



# Parallel Programming in Computational Engineering & Science

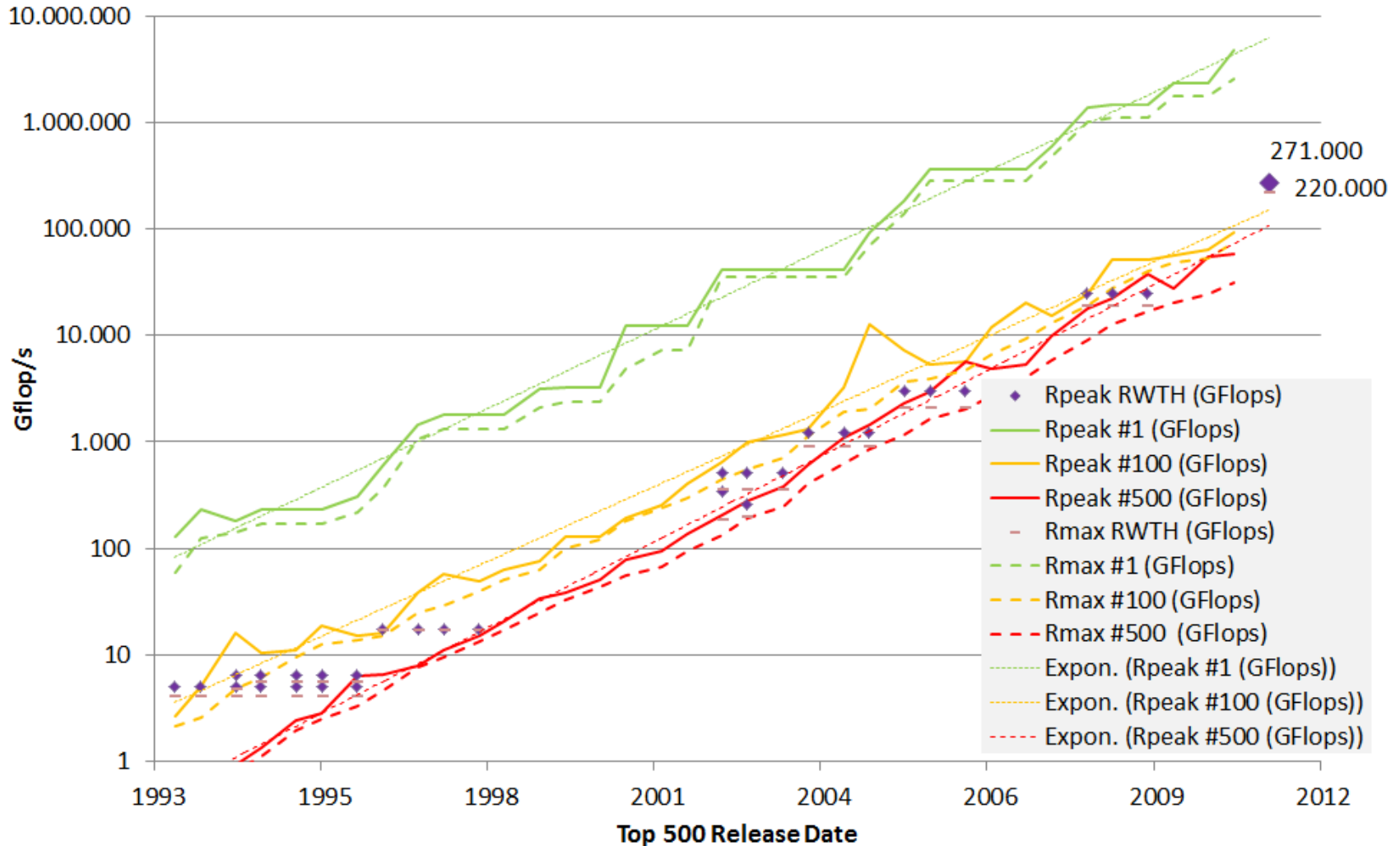
## Introduction

*Matthias Müller, Dieter an Mey*  
*Center for Computing and Communication*

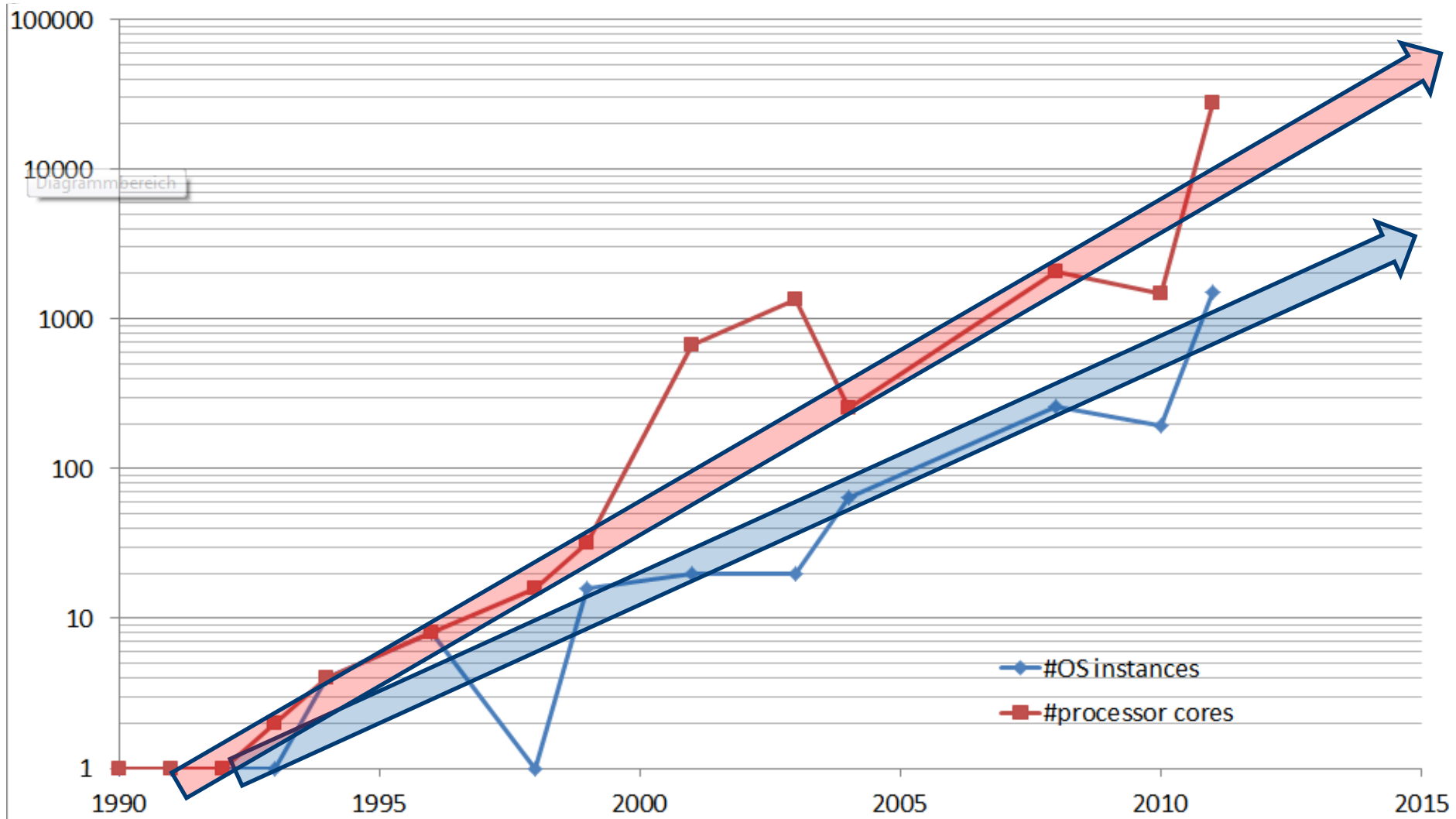
*Kindly sponsored by*

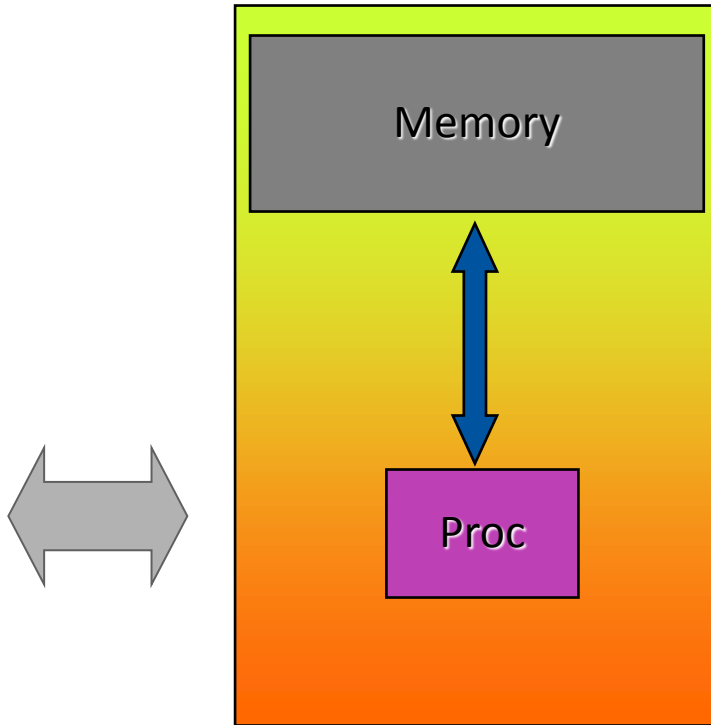


RWTH Systems in Top500 List over Time



# Growth of #OS instances / #processor cores





Main memory to store data and programs.

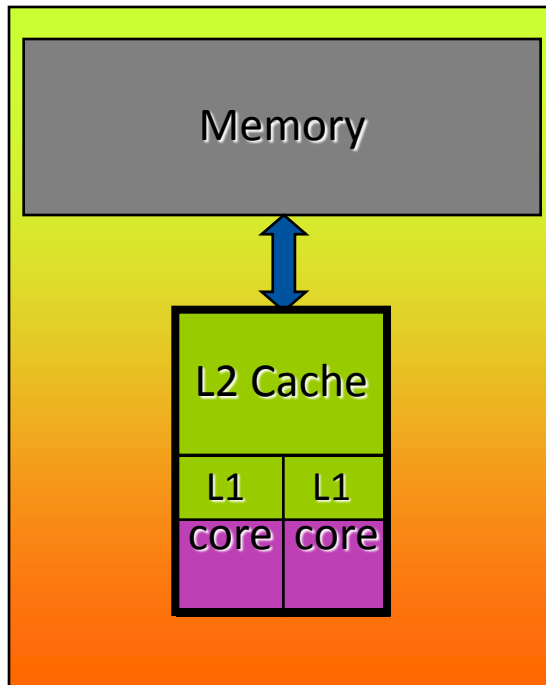
Processor to fetch program from memory, and execute program instructions:  
Load data from memory, process data and write results back to memory.

Accessing memory takes time.

Today memory bandwidth and latency frequently is a severe bottleneck!

Input/ output  
is not covered here.

# Computer Architecture: Refined View with Multiple Cache Levels



Since 2005/6 Intel and AMD are producing dualcore processors for the mass market.

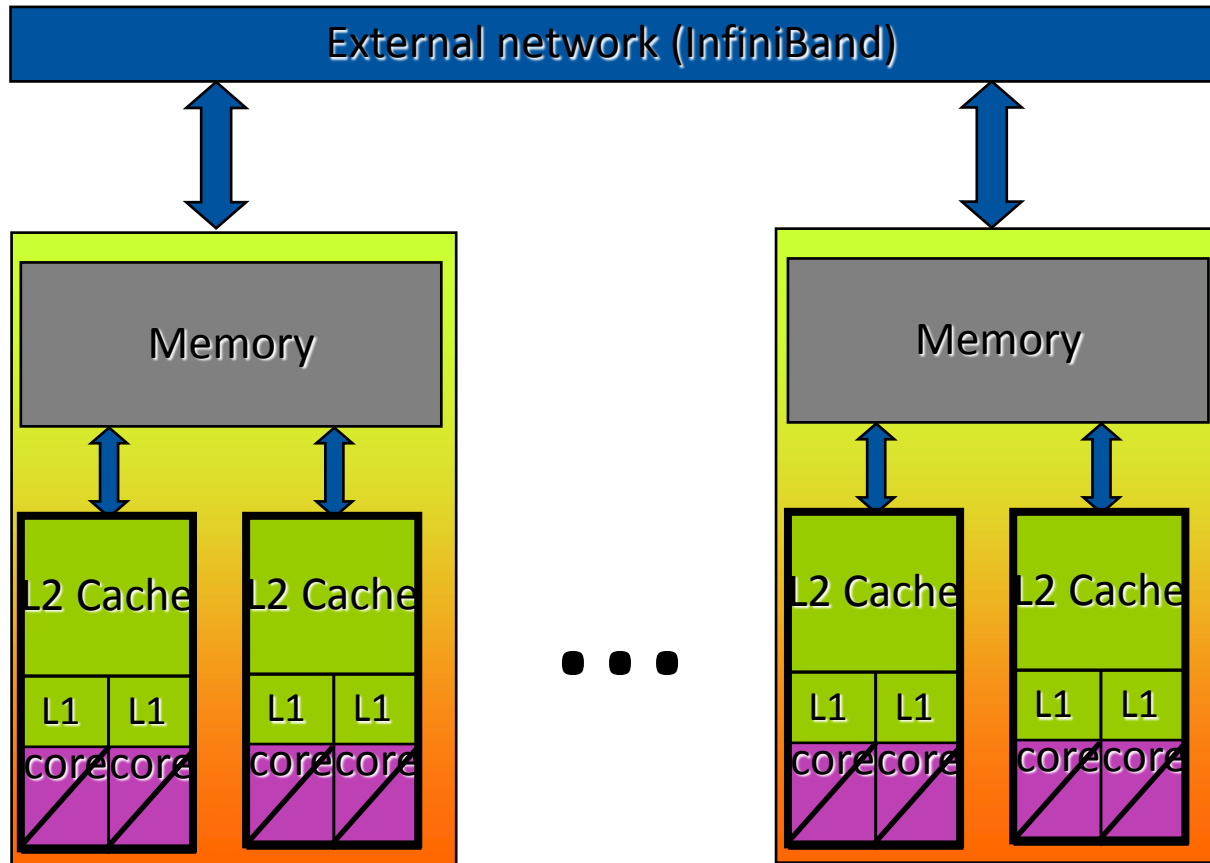
Today multicores are ubiquitous.

Currently 4 to 12 cores per chip are quite common.

Caches have been employed since long to remedy the memory bottleneck to a certain degree.

But with a growing number of cores, the memory bottleneck is still growing !

■ **Cluster of Multiprocessor Nodes with Multicore Processors**

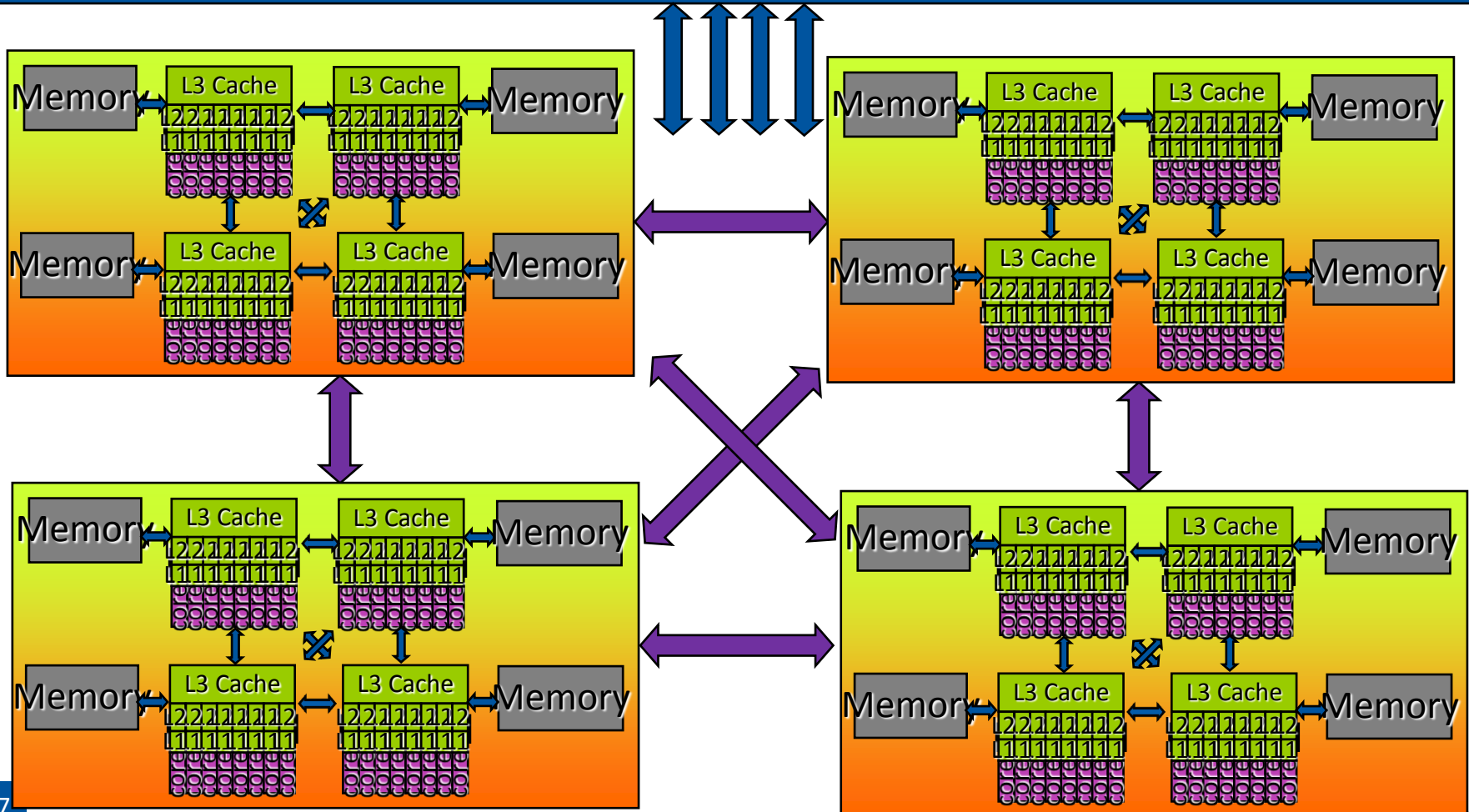


For High Performance Computing (HPC) large clusters of many nodes with multiple multicore processors are connected by fast networks like InfiniBand.

Each node is a shared memory parallel computer where all cores of all processors have access to one main memory.

■ Bull BCS System

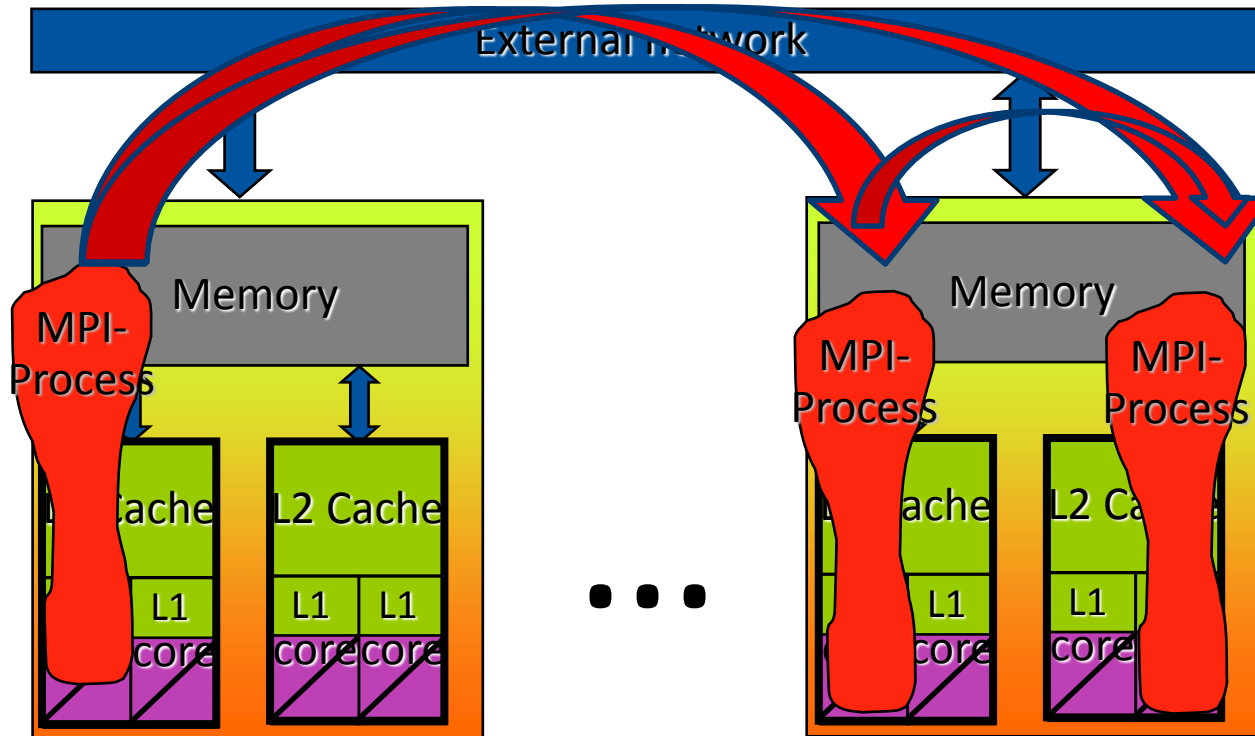
InfiniBand Network



# Message Passing with MPI

## On Distributed Memory Parallel Computers

Typically, when using Message Passing with MPI, one MPI process runs on each processor core



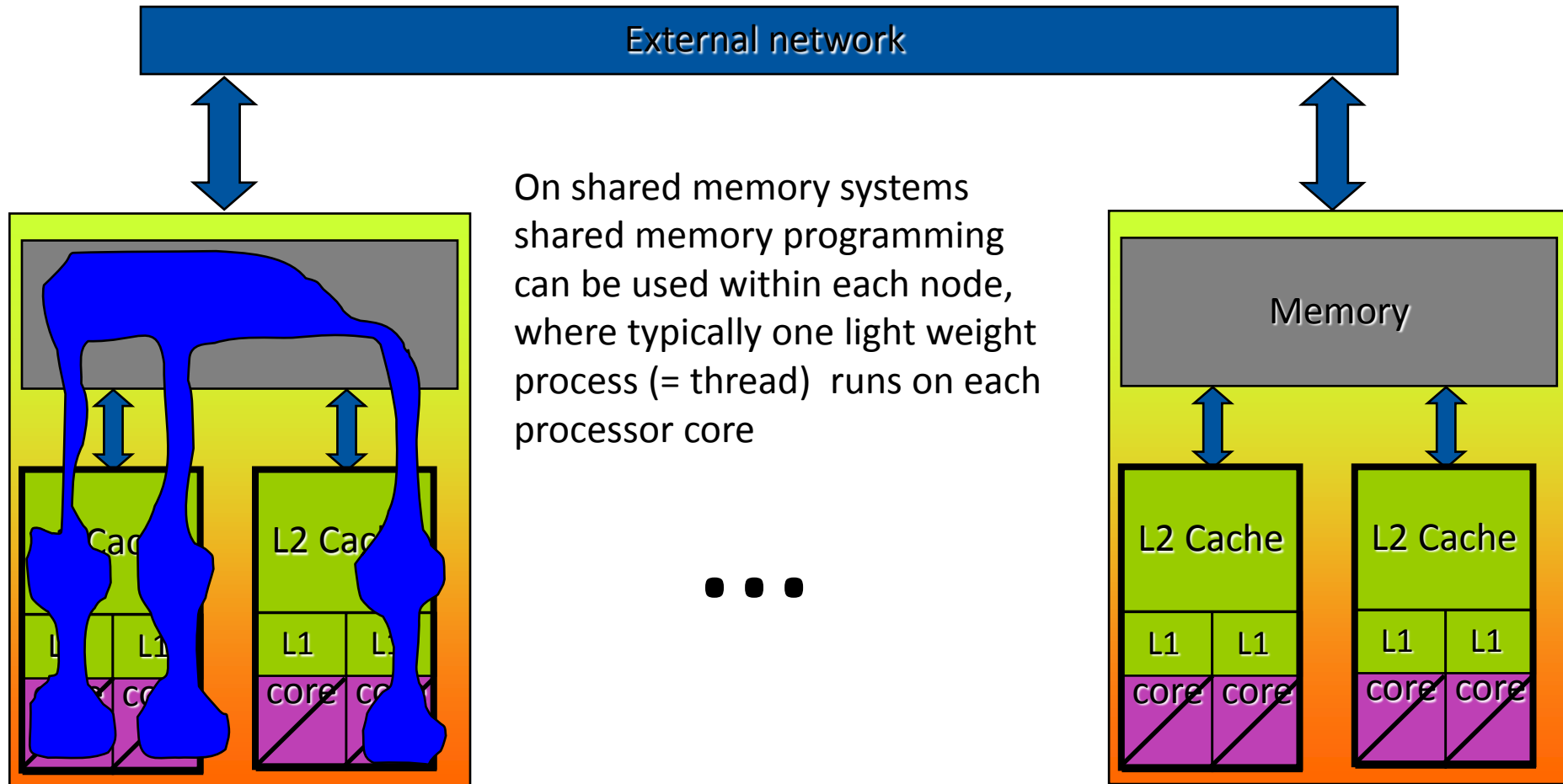
MPI is the de-facto standard for message passing.

MPI is a program library plus a mechanism to launch multiple cooperating executable programs.

Typically it is the same binary, which is started on multiple processors.

(SPMD=single program multiple data paradigm)

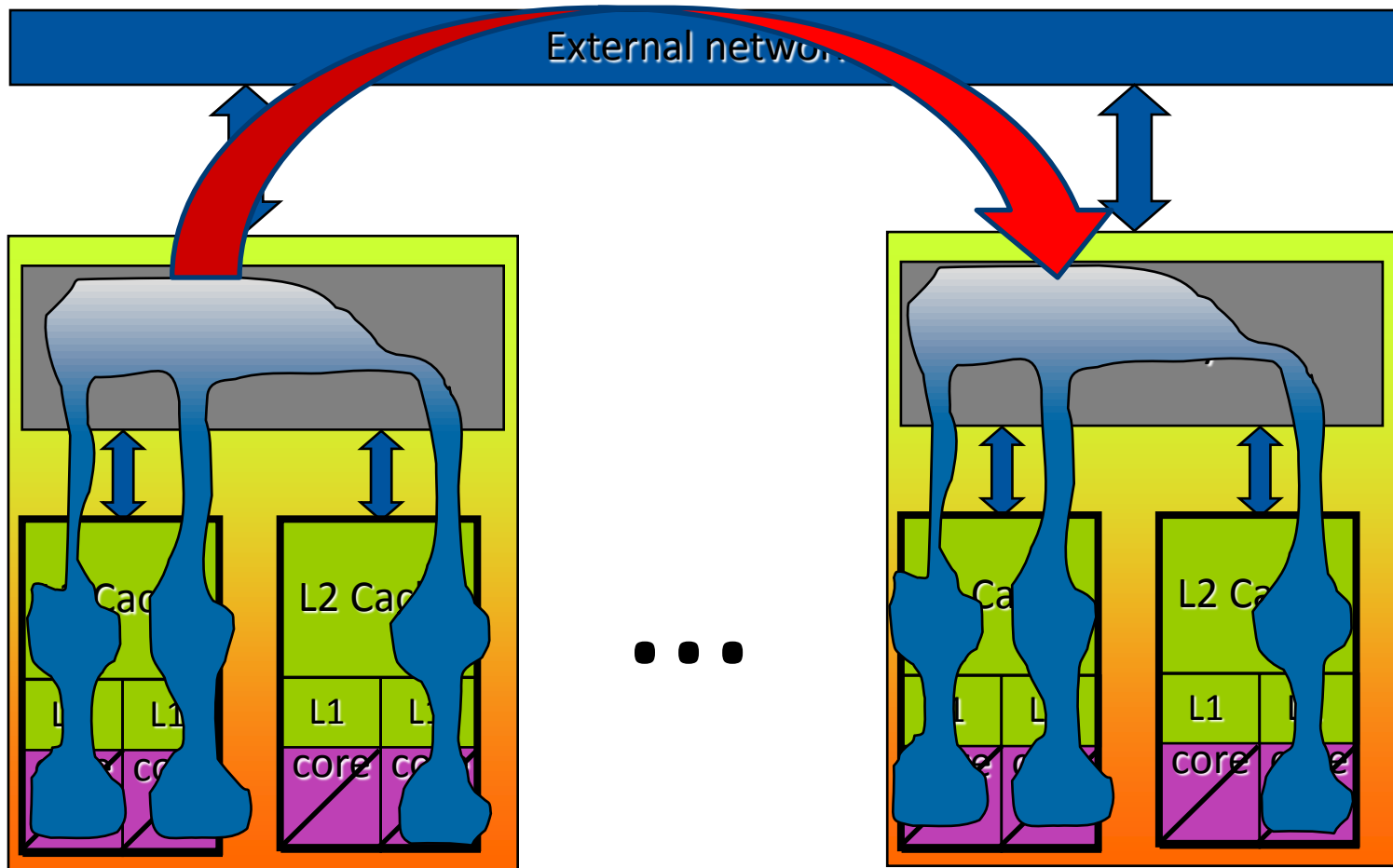




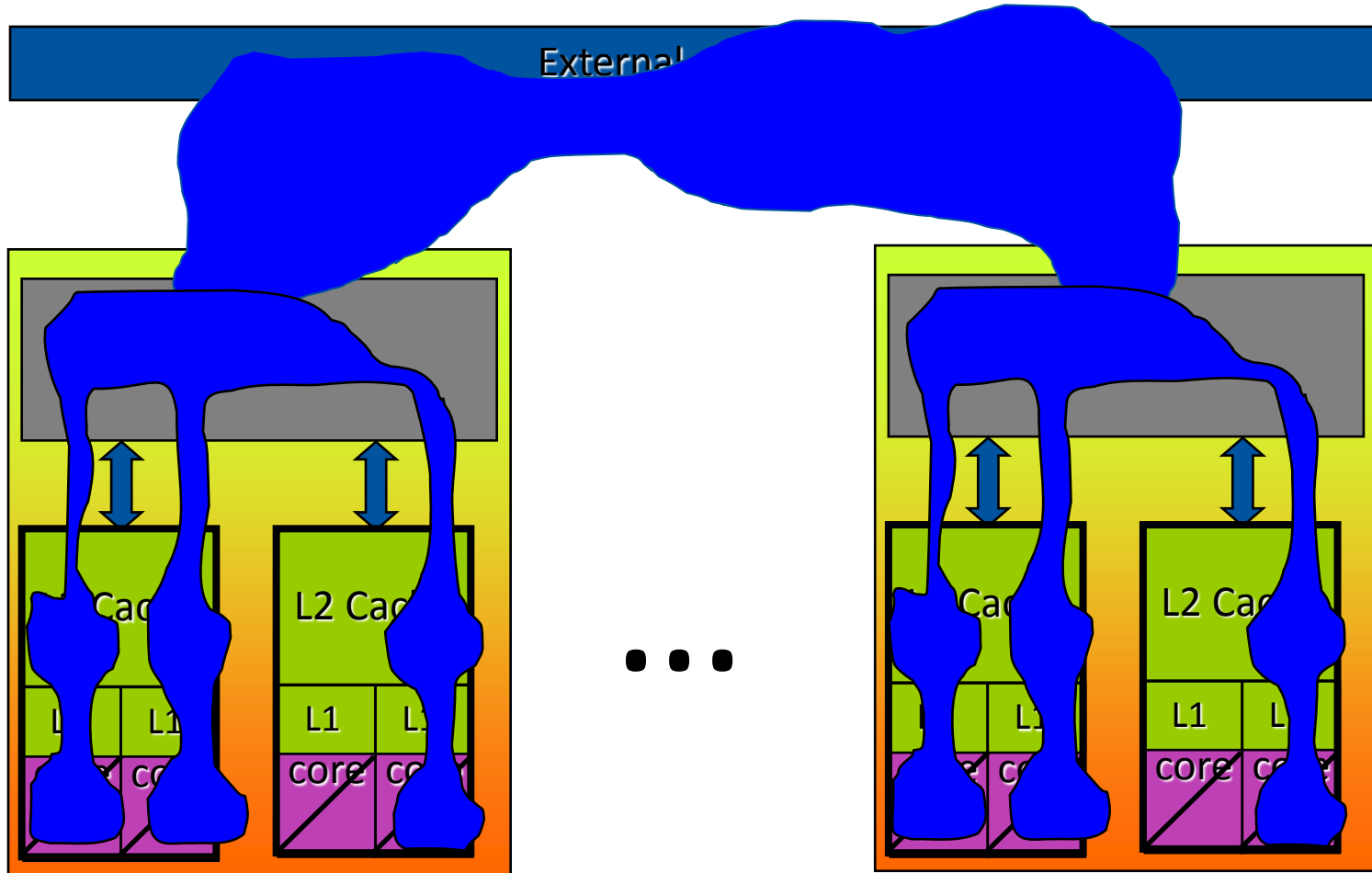
On shared memory systems shared memory programming can be used within each node, where typically one light weight process (= thread) runs on each processor core

...

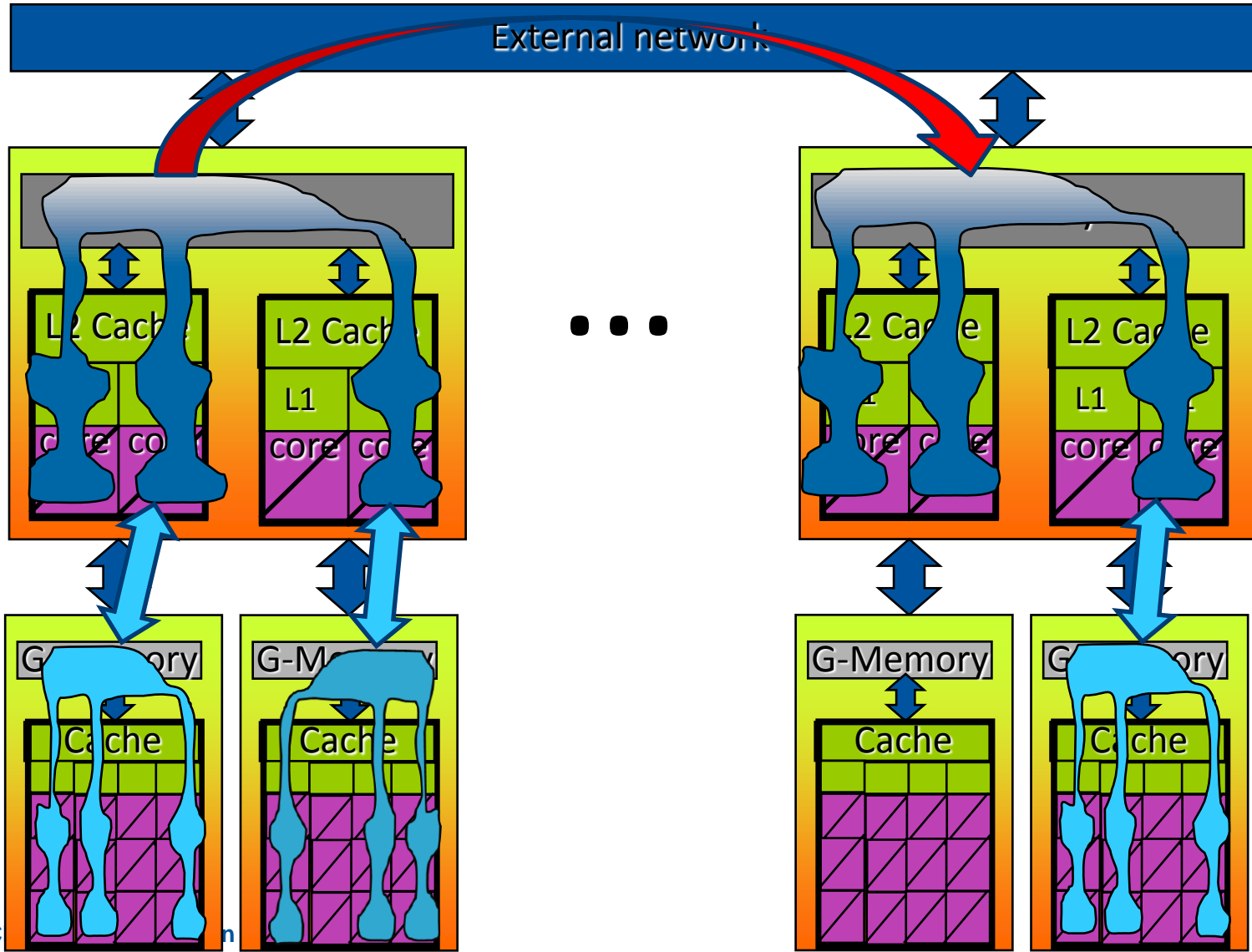
# MPI + OpenMP = Hybrid Parallelization



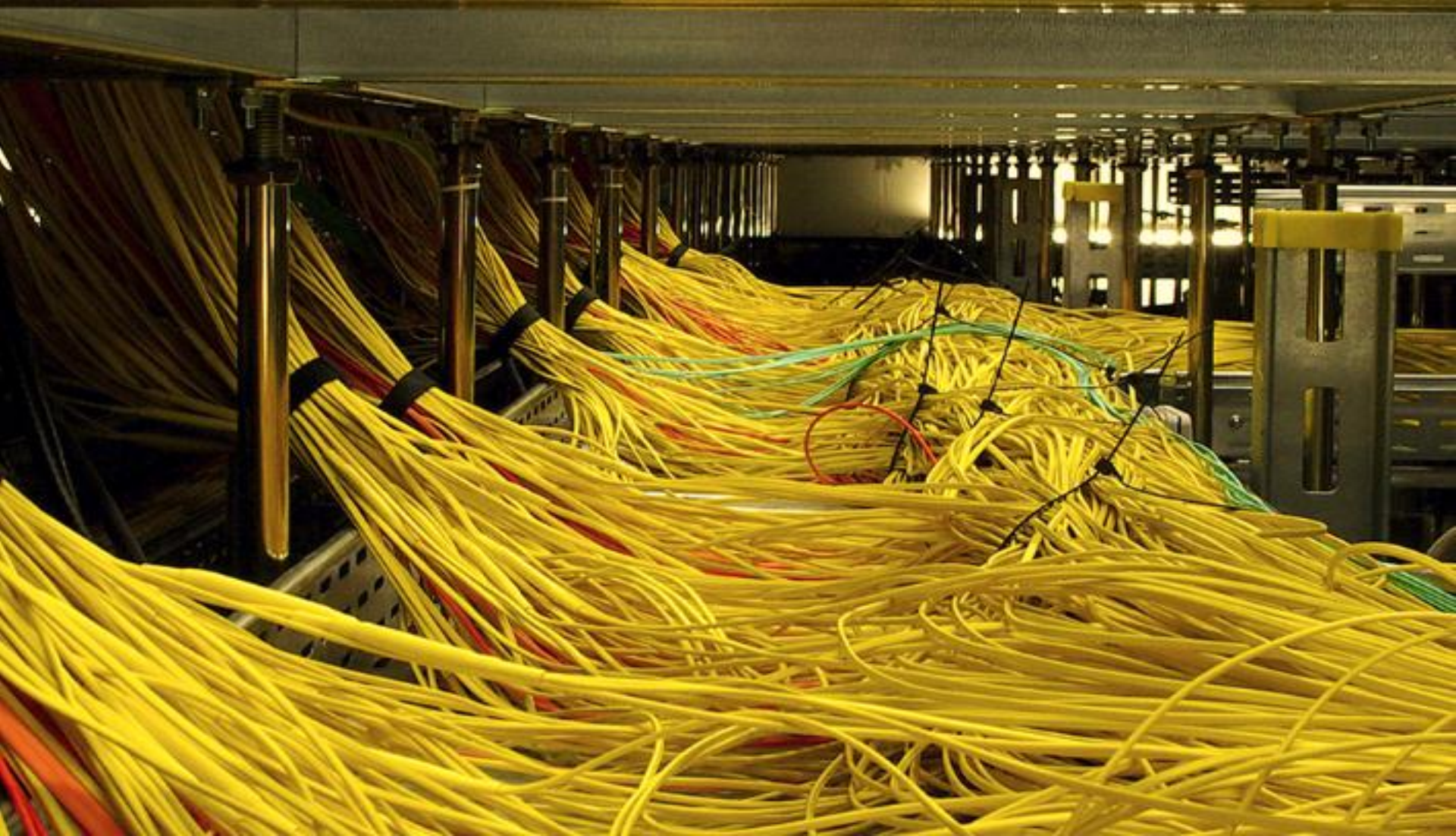
# Virtual Shared Memory Programming with OpenMP (using Software from ScaleMP)



and then there are Accelerators / Coprocessors  
( NVIDIA GPGPUs, Intel Xeon Phi) ...



# How to deal with this Complexity?



<b>Part I</b> Monday, March 11, 14-17:30	<b>Processor Architectures and Serial Programming</b> incl Labs
<b>Part II</b> Tuesday, March 12, 9-17:30	<b>Message Passing with MPI</b> incl Labs
<b>Part III</b> Wednesday, March 13, 9-17:30	<b>Shared Memory Programming with OpenMP</b> incl Labs
<b>Part IV</b> Thursday, March 14, 9-17:30	<b>GPGPU Programming</b> incl Labs
<b>Part V</b> Friday, March 15, 9-15:30	<b>Programming Intel Xeon Phi</b> incl Labs + Code Tuning

	Introduction Serial Programming, Tuning, Processor Architectures	Message Passing with MPI	Shared Memory Programming with OpenMP	GPGPU Programming with OpenACC	Intel Xeon Phi, Code tuning
	Mo, March 11	Tu, March 12	We, March 13	Th, March 14	Fr, March 15
9:00 - 10:30		<b>MPI Basics: Part I</b> <ul style="list-style-type: none"> <li>• General Concepts</li> <li>• Point-to-Point communication</li> </ul> <i>H. Iliev, RWTH</i>	<b>Introduction to Parallel Computing with OpenMP</b> <i>C. Terboven, RWTH</i>	<b>GPU Introduction, OpenACC Basics</b> <i>S. Wienke, RWTH</i>	<b>Programming the Intel® Xeon Phi™ Coprocessor</b> <i>T. Cramer, RWTH</i>
10:30 - 11:00		coffee break	coffee break	coffee break	coffee break
11:00 - 12:30		Lab: MPI	Lab: OpenMP Part I	Lab: OpenACC	Lab: Intel Xeon Phi, Bring your code tuning (not only for Xeon Phi)
12:30 - 14:00		lunch break	lunch break	lunch break	lunch break
14:00 - 15:30	<b>Welcome and Introduction</b> <i>15 min., Prof. M. Müller, RWTH</i> <b>Parallel Computing Architectures</b> <i>75 min., C. Terboven, RWTH</i>	<b>MPI Basics: Part II</b> <i>H. Iliev, RWTH</i>	<b>Getting OpenMP up to Speed</b> <i>R. v. d. Pas, Oracle</i>	<b>OpenACC Advanced Case Study</b> <i>70 min., S. Wienke, RWTH</i> <i>20 min., P. Springer, RWTH</i>	Lab: Intel Xeon Phi, Bring your code tuning (not only for Xeon Phi)
15:30 - 16:00	coffee break		coffee break	coffee break	
16:00 - 17:30	<b>The RWTH Compute Cluster</b> <i>25 min., T. Warschko, Bull</i> <b>RZ Environment</b> <i>20 min., T. Cramer, RWTH</i> <i>45 min., Lab: Performance Tuning for Cached-based Systems</i>	<b>Vampir</b> <i>15 min., H. Iliev (RWTH)</i> <b>TotalView</b> <i>30 min., T. Cramer, RWTH</i> <i>45 min., Lab: MPI and Tools</i>	<b>OpenMP Programming on ScaleMP</b> <i>25 min., Dirk Schmidl, RWTH</i> <b>Misc. Advanced OpenMP Programming</b> <i>20 min., C. Terboven, RWTH</i> <i>45 min., Lab: OpenMP Part II</i>	<b>Outlook on OpenMP for Accelerators</b> <i>30 min., C. Terboven, RWTH</i>  <i>60 min., Lab: OpenACC</i>	
19:00 -			<b>Social event in Palladion</b> Schmiedstraße 3		



Welcome to  
PPCES 2013

