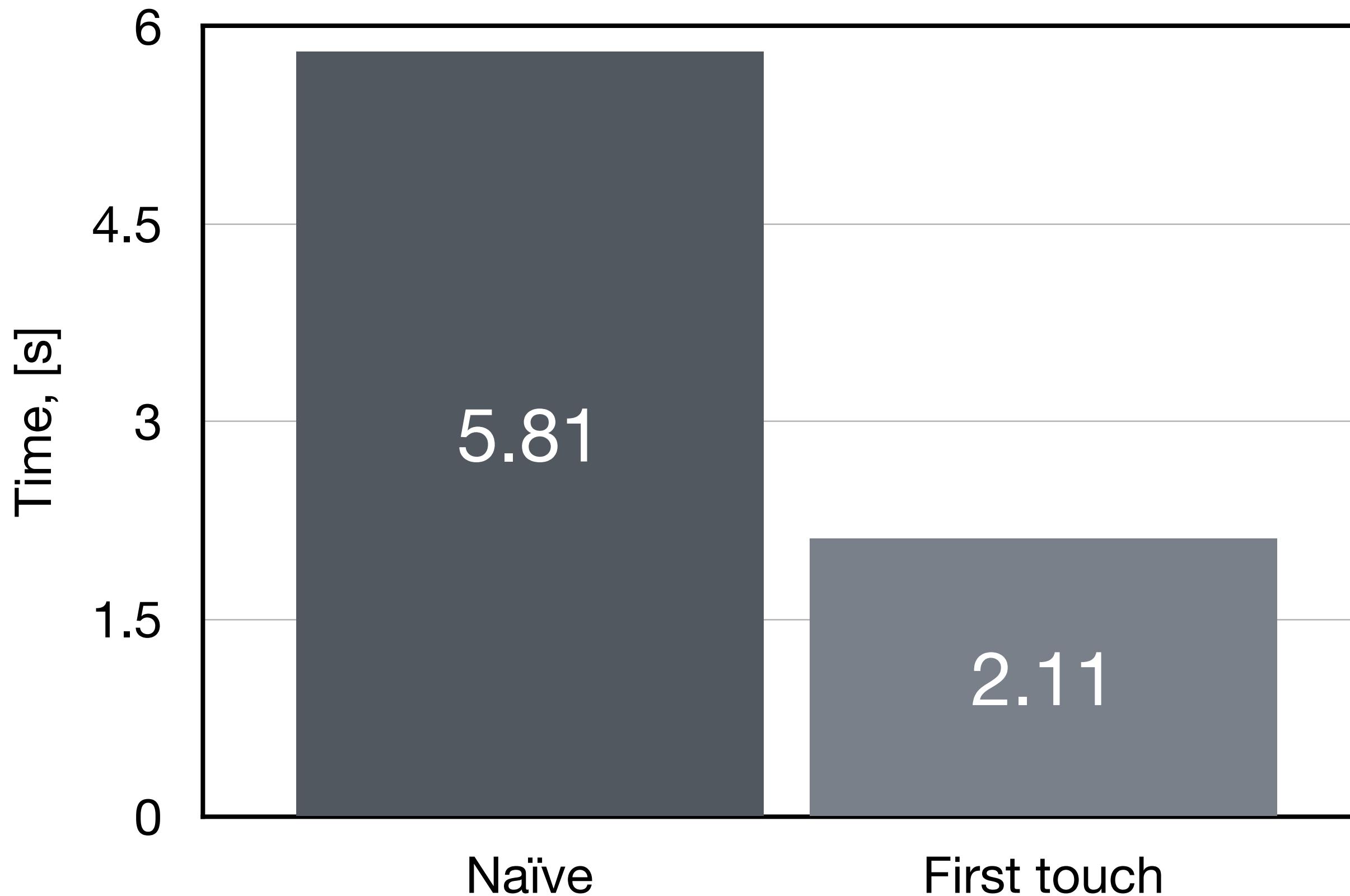


1. <https://www.openmp.org/resources/openmp-compilers-tools/>

OpenMP

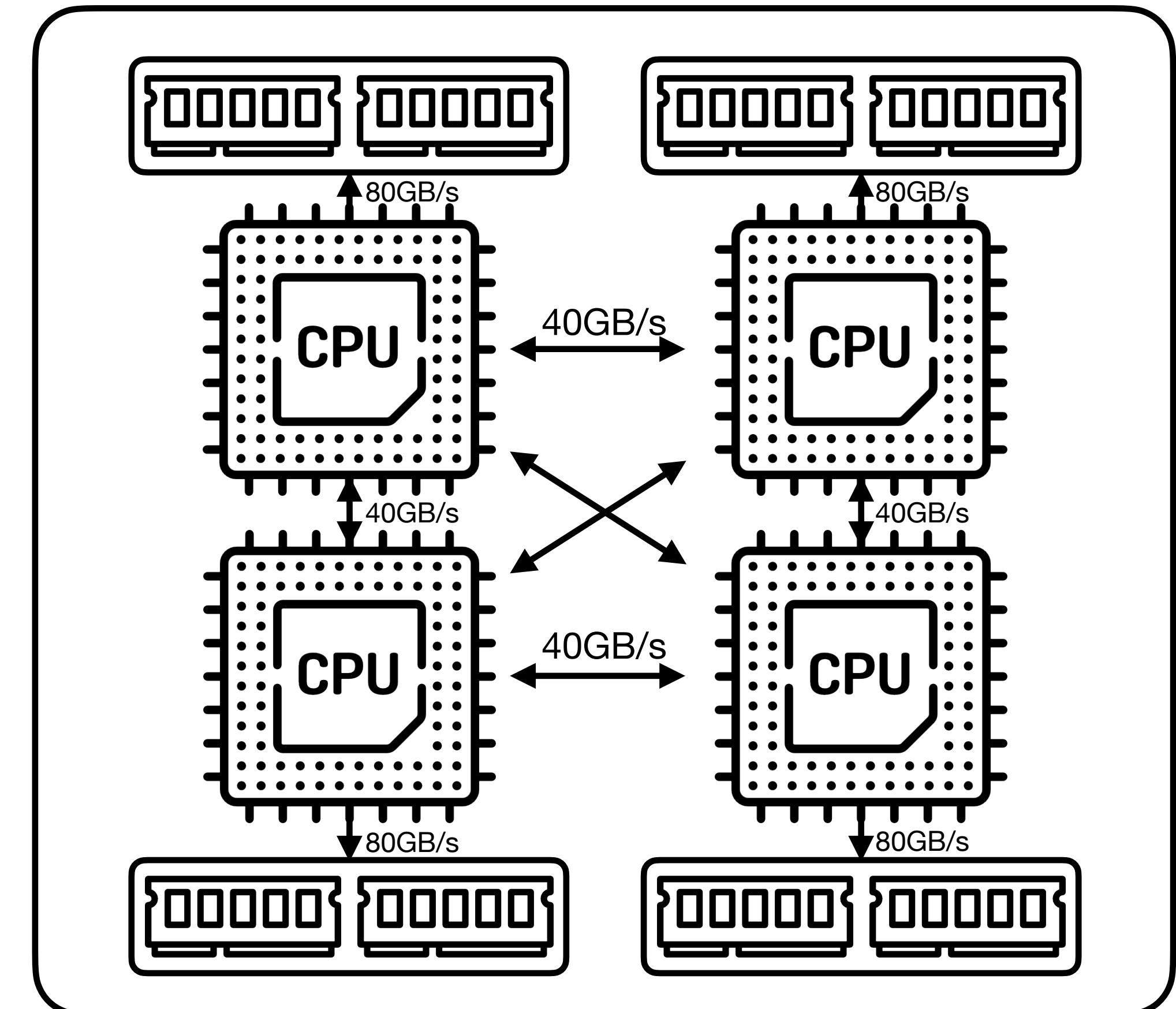
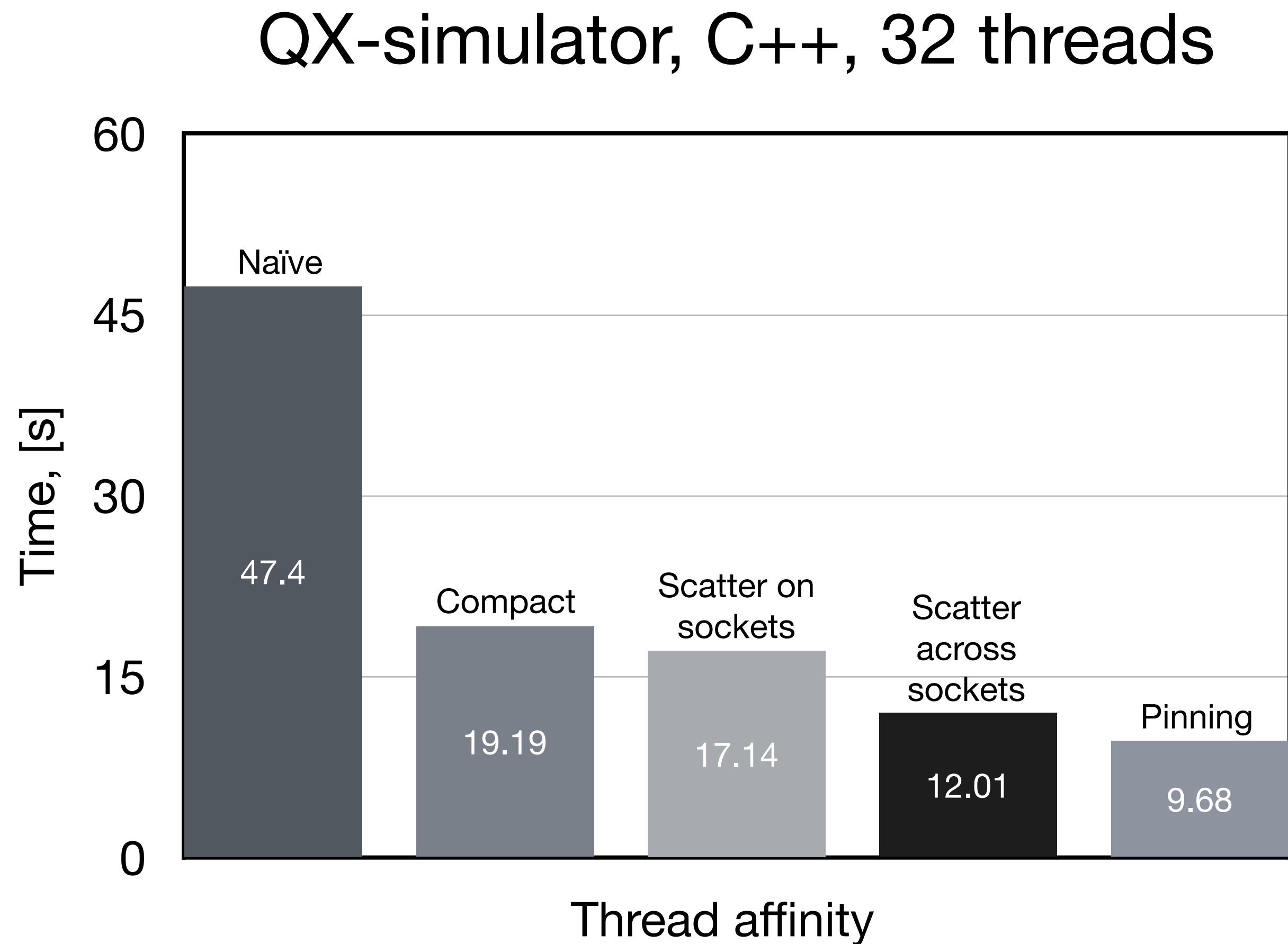
Memory placement

MKA, FORTRAN, 16 threads



OpenMP

Thread affinity

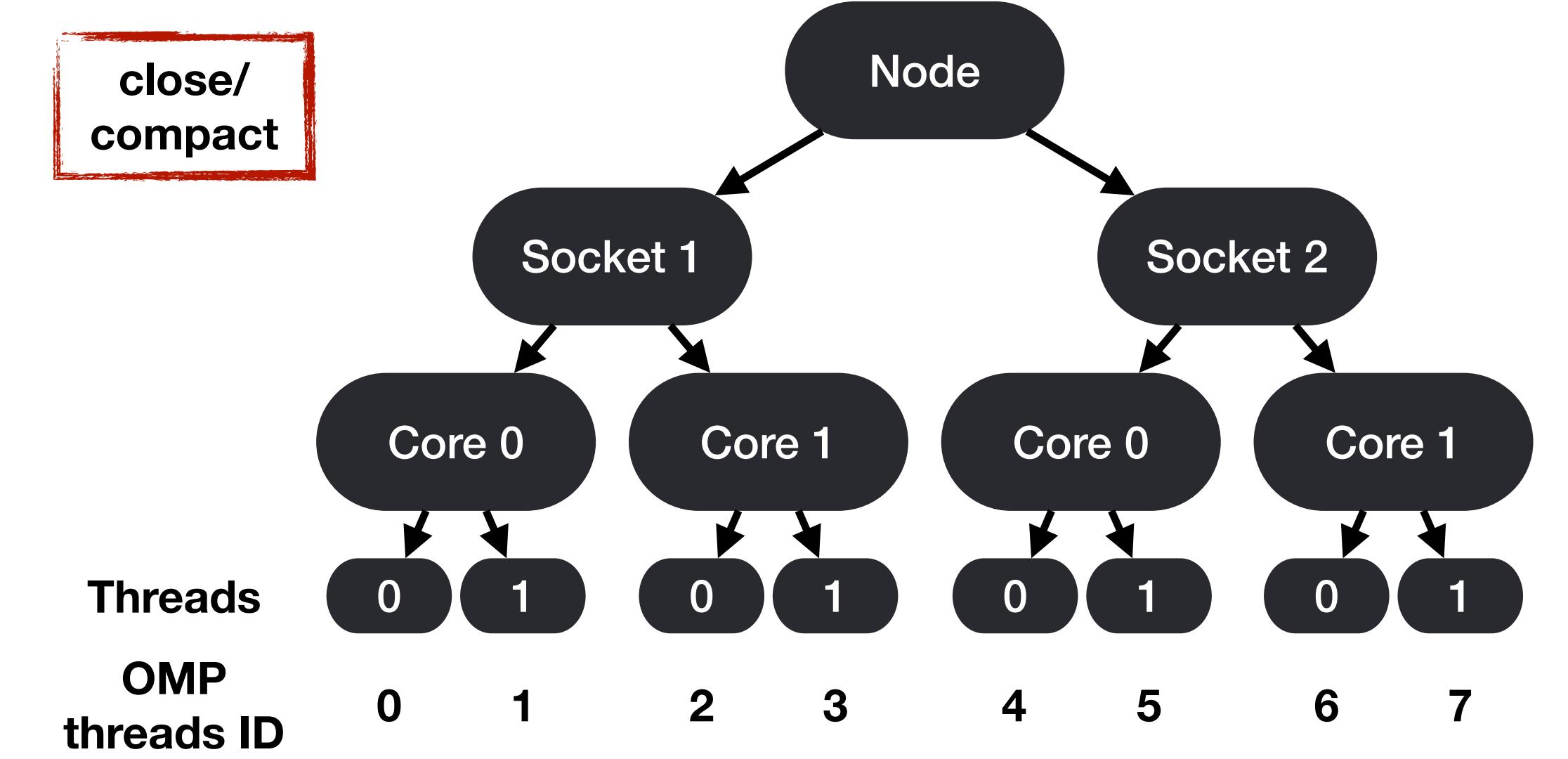


OpenMP

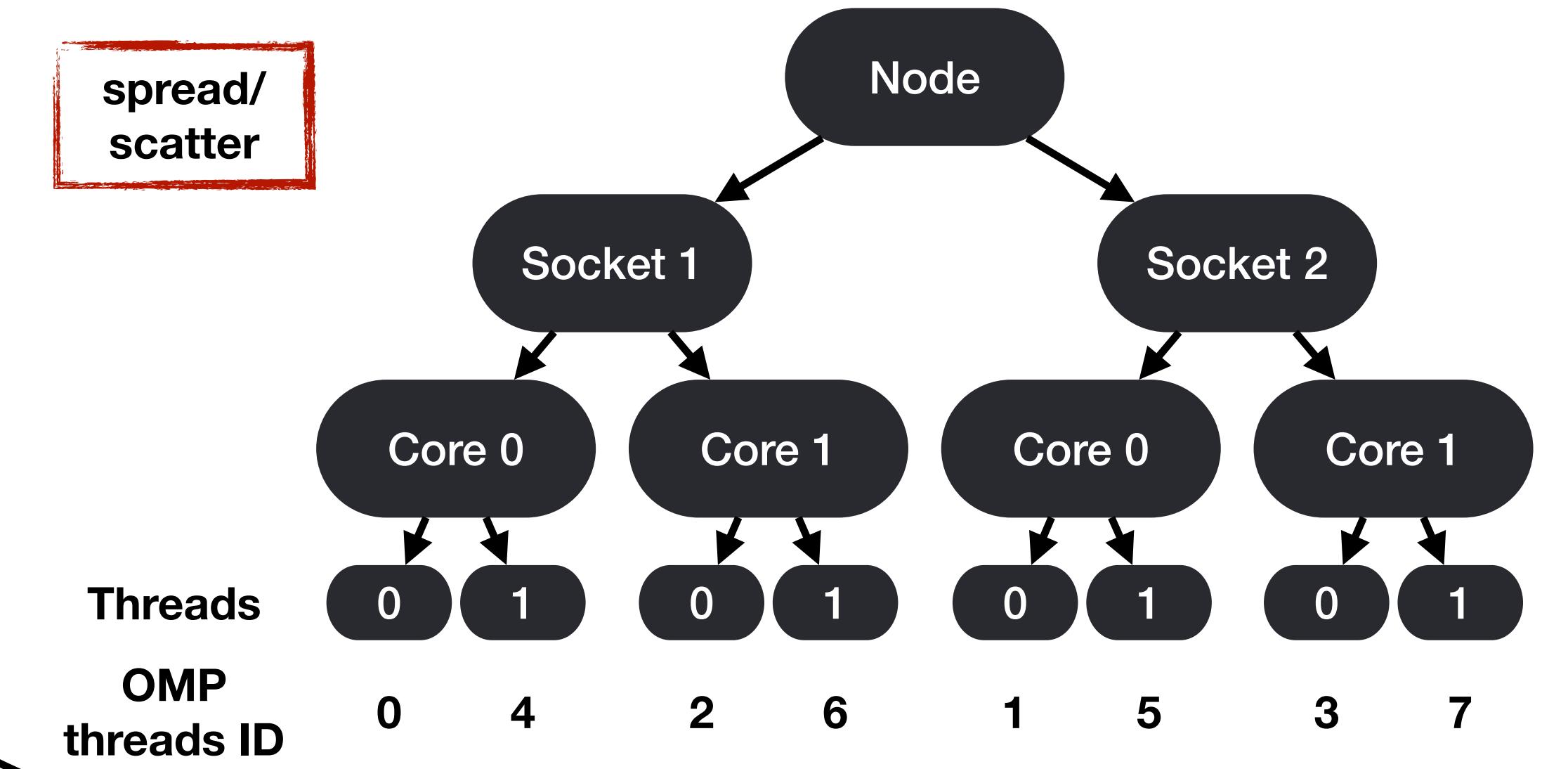
Thread affinity

- Common:
 - **OMP_PROC_BIND**=true | false | close | spread
 - Specifies whether threads may be moved between CPUs
 - **OMP_PLACES**=threads | cores | sockets
 - Specifies on which CPUs the threads should be placed
- GNU:
 - **GOMP_CPU_AFFINITY**="0 3 1-2 4-15:2"
 - Bind threads to specific CPUs
- Intel:
 - **KMP_AFFINITY**=[<modifier>,...]<type>[,<permute>][,<offset>]
 - modifier
 - *granularity = fine | thread | core | tile*
 - *type = balanced, compact, disabled, explicit, none, scatter*

close/
compact



spread/
scatter



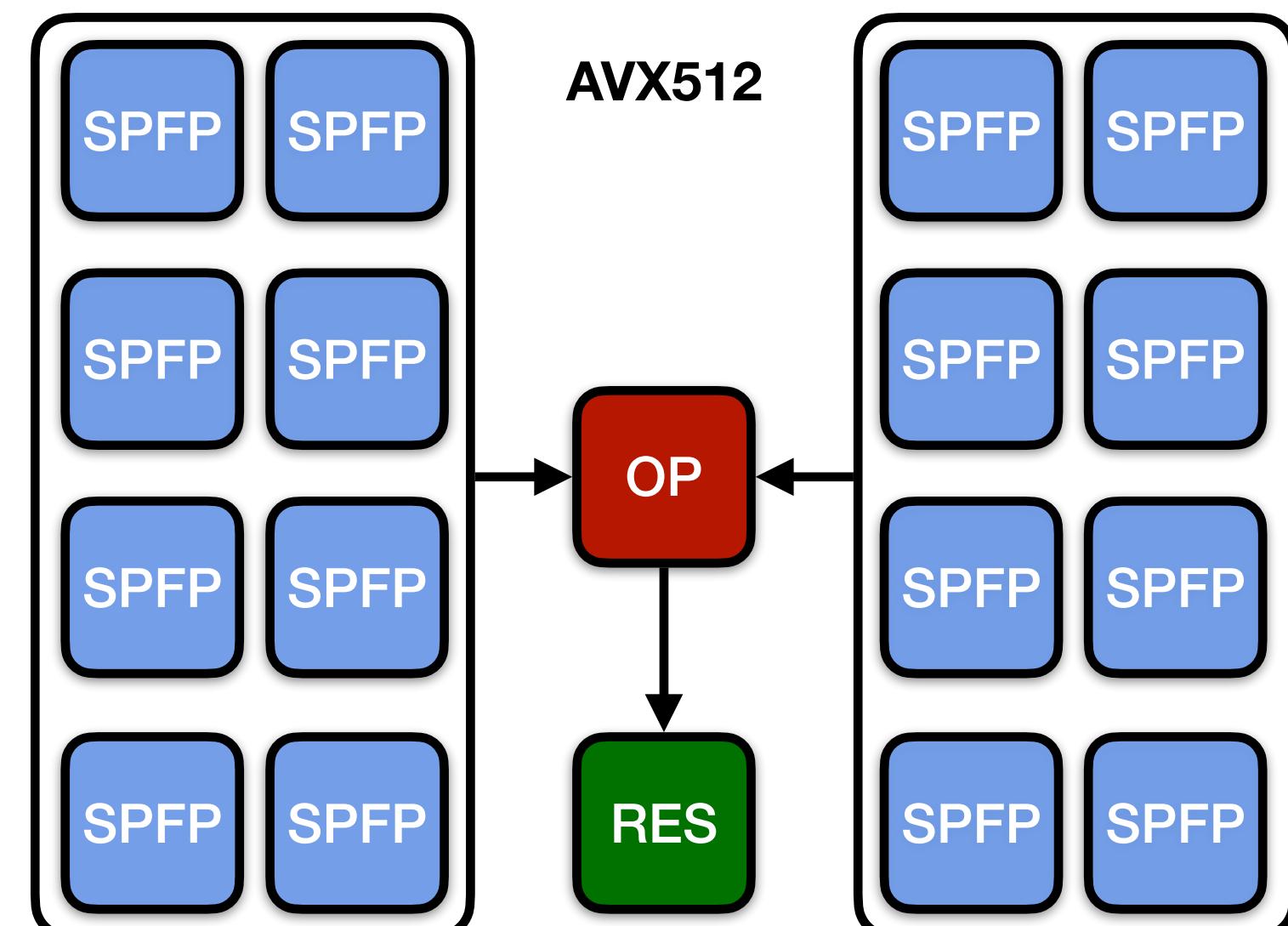
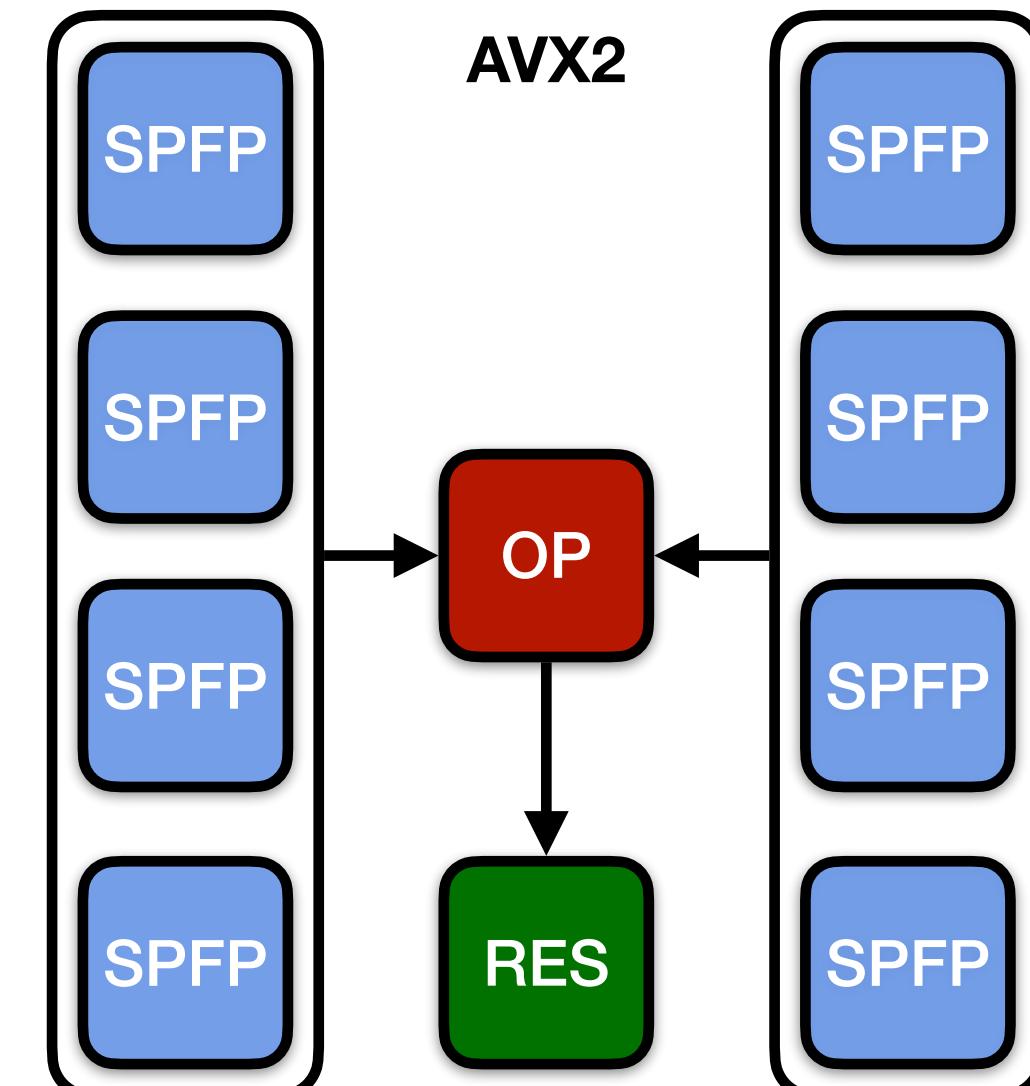
Read more: <https://software.intel.com/content/www/us/en/develop/documentation/cpp-compiler-developer-guide-and-reference/top/optimization-and-programming-guide/openmp-support/openmp-library-support/thread-affinity-interface-linux-and-windows.html>

OpenMP

Latest

- **SIMD directive:** multiple iterations of the loop can be executed concurrently using SIMD instructions
- Some useful options to check the vectorisation
 - **GNU:** *-fopt-info-vec-optimized*
 - **Intel:** *-fopt-report-phase=vectorize*

```
#pragma omp simd [clause[ [, clause] ... ] new-line
for (int n = 0; n < N; ++n) {
    compute(...);
}
```



Hands-on

Hands-on

Filling the empty space

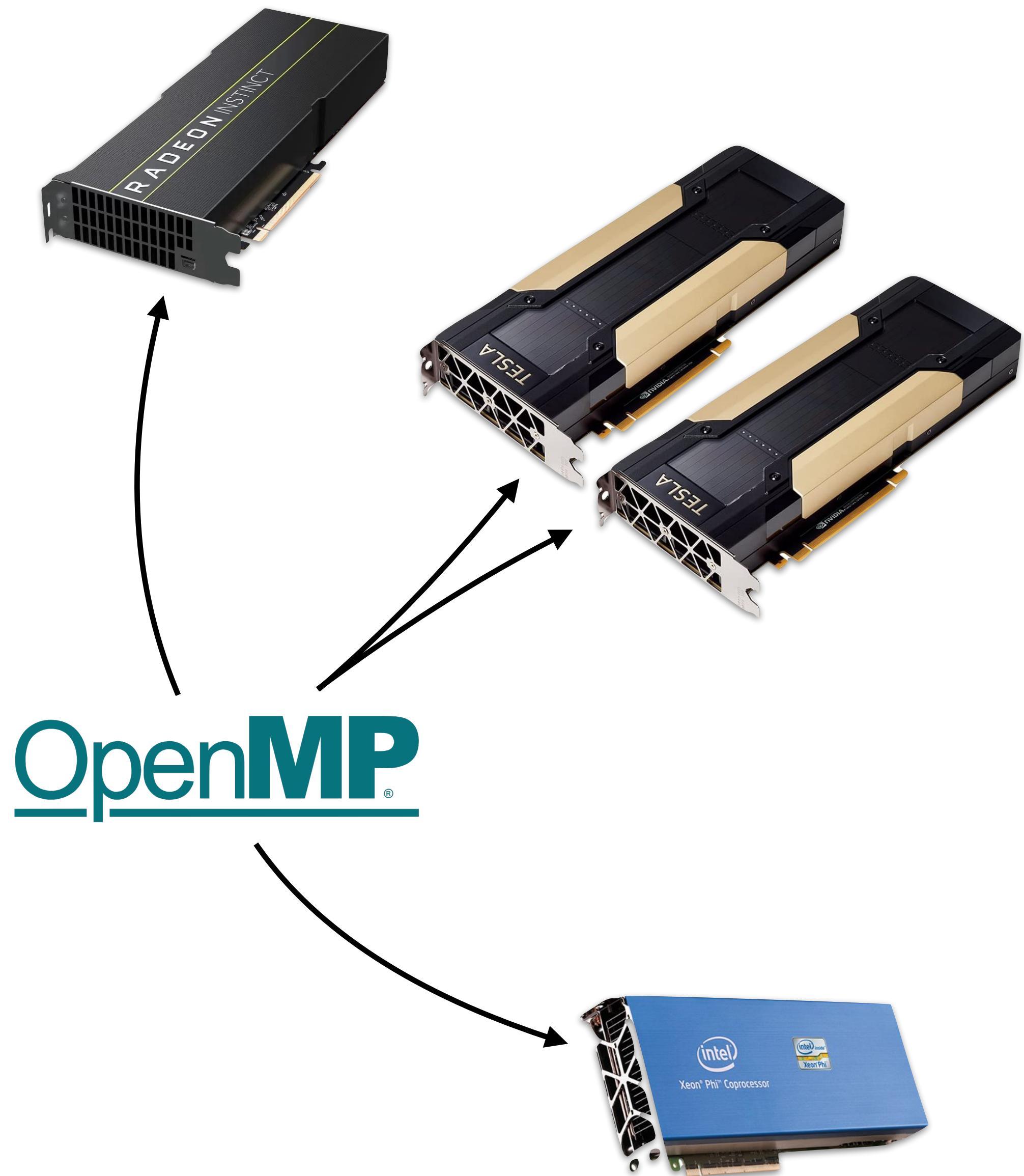
- Parallelise the main math operations in the Jacobi code (**Solver/solver.cpp**) with OpenMP
- Vectorise as many operations as possible and measure the elapsed time for 32x32 grid
- Compare performance of GNU and Intel compilers (modify **make_all.sh** accordingly)
 - For the GNU compiler (module load foss/2020a):
 - Set `extra_flags` variable in `omp` clause to ``(-fopenmp -fopenmp-simd -fopt-info-vec-optimized)`
 - For the Intel compiler (module load intel/2020a):
 - Set `compiler` variable to `icpc`
 - Set `extra_flags` variable in `omp` clause to ``(-qopenmp -qopenmp-simd -fopt-report-phase=vectorize)`

OpenMP-2

OpenMP

Offloading

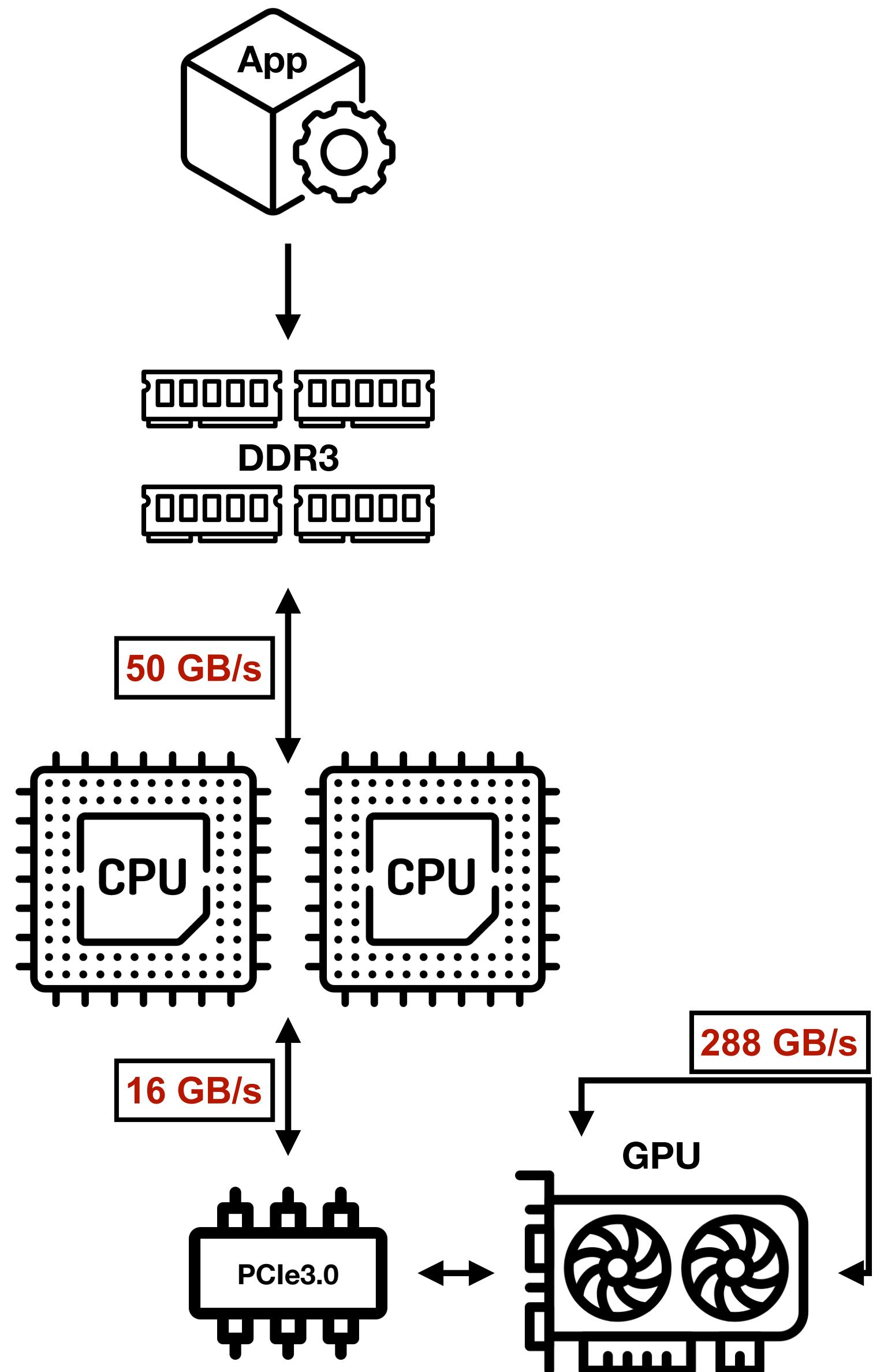
- The OpenMP-4.0/4.5 standard supports offloading to a device (GPU or MIC)
- **Pros:**
 - OpenMP native (no need for a 3rd party library)
 - Requires relatively simple modification of already parallelised code (if the code base is simple)
- **Cons:**
 - Not all compilers provide decent support
 - Not all GPUs are well supported
 - Not as efficient as low-level implementations (e.g. with CUDA)



OpenMP

Offloading

CPU	GPU
Task parallelism	Data parallelism
A few heavyweight cores	Many lightweight cores
High memory size	High memory throughput
Many diverse instruction sets	A few highly optimized instruction sets
Explicit thread management	Threads are managed by hardware

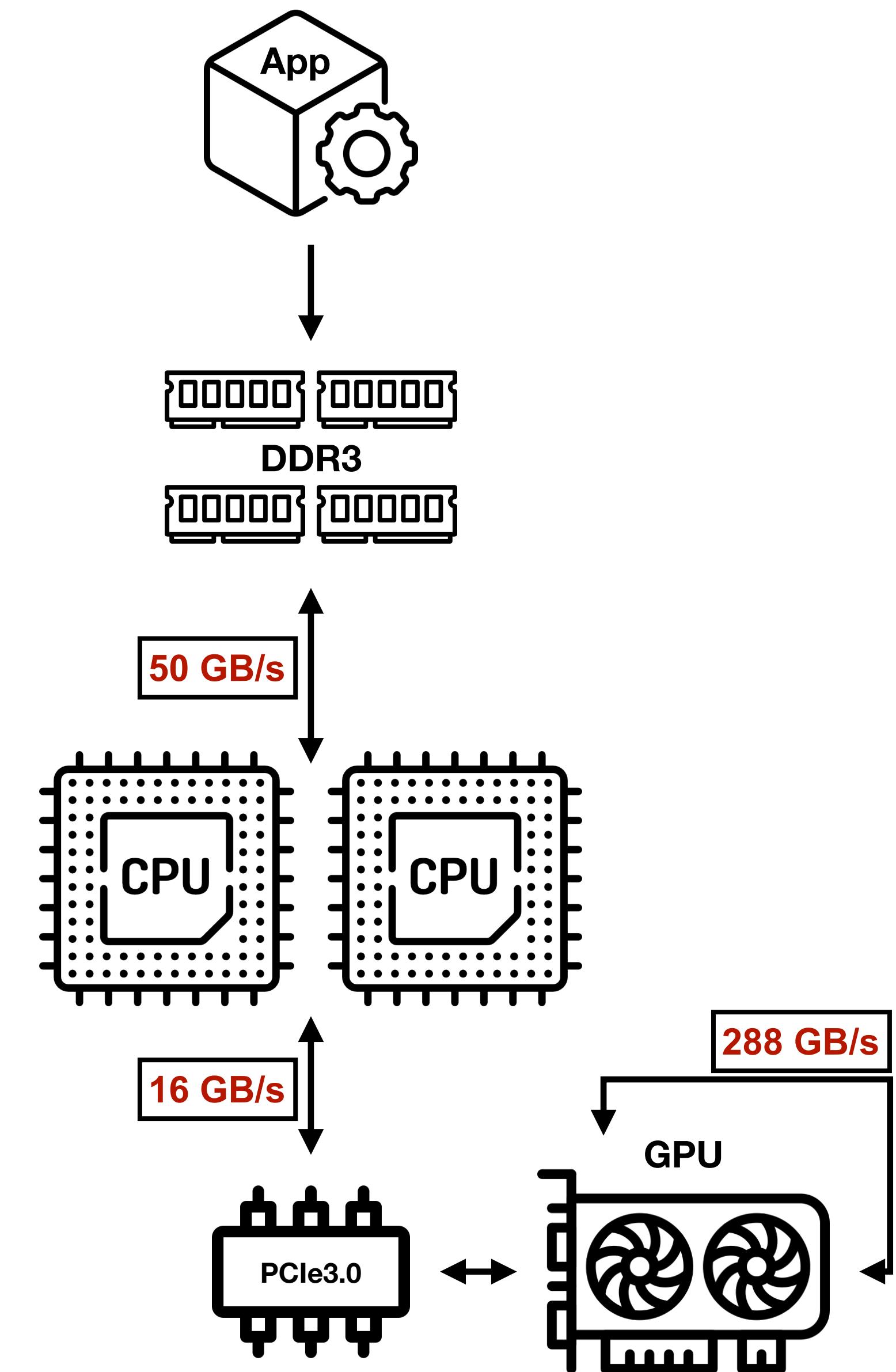
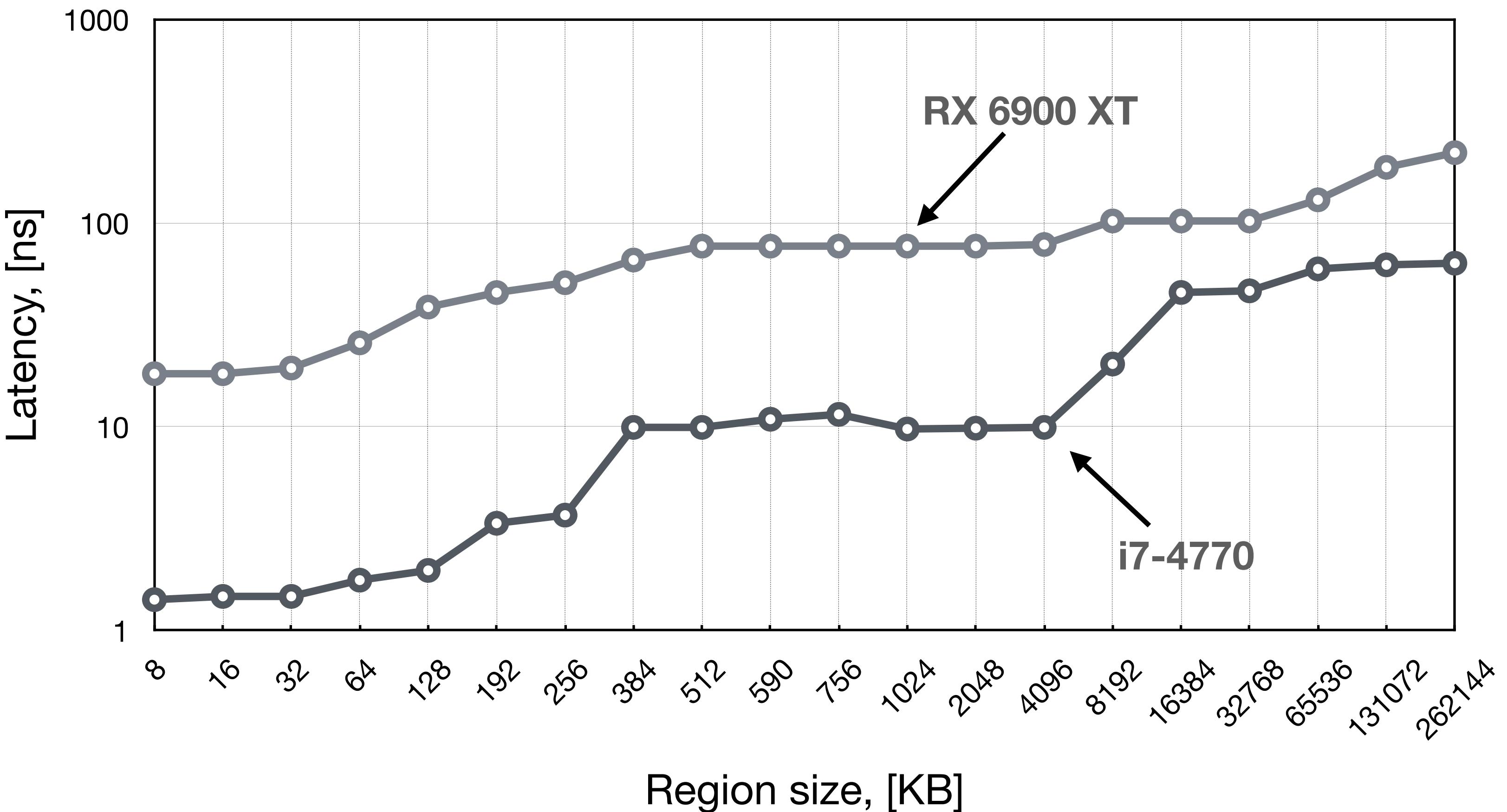


1. https://www.flaticon.com/free-icon/cpu_689379
2. https://www.flaticon.com/free-icon/graphics-card_2000522
3. https://www.flaticon.com/free-icon/ram_900330
4. https://www.flaticon.com/free-icon/3d-modeling_4229105

OpenMP

Offloading

CPU vs. GPU memory latency



1. https://www.flaticon.com/free-icon/cpu_689379

2. https://www.flaticon.com/free-icon/graphics-card_2000522

3. https://www.flaticon.com/free-icon/ram_900330

4. https://www.flaticon.com/free-icon/3d-modeling_4229105

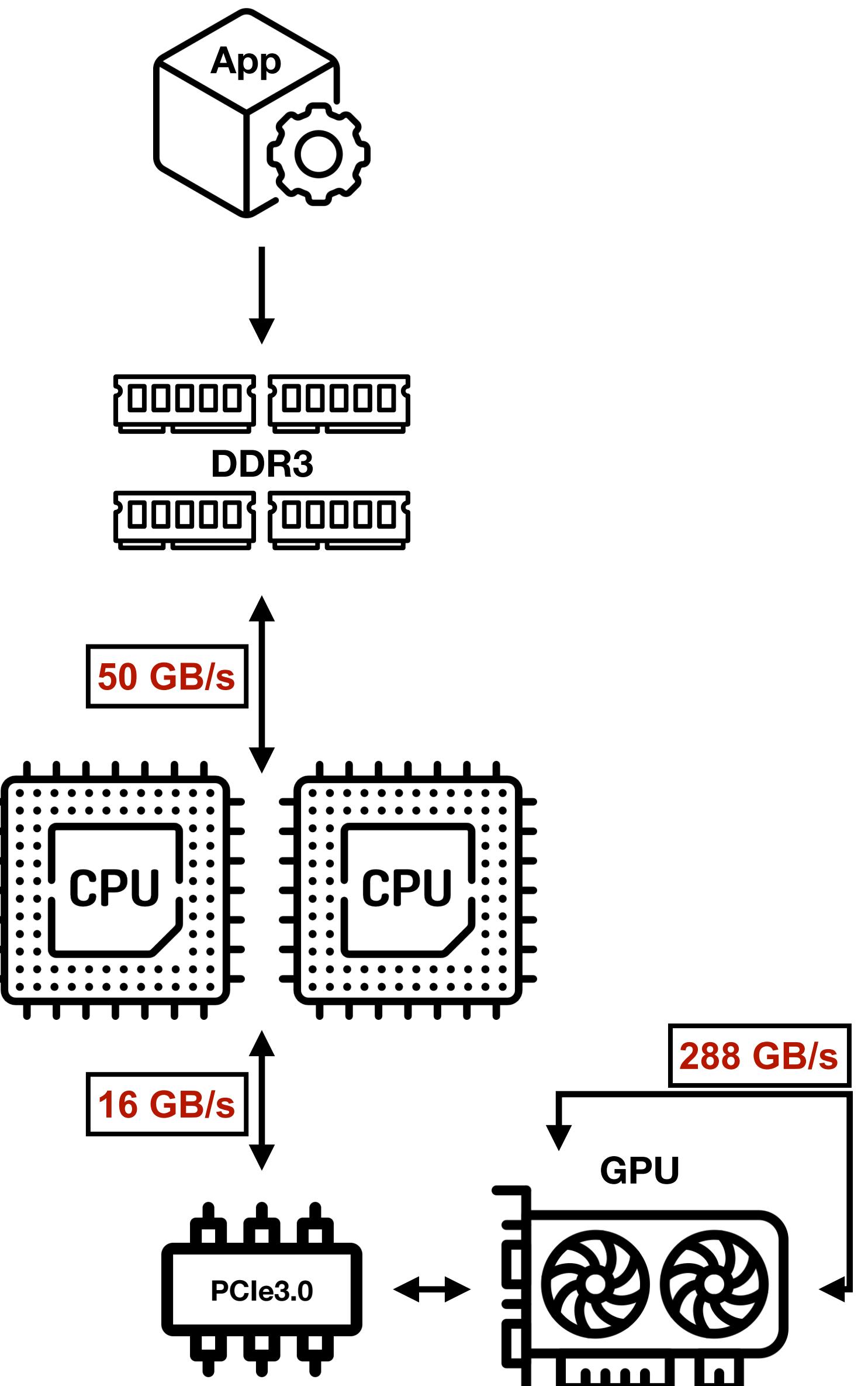
5. Data for the plot: <https://chipsandcheese.com/2021/04/16/measuring-gpu-memory-latency>

OpenMP

Offloading

Rules of thumb:

- Memory transfer is expensive, avoid it
- Offload as much of the work as possible
- Avoid branches
- Preallocate and reuse the memory on a device



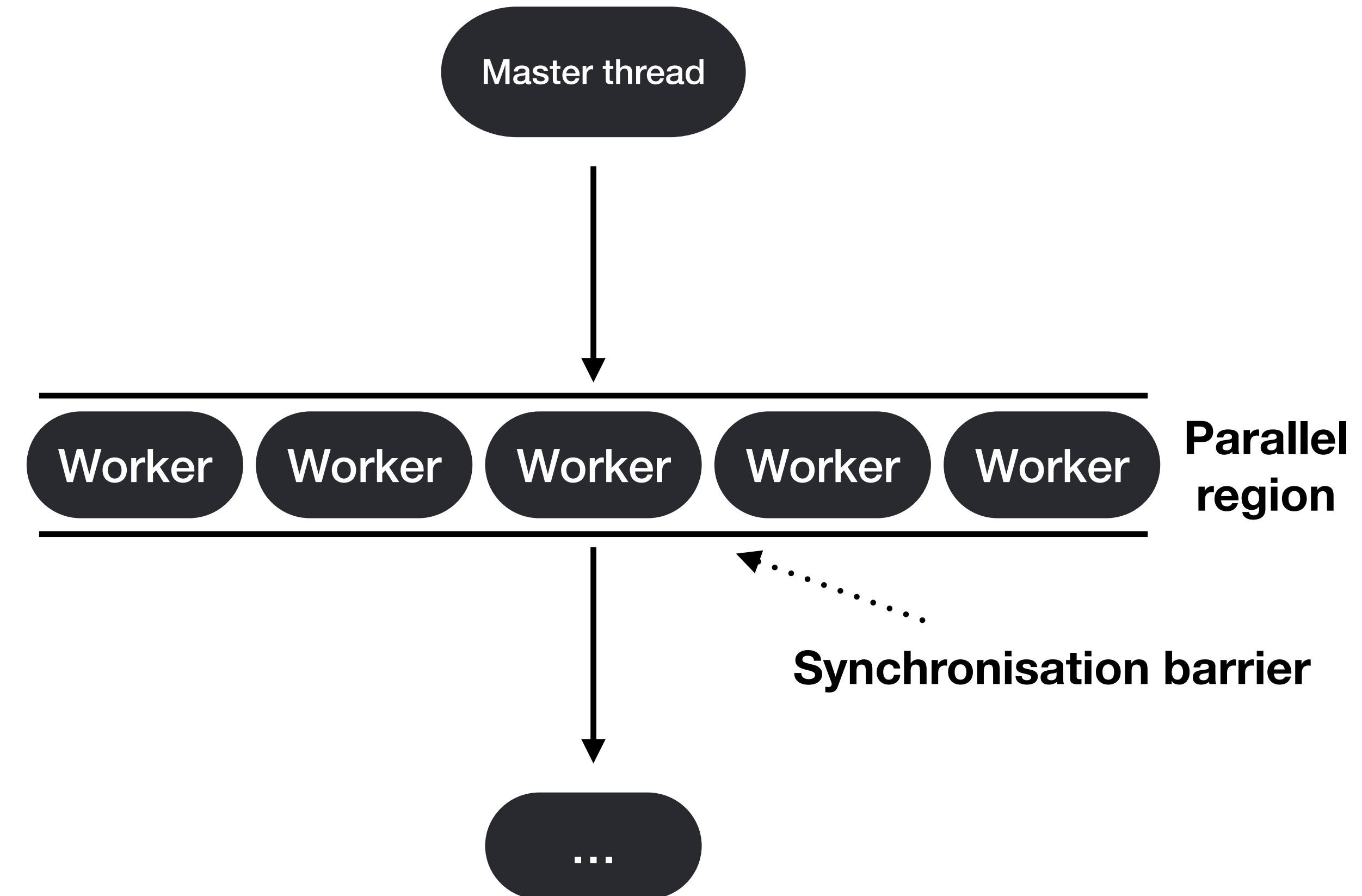
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3. https://www.flaticon.com/free-icon/ram_900330
4. https://www.flaticon.com/free-icon/3d-modeling_4229105

OpenMP

Offloading

```
int N = 64;
double A[N][N], B[N][N], C[N][N];

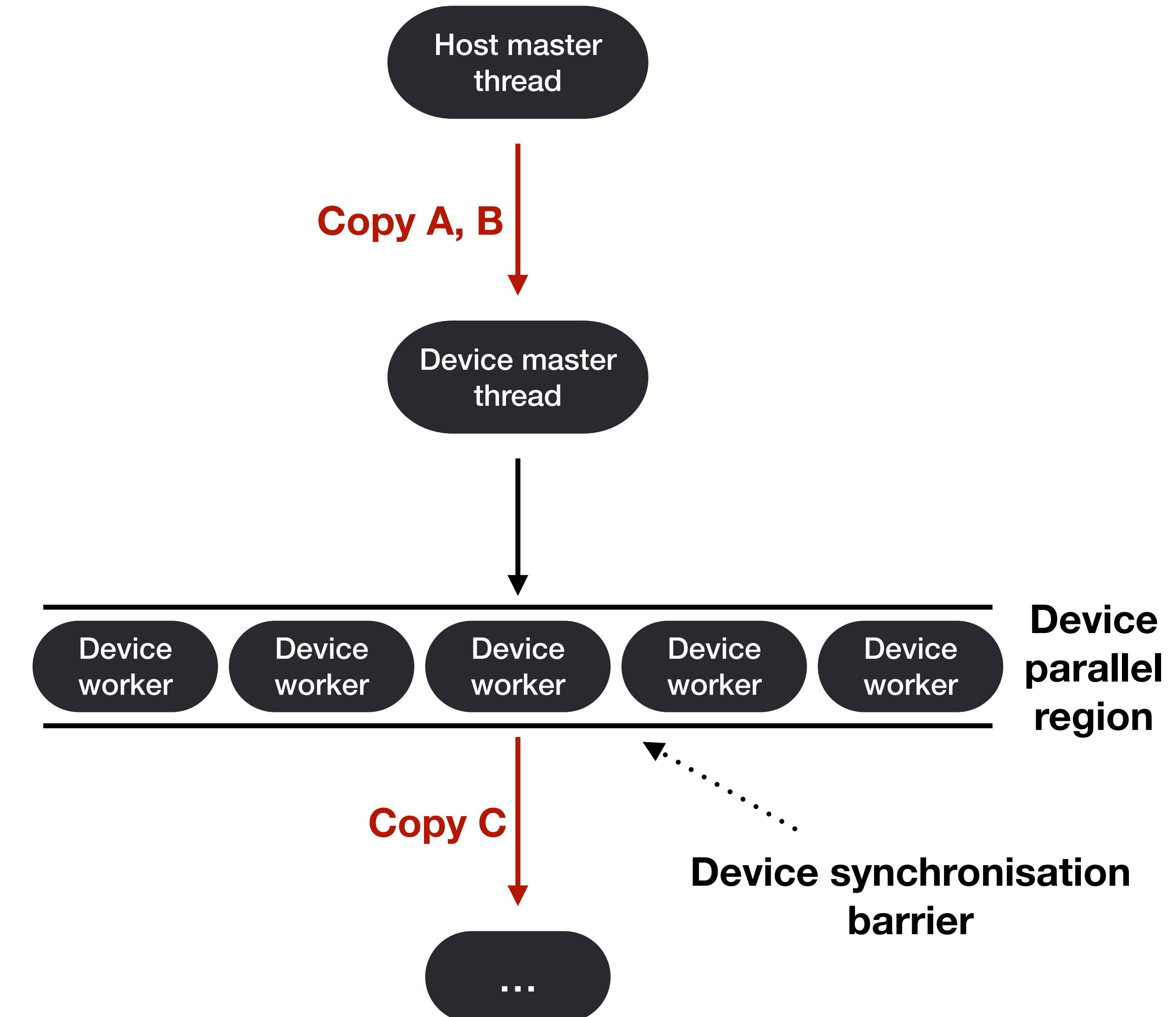
...
#pragma omp parallel for
for(int i = 0; i < N; ++i) {
    for(int j = 0; j < N; ++j) {
        for(int k = 0; k < N; ++k) {
            C[i][j] = A[i][k] * B[k][j];
        }
    }
}
```



OpenMP

Offloading

```
int N = 64;
double A[N][N], B[N][N], C[N][N];
...
#pragma omp target map(to: A, B) map(from: C)
{
    #pragma omp parallel for
    for(int i = 0; i < N; ++i) {
        for(int j = 0; j < N; ++j) {
            for(int k = 0; k < N; ++k) {
                C[i][j] = A[i][k] * B[k][j];
            }
        }
    }
}
```



OpenMP

Offloading

```
int N = 64;
double A[N][N], B[N][N], C[N][N];

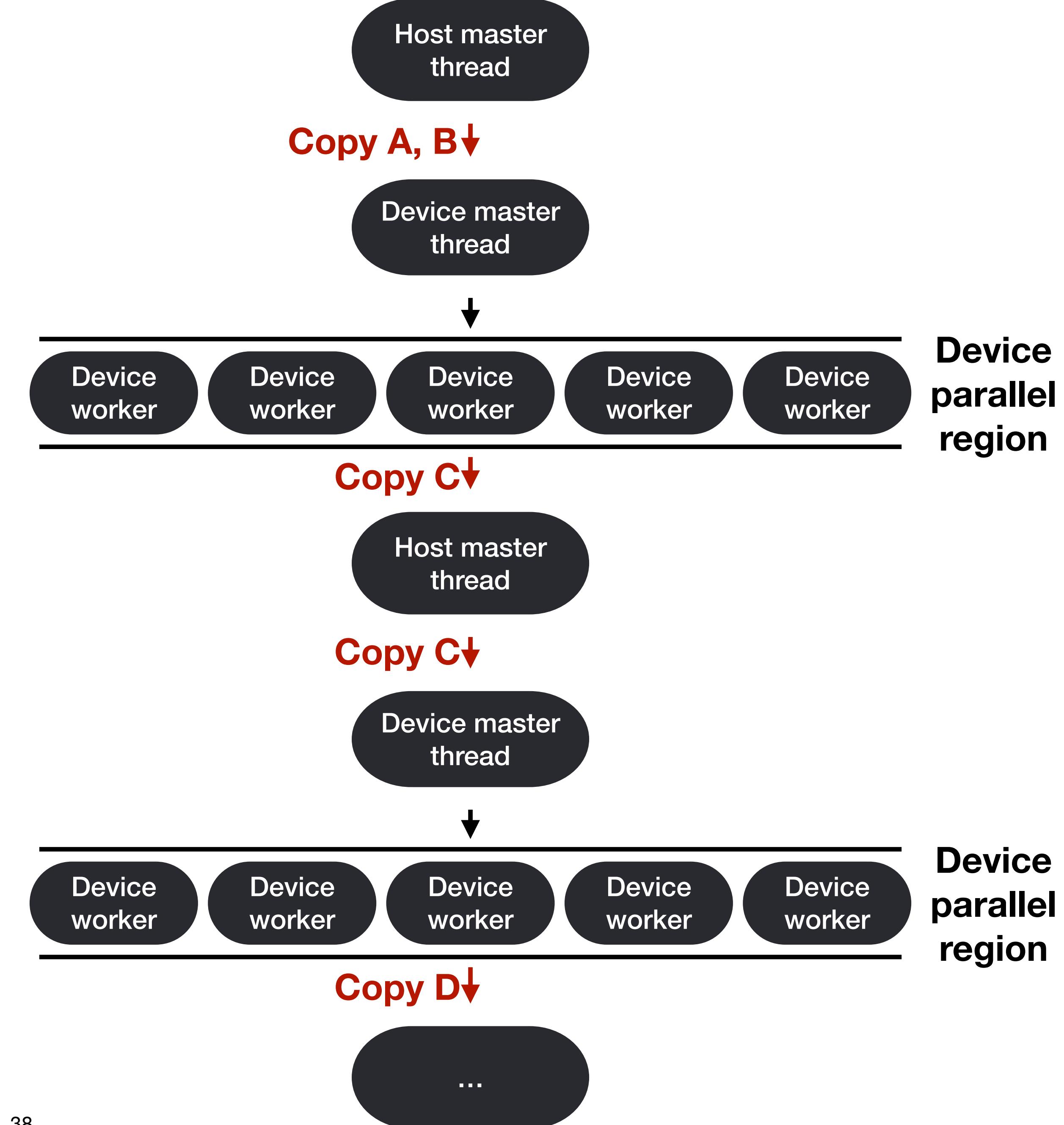
...
#pragma omp target map(to: A, B) map(from: C)
{
    #pragma omp parallel for
    for(int i = 0; i < N; ++i) {
        for(int j = 0; j < N; ++j) {
            for(int k = 0; k < N; ++k) {
                C[i][j] = A[i][k] * B[k][j];
            }
        }
    }
}
```

- **map(to:list)**: *read-only* data on the device. Variables in the list are initialised on the device using the original values from the host
- **map(from:list)**: *write-only* data on the device: initial value of the variable is not initialised. At the end of the target region, the values from variables in the list are copied into the original variables
- **map(tofrom:list)**: the effect of both a map-to and a map-from
- **map(alloc:list)**: data is allocated and uninitialised on the device
- **map(list)**: equivalent to **map(tofrom:list)**

OpenMP

Scope of data

```
int N = 64;  
double A[N][N], B[N][N], C[N][N], D[N][N];  
  
...  
  
#pragma omp target map(to: A, B) map(from: C)  
{  
    // Calculate C = f(A, B)  
}  
  
#pragma omp target map(to: C) map(from: D)  
{  
    // Calculate D = f(C)  
}
```



OpenMP

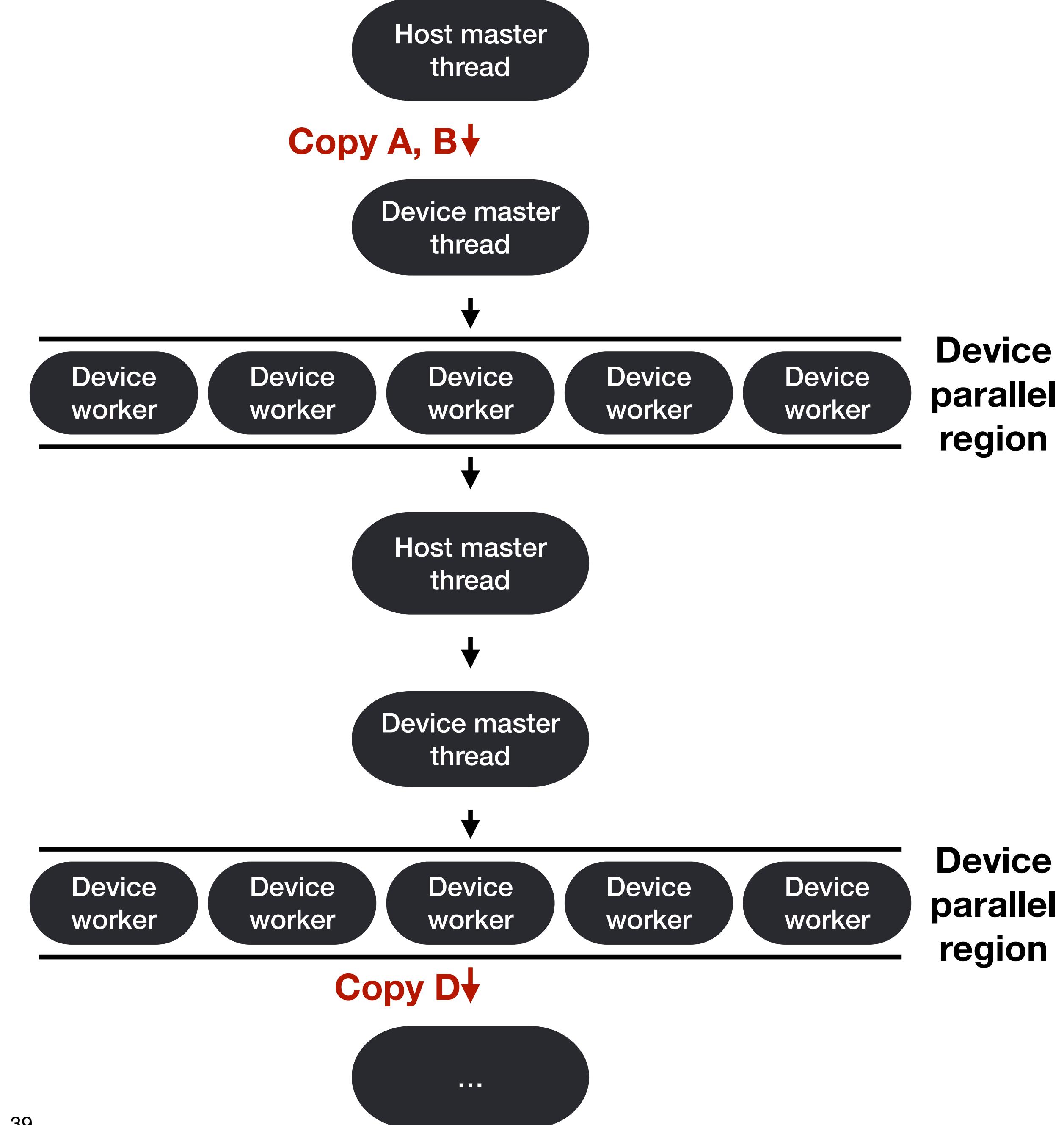
Scope of data

C is allocated and kept directly on the device

```
int N = 64;
double A[N][N], B[N][N], C[N][N], D[N][N];

...
#pragma omp target data map(alloc: C)
{
    #pragma omp target map(to: A, B)
    {
        // Calculate C = f(A, B)
    }

    #pragma omp target map(from: D)
    {
        // Calculate D = f(C)
    }
}
```



OpenMP

Offloading

- A device has at most one copy of each mapped variable
- The **map** clauses are ignored when data is already in the device scope
- The update of the data can be forced using the **update to/from** clause
- Data can be “pre-mapped” using **enter data** and **exit data** clauses

```
#pragma omp target map(tofrom: C)
{
    // Update C
}
#pragma omp target update from(C)
// Use C on the host
```

```
#pragma omp target enter data map(allo: C)
#pragma omp target map(to: C)
{
    // Use C
}
#pragma omp target exit data map(from: C)
```

OpenMP

Offloading

- Mapping rules:
 - for pointers **map(to:data[0:N])**
 - for static data **map(to:data)**
- If memory is allocated within a target region it cannot be brought to the host
- Use **target declare** to declare functions for offloading

```
// static array  
double C[N];  
...  
#pragma omp target map(tofrom: C)  
{  
    // Update C  
}
```

```
// dynamic array  
double* C = (double*) malloc(N * sizeof(double));  
...  
#pragma omp target map(tofrom: C[0:N])  
{  
    // Update C  
}
```

Allows to load a subset of an array!

```
#pragma omp declare target  
void foo() {  
    // Do some work  
}  
#pragma omp end declare target
```

OpenMP

Offloading

- In **C++** you can also **map an entire class** to the device
 - class can then be used on host or device
 - constructor/destructor used on host/device

- In **OpenMP5.0**

- can also map individual methods
- can map class static variables
- can map class that have virtual functions, as long as they are not used on the device

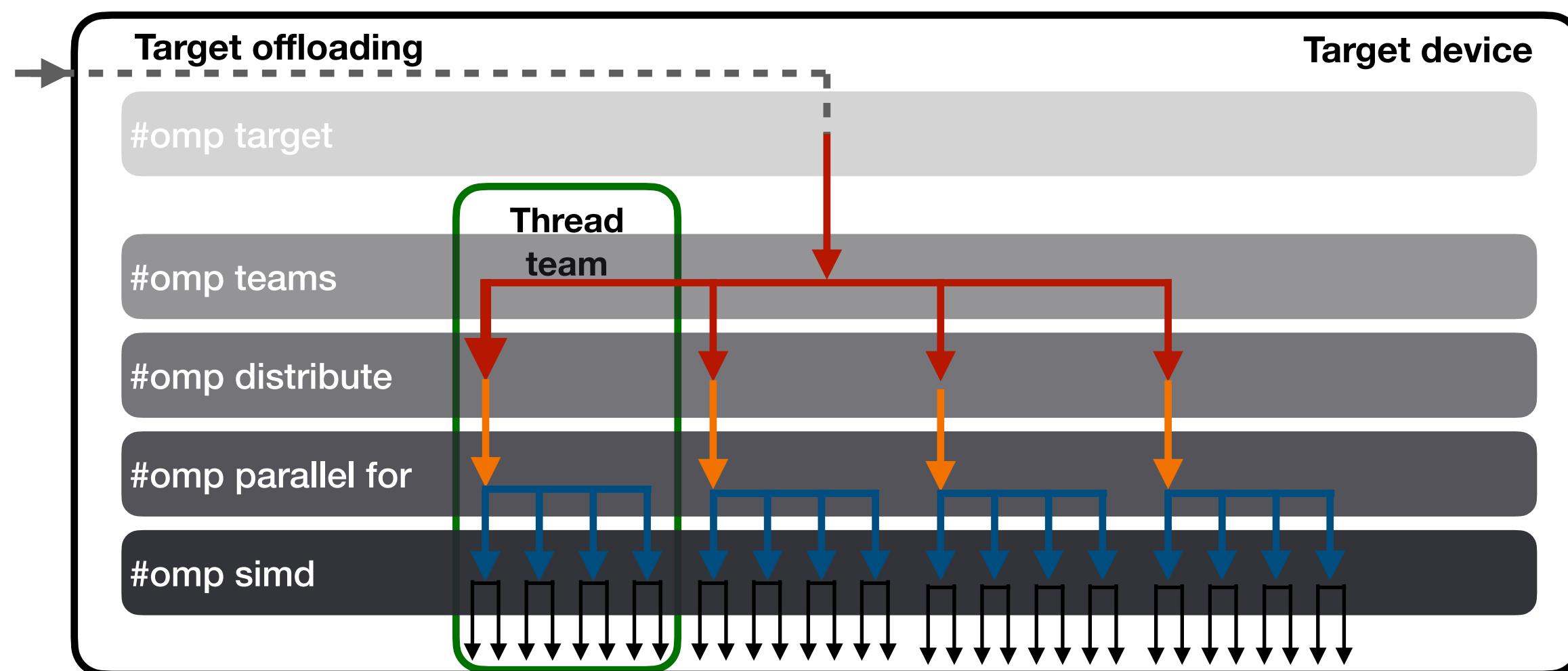
```
#pragma omp declare target
class Foo {
private:
    int a, b;
public:
    Foo() : a(1), b(2) { }
    ~Foo() { }
    int sum() { return a + b; }
};
#pragma omp end declare target
```

```
class Foo {
private:
    int a, b;
public:
    Foo() : a(1), b(2) { }
    ~Foo() { }
#pragma omp declare target
    int sum() { return a + b; }
#pragma omp end declare target
};
```

OpenMP

Offloading

- Threads can be combined in **teams**
- Work can be **distributed** across **teams**



```
int N = 64;
double A[N][N], B[N][N], C[N][N];

...
#pragma omp target map(to: A, B) map(from: C)
#pragma omp teams num_teams(4)
#pragma omp distribute
#pragma omp parallel for simd num_threads(3)
for(int i = 0; i < N; ++i) {
    for(int j = 0; j < N; ++j) {
        for(int k = 0; k < N; ++k) {
            C[i][j] = A[i][k] * B[k][j];
        }
    }
}
```

OpenMP

Compiler flags

- Compiler flags

```
$ module use /sw/arch/Debian10/EB_testing/modulefiles/compiler  
$ module load 2020  
$ module load GCC/10.2.0  
$ gcc -fopenmp -foffload=nvptx-none="-Ofast -misa=sm_35" main.cpp
```



- m32
- m64
- misa=*ISA-string*
- mmainkernel
- moptimize
- msoft-stack
- muniform-simt
- mgomp

- Profiling

```
$ #profile:  
$ module load CUDACore/11.0.2  
$ nvprof ./a.out -s 32 32 -d 1 1
```

OpenMP

GPU offloading

- Example of intensive memory allocations (*nvprof*)

Type	Time(%)	Time	Calls	Avg	Min	Max	Name
GPU activities:	98.93%	2.95501s	5744	514.45us	483.43us	541.73us	
_ZN6Solver13calculateNormER6Vector\$omp_fn\$0	0.62%	18.646ms	5744	3.2460us	2.8160us	13.600us	[CUDA memcpy DtoH]
	0.44%	13.271ms	5744	2.3100us	2.2400us	11.104us	[CUDA memcpy HtoD]
API calls:	85.39%	31.2376s	11488	2.7191ms	8.9400us	7.1071ms	cuMemAlloc
	8.22%	3.00754s	5744	523.60us	6.1710us	1.2464ms	cuCtxSynchronize
	4.40%	1.60891s	11488	140.05us	3.6850us	1.1687ms	cuMemFree
	0.51%	188.12ms	1	188.12ms	188.12ms	188.12ms	cuCtxCreate
	0.47%	171.97ms	5744	29.938us	25.523us	144.83us	cuMemcpyDtoH
	0.30%	110.65ms	5744	19.262us	13.155us	91.109us	cuMemcpyHtoD
	0.30%	109.78ms	5744	19.111us	16.459us	826.53us	cuLaunchKernel
	0.22%	79.001ms	1	79.001ms	79.001ms	79.001ms	cuCtxDestroy
	0.10%	35.027ms	24	1.4595ms	1.2342ms	2.6770ms	cuLinkAddData
	0.03%	11.231ms	22979	488ns	210ns	691.80us	cuCtxGetDevice
	0.03%	10.235ms	11488	890ns	381ns	669.70us	cuMemGetAddressRange

Hands-on

Hands-on

OpenMP offloading

- Offload the main operations in the Jacobi solver
- Compile code with the `gpu` flag
- Measure the performance
- Use decent domain size, e.g. 100x100

```
$ module use /sw/arch/Debian10/EB_testing/modulefiles/compiler  
$ module load 2020  
$ module load GCC/10.2.0  
$ gcc -fopenmp -foffload=nvptx-none="-Ofast -misa=sm_30" main.cpp
```

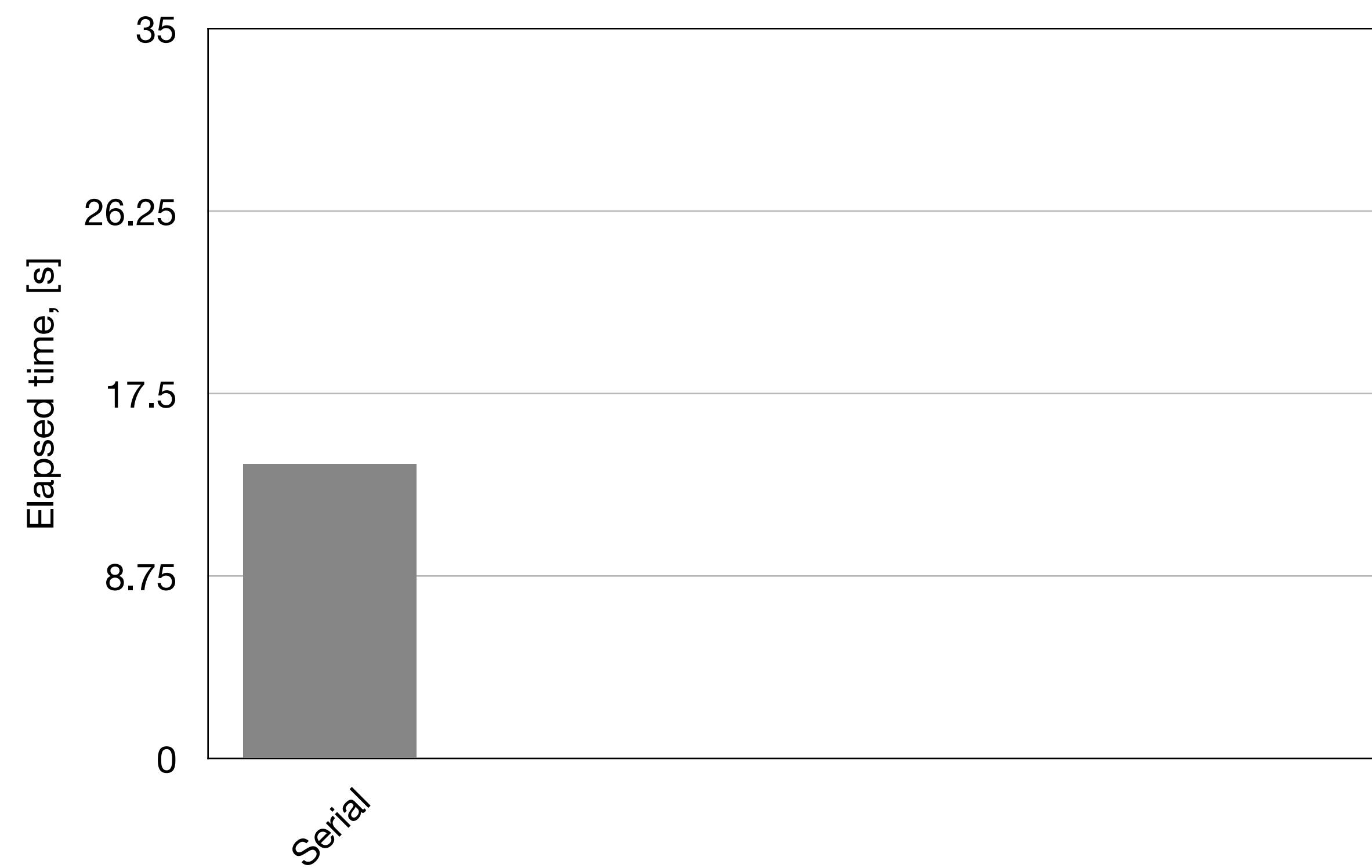
```
$ #profile:  
$ module load CUDACore/11.0.2  
$ nvprof ./a.out -s 32 32 -d 1 1
```

OpenMP

GPU offloading

The original code

100x100 grid points, 100 iterations with 1 thread



```
...
while ( (iter < max_iter) && (residual_norm > tolerance) ) {

#pragma omp parallel for
    for(int i = num_rows - 1; i >= 0; i--) {
        double diag = 1.;                                // Diagonal element
        double sigma = 0.0;                             // Just a temporary value

        x[i] = b[i];

#pragma omp simd reduction(+:sigma)
        for(int j = 0; j < num_cols; ++j) {
            sigma = sigma + A[j + i * num_cols] * x_old[j];
        }
        diag = A[i + i * num_cols];
        sigma -= diag * x_old[i];
        x[i] = (x[i] - sigma) * omega / diag;
    }

#pragma omp parallel for simd
    for(int i = 0; i < num_loc_elts_x; ++i) {
        x[i] += (1 - omega) * x_old[i];
        x_old[i] = x[i];
    }

calculateResidual(A, x, b, res, num_rows, num_cols);
residual_norm = calculateNorm(res, num_rows) / b_norm;

if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;

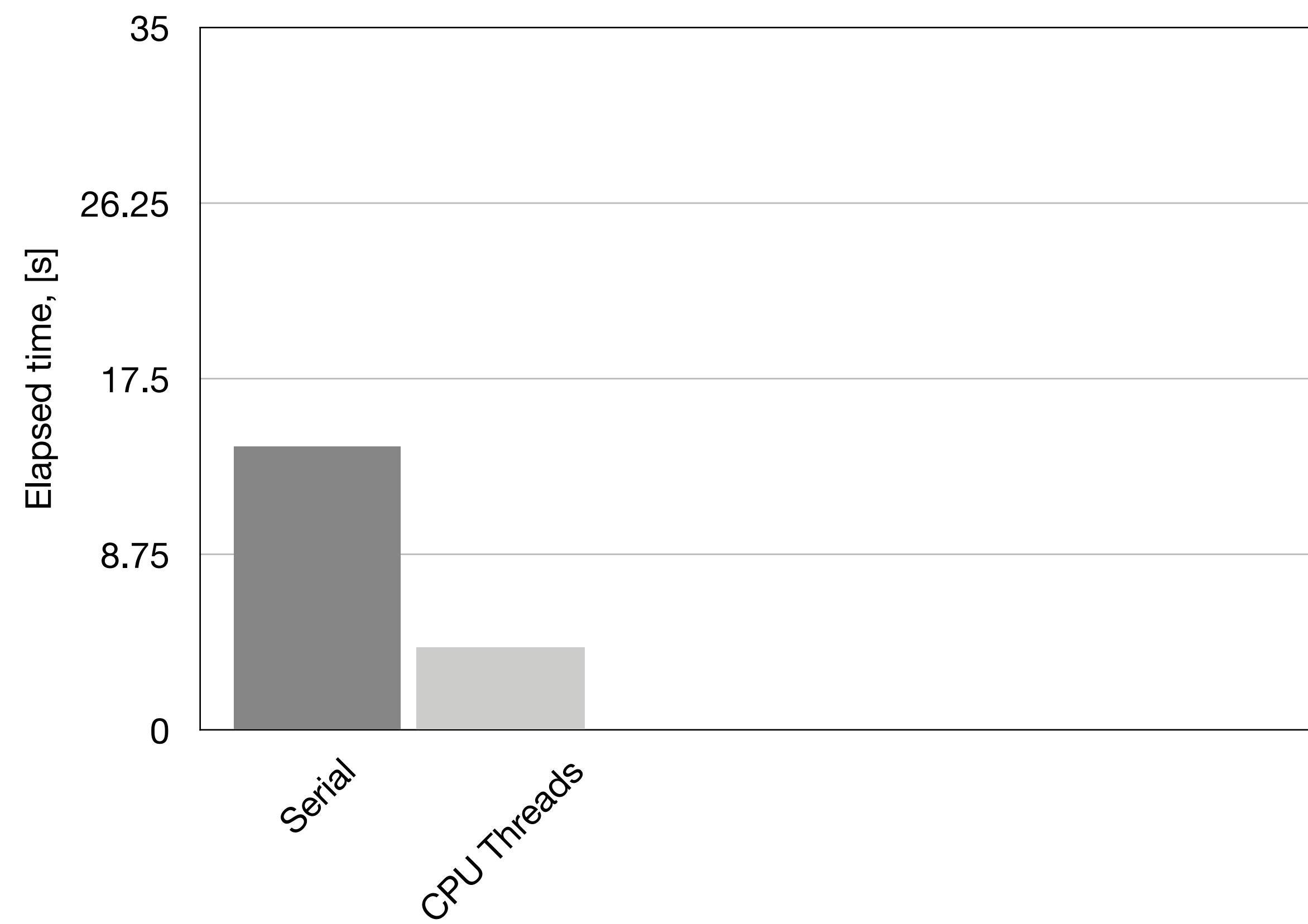
iter++;
}
```

OpenMP

GPU offloading

The original code

100x100 grid points, 100 iterations with 24 thread



```
...
while ( (iter < max_iter) && (residual_norm > tolerance) ) {

#pragma omp parallel for
    for(int i = num_rows - 1; i >= 0; i--) {
        double diag = 1.;                                // Diagonal element
        double sigma = 0.0;                            // Just a temporary value

        x[i] = b[i];

#pragma omp simd reduction(+:sigma)
        for(int j = 0; j < num_cols; ++j) {
            sigma = sigma + A[j + i * num_cols] * x_old[j];
        }
        diag = A[i + i * num_cols];
        sigma -= diag * x_old[i];
        x[i] = (x[i] - sigma) * omega / diag;
    }

#pragma omp parallel for simd
    for(int i = 0; i < num_loc_elts_x; ++i) {
        x[i] += (1 - omega) * x_old[i];
        x_old[i] = x[i];
    }

calculateResidual(A, x, b, res, num_rows, num_cols);
residual_norm = calculateNorm(res, num_rows) / b_norm;

if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;

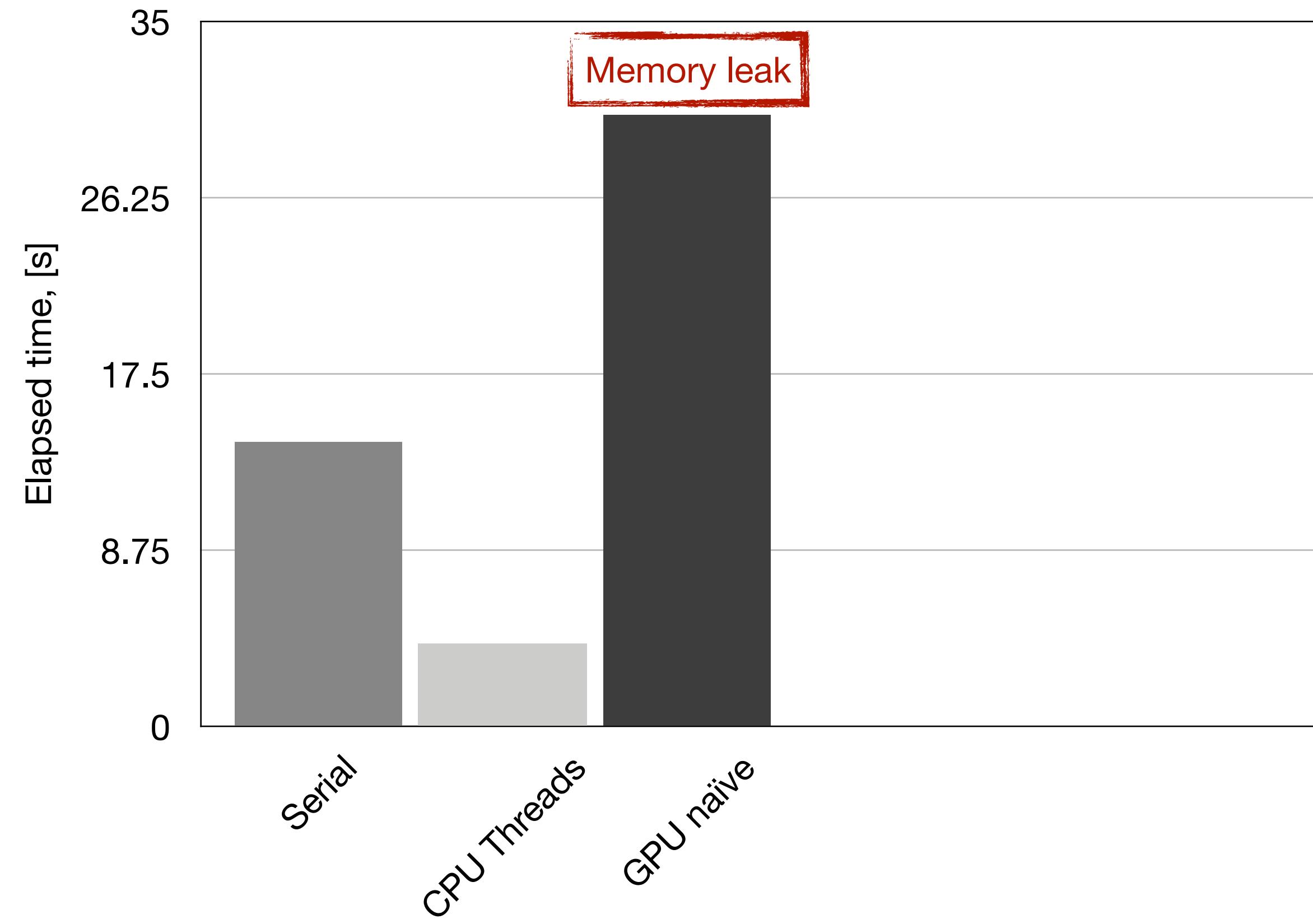
iter++;
}
```

OpenMP

GPU offloading

GPU offload: naïve

100x100 grid points, 100 iterations with 1 thread



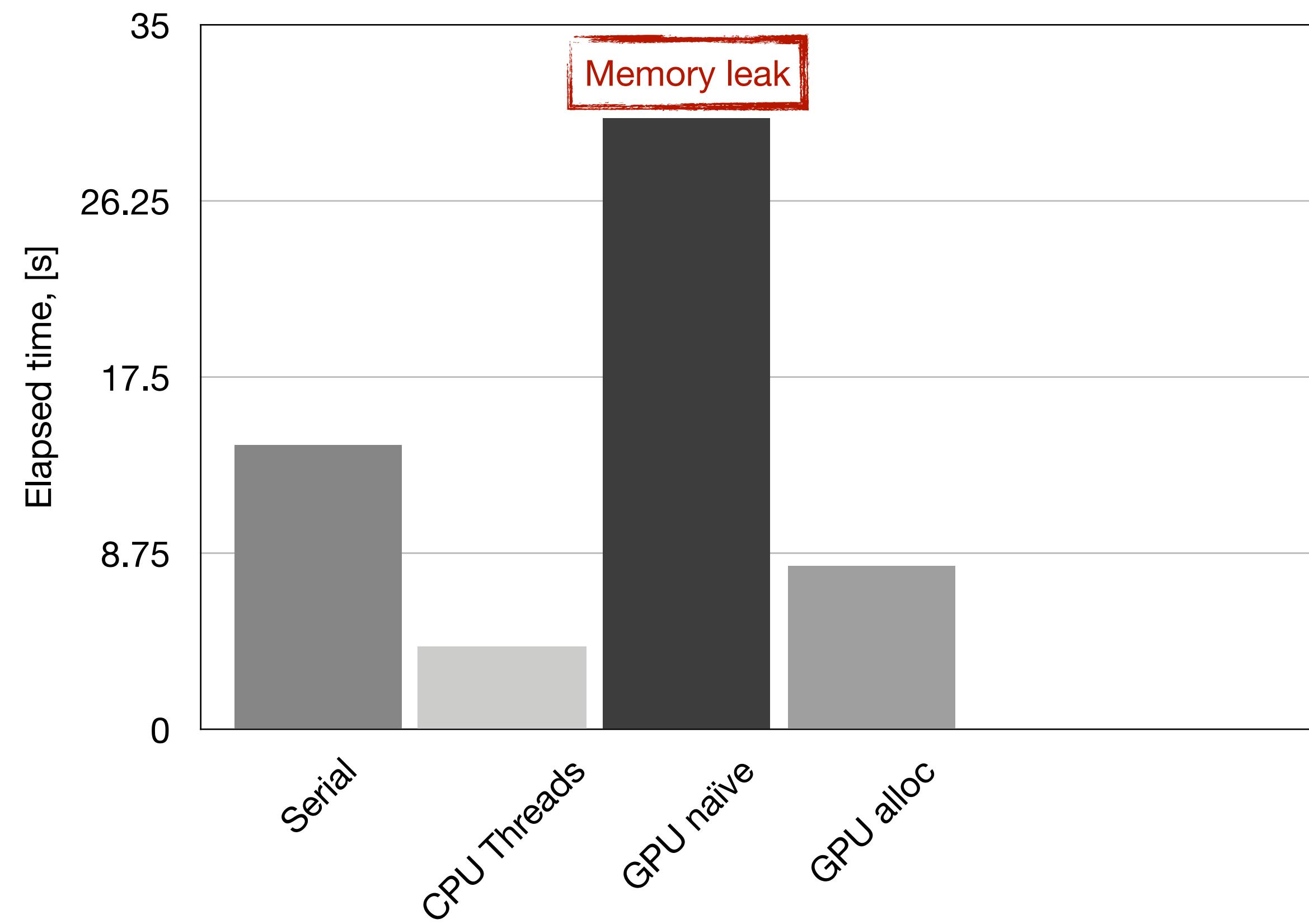
```
...  
while ( (iter < max_iter) && (residual_norm > tolerance) ) {  
  
#pragma omp target map(to: A[0:num_elts_A], b[0:num_loc_elts_x],  
// x_old[0:num_loc_elts_x]) \  
map(tofrom: x[0:num_loc_elts_x])  
#pragma omp parallel for  
for(int i = num_rows - 1; i >= 0; i--) {  
    double diag = 1.; // Diagonal element  
    double sigma = 0.0; // Just a temporary value  
  
    x[i] = b[i];  
  
#pragma omp simd reduction(+:sigma)  
for(int j = 0; j < num_cols; ++j) {  
    sigma = sigma + A[j + i * num_cols] * x_old[j];  
}  
diag = A[i + i * num_cols];  
sigma -= diag * x_old[i];  
x[i] = (x[i] - sigma) * omega / diag;  
}  
  
#pragma omp parallel for simd  
for(int i = 0; i < num_loc_elts_x; ++i) {  
    x[i] += (1 - omega) * x_old[i];  
    x_old[i] = x[i];  
}  
  
calculateResidual(A, x, b, res, num_rows, num_cols);  
residual_norm = calculateNorm(res, num_rows) / b_norm;  
  
if (my_rank == 0)  
    cout << iter << '\t' << residual_norm << endl;  
}  
iter++;
```

OpenMP

GPU offloading

GPU offload: proper memory allocation

100x100 grid points, 100 iterations with 1 thread



```
...
#pragma omp target data map(to: A[0:num_elts_A],
                           b[0:num_loc_elts_x],
                           x_old[0:num_loc_elts_x]) \
                           map(tofrom: x[0:num_loc_elts_x])
while ( (iter < max_iter) && (residual_norm > tolerance) ) {
#pragma omp target
#pragma omp parallel for
    for(int i = num_rows - 1; i >= 0; i--) {
        double diag = 1.;                         // Diagonal element
        double sigma = 0.0;                        // Just a temporary value
        x[i] = b[i];
    }
#pragma omp simd reduction(+:sigma)
    for(int j = 0; j < num_cols; ++j) {
        sigma = sigma + A[j + i * num_cols] * x_old[j];
    }
    diag = A[i + i * num_cols];
    sigma -= diag * x_old[i];
    x[i] = (x[i] - sigma) * omega / diag;
}

#pragma omp target update from(x[0:num_loc_elts_x])

#pragma omp parallel for simd
    for(int i = 0; i < num_loc_elts_x; ++i) {
        x[i] += (1 - omega) * x_old[i];
        x_old[i] = x[i];
    }

calculateResidual(A, x, b, res, num_rows, num_cols);

residual_norm = calculateNorm(res, num_rows) / b_norm;

if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;

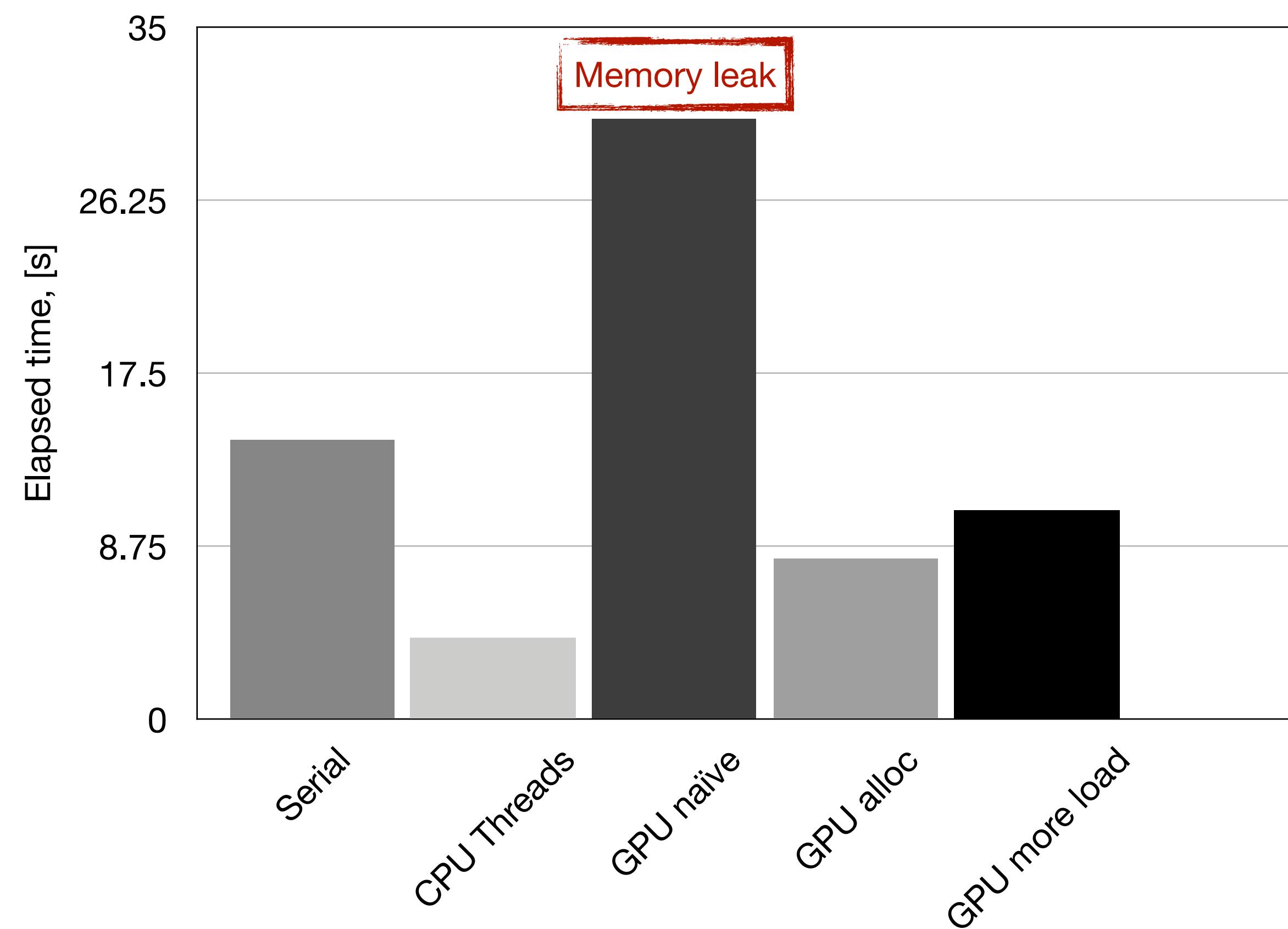
iter++;
}
```

OpenMP

GPU offloading

GPU offload: more workload

100x100 grid points, 100 iterations with 1 thread



```
...
#pragma omp target data map(to: A[0:num_elts_A],
                           b[0:num_loc_elts_x],
                           x_old[0:num_loc_elts_x],
                           res[0:num_loc_elts_x]) \
                           map(tofrom: x[0:num_loc_elts_x])
while ( (iter < max_iter) && (residual_norm > tolerance) ) {
#pragma omp target
#pragma omp parallel for
for(int i = num_rows - 1; i >= 0; i--) {
    double diag = 1.; // Diagonal element
    double sigma = 0.0; // Just a temporary value
    x[i] = b[i];
}

#pragma omp simd reduction(+:sigma)
for(int j = 0; j < num_cols; ++j) {
    sigma = sigma + A[j + i * num_cols] * x_old[j];
}
diag = A[i + i * num_cols];
sigma -= diag * x_old[i];
x[i] = (x[i] - sigma) * omega / diag;
}

#pragma omp target
#pragma omp parallel for simd
for(int i = 0; i < num_loc_elts_x; ++i) {
    x[i] += (1 - omega) * x_old[i];
    x_old[i] = x[i];
}

#pragma omp target
calculateResidual(A, x, b, res, num_rows, num_cols);

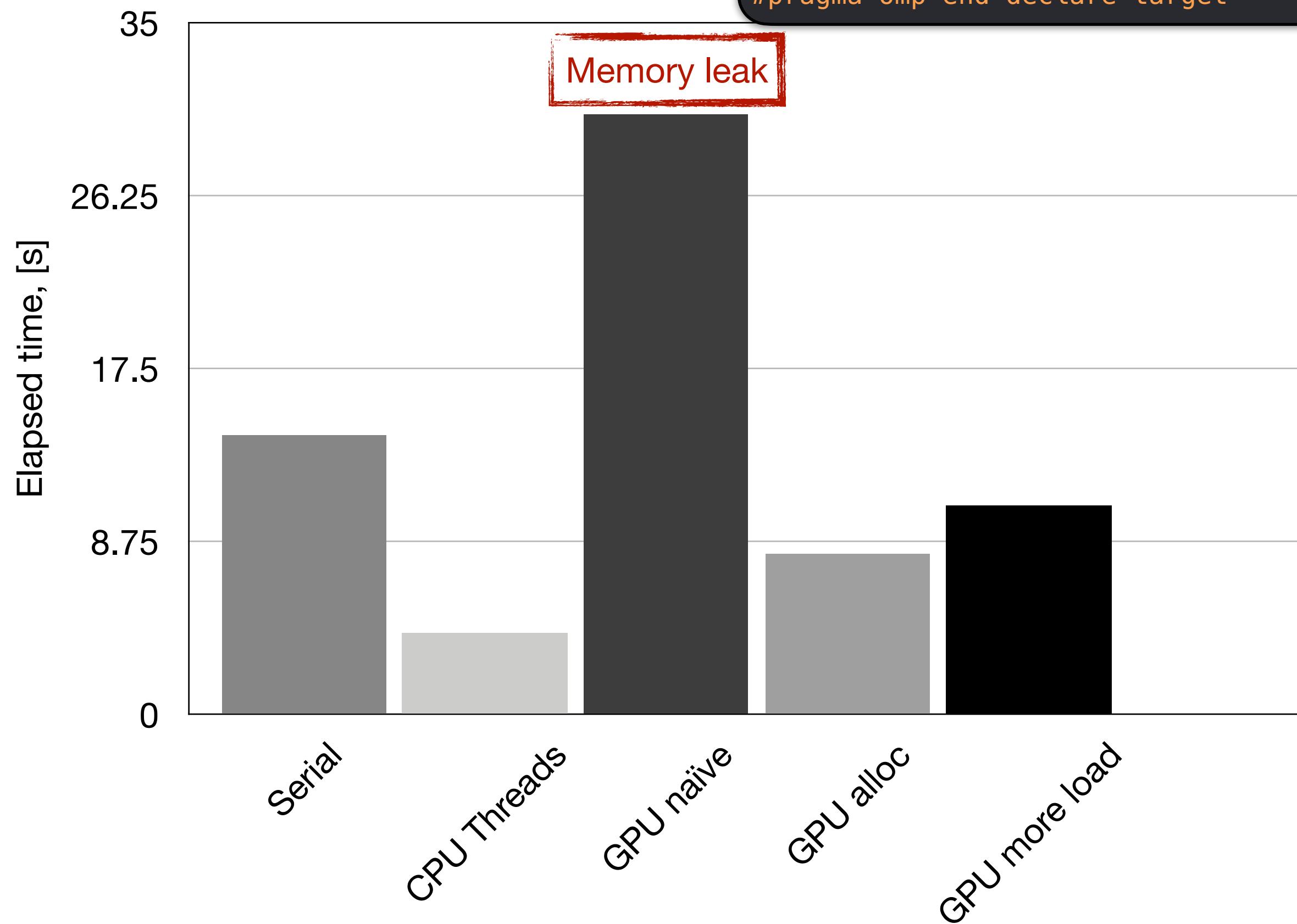
#pragma omp target map(from:residual_norm)
residual_norm = calculateNorm(res, num_rows) / b_norm;

if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;
    iter++;
}
```

OpenMP

GPU offloading

GPU offload:
100x100 grid points, 10



```
#pragma omp declare target
void Solver::calculateResidual(double *A, double *x, double *b,
                                double *res, int num_rows,
                                int num_cols) {
    copyVector(b, res, num_rows);

#pragma omp parallel for
    for(int i = 0; i < num_rows; ++i) {
        double sum = 0.0;
#pragma omp simd reduction(+:sum)
        for(int j = 0; j < num_cols; ++j) {
            sum += A[j + i * num_cols] * x[j];
        }
        res[i] -= sum;
    }
#pragma omp end declare target
```

```
data map(to: A[0:num_elts_A],
         b[0:num_loc_elts_x],
         x_old[0:num_loc_elts_x],
         res[0:num_loc_elts_x]) \
        map(tofrom: x[0:num_loc_elts_x])
max_iter) && (residual_norm > tolerance) ) {

l for
    num_rows - 1; i >= 0; i--) {
    diag = 1.; // Diagonal element
    sigma = 0.0; // Just a temporary value
    b[i];
    reduction(+:sigma)
    for(int j = 0; j < num_cols; ++j) {
        sigma = sigma + A[j + i * num_cols] * x_old[j];
    }
    diag = A[i + i * num_cols];
    sigma -= diag * x_old[i];
    x[i] = (x[i] - sigma) * omega / diag;
}

#pragma omp target
#pragma omp parallel for simd
for(int i = 0; i < num_loc_elts_x; ++i) {
    x[i] += (1 - omega) * x_old[i];
    x_old[i] = x[i];
}

#pragma omp target
calculateResidual(A, x, b, res, num_rows, num_cols);

#pragma omp target map(from:residual_norm)
residual_norm = calculateNorm(res, num_rows) / b_norm;

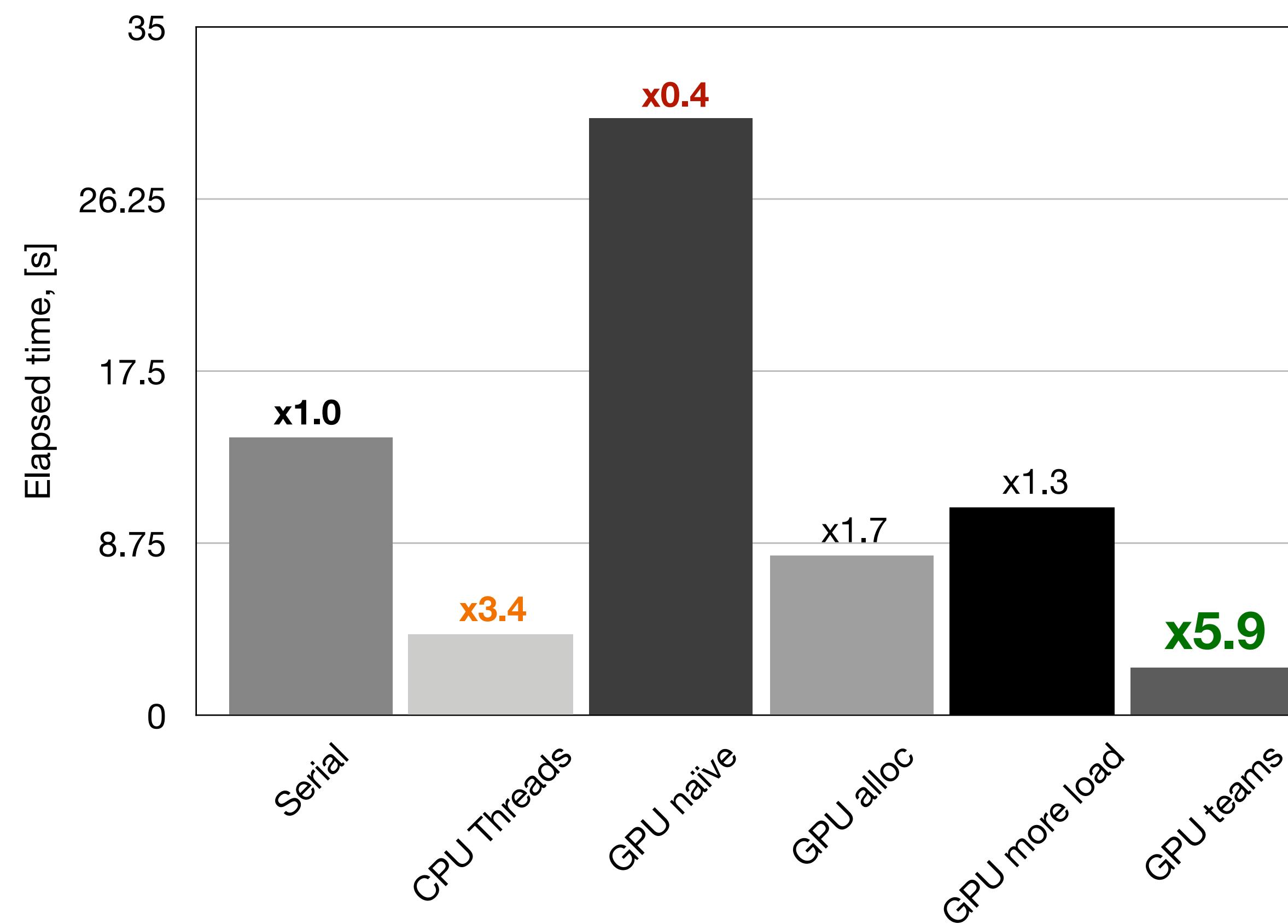
if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;
    iter++;
}
```

OpenMP

GPU offloading

GPU offload: teams

100x100 grid points, 100 iterations with 1 thread



```
...
#pragma omp target data map(to: A[0:num_elts_A],
                           b[0:num_loc_elts_x],
                           x_old[0:num_loc_elts_x],
                           res[0:num_loc_elts_x]) \
                           map(tofrom: x[0:num_loc_elts_x])
while ( (iter < max_iter) && (residual_norm > tolerance) ) {
#pragma omp target teams
#pragma omp distribute parallel for
for(int i = num_rows - 1; i >= 0; i--) {
    double diag = 1.; // Diagonal element
    double sigma = 0.0; // Just a temporary value
    x[i] = b[i];
}

#pragma omp simd reduction(+:sigma)
for(int j = 0; j < num_cols; ++j) {
    sigma = sigma + A[j + i * num_cols] * x_old[j];
}
diag = A[i + i * num_cols];
sigma -= diag * x_old[i];
x[i] = (x[i] - sigma) * omega / diag;
}

#pragma omp target teams
#pragma omp distribute parallel for simd
for(int i = 0; i < num_loc_elts_x; ++i) {
    x[i] += (1 - omega) * x_old[i];
    x_old[i] = x[i];
}

#pragma omp target teams
calculateResidual(A, x, b, res, num_rows, num_cols);

#pragma omp target map(from:residual_norm)
residual_norm = calculateNorm(res, num_rows) / b_norm;

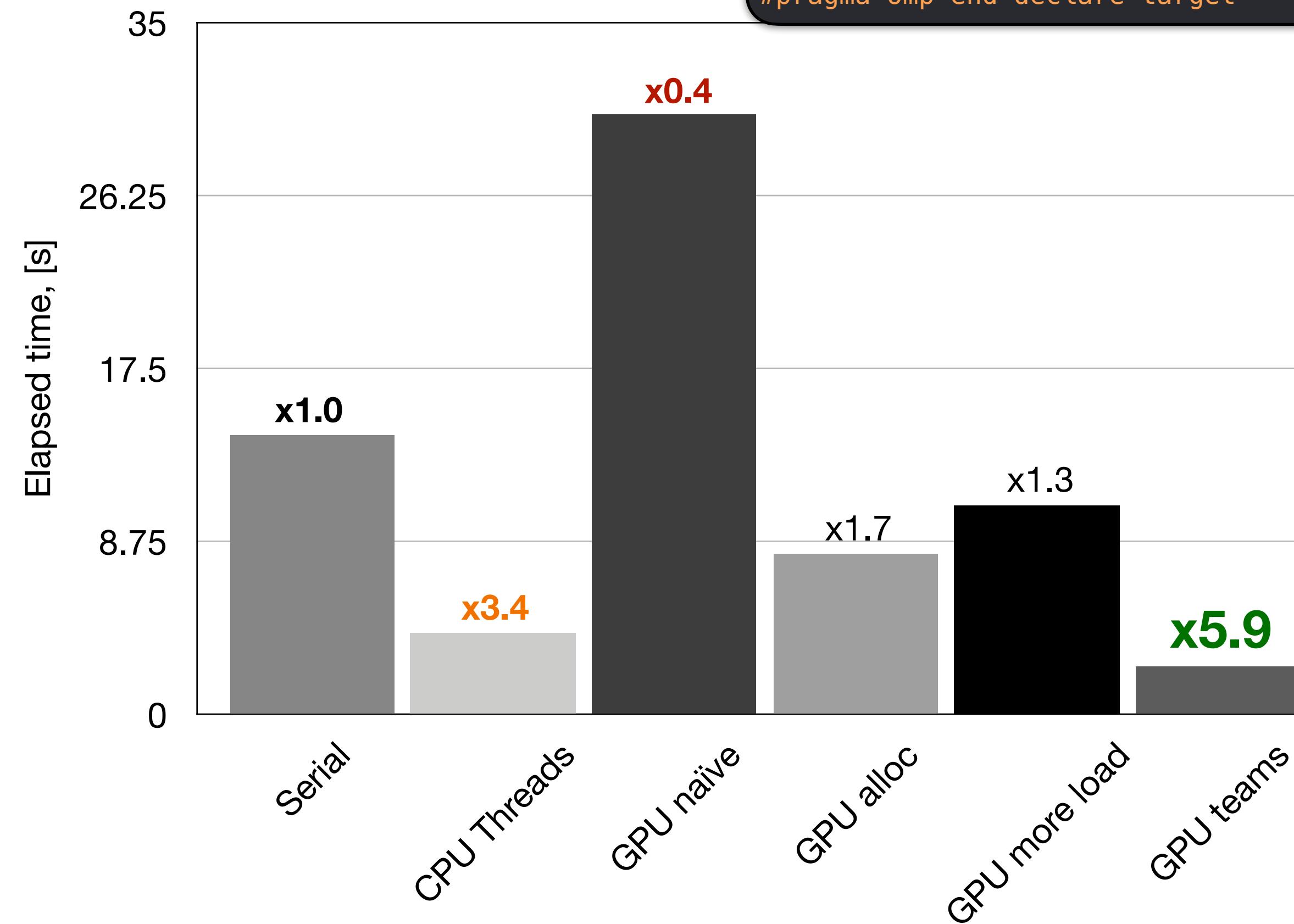
if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;
    iter++;
}
```

OpenMP

GPU offloading

GPU offload

100x100 grid points, 100 iterations



```
#pragma omp declare target
void Solver::calculateResidual(double *A, double *x, double *b,
                                double *res, int num_rows,
                                int num_cols) {
    copyVector(b, res, num_rows);

#pragma omp distribute parallel for
    for(int i = 0; i < num_rows; ++i) {
        double sum = 0.0;
#pragma omp simd reduction(+:sum)
        for(int j = 0; j < num_cols; ++j) {
            sum += A[j + i * num_cols] * x[j];
        }
        res[i] -= sum;
    }
#pragma omp end declare target
```

```
data map(to: A[0:num_elts_A],
         b[0:num_loc_elts_x],
         x_old[0:num_loc_elts_x],
         res[0:num_loc_elts_x]) \
        map(tofrom: x[0:num_loc_elts_x])
max_iter) && (residual_norm > tolerance) ) {
teams
ute parallel for
num_rows - 1; i >= 0; i--) {
diag = 1.; // Diagonal element
sigma = 0.0; // Just a temporary value
b[i];
duction(+:sigma)
... ... j = 0; j < num_cols; ++j) {
sigma = sigma + A[j + i * num_cols] * x_old[j];
}
diag = A[i + i * num_cols];
sigma -= diag * x_old[i];
x[i] = (x[i] - sigma) * omega / diag;

#pragma omp target teams
#pragma omp distribute parallel for simd
for(int i = 0; i < num_loc_elts_x; ++i) {
    x[i] += (1 - omega) * x_old[i];
    x_old[i] = x[i];
}

#pragma omp target teams
calculateResidual(A, x, b, res, num_rows, num_cols);

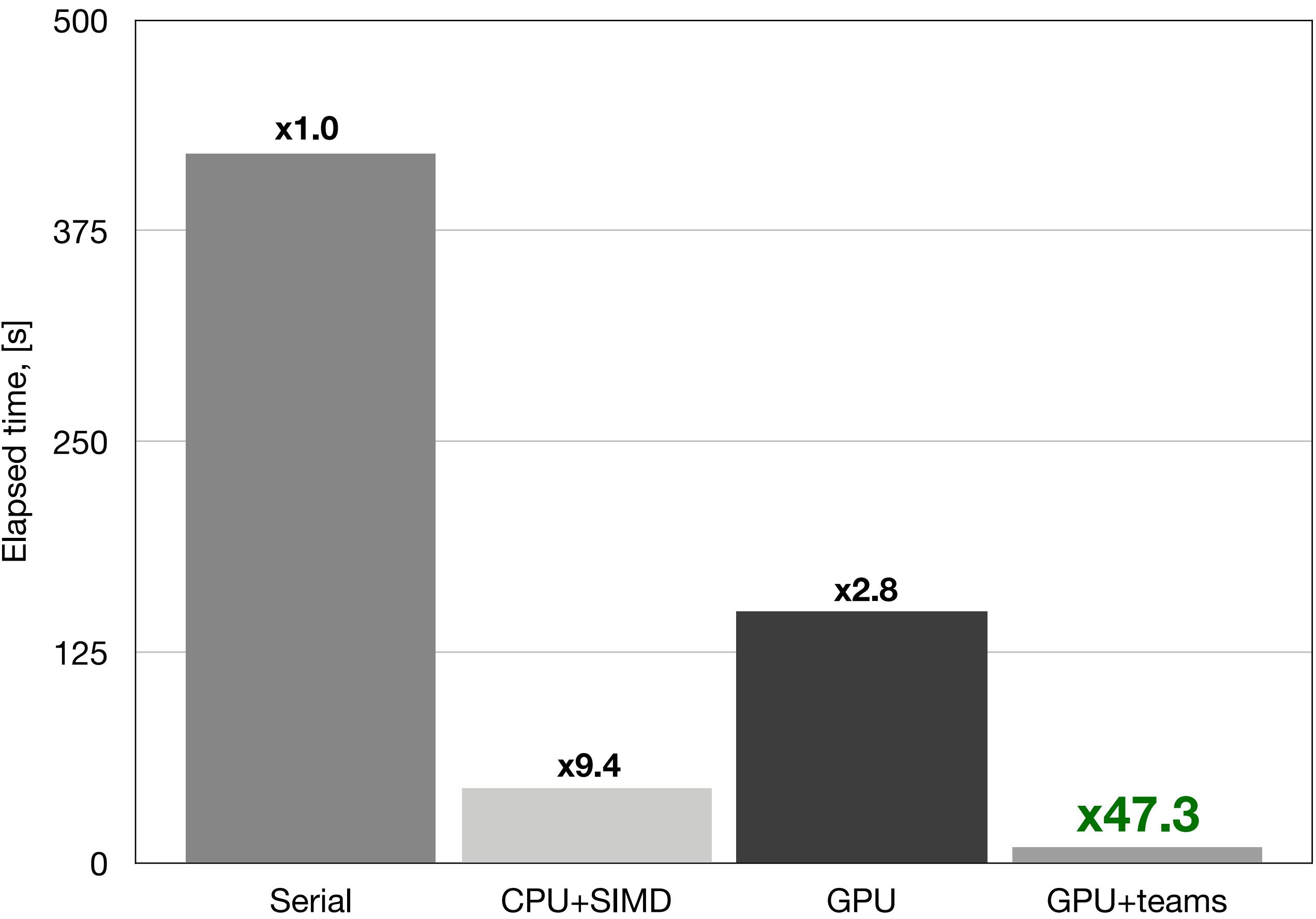
#pragma omp target map(from:residual_norm)
residual_norm = calculateNorm(res, num_rows) / b_norm;

if (my_rank == 0)
    cout << iter << '\t' << residual_norm << endl;
iter++;
}
```

OpenMP

Offload

- Large case: 200x200 grid points
- Performance of the Jacobi solver on host machine (CPU) and on the device (GPU)
- CPU: Xeon Gold 5118, 2.30GHz,
2x12 cores
- GPU: Nvidia Titan RTX
- Evaluated iterations: 100

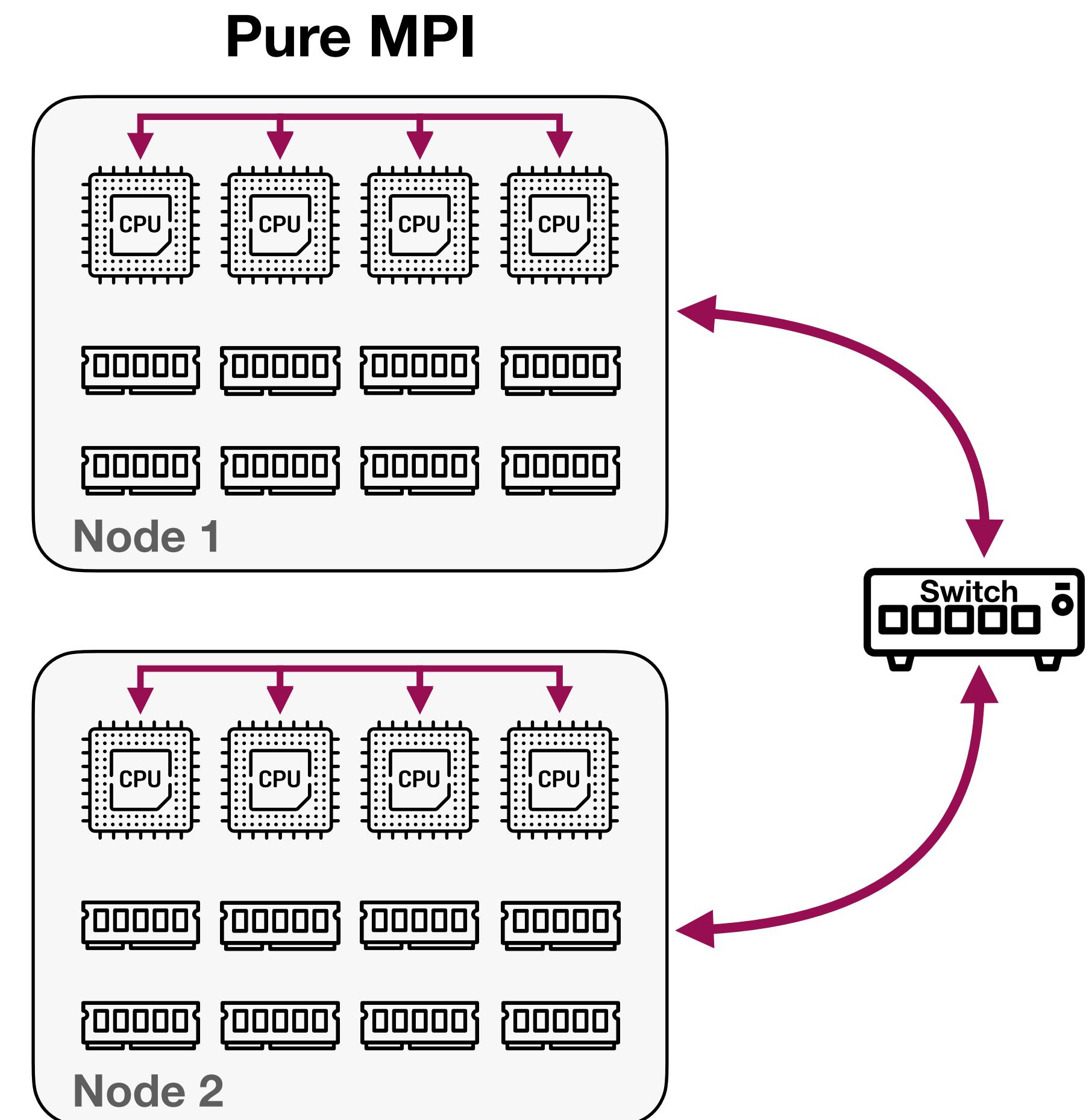


MPI+OpenMP

MPI+OpenMP

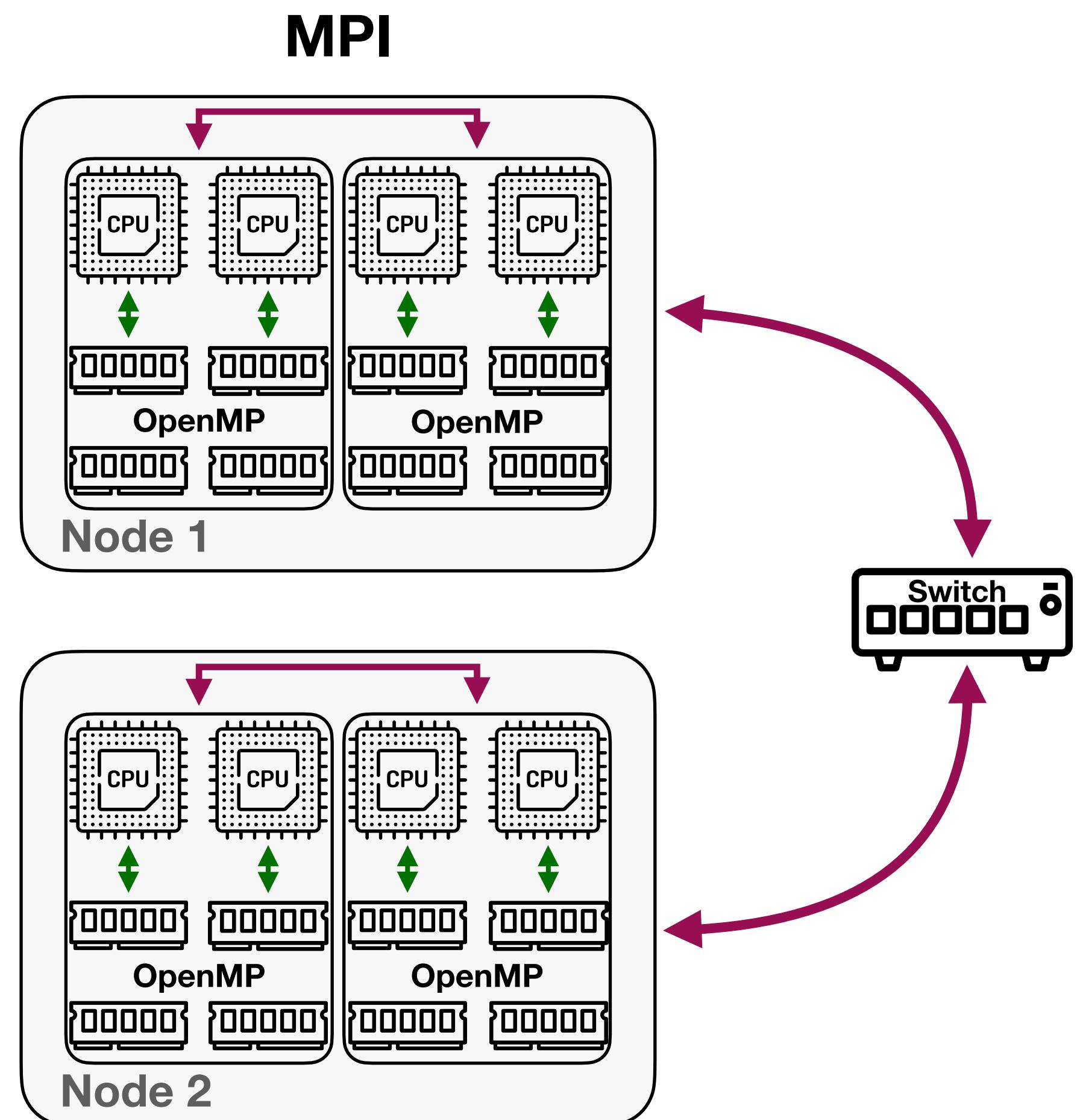
Hybrid

- Communications are expensive
- Intra-node communications can be reduced by using threads
- Often easy to implement with already MPI-parallelised code
- Often used in particle-based simulations



MPI+OpenMP Hybrid

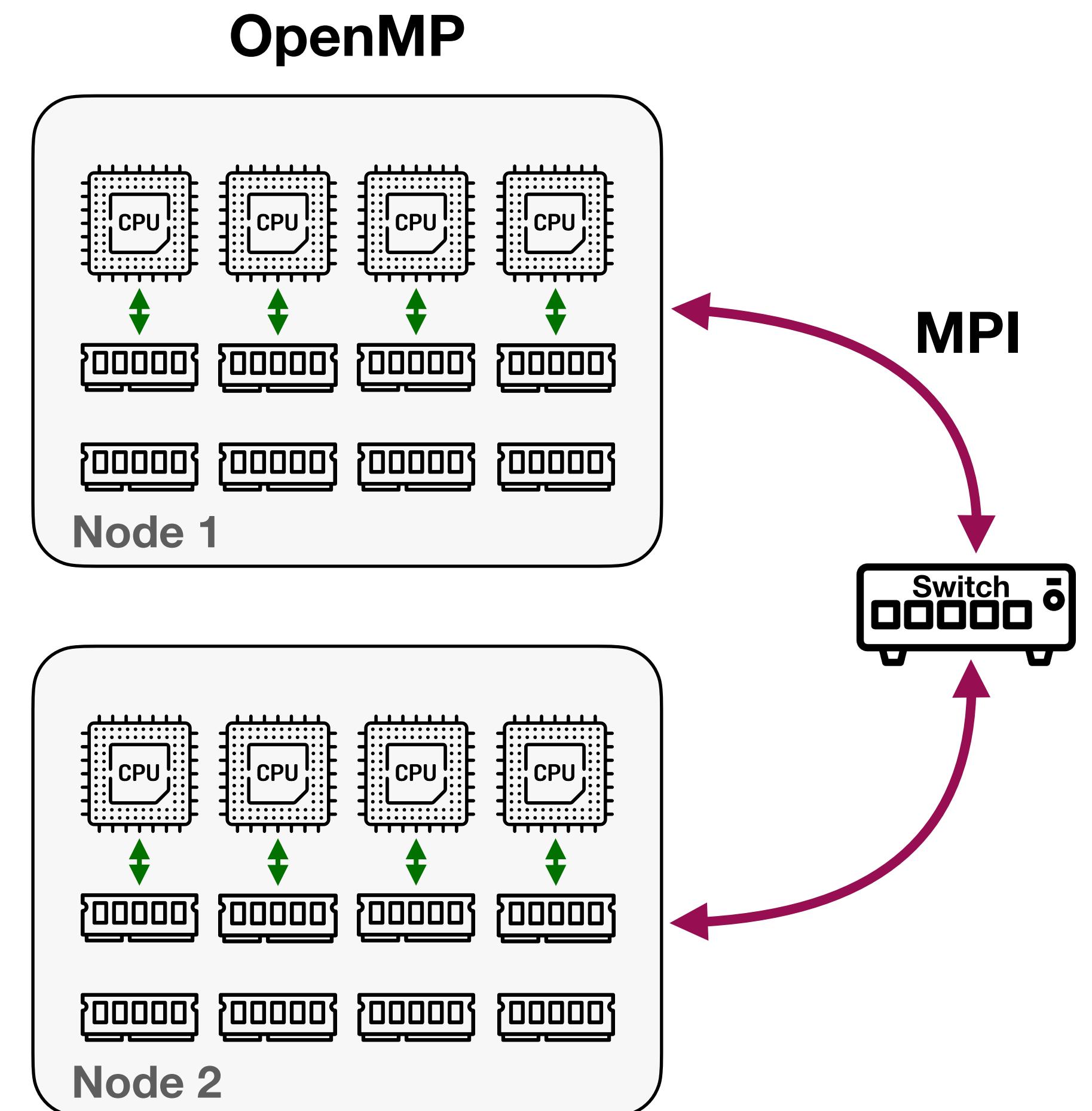
- Idea - some (every) MPI ranks spawn a few threads
- Sometimes even using hyperthreading may pay off
- May help to reduce impact of the load imbalance
- MPI library may already have optimal implementation on a shared-memory node (hard to optimise)



MPI+OpenMP

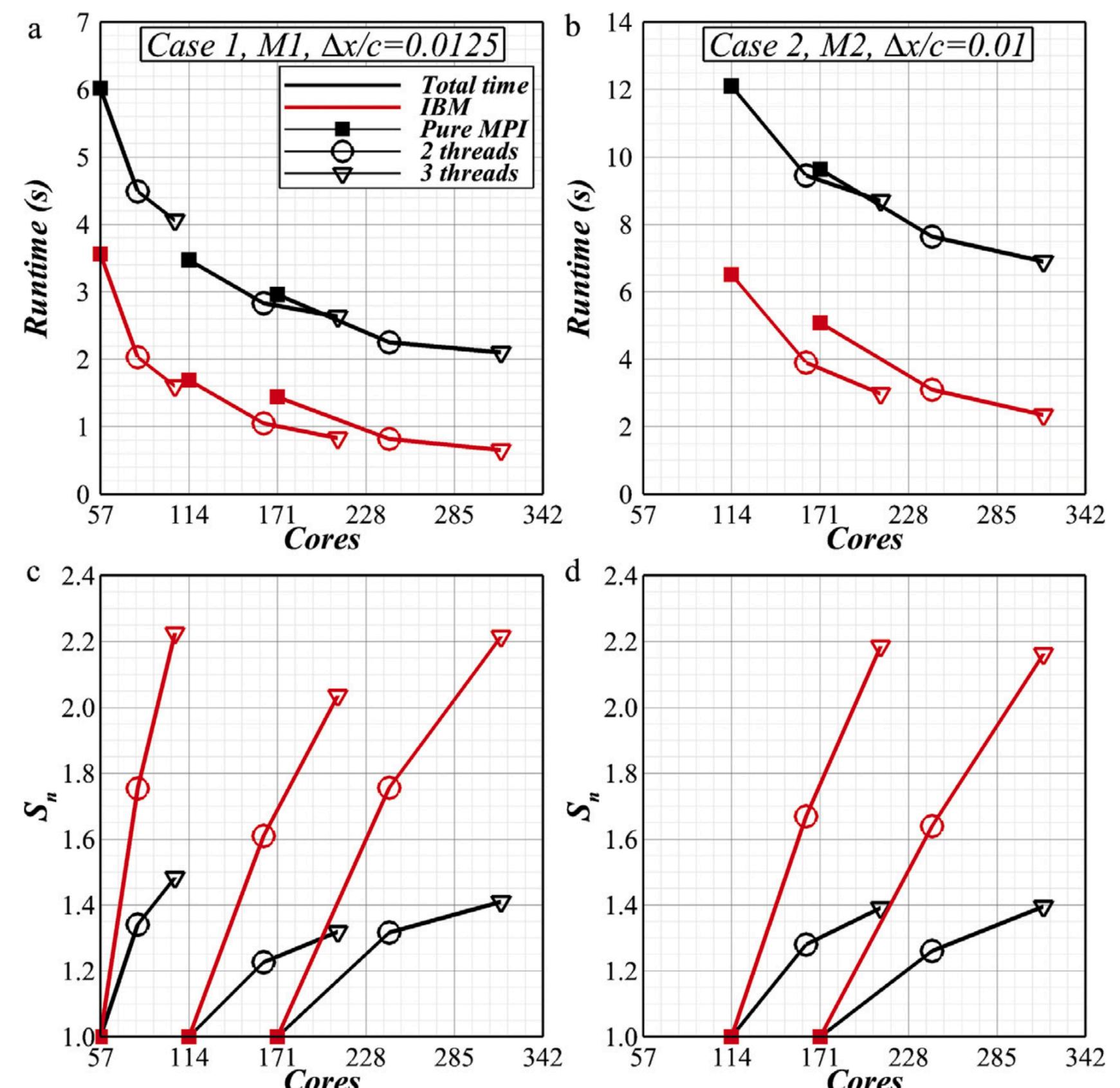
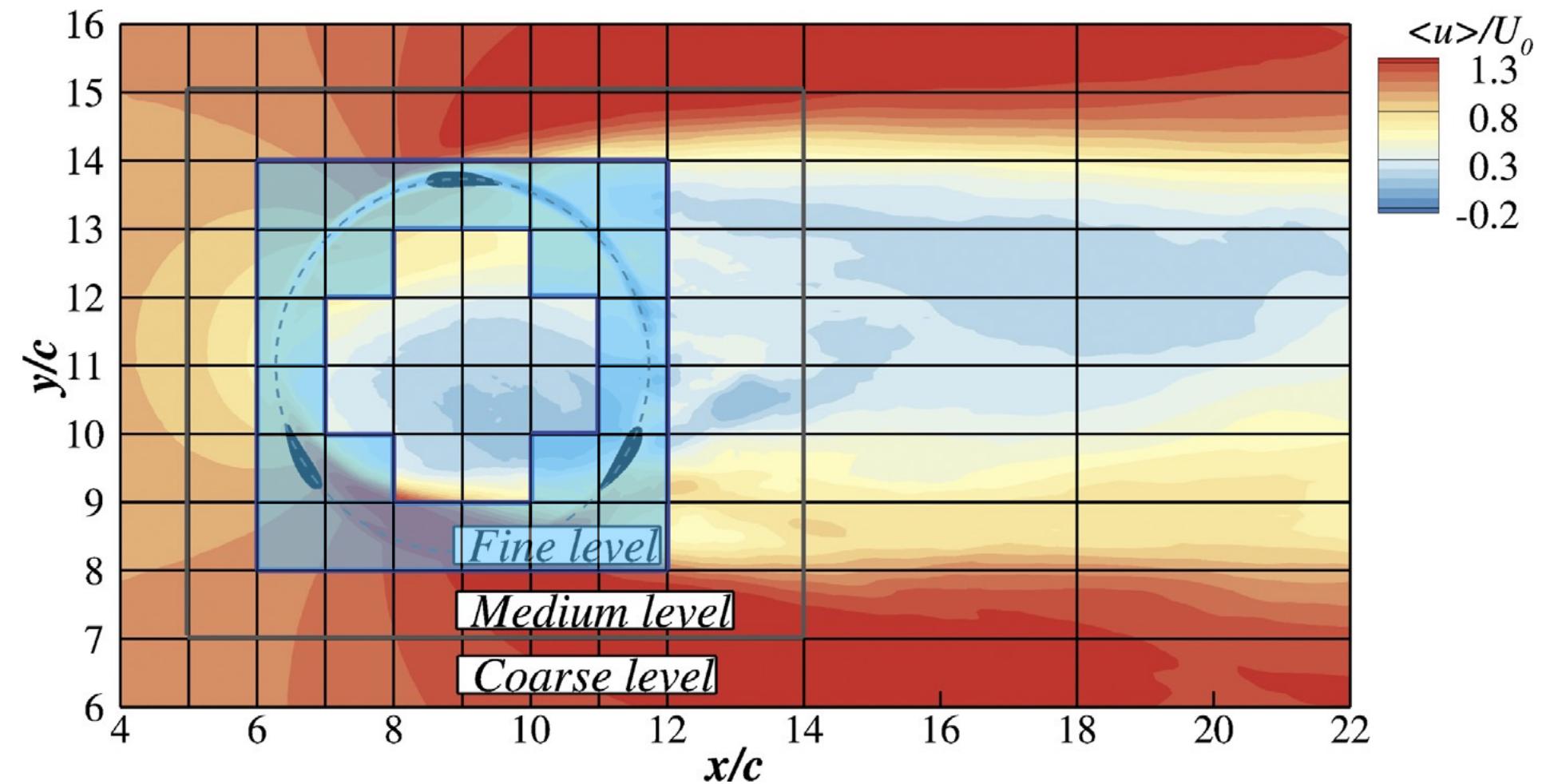
Hybrid

- Idea - some (every) MPI ranks spawn a few threads
- Sometimes even using hyperthreading may pay off
- May help to reduce impact of the load imbalance
- MPI library may already have optimal implementation on a shared-memory node (hard to optimise)



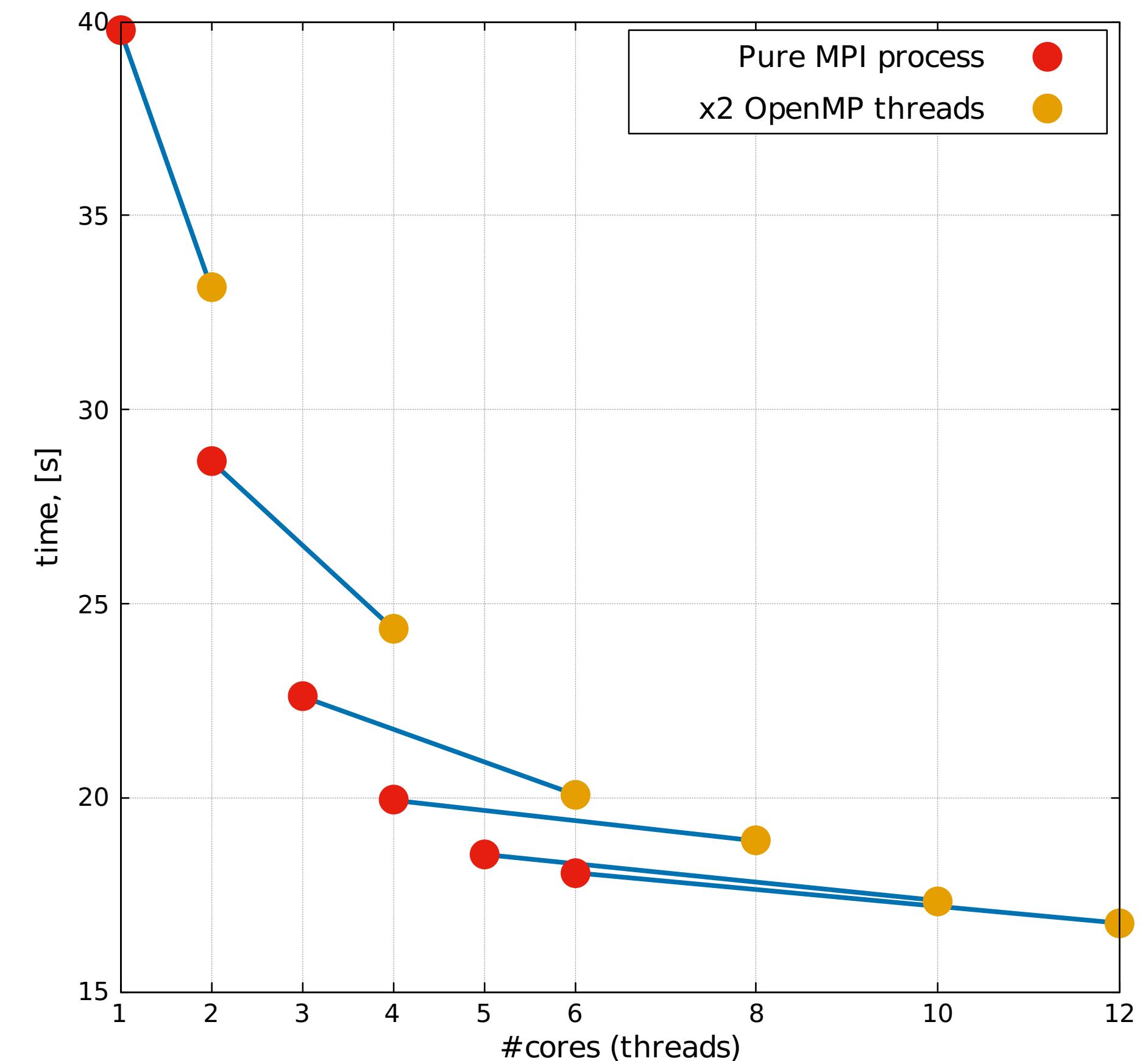
MPI+OpenMP Hybrid

- Example: CFD + IBM¹
- The whole domain is distributed across multiple processes
- However, only the blue region (Lagrangian grid) around the blades is evaluated with multiple threads
- This helped to improve the load imbalance



MPI+OpenMP Hybrid

- Example: FoxBerry, multiphase CFD code
- Duct flow, 300 DoF, structured grid
- BiCGStab(2) + AMG for solving PPE
- MPI tasks correspond to physical cores
- OpenMP threads correspond to hyperthreads
- Performance with 6 MPI tasks and 2 hyperthreads is ~8% better, compared to pure MPI



Hands-on

Hands-on

MPI+OpenMP

```
$ ./make_all hybrid
$ sbatch hybrid.sh
$
$ cat hybrid.sh
#!/bin/bash
#SBATCH --job-name=hybrid
#SBATCH --output=hybrid.out
#SBATCH -N 4
#SBATCH --ntasks-per-node=12
#SBATCH --cpus-per-task=2
#SBATCH --partition=short
#SBATCH --time 10

# Placement of threads as close as possible together
#SBATCH --distribution=block:block

module load 2020 foss/2020a

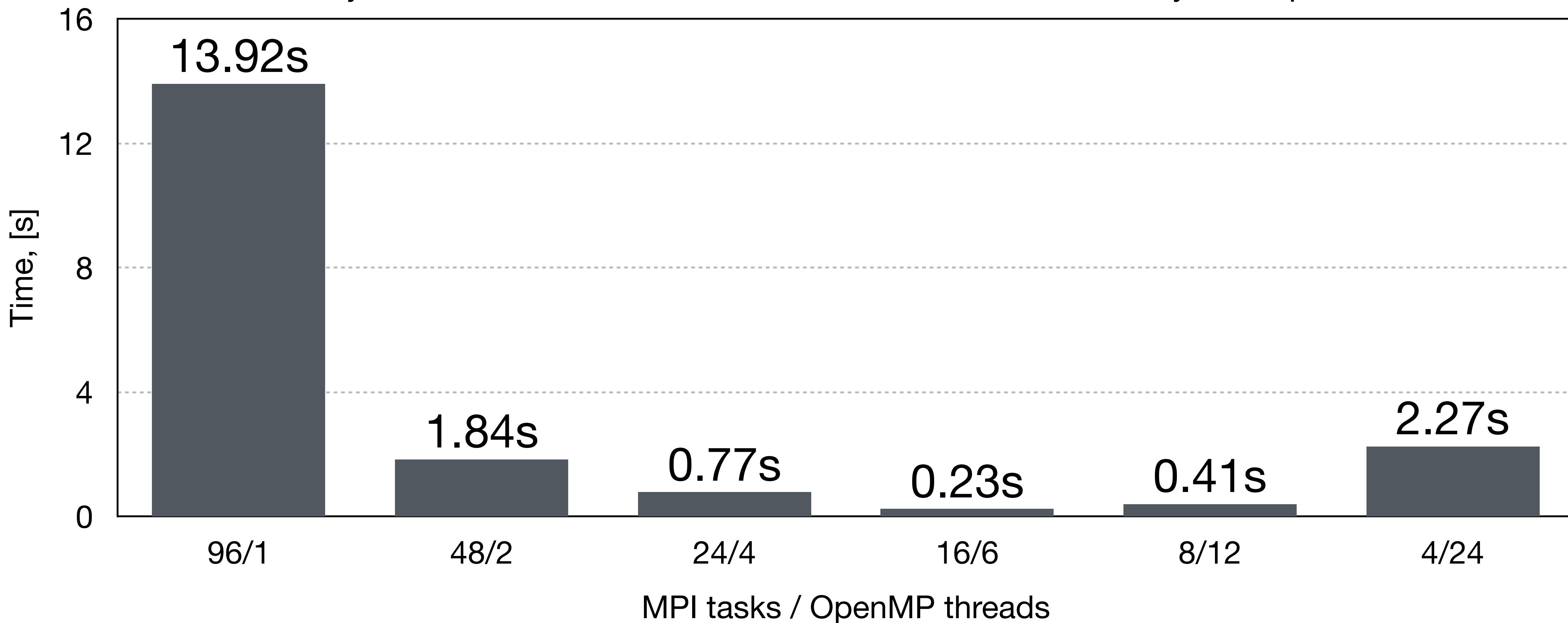
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

echo "Running $SLURM_NTASKS tasks with $SLURM_CPUS_PER_TASK threads"
srun ./a.out -s 256 256 -d 1 $SLURM_NTASKS
```

- Compile the Jacobi code in a hybrid way
- Use this batch script on Cartesius, or modify the script accordingly for Lisa
- Measure the performance with 2 and 4 threads per MPI process

Hands-on MPI+OpenMP

Performance of the hybrid Jacobi solver (**256² DoF**), time represents execution of **only 20! iterations**. System: Cartesius, Haswell nodes, 2x12 cores. Job always occupied 4 full nodes



Invited talk