HPC Programming

Message Passing Interface (MPI), Part I

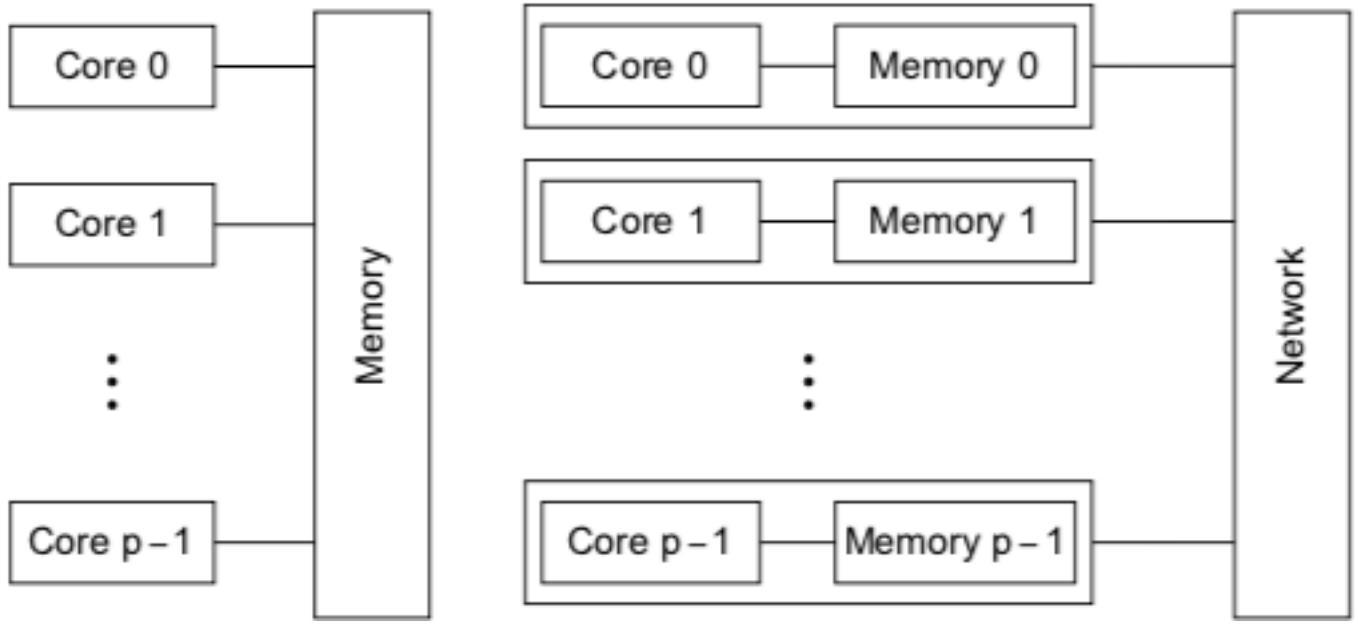
Peter-Bernd Otte, 12.11.2019

Shared System: Why two C extensions?

(a) Shared-Memory system:
- Each core can read/write each memory location
- Coordination of cores via shared-memory locations
- Use OpenMP
- Small projects. HIMster2: up to 32 cores/node

(b) Distributed-Memory system:
- Each core has private memory
- Cores explicitly sending messages for data exchange and coordination
- MPI
- Several nodes of a cluster

- Hybrid-Programming:
  - OpenMP+MPI



(a) (b)

Worked out example: bandwidth (CPU: i7-4790)

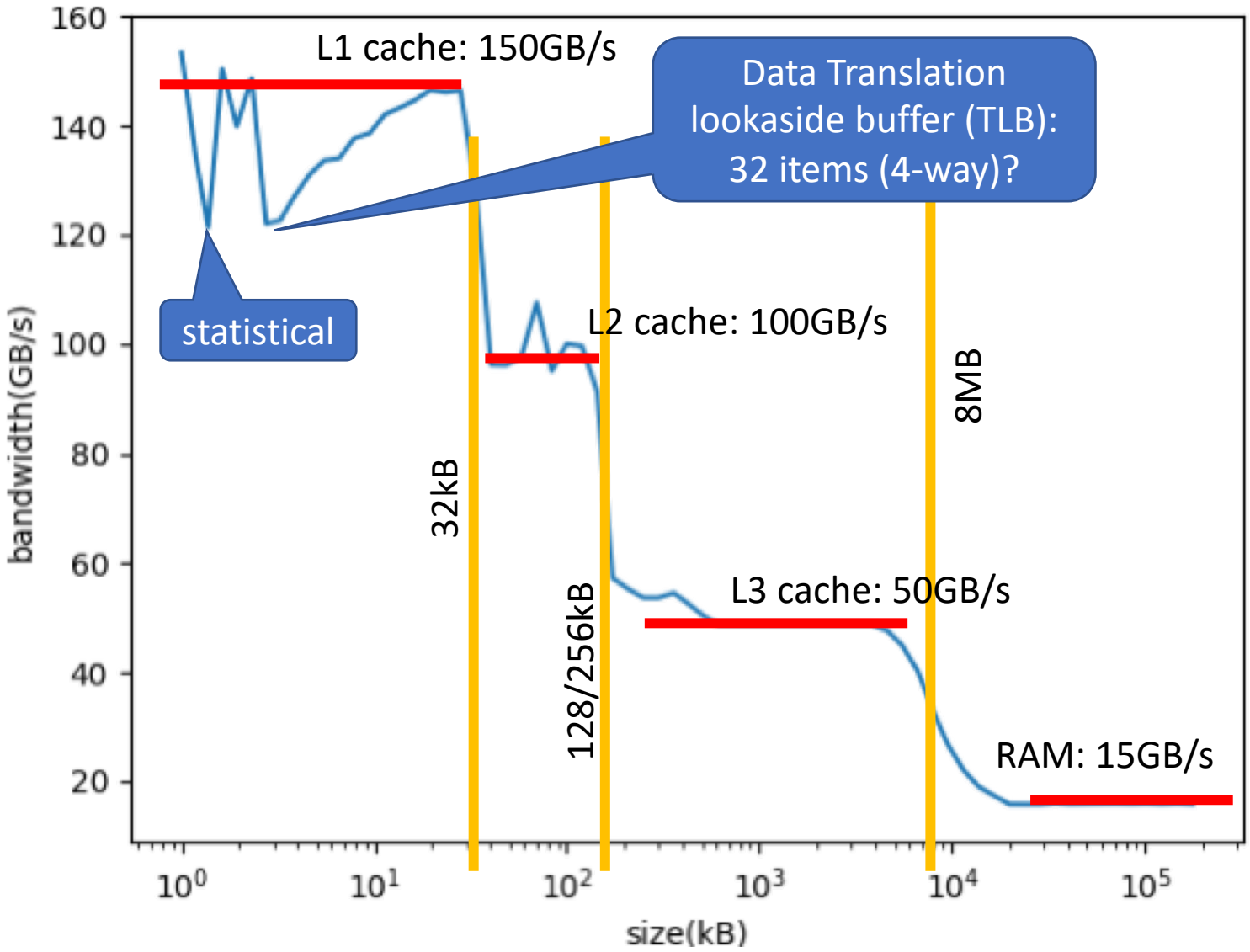
cache line block size = 64 bytes = 16 ints

main routine:

```
int *mem;
for(int i=0;i<n;i+=16) {
    result+=mem[i];
}
```

```
git clone –recursive
https://github.com/realead/memmeter
bash run_test.sh band_width
```

CPU under test: i7-4790 CPU @ 3.90GHz (cat /proc/cpuinfo | grep MHz)



Worked out example: latency (CPU: i7-4790)

main routine:

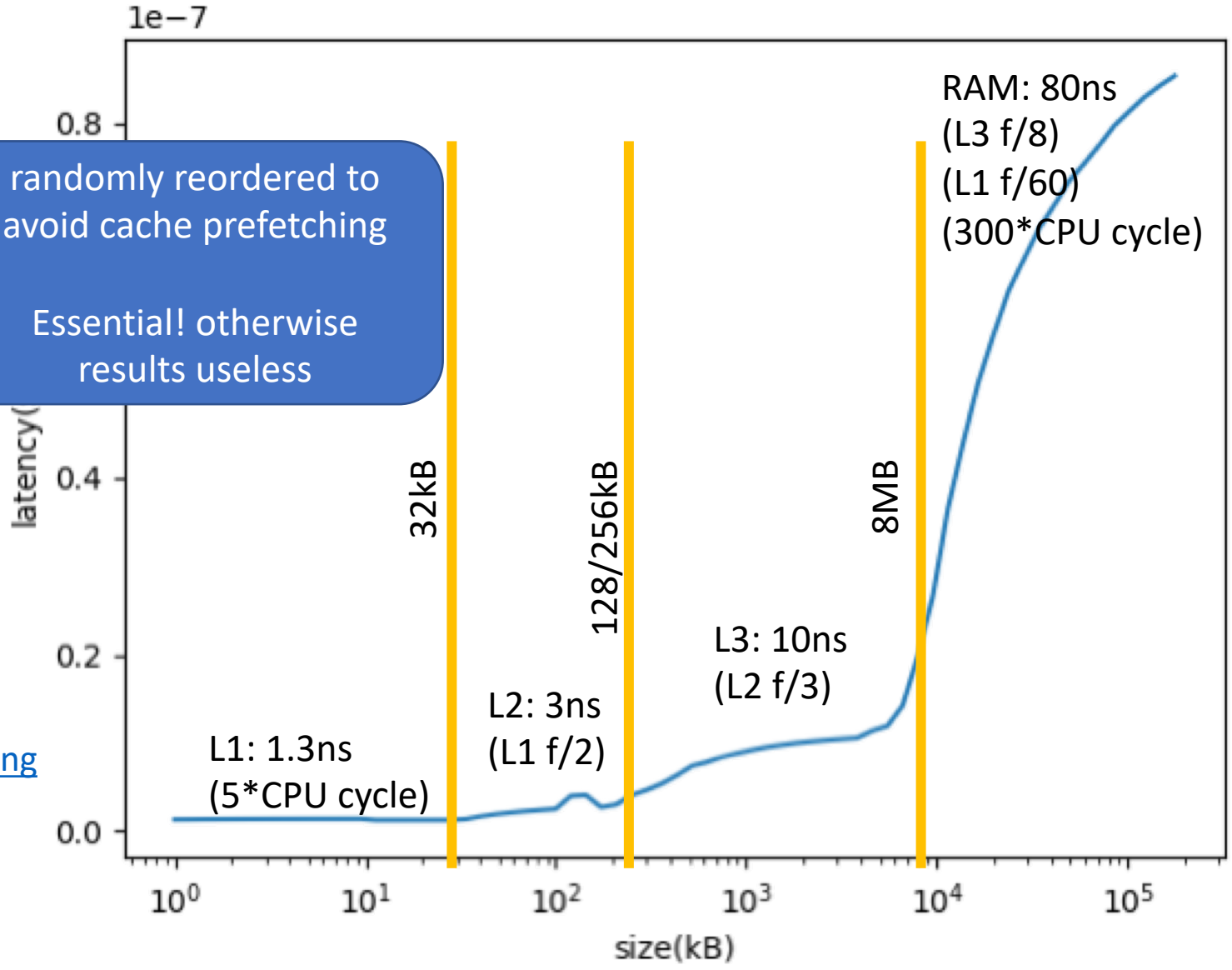
```
int *mem[STEPS] = 0..STEPS
reorder_randomly(mem);

for(unsigned int
i=0;i<steps;i++){

    index=mem[index];

}
```

randomly reordered to avoid cache prefetching

Essential! otherwise results useless

```
bash run_test.sh latency
```

see:
https://en.wikipedia.org/wiki/Cache_prefetching



Introduction MPI

1. Overview / Getting Started
2. Messages & Point-to-point Communication
3. Nonblocking Communication
4. Collective Communication
5. Dealing with I/O
6. Groups & Communicators
7. MPI Derived Datatypes
8. Common pitfalls and good practice (“need for speed”)

3x lecture with c

1x lecture with Python

MPI: Getting Started (1)

- Message Passing Interface (MPI) by MPI Forum (mpi-forum.org)
  - underlying: Distributed Memory Model
- De facto standard in parallel computing
  - Developed by academia and industry since 1991
  - C and Fortran in version 3.1 (2015, MPI 4 in development)
  - Several well-tested and efficient implementations available

- Other attempts (will not be covered by this lecture):
  - PGAS (Partitioned Global Address Space):
    - parallel programming model: assumes global memory, logically partitioned and a portion of it is local to each process
    - Library based: Global Arrays, OpenSHMEM
    - Compile based: Unified Parallel C (UPC), Co-Array Fortran (CAF)
    - HPCS (High Productivity Computing Systems) PGAS, Language-based: Chapel (Cray), X10 (IBM)
  - PVM (Parallel Virtual Machine, last update 2011) for set of heterogenous machines

MPI: Getting Started (2)

„MPI = Sending and receiving messages“

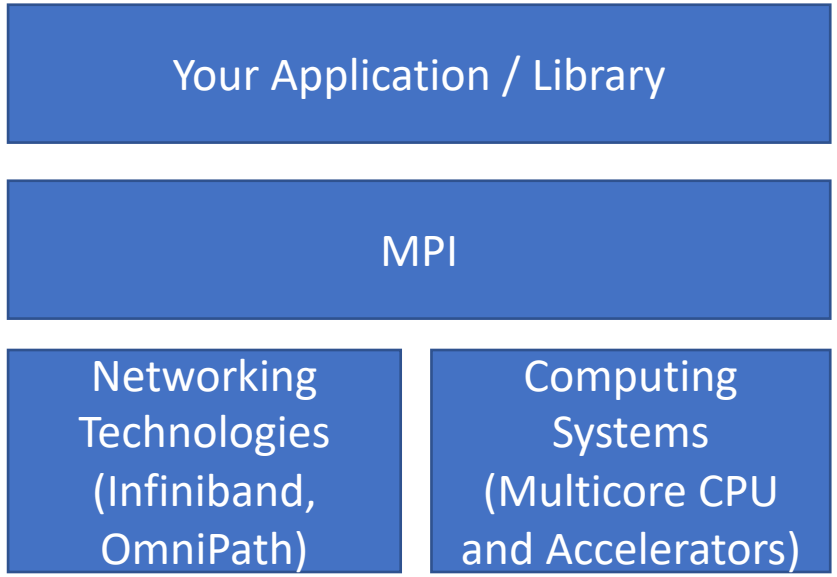
rank 0

rank 1

MPI: Getting Started (3)

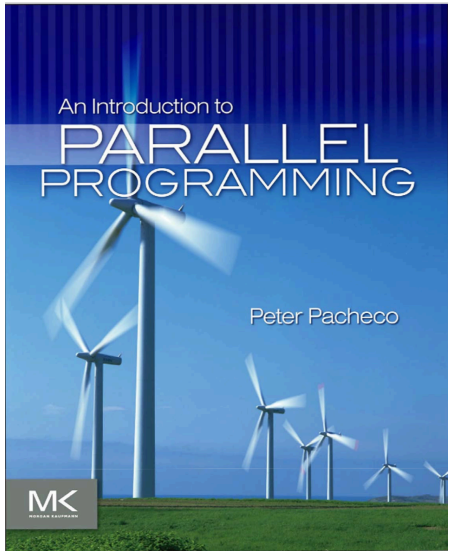
- Major MPI Features
  - Point to point Two sided Communication
  - Collective Communication
  - One-sided Communication
  - Job Startup
  - Parallel I/O

- Why?
  - Abstract message and file I/O exchange
    - simplifies your programming
  - Overlap computation and communication:
    - e.g. Non-blocking collectives and sending/receiving
  - Resiliency:
    - integrated failure detection

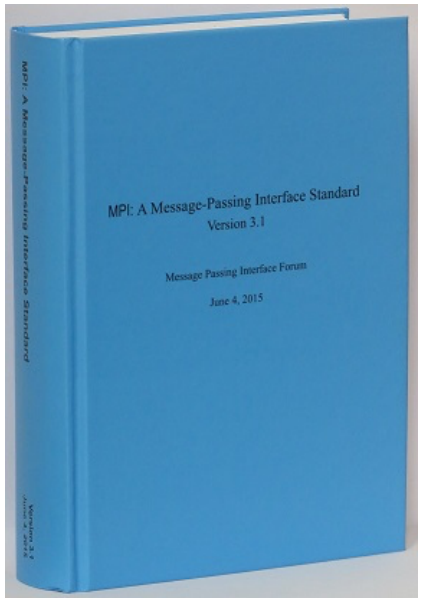


MPI: Getting Started (3)

- Good reads:
  - An Introduction to Parallel Programming by Peter Pacheco



  - MPI-3.1 Standard



MPI: Fast lane to “Hello World”

- Compilation of a MPI program:
  - mpicc
  - wrapper script for the C compiler
- Executing a MPI program:
  - mpirun -n [NumberOfRanks] ./Executable
  - (machine dependent: mpiexec, srun, …)
- But: to have MPI available on HIMster2: first load corresponding module
  - module load mpi/OpenMPI/3.1.0-GCC-6.3.0
  - On head node and on compute node, put in submit script
  - → see next slide

MPI libraries on HIMster2

```
$ module load mpi/
mpi/impi/2017.2.174-iccifort-2017.2.174-GCC-6.3.0  mpi/OpenMPI/2.1.2-GCC-6.3.0
mpi/impi/2018.0.128-iccifort-2018.0.128-GCC-6.3.0  mpi/OpenMPI/3.0.0-GCC-6.3.0
mpi/impi/2018.1.163-iccifort-2018.1.163-GCC-6.3.0  mpi/OpenMPI/3.0.1-GCC-6.3.0
mpi/impi/2018.2.199-iccifort-2018.2.199-GCC-6.3.0  mpi/OpenMPI/3.0.1-GCC-6.4.0
mpi/impi/2018.3.222-iccifort-2018.3.222-GCC-6.3.0  mpi/OpenMPI/3.0.1-GCC-8.1.0
mpi/MVAPICH2/2.2-GCC-6.3.0                         mpi/OpenMPI/3.0.1-iccifort-2018.2.199-GCC-6.3.0
mpi/OpenMPI/1.10.4-GCC-6.3.0                       mpi/OpenMPI/3.1.0-GCC-6.3.0
mpi/OpenMPI/2.0.2-GCC-6.3.0                        mpi/OpenMPI/3.1.1-iccifort-2018.3.222-GCC-6.3.0
```

MPI: Basics

- `int MPI_Init(int *argc_p, char ***argv_p)`
  - tells MPI system to setup (eg allocate storage for message buffers, decides which process gets which rank, creates MPI_COMM_WORLD communicator)
  - MPI_Init(Null, Null) just fine for beginning.
  - no other MPI function call before this
- `int MPI_Finalize(void)`
  - tells MPI system: we are done using MPI, free resources allocated for MPI
  - no MPI functions after this call, also no MPI_Init!

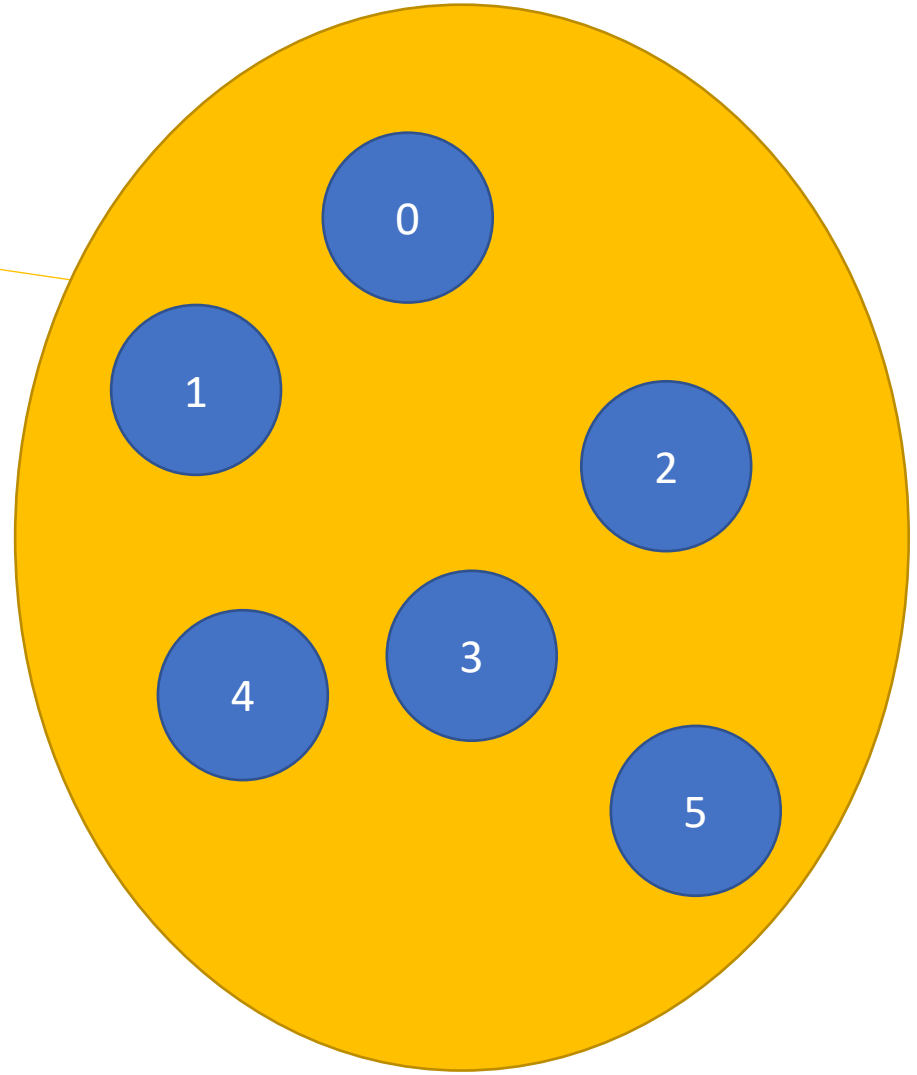
MPI: Communicators

- MPI Communicator
  = group of processes that can send messages to each other.
- All processes are in `MPI_COMM_WORLD` communicator
  - Defining sub groups → see future lecture
- Number of members in communicator with

```
int MPI_Comm_size (
      MPI_Comm comm    /*in*/,
      int *comm_size_p /*out*/)
```

- Get rank of sub_process with

```
int MPI_Comm_rank (
      MPI_Comm comm   /*in */,
      int * my_rank_p /*out*/)
```



Single Program, Multiple Data (SPMD)

- Standard MPI programming:
  - Write single executable
  - behaviour depends on its rank
    - eg rank=0: message collecting master,
      ranks>0: computing
  - Number of ranks from 1 to O(10^4) on Himster2
    - O(10^6) on extreme machines
  - called “Single Program, multiple Data”
- ⇔ Multiple-Program Multiple-Data (MPMD)
  - even mixture of different software possible with MPI:
    Fortran and C executable communicating fine

```
MPI_Comm_rank(MPI COMM WORLD, &my_rank);

if (my_rank == 0) {
  ...
} else {
  ...
}
```

MPI: MPI_Send

- Sending a message to another receiving rank
- Syntax:

```
int MPI_Send(
      void           *msg_buf_p     /*in*/,
      int            msg_size       /*in*/,
      MPI_Datatype   msg_type       /*in*/,
      int            dest           /*in*/,
      int            tag            /*in*/,
      MPI_Comm       communicator   /*in*/);
```

defines contents of message

defines destination of message

- dest = receiving rank (defined in communicator)
- tag to distinguish messages
- defines the “communication universe”,
  all processes are in: `MPI_COMM_WORLD`

MPI: MPI_Recv

- Receiving a message from another rank
- Syntax:

```
int MPI_Recv(
      void           *msg_buf_p     /*out*/,
      int            msg_size       /*in*/,
      MPI_Datatype   msg_type       /*in*/,
      int            source         /*in*/,
      int            tag            /*in*/,
      MPI_Comm       communicator   /*in*/,
      MPI_Status     *status_p      /*out*/);
```

defines contents of message

defines destination of message

- source = sender rank (defined in communicator). To accept all: MPI_ANY_SOURCE
- tag to distinguish messages. To accept from all: MPI_ANY_TAG
- defines the “communication universe”, no wildcard available, all processes are in: `MPI_COMM_WORLD`
- `status_p` to retrieve error information, or: `MPI_STATUS_IGNORE`

MPI: Make a match

- rank s calls: `MPI_Send(send_buf, send_buf_size, send_type, dest, send_tag, send_comm);`
- rank q calls: `MPI_Recv(recv_buf, recv_buf_size, recv_type, src, recv_tag, recv_comm, &status);`

- All 5 “green” parameters need to match to get message successfully through.
  - all mandatory to be equal, except recv_buf_size >= send_buf_size

MPI: Elementary datatypes

- C types can't be passed
  → use MPI datatypes
- Advantage: interoperability with other software and hardware

MPI datatype	C equivalent
MPI_SHORT	short int
MPI_INT	int
MPI_LONG	long int
MPI_LONG_LONG	long long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_UNSIGNED_LONG_LONG	unsigned long long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_CHAR	char

MPI exercises 1 and 2

- Setup your workspace: https://gitlab.rlp.net/pbotte/learnhpc/tree/master/mpi

- Try out exercises 1 and 2