HPC/Exascale Centre of Excellence in Personalised Medicine

Centre of Excellence for Computational Biomolecular Research

PATC course

Introduction to HPC for Life Scientists

31 January - 02 February 2022

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Parallel programming models

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PATC course: Introduction to HPC for Life Scientists, 31 January - 02 February 2022

Partners

Funding
Horizon 2020 European Union Funding for Research & Innovation

Parallel Programming models

Different ways to exploit parallelism

Partners

Funding

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Reusing this material

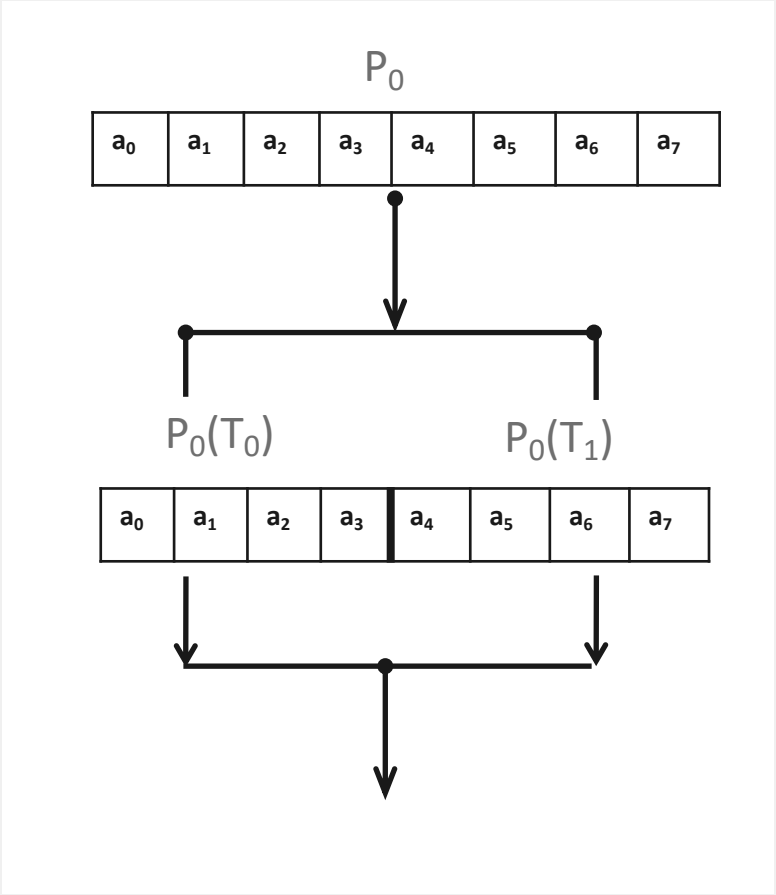
Outline

- Shared-memory parallelism
  - Threads
  - OpenMP
  - Shared-memory in HPC machines
- Message-passing (distributed) parallelism
  - Processes
  - MPI libraries
  - Distributed-memory in HPC machines
- Hybrid (MPI+OpenMP) parallelism
  - A combination of the above
- Exploiting GPU parallelism

Shared Memory
Thread-based parallelism

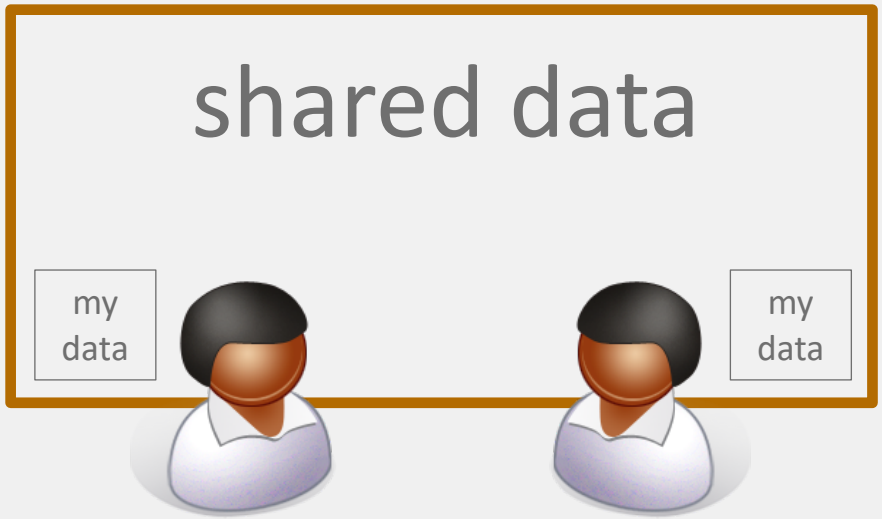
Shared-memory concepts

- Imagine some data which lives on a process
- Each thread can see the data of the parent process – they share the same memory
- These threads are assigned to different physical cores on the processor
- The threads can operate on different parts of the data – this allows for parallel speed up



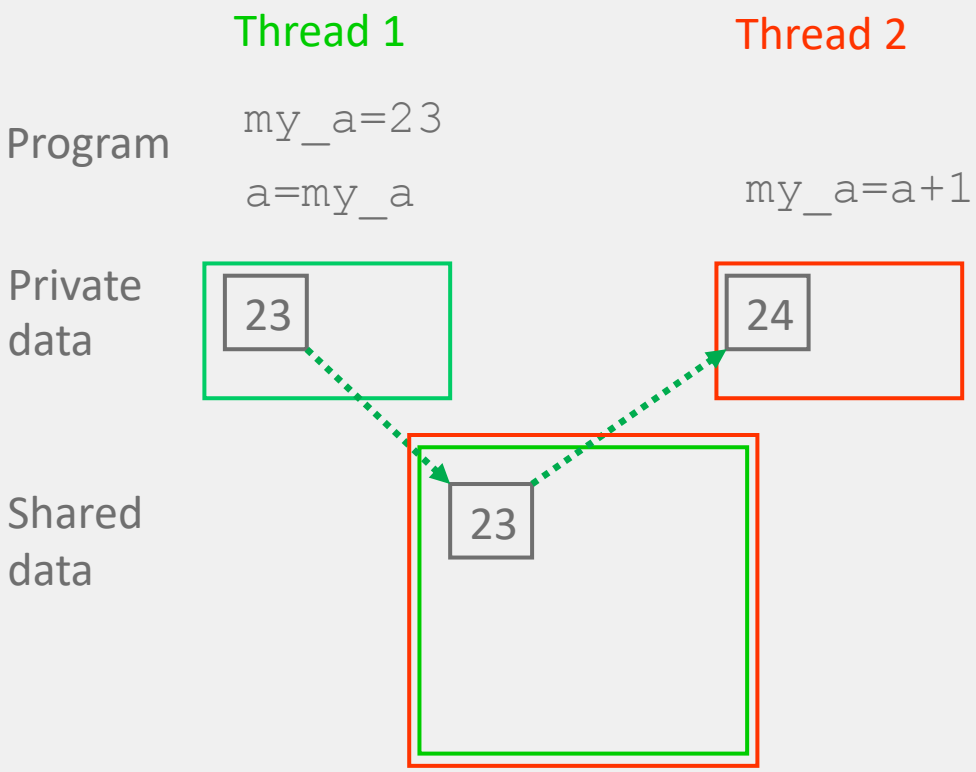
Analogy

- One very large whiteboard in a two-person office
  - the shared memory
- Two people working on the same problem
  - the threads running on different cores attached to the memory
- How do they collaborate?
  - working together
  - but not interfering
- Also need *private* data



Thread communication

- Each thread can read and write to the shared data
- Therefore they can communicate by reading and writing to this shared space.
- Synchronisation crucial for shared variables approach.
  - thread 2's code must execute *after* thread 1



OpenMP

- OpenMP is an Application Program Interface (API) for shared memory programming using threads
  - You can expect OpenMP to be supported by all compilers on all HPC platforms
  - Example usage: `gcc –fopenmp mycode.c –o mycode`
- Parallelism is implicit ie. a lot is abstracted from the programmer
  - You specify which parts of the program you want to parallelise and the compiler produces a parallel executable

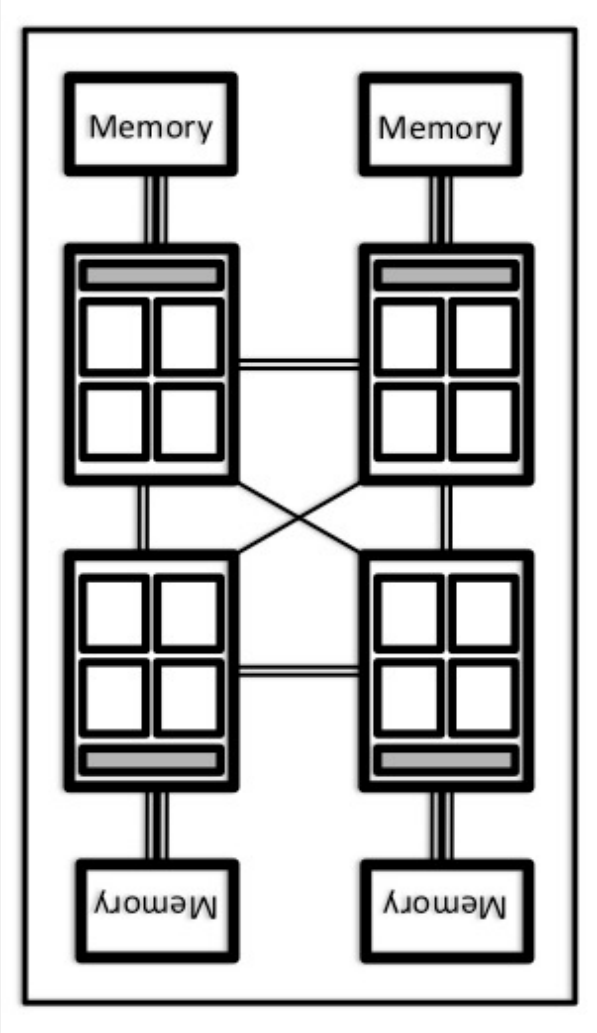
Example: OpenMP Loop parallelism

- The most common form of OpenMP parallelism is to parallelise the work in a loop
  - The OpenMP directives tell the compiler to divide the iterations of the loop between the threads

```
#pragma omp parallel shared(a,b,c) private(i)
{
   #pragma omp for
   for (i=0; i < N; i++) {
     c[i] = a[i] + b[i];
   }
}
```

Hardware

- Shared-memory parallelism can only take place on cores that share memory i.e a single node or memory region.
- Would expect poor performance if used across multiple memory regions.
- We are usually restricted to only a few 10s of threads on most machines



Usage

- Number of threads set by using the environment variable OMP_NUM_THREADS e.g.

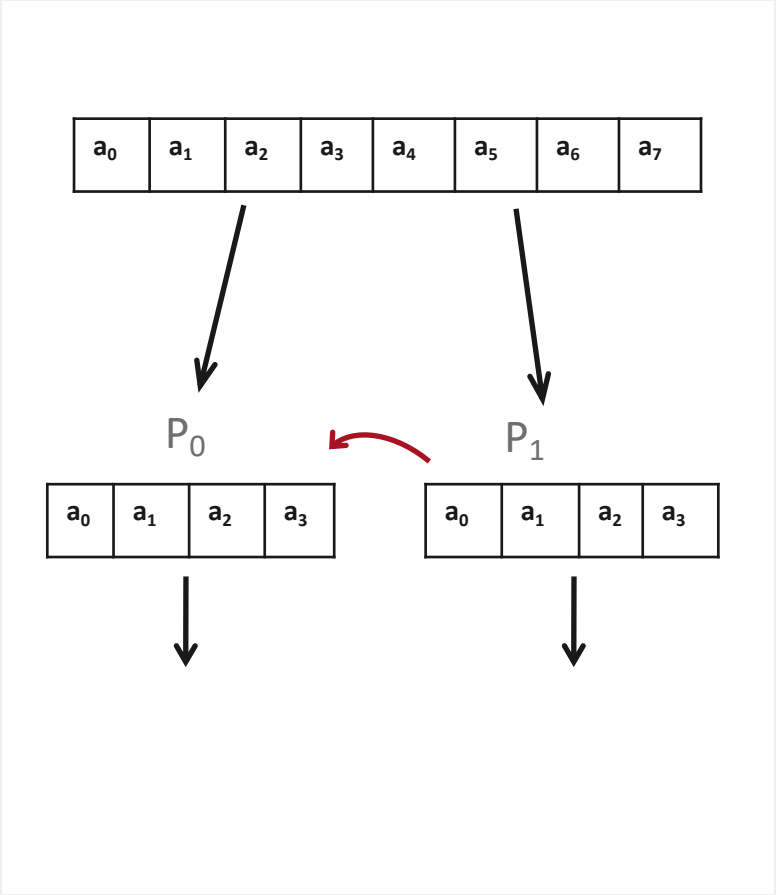
```
export OMP_NUM_THREADS=2
```

- When using Slurm you must also set the SBATCH option `--cpus-per-task`. This is the number of cores allocated to a single process (task) and should be the same as the number of threads to ensure one core per thread.

Message Passing
Distributed parallelism

Distributed memory parallelism

- The data is distributed amongst different processes.
- Create smaller sub-problems - parallelism
- Processes can only see their own data
- Communication between them is done via messages.
  - One process can send data to another process

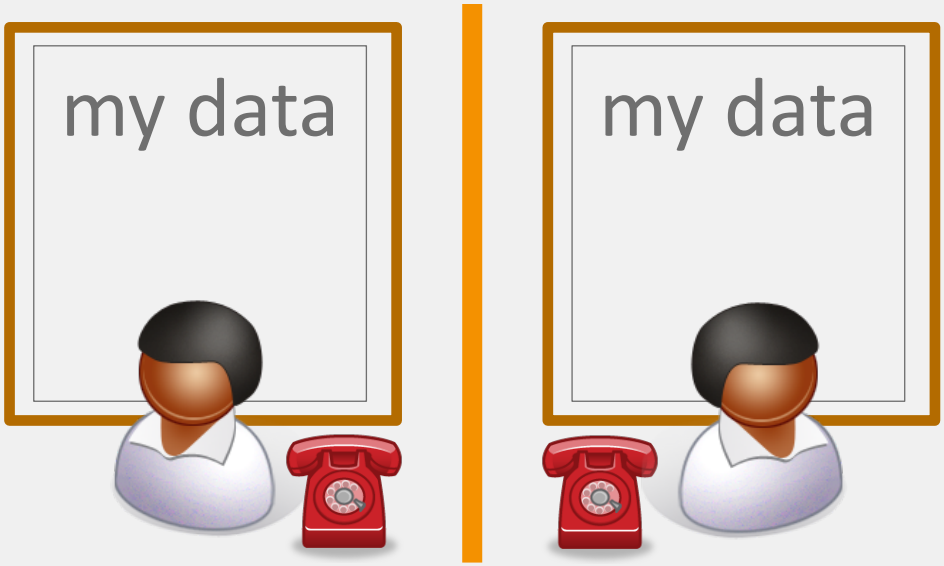


Analogy

- Two whiteboards in different single-person offices
  - the distributed memory
- Two people working on the same problem
  - the processes on different nodes attached to the interconnect

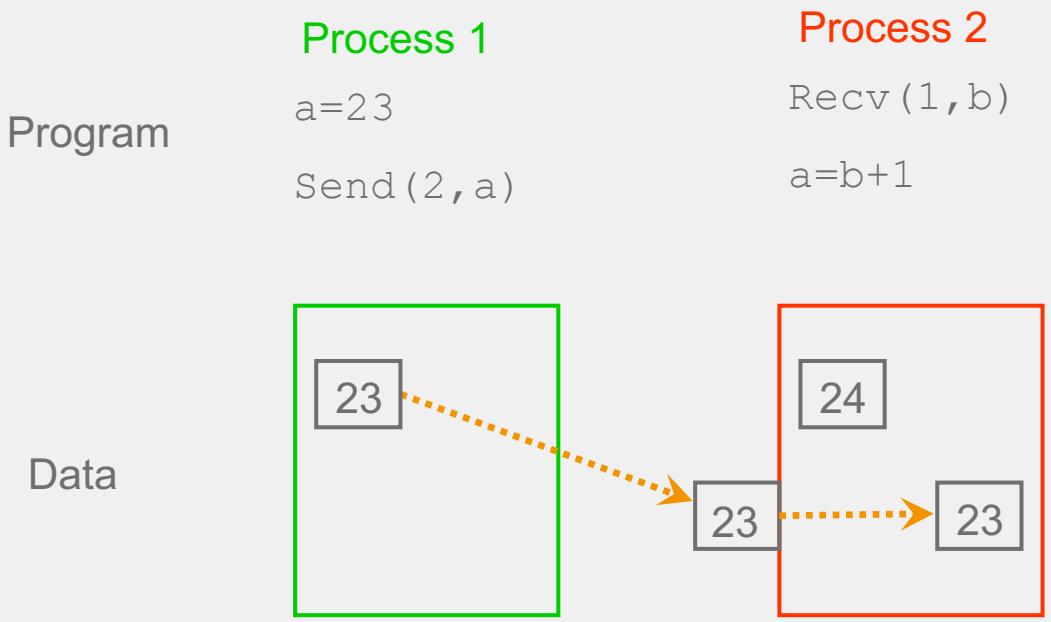
- How do they collaborate?
  - to work on single problem

- Explicit communication
  - e.g. by telephone
  - no shared data



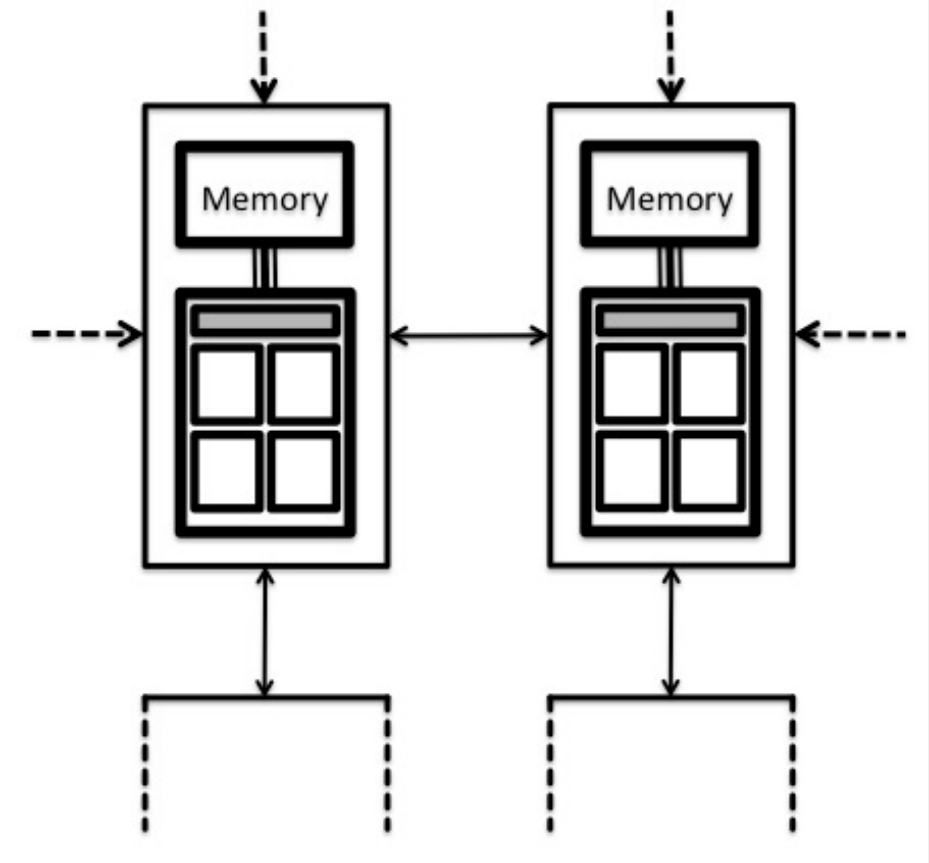
Process communication

- Explicit messages between processes.
- Messages are two-sided, they require a send and a receive.
- To send a message must specify the data to send and the destination process.
- The receive counterpart must match the sender process number.



Hardware

- Processes can be distributed across multiple nodes with one process per core, and messages across in the interconnect
- Intra-node messages are fast.
- Message passing is the standard parallelism for modern machines as it can exploit cores across multiple nodes.



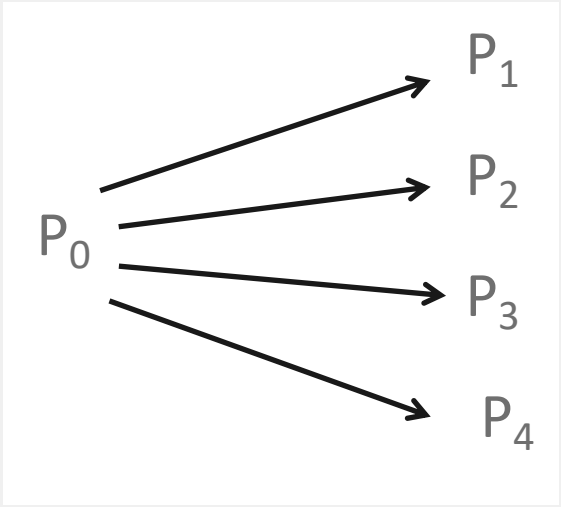
Message passing interface (MPI)

- MPI is a portable **library** used for writing parallel programs using the message passing model
- There are a number of different implementations, but all should support the MPI standard
  - Examples: MPICH, Open MPI, Intel MPI
- In message-passing all the parallelism is explicit
  - The programmer needs to decide how to decompose the problem over processes
  - Then **what** to send/receive and **when/how often**

Communications

- Point-to-point communications
  - A message sent by one process and received by another

- Collective communications
  - Involve “all” processes
  - E.g. Broadcasting data to all processes
  - More efficient than many point-to-point messages



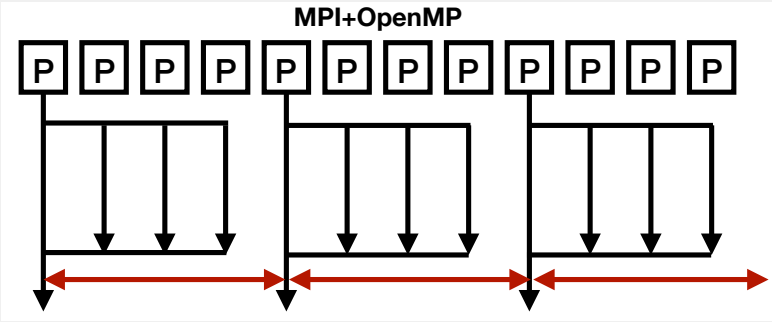
Usage

- For pure MPI one process is associated with one physical core
- The job launcher launches the same program across multiple processes.
  - e.g. srun, mpirun, mpiexec, aprun
- Need to specify the number of processes in the job
  - `--ntasks-per-node` or `--ntasks`
  - This is the number of copies of the program created

MPI+OpenMP
Mixed mode parallelism

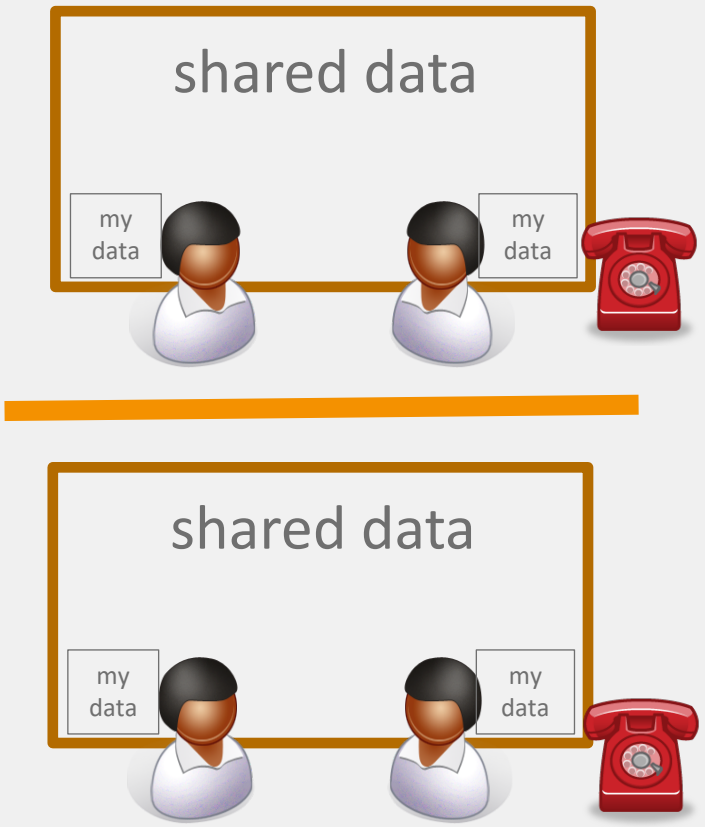
Hybrid MPI+OpenMP

- Modern HPC machines are distributed clusters
  - Cannot use shared memory (threads) across nodes – limited to a single node
  - Can instead use shared memory within a node and message passing between nodes. i.e. each process spawns multiple threads
- This is known as MPI+OpenMP
  - Has the possibility to improve the performance
  - Can also decrease the overall memory requirements
    - Less copies of data on a node



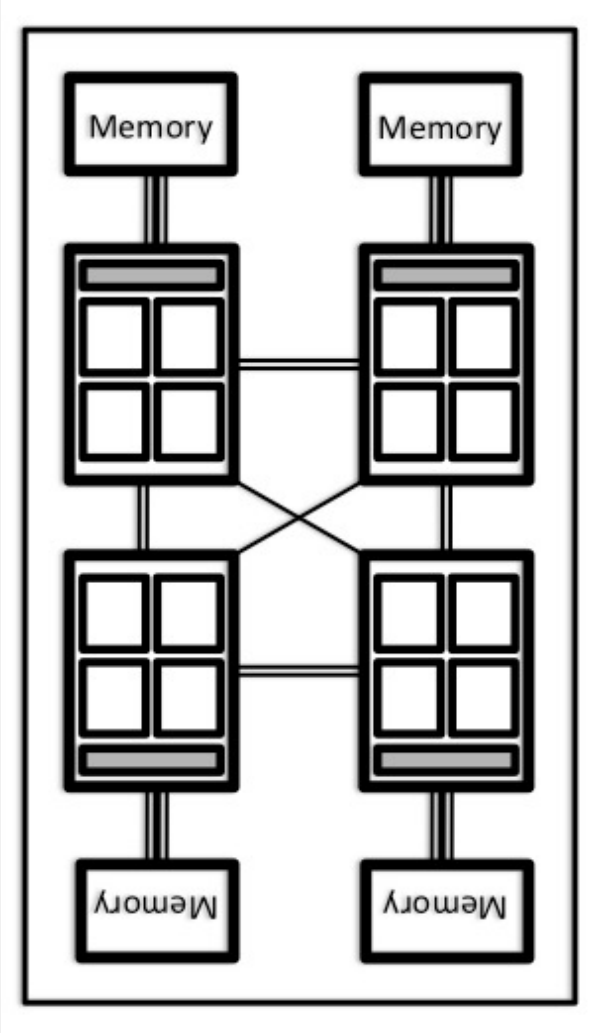
Analogy

- Groups of people working in separate offices
  - They all work on parts of the same problem
- In the same office they can work on the whiteboard
  - Working together i.e. sharing memory
- Across different offices they must communicate with each other
- But they only have to send one message per office instead of one per person



MPI+OpenMP Usage

- Implemented in lots of HPC applications
  - However not always more performant than using a single thread (e.g. pure MPI)
  - Number of threads to use needs to be tuned to the use case and the machine
  - Need to be aware of the underlying node structure when running e.g. regions when memory is shared
  - More complex to implement for a programmer



Usage

- Need to think about the placement of processes and threads on the node architecture
  - Ensure each thread is placed on a separate core
  - Want to populate entire nodes
- Set $N_{tasks} \times N_{threads} = N_{cores\_per\_node}$
  - Options in the job script to do this
  - E.g for 2 threads per process on MN

```
#SBATCH --ntasks-per-node=24
#SBATCH --cpus-per-task=2
export OMP_NUM_THREADS=2
```

- The shared memory portion (i.e. groups of threads) should not span more than one NUMA region – see exercise

GPU parallelism

GPU based parallelism

- GPUs ideal for some HPC applications as they are designed for doing many numerical operations at once
  - Many many threads (many many cores)
  - Ideal if cores execute same operations (e.g. on different subsets of data)
- Specific numerically intense calculations offloaded to GPU
  - Rest of code runs on CPU
- GPU ("device") memory is separate from main ("host") memory
  - Requires copying data onto and off the GPU
- Application may run on multiple GPUs per node, and on many nodes
  - Communication between GPUs typically MPI between host memory spaces
  - NVLINK enables fast communication directly between GPU memory spaces (i.e. bypassing host memories)

GPU programming

- Nvidia GPUs: CUDA
  - Proprietary Nvidia software (available on all systems with Nvidia GPUs)
  - Application Programming Interface (API) and runtime platform
  - Rewrite numerically intensive code as GPU-specific function: ***kernel***
  - Includes functions to shift data between CPU and GPU memory
- Most recent OpenMP standard (4.0) incorporates simple syntax for offloading execution to GPUs
- HIP – kernel language for Nvidia and AMD GPUs
  - Can convert CUDA code to HIP (increased portability)

Scientific libraries

- Scientific libraries contain highly optimised code used by different scientific (HPC) applications
  - Library code contains implementations of common mathematical routines
  - Dense & sparse linear algebra, fast fourier transforms, etc.

- Parallel (MPI & thread-based) versions of many of these libraries are available
  - Critical for performance of many large-scale HPC applications
  - Includes parallel IO (writing and reading large amounts of data quickly in parallel)
  - More recently, versions that offload to GPU using CUDA increasingly available

Summary

- Shared-variables parallelism e.g. with OpenMP
  - uses threads
  - requires shared-memory
  - easy to implement but limited scalability
- Distributed memory e.g with MPI
  - uses processes
  - can run on any machine: messages can go over the interconnect
  - harder to implement but better scalability
- MPI+OpenMP
  - Shared memory within a node, message passing across nodes
  - Can have advantages over pure MPI, but not always
- GPU parallelism
  - Using GPUs for HPC