



Summer Term 2013
OvGU Magdeburg

Scientific Computing II

Parallel Methods

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Computational Methods in Systems and Control Theory (CSC)
Max Planck Institute for Dynamics of Complex Technical Systems



Preface

Why are you here?

Parallel Computing Basics



What is a Parallel Computer?

Characterization

A parallel computer is a

- collection of processing elements
- communicating and
- cooperating

for the fast solution of a large problem.

Parallel Computing Basics

Basic Types of Parallelism



- Pseudo Parallelism, or Multitasking



modern operating systems simulate parallel execution by time slicing

Parallel Computing Basics

Basic Types of Parallelism



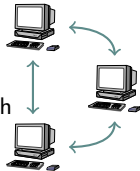
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- Distributed Memory

Computations executed on single unit with exclusive memory each



Parallel Computing Basics

Basic Types of Parallelism



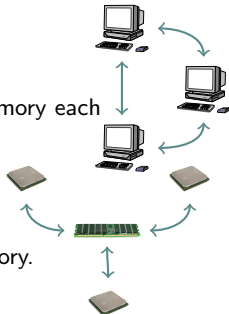
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- Distributed Memory

Computations executed on single unit with exclusive memory each



- Shared memory

Several computational units share a common main memory.

Parallel Computing Basics

Common Pitfalls in Parallel Computing



Most errors and misunderstandings in parallel computing are related to one of the following issues:

- race conditions,

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- data interdependence,

Parallel Computing Basics

Common Pitfalls in Parallel Computing



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- race conditions,
- execution order based accuracy issues,
- deadlocks,
- data interdependence,
- blocking problems on hardware level.

Chapter 1



Introduction: Part I

Why Parallel Computing?



- 1 **Problem size exceeds desktop capabilities.**

Why Parallel Computing?



- ① **Problem size exceeds desktop capabilities.**
- ② **Problem is inherently parallel (e.g. Monte-Carlo simulations).**

Why Parallel Computing?



- 1 **Problem size exceeds desktop capabilities.**
- 2 **Problem is inherently parallel (e.g. Monte-Carlo simulations).**
- 3 **Modern architectures require parallel programming skills to be optimally exploited.**

Flynn's Taxonomy of Parallel Architectures



[FLYNN '72]

The basic definition of a parallel computer is very vague in order to cover a large class of systems. Important details that are not considered by the definition are:

Flynn's Taxonomy of Parallel Architectures



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- How many processing elements?
- How complex are they?
- How are they connected?
- How is their cooperation coordinated?
- What kind of problems can be solved?

The basic classification allowing answers to most of these questions is known as [Flynn's taxonomy](#). It distinguishes four categories of parallel computers.

Flynn's Taxonomy of Parallel Architectures



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- 3 Single-Instruction, Multiple-Data (SIMD)

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- 3 Single-Instruction, Multiple-Data (SIMD)
- 4 Multiple-Instruction, Multiple-Data (MIMD)

Flynn's Taxonomy of Parallel Architectures



Single-Instruction, Single-Data (SISD)

The SISD model is characterized by

- a single processing element,

Flynn's Taxonomy of Parallel Architectures



Single-Instruction, Single-Data (SISD)

The SISD model is characterized by

- **a single processing element,**
- **executing a single instruction,**
- **on a single piece of data,**
- **in each step of the execution.**



Flynn's Taxonomy of Parallel Architectures



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It is thus in fact the standard sequential computer implementing, e.g., the *von Neumann* model.

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Examples

- desktop computers until Intel[®] Pentium[®] 4 era,
- early netBooks on Intel[®] Atom[™] basis,
- pocket calculators,
- abacus,
- embedded circuits

Flynn's Taxonomy of Parallel Architectures



Single-Instruction, Single-Data (SISD)

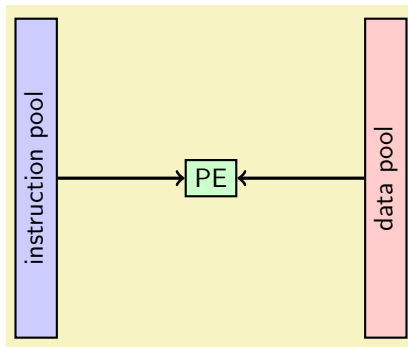


Figure: Single-Instruction, Single-Data (SISD) machine model

Flynn's Taxonomy of Parallel Architectures

Multiple-Instruction, Single-Data (MISD)



In contrast to the SISD model in the MISD architecture we have

- **multiple processing elements,**

Flynn's Taxonomy of Parallel Architectures



Multiple-Instruction, Single-Data (MISD)

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Flynn's Taxonomy of Parallel Architectures



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In contrast to the SISD model in the MISD architecture we have

- **multiple processing elements,**
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The MISD model is usually not considered very useful in practice.

Flynn's Taxonomy of Parallel Architectures



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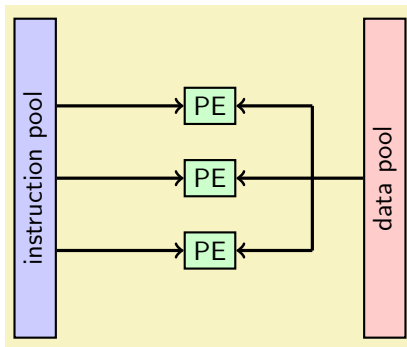


Figure: Multiple-Instruction, Single-Data (MISD) machine model

Flynn's Taxonomy of Parallel Architectures



Single-Instruction, Multiple-Data (SIMD)

Here the characterization is

- **multiple processing elements,**
- **execute the same instruction,**
- **on a multiple pieces of data,**
- **in each step of the execution.**

This model is thus the ideal model for all kinds of vector operations

$$c = a + \alpha b.$$

Examples

- Graphics Processing Units,
- Vector Computers,
- SSE (Streaming SIMD Extension) registers of modern CPUs. ^a

^aSee talk by Maximilian Behr in the selected topics seminar.

Flynn's Taxonomy of Parallel Architectures

Single-Instruction, Multiple-Data (SIMD)



The attractiveness of the SIMD model for vector operations, i.e., linear algebra operations, comes at a cost.

Consider the simple conditional expression

```
if (b==0) c=a; else c=a/b;
```

The SIMD model requires the execution of both cases sequentially. First all processes for which the condition is true execute their assignment, then the other do the second assignment. Therefore, conditionals need to be avoided on SIMD architectures to guarantee maximum performance.

Flynn's Taxonomy of Parallel Architectures



Single-Instruction, Multiple-Data (SIMD)

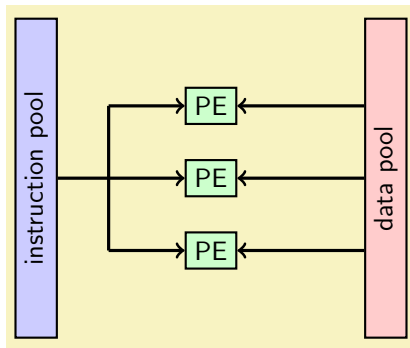


Figure: Single-Instruction, Multiple-Data (SIMD) machine model

Flynn's Taxonomy of Parallel Architectures



Multiple-Instruction, Multiple-Data (MIMD)

MIMD allows

- **multiple processing elements,**
- **to execute a different instruction,**
- **on a separate piece of data,**
- **at each instance of time.**

Flynn's Taxonomy of Parallel Architectures



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Examples

- multicore and multi-processor desktop PCs,
- cluster systems.

Flynn's Taxonomy of Parallel Architectures



Multiple-Instruction, Multiple-Data (MIMD): Hardware classes

MIMD computer systems can be further divided into three class regarding their memory configuration:

distributed memory

Every processing element has a certain exclusive portion of the entire memory available in the system. Data needs to be exchanged via an interconnection network.

shared memory

All processing units in the system can access all data in the main memory.

hybrid

Certain groups of processing elements share a part of the entire data and instruction storage.

Flynn's Taxonomy of Parallel Architectures



Multiple-Instruction, Multiple-Data (MIMD): Programming models

Single Program, Multiple Data (SPMD)

SPMD is a programming model for MIMD systems. “In SPMD multiple autonomous processors simultaneously execute the same program at independent points.”^a This contrasts to the SIMD model where the execution points are not independent.

^aWikipedia: <http://en.wikipedia.org/wiki/SPMD>

This is opposed to

Multiple Program, Multiple Data (MPMD)

A different programming model for MIMD systems, where multiple autonomous processing units execute different programs at the same time. Typically Master/Worker like management methods of parallel programs are associated with this class.

Flynn's Taxonomy of Parallel Architectures



Multiple-Instruction, Multiple-Data (MIMD)

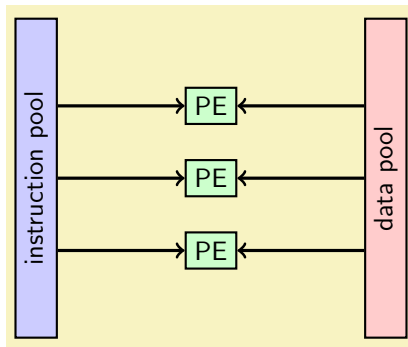


Figure: Multiple-Instruction, Multiple-Data (MIMD) machine model

Memory Hierarchies in Parallel Computers



Repetition Sequential Processor

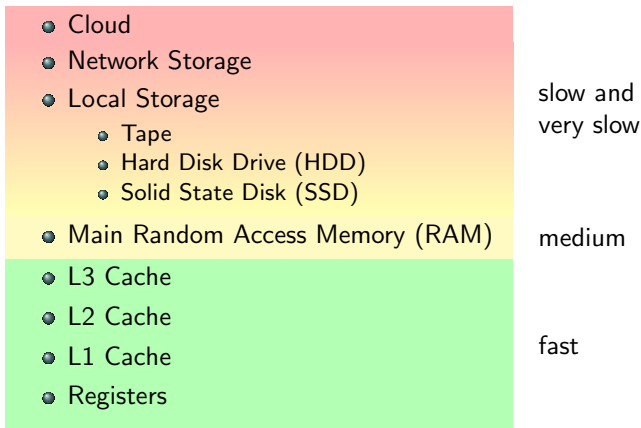


Figure: Basic memory hierarchy on a single processor system.

Memory Hierarchies in Parallel Computers



Shared Memory: UMA

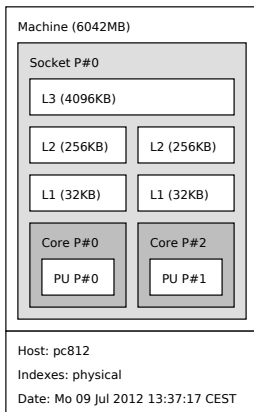


Figure: A sample dual core Xeon[®] setup

Memory Hierarchies in Parallel Computers

Shared Memory: UMA+GPU

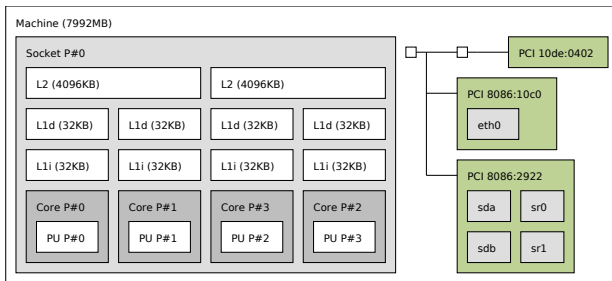


Figure: A sample Core™2Quad setup

Memory Hierarchies in Parallel Computers

Shared Memory: NUMA

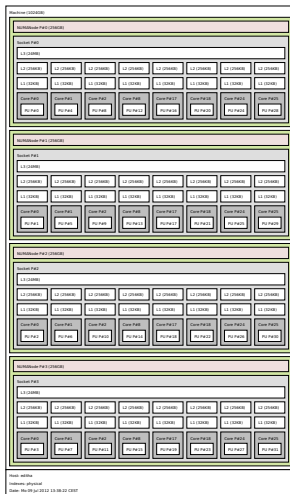
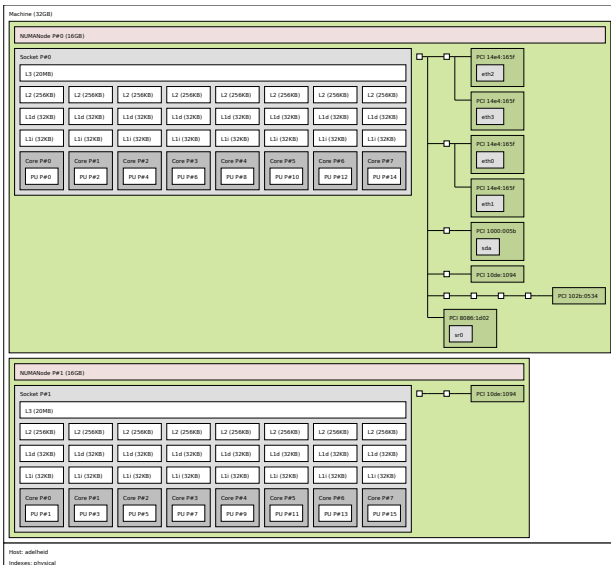


Figure: A four processor octa-core Xeon[®] system



Memory Hierarchies in Parallel Computers

Shared Memory: NUMA+2GPUs



Memory Hierarchies in Parallel Computers



General Memory Setting

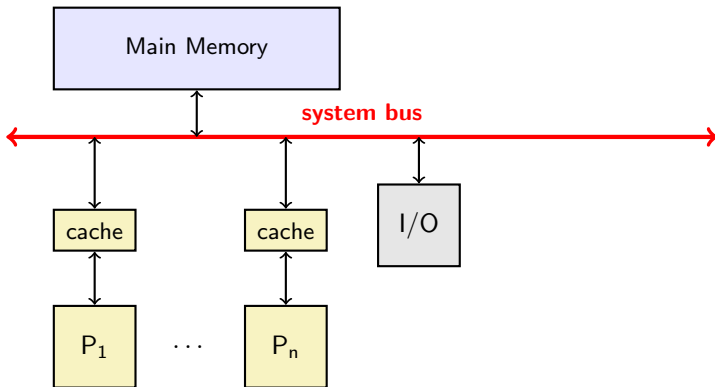


Figure: Schematic of a general parallel system

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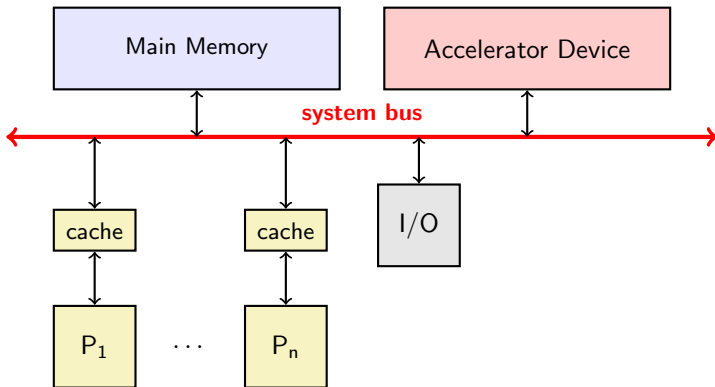


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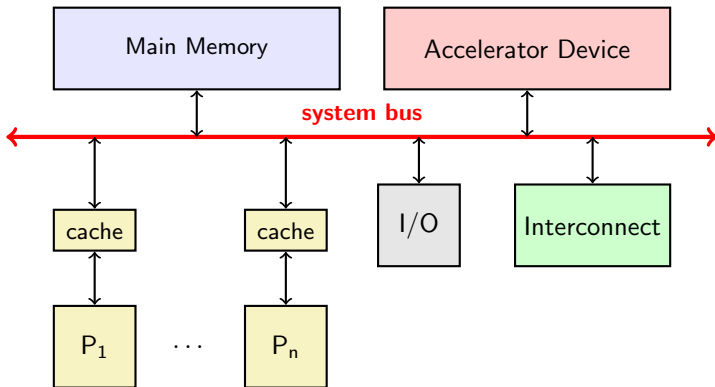


Figure: Schematic of a general parallel system

Communication Networks



The **Interconnect** in the last figure stands for any kind of Communication grid. This can be implemented either as

- **local hardware interconnect,**

or in the form of

- **network interconnect.**

In classical supercomputers the first was mainly used, whereas in today's cluster based systems often the network solution is used in the one form or the other.

Communication Networks



Hardware

MyriNet

- shipping since 2005
- transfer rates up to 10Gbit/s
- lost significance (2005 28.2% TOP500 down to 0.8% in 2011)

Infiniband

- transfer rates up to 300Gbit/s
- most relevant implementation driven by OpenFabrics Alliance^a, ↪ usable in Linux, BSD , Windows.
- features remote direct memory access (RDMA) ↪ reduced CPU overhead

^a<http://www.openfabrics.org/>

Communication Networks



Topologies

- 1 **Linear array:**
nodes aligned on a string each being connected to at most two neighbors.

Communication Networks



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every node is connected to all other nodes

Communication Networks



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- ④ **Mesh and Torus:**
Every node is connected to a number of neighbours (2-4 in 2d mesh, 4 in 2d torus).

Communication Networks



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- 4 **Mesh and Torus:**
Every node is connected to a number of neighbours (2-4 in 2d mesh, 4 in 2d torus).
- 5 **k-dimensional cube / hypercube:**
Recursive construction of a well connected network of 2^k nodes each connected to k neighbors. Line for two, square for four, cube for eight.

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Recursive construction of a well connected network of 2^k nodes each connected to k neighbors. Line for two, square for four, cube for eight.
- 6 **Tree:**
Nodes are arranged in groups, groups of groups and so forth until only one large group is left, which represents the root of the tree.