HPC.NRW

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MPI in Small Bites

PPCES 2024

HPC.NRW Competence Network

Message Passing Basics

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Parallel Architectures

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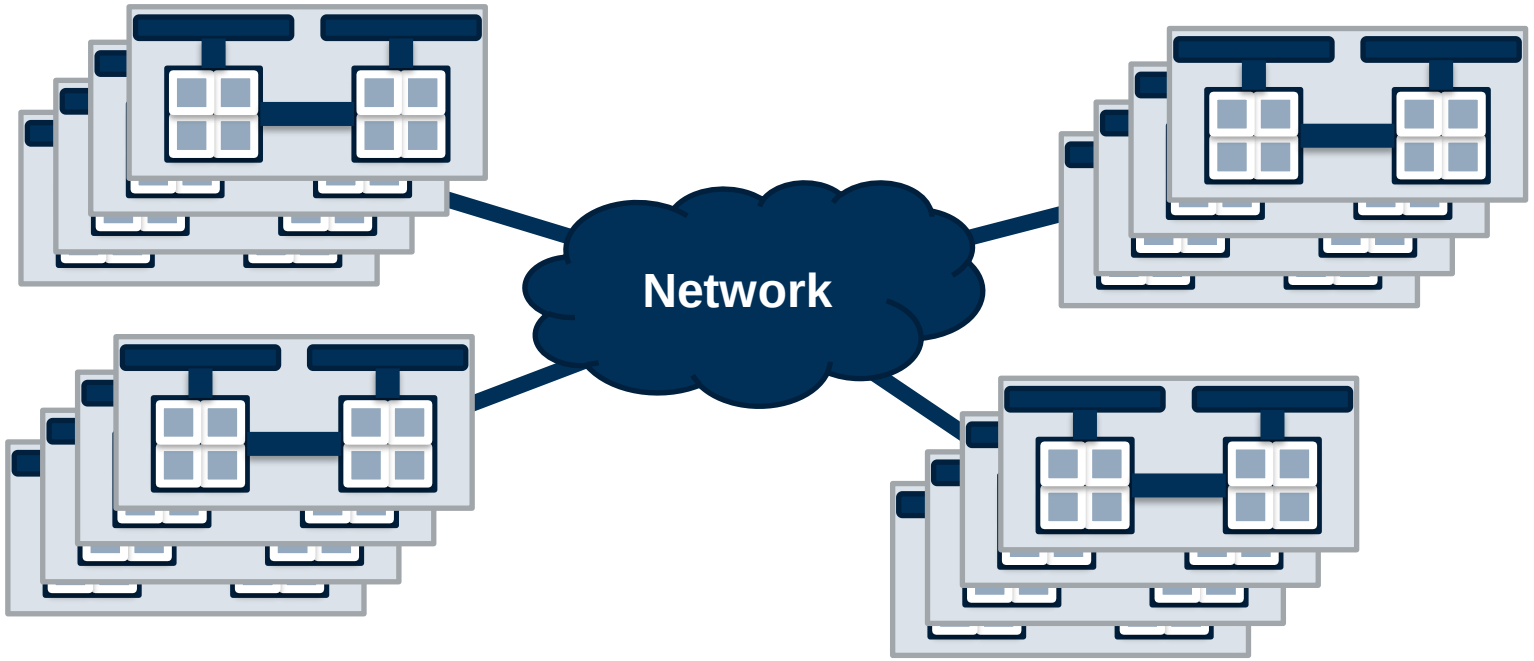
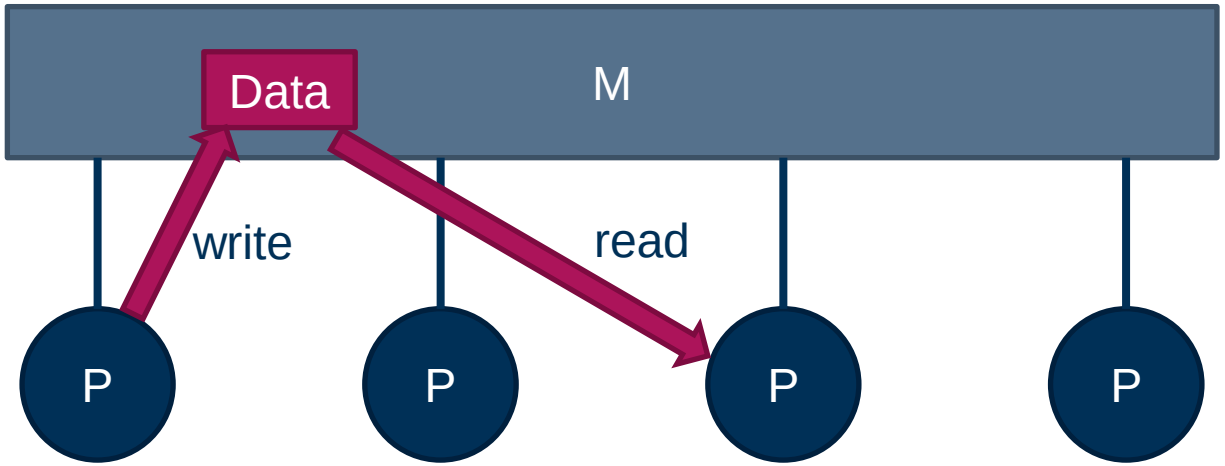
- Clusters
  - HPC market dominated by distributed memory *multi-computers*
  - Nodes have no direct access to other nodes' memory
  - Nodes run a separate copy of the (possibly stripped down) OS



– All processing elements (P) have direct access to the main memory block (M)



– Data exchange is achieved through read/write operations on shared variables located in the global address space

Parallel Architectures – Distributed Memory

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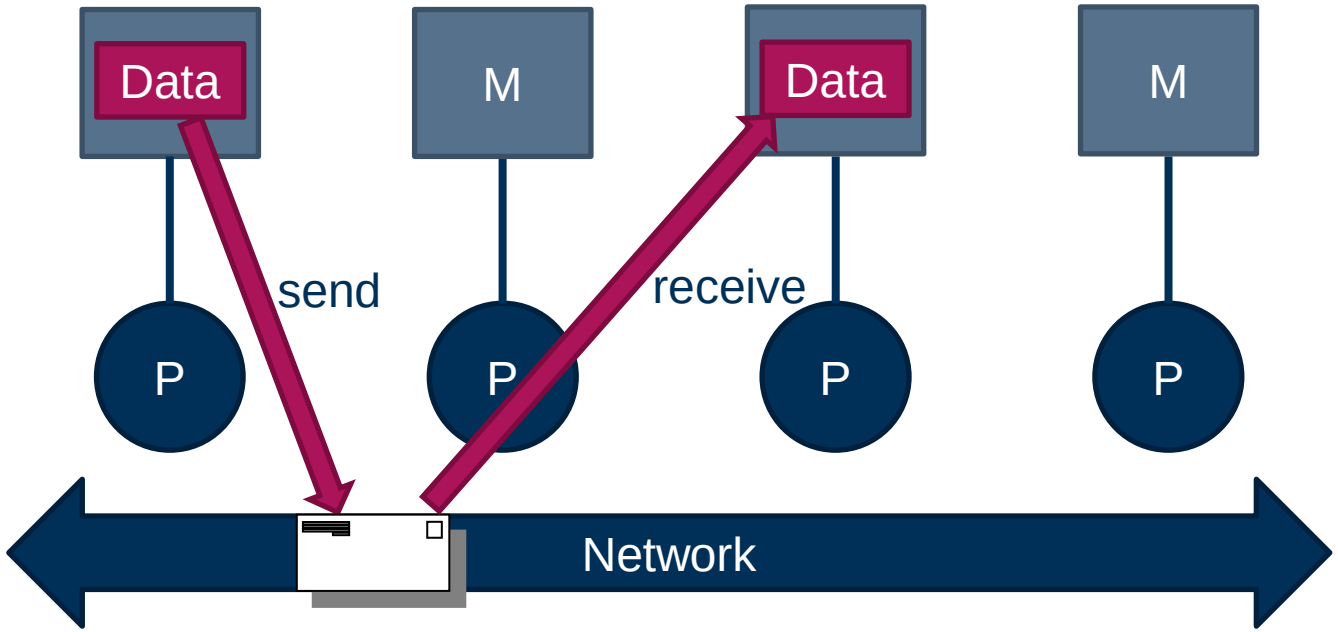
– Each processing element (P) has its separate main memory block (M)



– Data exchange is achieved through message passing over the network
– Two distinct copies of the data at sender and receiver

Distributed Memory Overview

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- Each processing element (P) works on a separate main memory block (M)
  - Processes typically have own (virtual) address space
- Data exchange is achieved through message passing (data copy)
- Message passing can be either explicit (MPI) or implicit (PGAS)
  - PGAS provides shared-memory abstractions, but may use message passing at runtime.
- No shared variables
  - No data races
- Implicit synchronisation with message exchange

Processes

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- A process is a running in-memory instance of an executable file
  - Executable code, e.g., binary machine instructions
  - One or more threads of execution sharing memory address space
  - Memory: data, heap, stack, processor state (CPU registers and flags)
  - Operating system context (e.g., signals, I/O handles, etc.)
  - Process ID (PID)
- Isolation and protection
  - Without OS support, a process cannot …
    - interoperate with other processes
    - access their context (even on the same node)
  - No direct inter-process data exchange (isolated/virtual address spaces)
  - No direct inter-process synchronisation

SPMD Model

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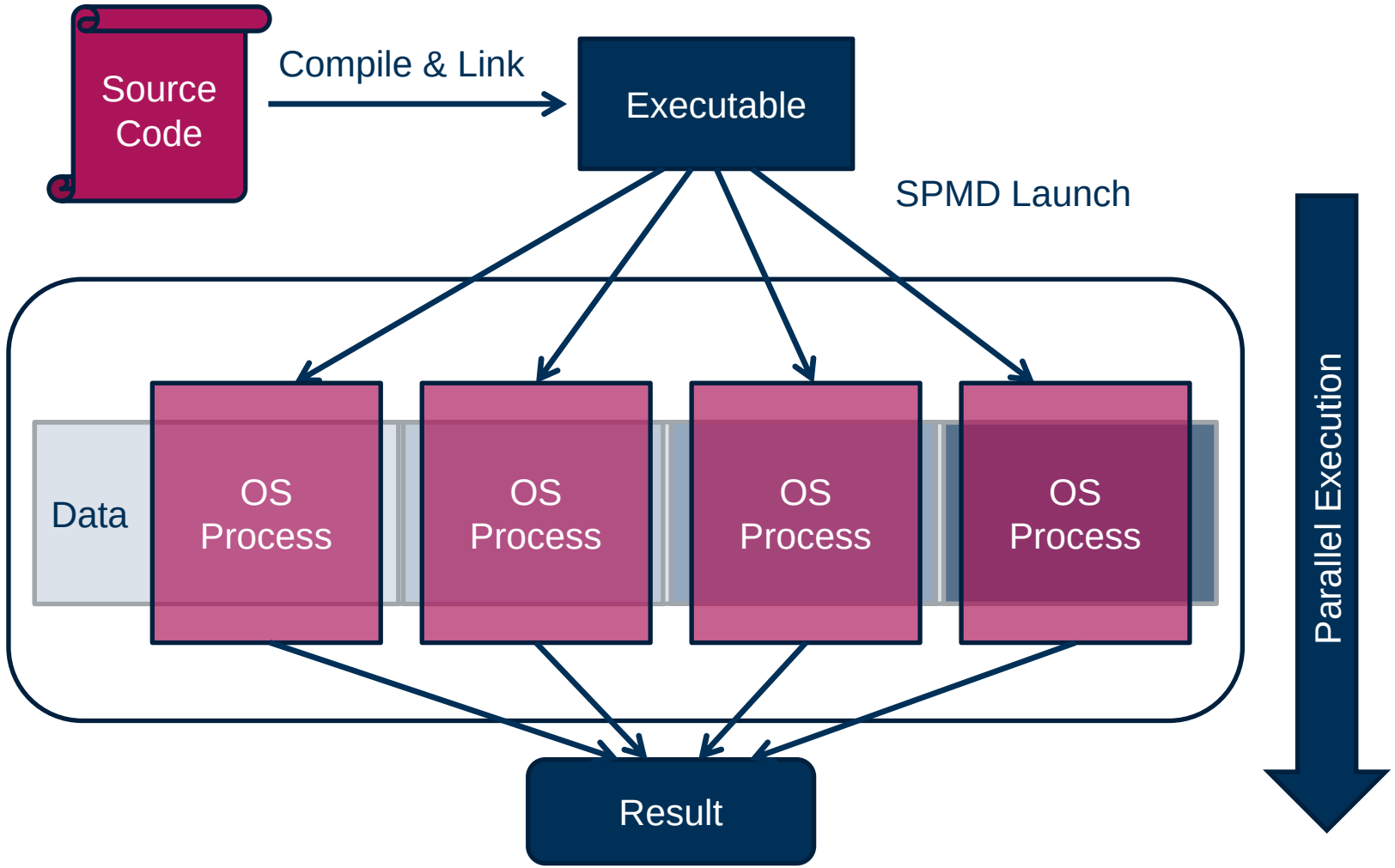
- Abstractions ease programming and understanding
- Single Program Multiple Data
  - Single Program (executable)
  - Multiple (different parts of) Data
- Multiple instruction flows (instances)
  - E.g., threads (OpenMP, Pthreads) and/or processes (MPI)
  - Unique instance IDs can be used for flow control

```
if (myID == specificID)
{
    do_something();
}
else
{
    do_something_different();
}
```

SPMD Program Lifecycle – multiple processes (e.g. MPI)



Requirements for SPMD Environments

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1. Provide dynamic identification of all peers
   - Who else is also working on this problem?
2. Provide robust mechanisms to exchange data
   - Whom to send data to / From whom to receive the data?
   - How much data?
   - What kind of data?
   - Has the data arrived?
3. Provide synchronisation mechanisms
   - Have all processes reached same point in the program execution flow?
4. Provide methods to launch and control a set of processes
   - How do we start multiple processes and get them to work together?
5. Portability

MPI Overview

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- Message Passing Interface
  - The de-facto standard API for explicit message passing nowadays
  - A moderately large standard (v4.1 has 1,166 pages)
  - Maintained by the non-profit Message Passing Interface Forum: https://www.mpi-forum.org/
- Many specific implementations of the MPI standard
  - Open MPI, MPICH, Intel MPI, MVAPICH, MS-MPI, etc.
- Application Programming Interface (API) to exchange messages in distributed memory
- MPI does not specify ABI compatibility!
  - Applications need to be compiled against a specific implementation

MPI Overview II

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- Language-independent specification (LIS)
  - Standard bindings for C and Fortran
    - Specific function prototypes / interfaces
  - Non-standard bindings for other languages exist:
    - C++ Boost.MPI, MPL
    - Java Open MPI, MPJ Express
    - Python mpi4py

- No extension of the base language
  - Set of libraries, header files, and auxiliary programs
  - Standard compilers can be used to compile and link a program

Further Reading

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- The MPI Forum document archive (free standards for everyone!)
  - http://www.mpi-forum.org/docs/
- Manual pages
  - man MPI_Xxx_yyy_zzz (for all MPI calls)
- Tutorials (like this one)