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Hybrid MPI+OpenMP Programming

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www.hp-see.eu

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High-Performance Computing Infrastructure
for South East Europe's Research Communities

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Agenda

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- Introduction: HPC, performance, speedup
- Parallel computing and memory models
- Programming models and Flynn's taxonomy
- MPI vs. OpenMP
- Hybrid programming model and mismatch problems
- Thread safety
- Hybrid parallelism and programming strategies
- Library stack
- Hybrid programming in practice
- Examples and exercises

What HPC stands for?

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- High Performance Computing
- The term is most commonly associated with computing used for scientific research. [from Wikipedia]
- It involves not only hardware, but software and people as well!
- HPC encompasses a collection of powerful:
  - hardware systems
  - software tools
  - programming languages
  - parallel programming paradigms

which make previously unfeasible calculations possible

Only performance?

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- High Throughput Computing
- High Availability Computing
- Capacity Computing
- Capability computing
- To reflect a greater focus on the productivity, rather than just the performance, of large-scale computing systems, many believe that HPC should now stand for High Productivity Computing

Performance vs. Productivity

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- A definition:
  - Productivity = (application performance) / (application programming effort)
- Scientists in HPC arena have different goals in mind thus different expectations and different definitions of productivity.
- Which kind of productivity are you interested in?

Measures of performance

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- How fast can I crunch numbers on my CPU?
- How much data can I store?
- How fast can I move the data around?
  - from CPUs to memory; from CPUs to disk; from CPUs to/on different machines
  - among computers: networks
    - default (commodity): 1 Gb/s
    - custom (high speed): 10Gb/s, 20 Gb/s and now 40Gb/s
  - within the computer:
    - CPU – Memory: thousands of Mb/s: 10 - 100 Gb/s
    - CPU - Disks: MByte/s: 50 ~ 100 MB/s up to 1000 MB/s

Parallel performance

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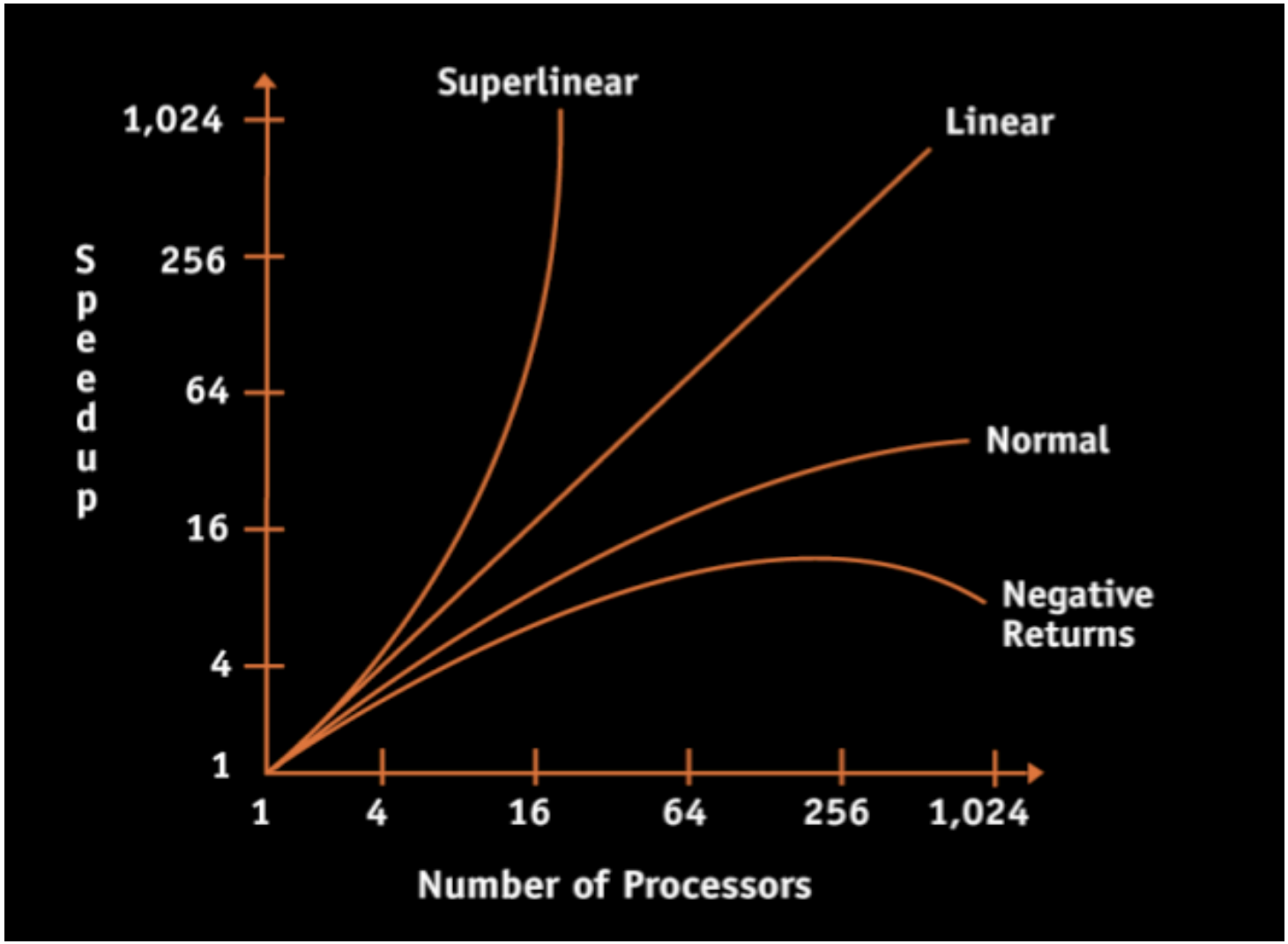
- The speedup of a parallel application is
  Speedup(p) = Time(1) / Time(p)
  where:
  Time(1) = execution time for a single processor
  Time(p) = execution time using p parallel processors
- If **Speedup(p) = p**, we have a perfect speedup (also called linear scaling)
- Speedup compares performance of an application with itself on one and on p processors
- More useful to compare:
  - The execution time of the best serial application on 1 processor vs.
  - The execution time of the best parallel algorithm on p processors

Speedup


Superlinear
Linear
Normal
Negative
Returns
1,024
256
64
16
4
1
Speedup
1
4
16
64
256
1,024
Number of Processors

Superlinear speedup?

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- Can we find **superlinear** speedup, i.e.

  Speedup(p) > p
- Yes, we can:
  - Choosing a bad "baseline" for T(1)
    - Old serial code has not been updated with optimizations
  - Shrinking the problem size per processor
    - May allow it to fit in small fast memory (cache)
    - Total time decreased because memory optimization tricks can be played.

Question

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- Algorithm A and algorithm B solve in parallel the same problem
- We know that on 64 core:
  - Program A gets a speedup of 50
  - Program B gets a speedup of 4
- Which one do you choose ?
  - 1) program A
  - 2) program B
  - 3) None of the above

Answer

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- None of the above, since we do not know the **overall execution time** of each of them!
- What if A is sequentially 1000 time slower than B?
- Always use the best sequential algorithm for computing speedup (absolute speedup)
- And the best compiler to produce the executable, for both serial and parallel version of the application!

Limits to speedup

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- All parallel programs contain:
  - Parallel sections
  - Serial sections
- Serial sections limit the speed-up:
  - Lack of perfect parallelism in the application or algorithm
  - Imperfect load balancing (some processors have more work)
  - Cost of communication
  - Cost of contention for resources, e.g., memory bus, I/O
  - Synchronization time
- Understanding why an application is not scaling linearly will help finding ways improving the applications performance on parallel computers.

Amdahl's law (1)

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- Let *S* be the fraction in an application representing the work done serially
- Then, 1-*S* = *P* is fraction done in parallel
- What is the maximum speedup for N processors?

$$speedup = \frac{1}{(1-P) + \frac{P}{N}} \Rightarrow \lim_{N \to \infty} \frac{1}{1-P}$$

- Even if the parallel part scales perfectly, we may be limited by the sequential portion of the code!

Amdahl's law (2)

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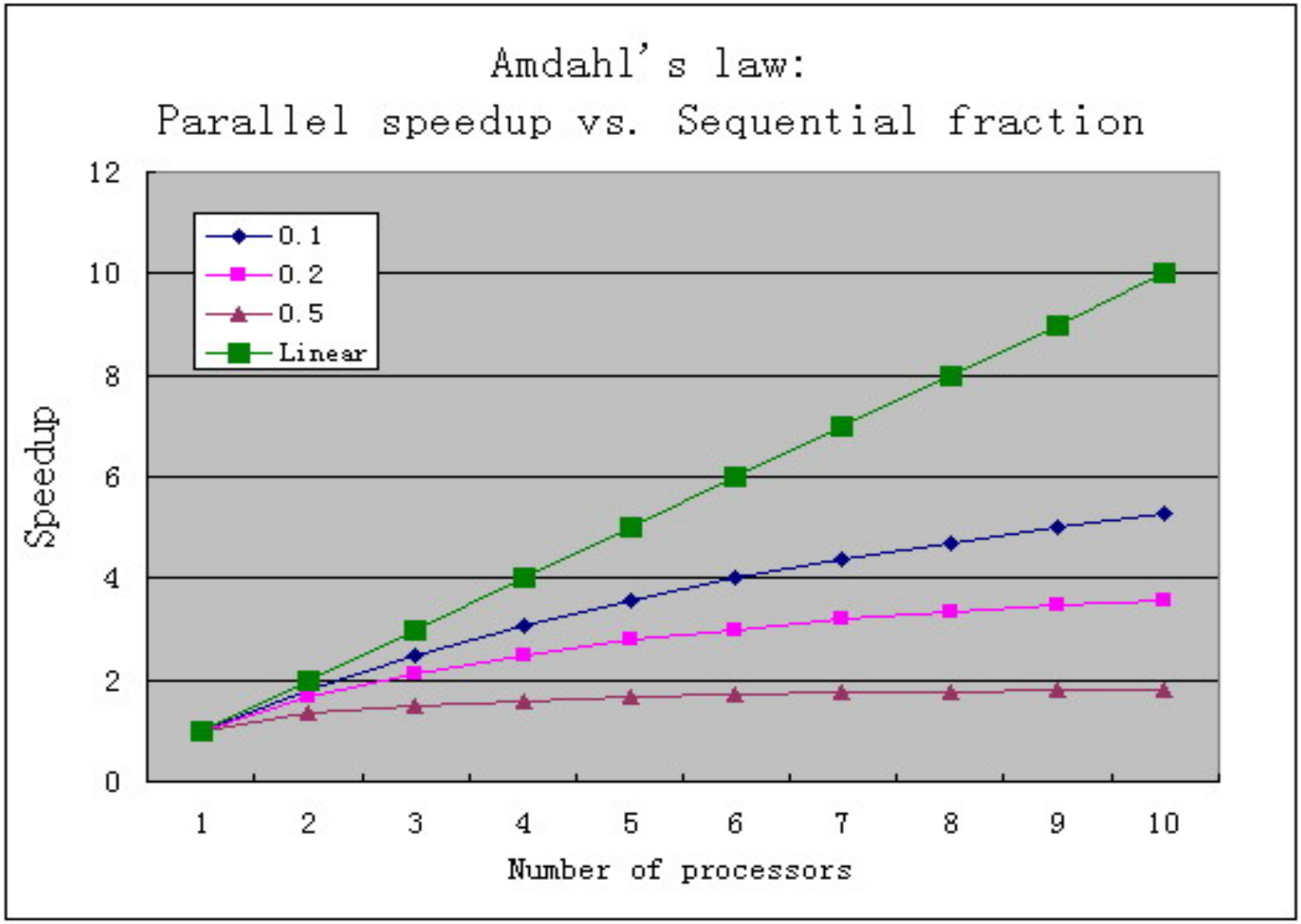
- The presence of a serial part of the code is quite limiting in practice:

>	2	4	8	32	64	256	512	1024
5%	1.91	3.48	5.93	12.55	15.42	18.62	19.28	19.63
2%	1.94	3.67	6.61	16.58	22.15	29.60	31.35	32.31
1%	1.99	3.88	7.48	24.43	39.29	72.11	83.80	91.18

- Amdahl's Law is relevant only if serial fraction is independent of the problem size
- Fortunately, the proportion of the computations that are sequential (non parallel) usually decreases as the problem size increase (a.k.a. Gustafson's law)

Effective parallel performance



How to run applications faster ?

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- There are 3 ways to improve performance:
  - Work Harder
  - Work Smarter
  - Get Help
- Analogy in computer science
  - Use faster hardware
  - Optimize algorithms and techniques used to solve computational tasks
  - Use multiple computers to solve a particular task
- All 3 strategies can be used simultaneously!

What is parallel computing?

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- Parallel computing is the simultaneous execution of the same task (split up and specially adapted) on multiple processors in order to obtain results faster
- The process of solving a problem usually can be divided into smaller tasks, which may be carried out simultaneously with some coordination

[from Wikipedia]

High performance problem:

picture from http://www.f1nutter.co.uk/tech/pitstop.php

Analysis of a parallel solution

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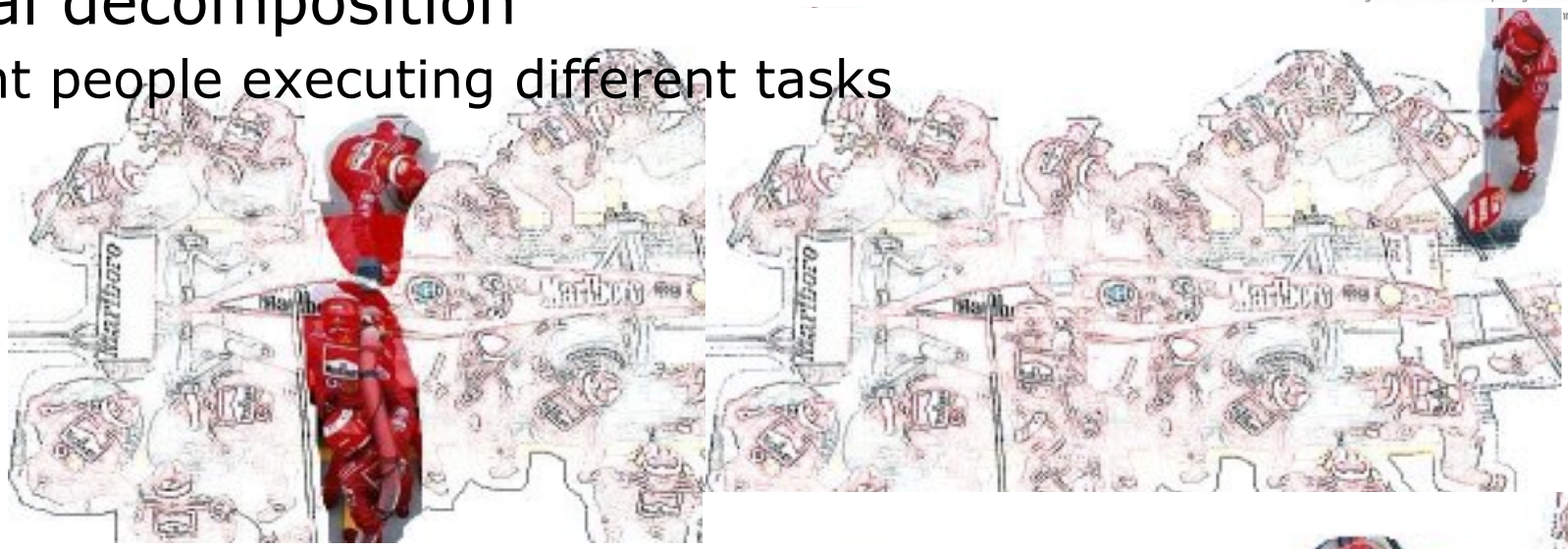
- Functional decomposition
  - Different people executing different tasks



- Domain decomposition
  - Different people executing the same tasks

HPC parallel computers

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- The simplest and most useful way to classify modern parallel computers is by their memory model.

- How CPUs view and can access the available memory?
  - Shared memory
  - Distributed memory

Shared vs. Distributed

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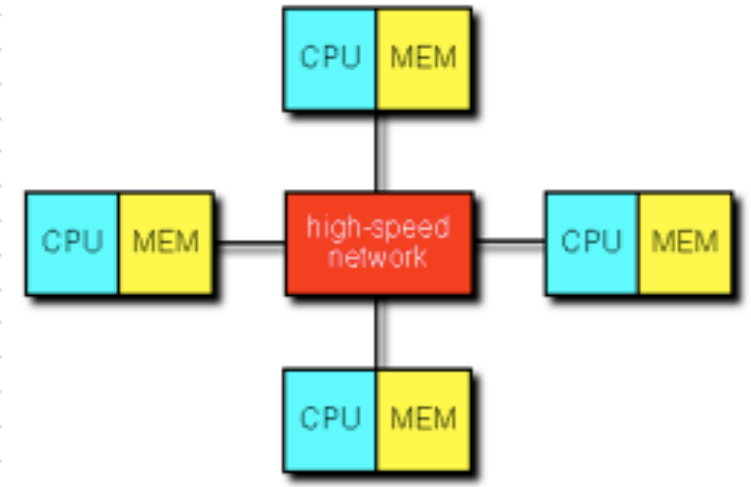
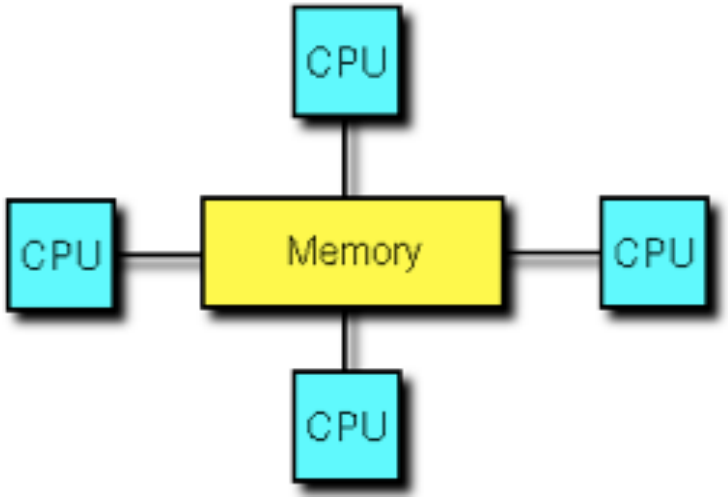
- Distributed Memory:
  - Each processor has its own local memory. Must do message passing to exchange data between processors.
  - Multi-computers



- Shared Memory
  - Single address space. All processors have access to a pool of shared memory.
  - Multi-processors



Shared Memory: UMA vs. NUMA

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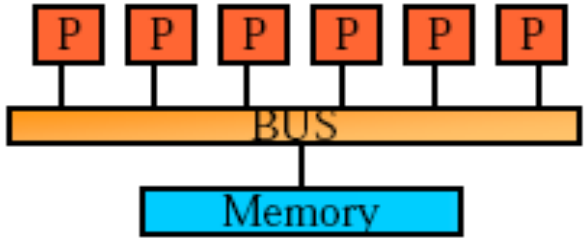
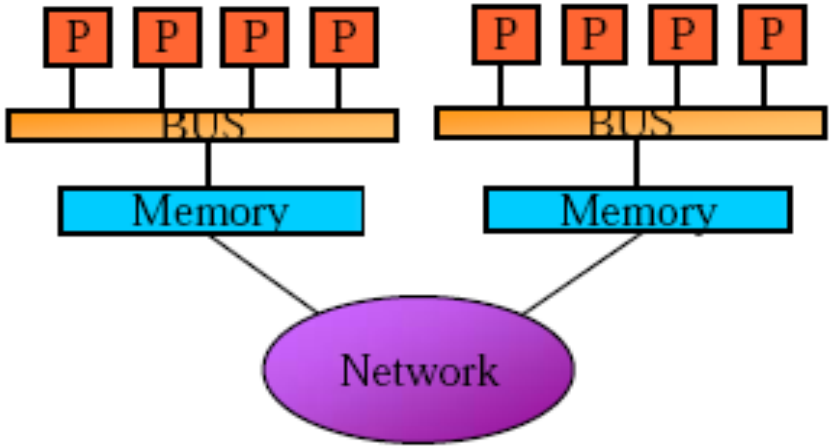
- **Uniform memory access (UMA):** Each processor has uniform access to memory. Also known as symmetric multiprocessors (SMP).



- **Non-uniform memory access (NUMA):** Time for memory access depends on location of data. Local access is faster than non-local access.



Clusters: distributed memory

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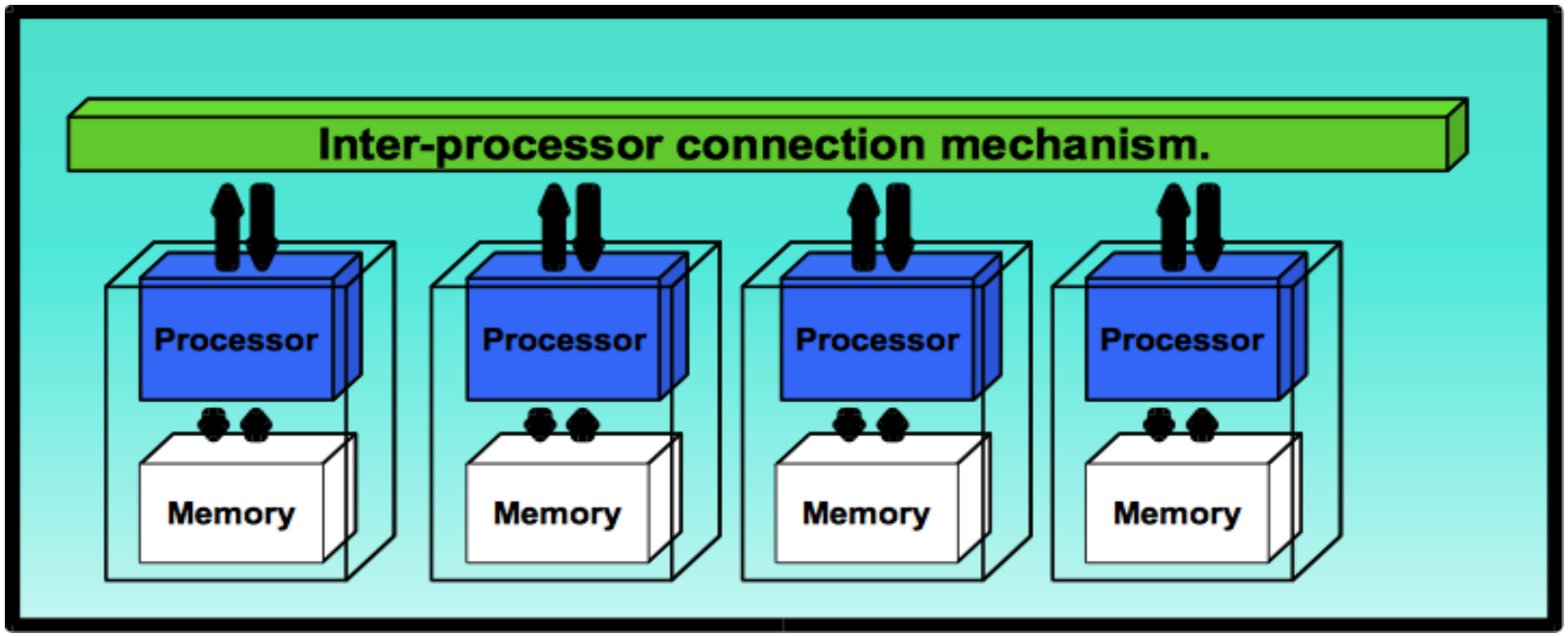
- Independent machines combined into a unified system through software and networking



Hybrid architecture

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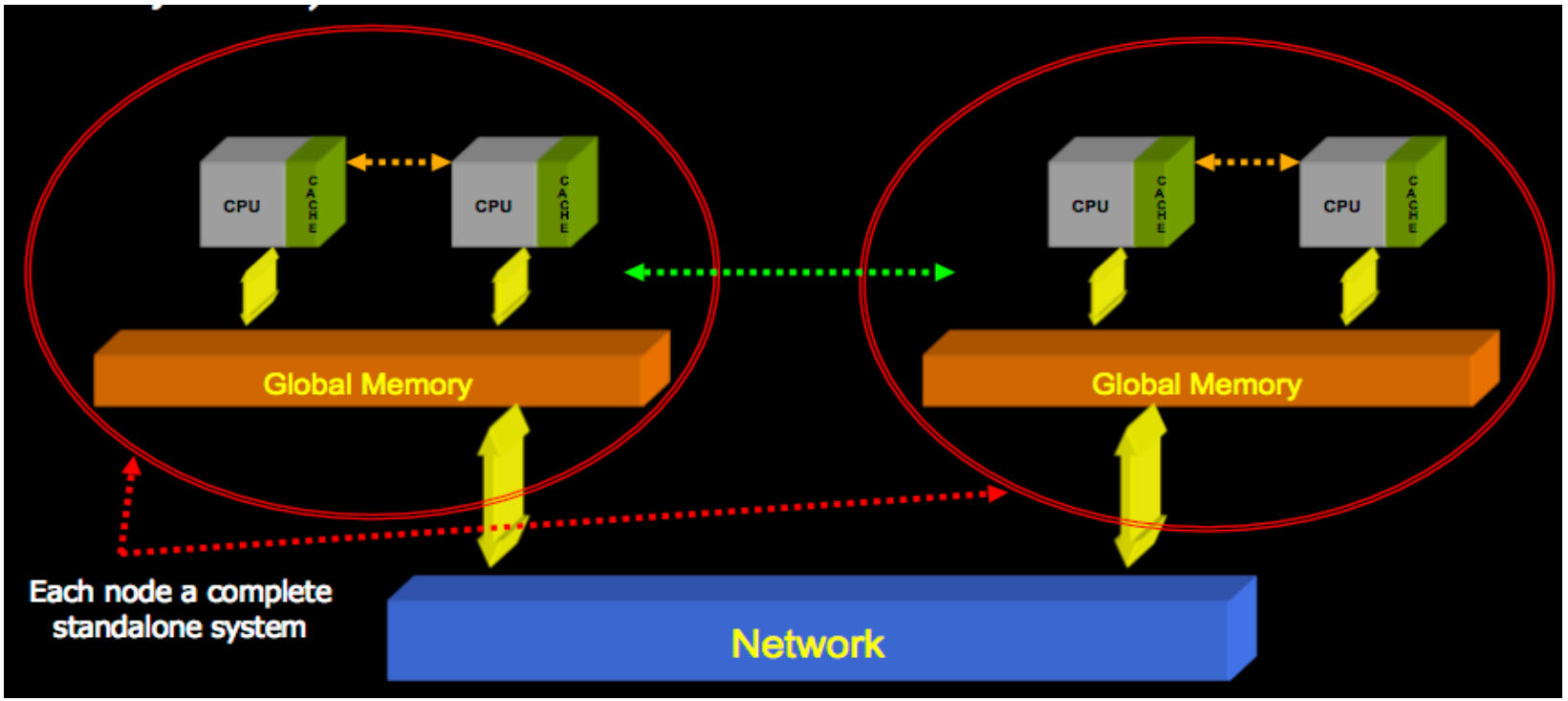
- All modern clusters have hybrid architecture
- Many-core CPUs make each node a small SMP system



Parallel Programming Paradigms

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- Memory models determine programming paradigms

Parallel machines	
Distributed memory	Shared memory
Parallel paradigms	
Message passing	Data parallel
All processes could **directly access only their local memory.** Explicit messages are requested to access remote memory of different processors.	Single memory view. all processes (usually threads) could **directly access the whole memory.**

Architecture vs. Paradigm

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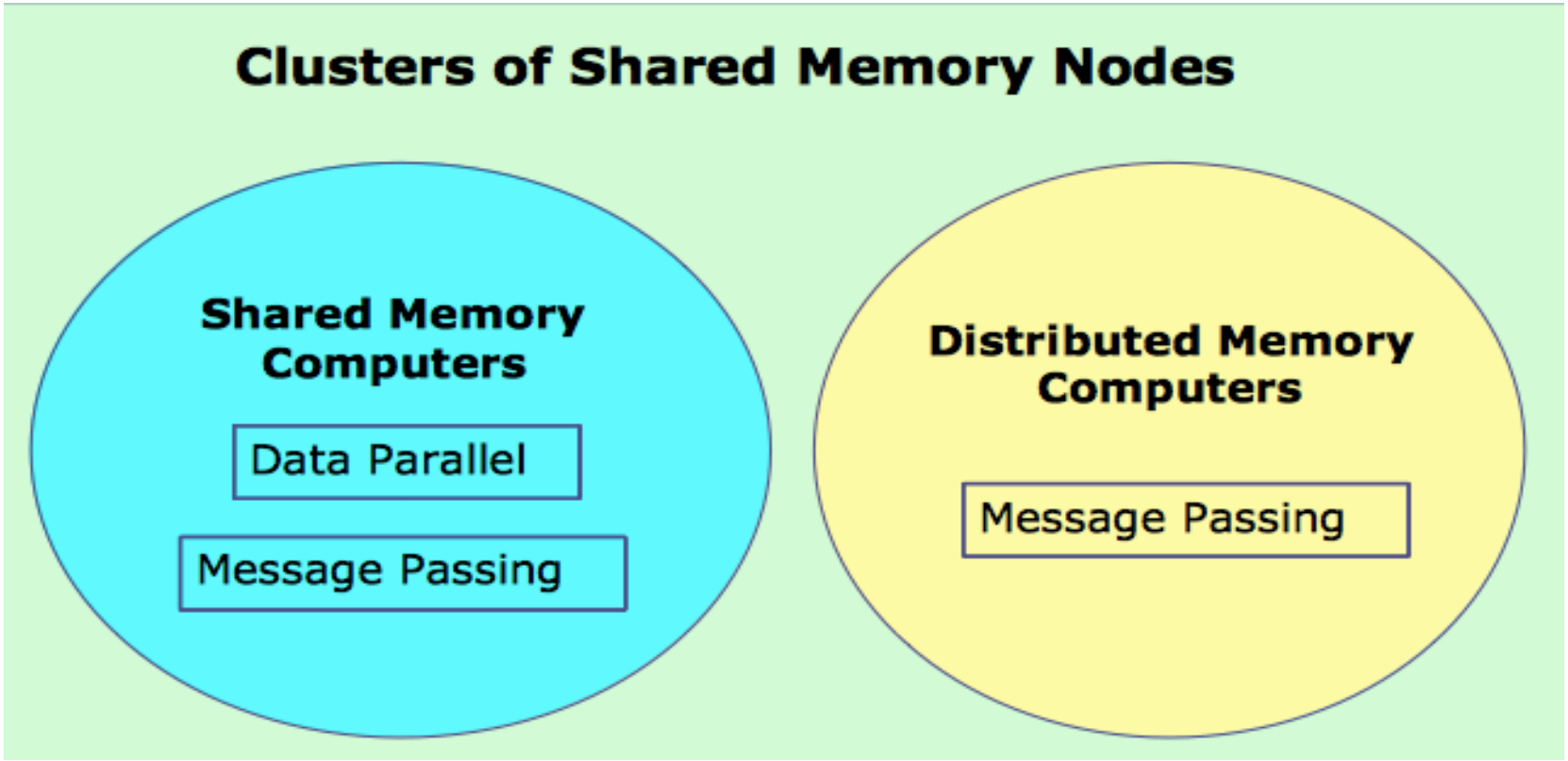

Architecture, Paradigm, Model

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Architecture	
Distributed memory	Shared memory
Programming paradigm	
Message passing	Data parallel
Programing model	
Domain decomposition	Functional decomposition

Programming models

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- Domain decomposition
  - Data divided into equal chunks and distributed to available CPUs
  - Each CPU process its own local data
  - Exchange of data if needed
- Functional decomposition
  - Problem decomposed into many sub-tasks
  - Each CPU performs one of sub-tasks
  - Similar to server/client paradigm

Flynn's taxonomy (1)

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- SISD (Single instruction, single data)
- **SIMD (Single instruction, multiple data)**
  - the same instructions are carried out simultaneously on multiple data items
  - SSE is a good example
- **MISD (Multiple instruction, single data)**
- **MIMD (Multiple instruction, multiple data)**
  - different instructions on different data
- **SPSD (Single program, single data)**
- **SPMD (Single program, multiple data)**
  - not synchronized at individual operation level
  - equivalent to MIMD since each MIMD program can be made SPMD

Flynn's taxonomy (2)

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- SPSD (Single program, single data)
- **SPMD (Single program, multiple data)**
- **MPSD (Multiple program, single data)**
- **MPMD (Multiple program, multiple data)**

Model	Paradigm	Flynn's taxonomy
Domain decomposition	Message Passing	**SPMD**
	Data Parallel - HPF	
Functional decomposition	Data Parallel - OpenMP	**MPSD**
	Message Passing	**MPMD**

Parallelism requires…

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- Balancing of the load
  - Applies to computation, I/O operations, network communication
  - Relatively easy for domain decomposition, not so easy for functional decomposition
- Minimizing communication
  - Join individual communications
  - Eliminate synchronization – the slowest process dominates
- Overlap of computation and communication
  - This is essential for true parallelism!

Message Passing Interface

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- Parallel programs consist of separate processes, each with its own address space
  - Programmer manages memory by placing data in a particular process
- Data sent explicitly between processes
  - Programmer manages memory movement
- Collective operations
  - On arbitrary set of processes
- Data distribution
  - Also managed by the programmer

Distributed memory

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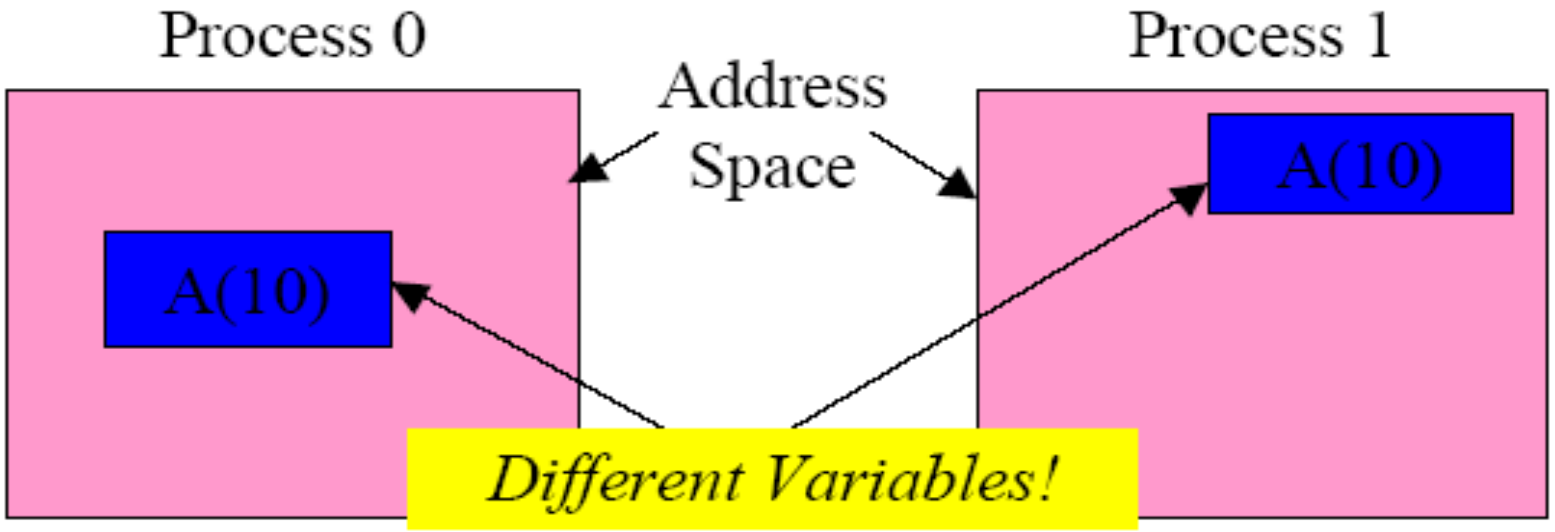
- Nothing is shared between processes



OpenMP

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- Shared memory necessary
- Good for SMP nodes, but also possible on clusters via distributed shared virtual memory systems
- Parallelism achieved through the memory sharing
- Programmer responsible for proper synchronization
- Programmer also responsible for management of memory (locks)

MPI vs. OpenMP

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- Pure MPI pro:
  - Portable to distributed & shared memory machines
  - Scales beyond one node
  - No data placement problem
- Pure MPI cons:
  - Difficult to develop & debug
  - High latency, low bandwidth
  - Explicit communication
  - Large granularity
  - Difficult load balancing
- Pure OpenMP pro:
  - Easy to implement parallelism
  - Low latency, high bandwidth
  - Implicit communication
  - Coarse & fine granularity
  - Dynamic load balancing
- Pure OpenMP cons:
  - Only on shared memory machines
  - Scales within one node
  - Possible data placement problem
  - No specific thread order

Standards

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- MPI inter-node
  - Message passing
  - Data distribution model
  - Version 2.2 (09/2009)
  - API for C/C++ and Fortran
- OpenMP intra-node
  - Threads
  - Relaxed-consistency model
  - Version 3.1 (07/2011)
  - Compiler directives for C/C++ and Fortran

Why hybrid?

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- Hybrid MPI/OpenMP paradigm is the parallel approach for clusters of SMP architectures.
- Elegant in concept and architecture: using MPI across nodes and OpenMP within nodes.
- Good usage of shared memory system resource (memory, latency, and bandwidth).
- Avoids the extra communication overhead with MPI within node.
- OpenMP adds fine granularity (larger message sizes) and allows increased and/or dynamic load balancing.
- Some problems have two-level parallelism naturally.
- Some problems could only use restricted number of MPI tasks.
- Could have better scalability than both pure MPI and pure OpenMP.

Mismatch problems

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- Topology problem (with pure MPI)
- Unnecessary intra-node communication (with pure MPI)
- Saturation problem (with pure MPI)
- Sleeping threads (with OpenMP)
- Inter-node bandwidth problem (with hybrid)
- Additional OpenMP overhead (with hybrid)
  - Thread startup / join
  - Cache flush (data source thread)
- Overlapping communication and computatio
  - application problem
  - programming problem
  - load balancing problem
- **no silver bullet – each parallelization scheme has its problems**

Thread safety

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- The MPI-2 standard defines four different levels of thread safety, in the form of how an MPI implementation can perform communication between processes:
  - MPI_THREAD_SINGLE: there is only one thread in the application.
  - MPI_THREAD_FUNNELED: only one thread may make MPI calls.
  - MPI_THREAD_SERIALIZED: any threads may make MPI calls, but only one at a time.
  - MPI_THREAD_MULTIPLE: any thread may make MPI calls at any time.
- The level of multi-threading stronly depends on the hardware and MPI implementation.
- All MPI implementations support MPI_THREAD_SINGLE (MPI-1 too).
- Usually when people refer to an MPI implementation as thread-safe, they mean that the implementation supports the maximum level of functionality

Relationship

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- In parallelizing a code with the hybrid paradigm, MPI is used for coarse-grain parallelism (i.e. principal data decomposition), while OpenMP provides fine-grain parallelism inside each MPI process.
- There are three main different mixed mode programming models depending on the way the MPI communication is being handled:
  - Master-only, where all MPI communication takes place outside of OpenMP parallel regions.
  - Funnelled, where communication may occur inside parallel regions, but is restricted to a single thread.
  - Multiple, where more than one thread can call MPI communication routines.

Classification of hybrid parallelism

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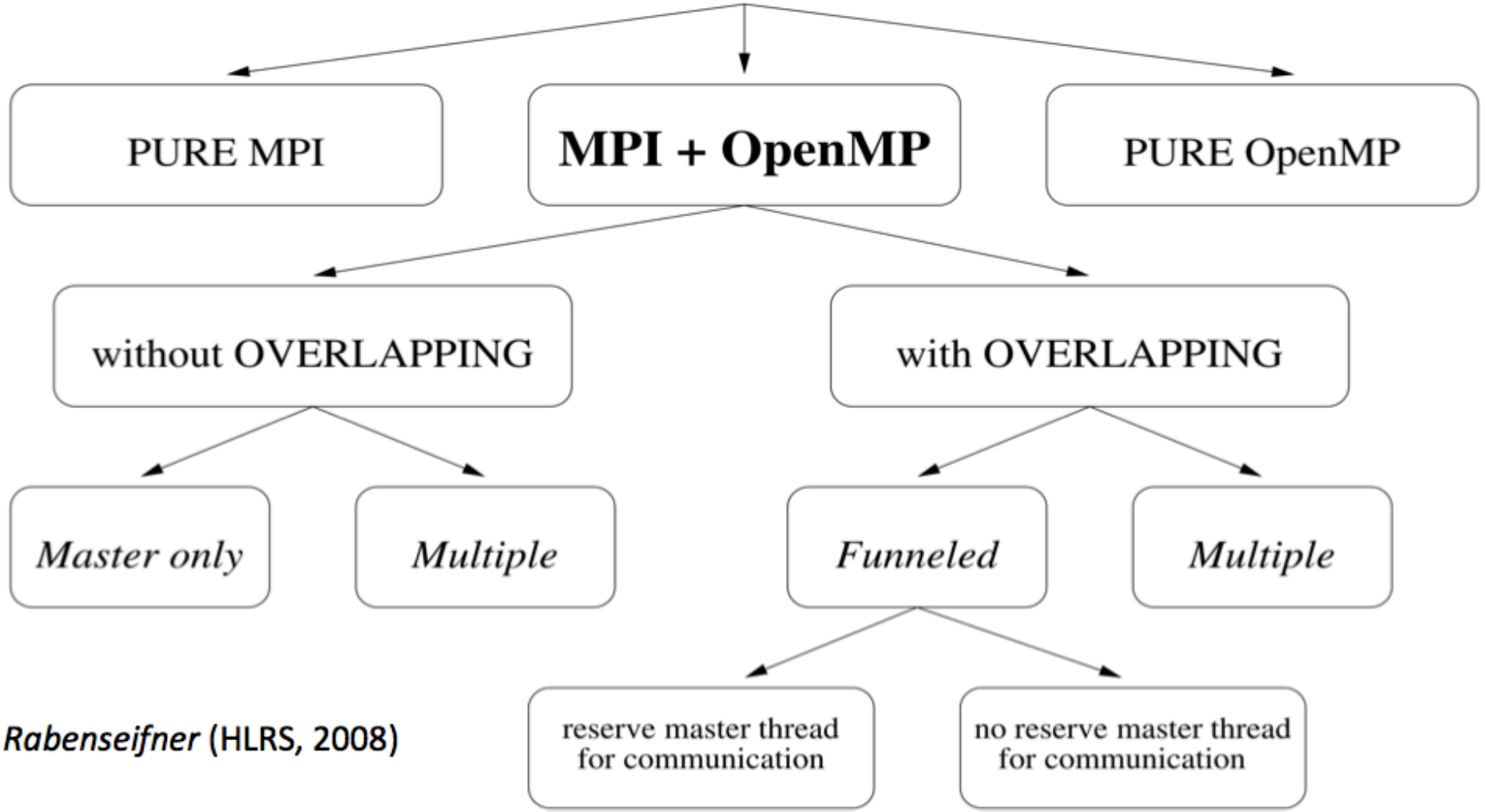

R. Rabenseifner (HLRS, 2008)

Programming strategies

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- Implicit
  - Use of threaded numerical libraries, which are then linked after compilation
  - No control over thread overhead
  - Very simple
- Explicit
  - Use of explicit OpenMP syntax
  - Full control
  - More complex, but also more efficient

Library stack for linear algebra

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- Implicit (thread level)
  - BLAS, LAPACK, FFTW
  - ESSL (IBM AIX)
  - MKL (Intel)
  - ACML (AMD)
- Explicit (MPI level)
  - PBLAS
  - SCALAPACK

Hybrid programming in practice

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- Things we need:
  - Thread-safe MPI / MPI with multithread support
  - OpenMP compiler/ OpenMP libraries
  - Hybrid programming aware Resource Manager (e.g. Torque)
- How to compile:
  - Using the MPI wrapper
  - Using the right compiler flag for OpenMP
  - Linking (the right MPI library)
- How to run:
  - Define correct task placement (One MPI task and as many threads as cores per node)
  - Execution environment (number of MPI task, number of OpenMP threads)

Examples

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- Example:
  mpicc –fopenmp –O3 –o hybrid hybrid.c

- Running the code on 4 nodes, each with 8 cores:
  export OMP_NUM_THREADS=8
  mpirun -np 4 -npernode 1 hybrid

- Batch system directive example:
  #PBS -l nodes=4:ppn=8

Exercise 1: pi

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- pi.c or pi.cpp calculates pi by integrating $f(x)=4/(1+x^2)$
- Compile and run the program
- Write MPI version and measure its speedup
- Write OpenMP version and measure its speedup
- Write hybrid version and measure its speedup

Exercise 2: trapez.c

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- trapez.c integrates given function by trapezoid rule
- Compile and run the program
- Write MPI version and measure its speedup
- Write OpenMP version and measure its speedup
- Write hybrid version and measure its speedup

Exercise 3: poisson_mpi.c

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- Poisson_mpi.c solves Poisson equation by Jacobi iteration solver (MPI implementation)
- Compile and run the program, measure its speedup
- Study the code and write hybrid version
- Measure its speedup on one node, by combining number of MPI processes and threads
- Measure speedup of the hybrid code in the preferred setup (one MPI process per node, with varying number of threads per node)
- Optimize hybrid code and measure its speedup