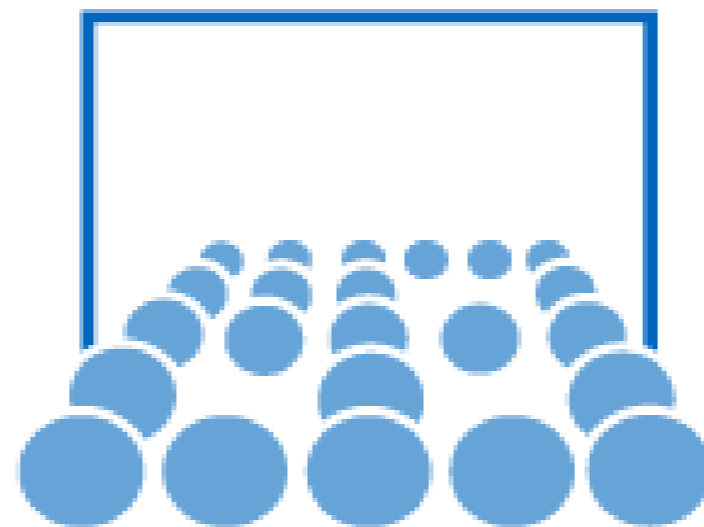


PSE Molekulardynamik

OpenMP, bigger Applications

Alex Breuer, Benjamin Uekermann

12.12.2014



Outline

- Schedule
- Presentations: Worksheet 4
- OpenMP
- Multicore Architectures
- Membrane, Crystallization
- Preparation: Worksheet 5

Schedule

10.10.2014	Intro 1 WS
24.10.2014	Review 1 WS / Intro 2 WS
07.11.2014	Review 2 WS / Intro 3 WS
28.11.2014	Review 3 WS / Intro 4 WS
12.12.2014	Review 4 WS / Intro 5 WS
16.01.2015	Review 5 WS

Presentations: Worksheet 4

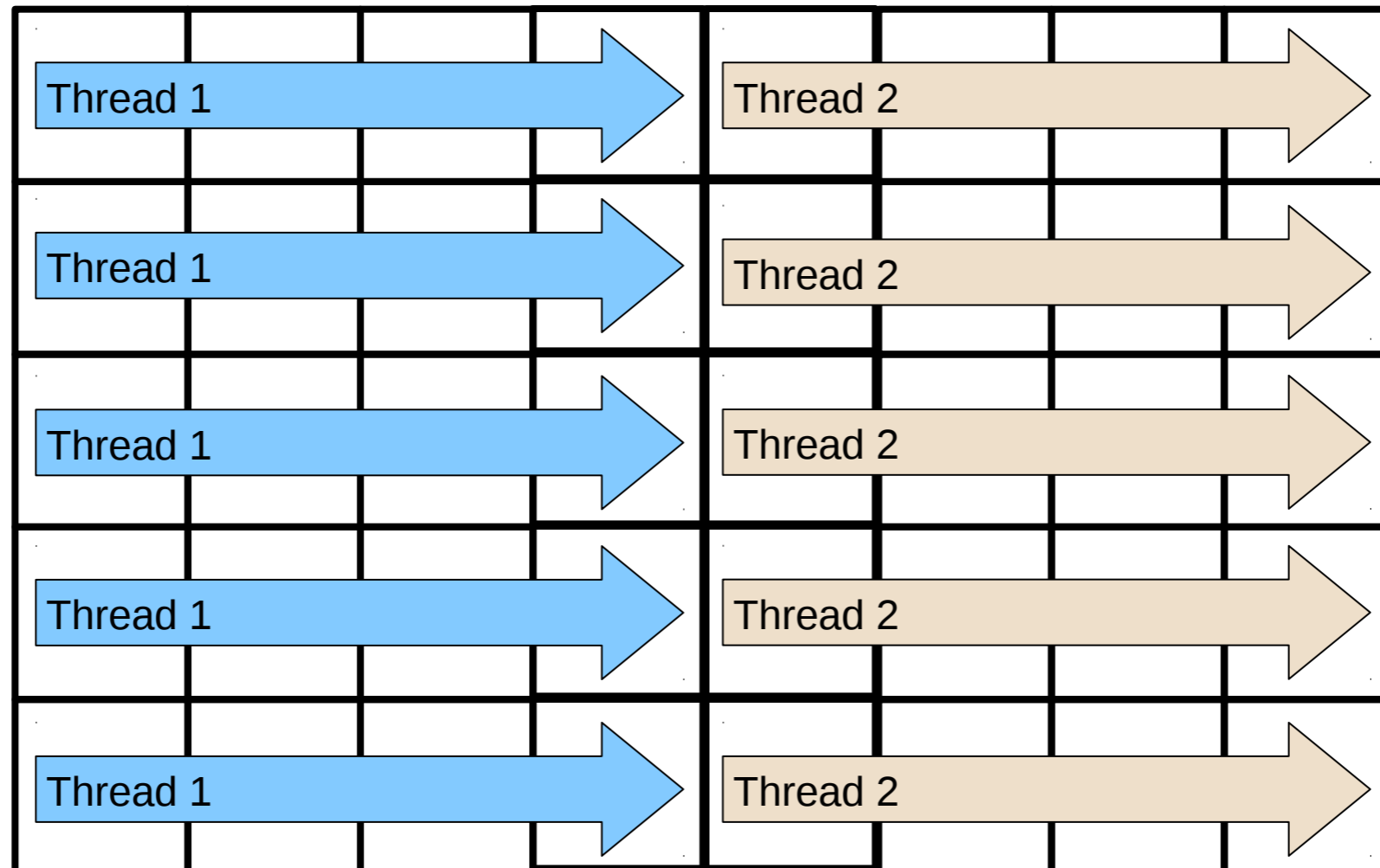
OpenMP

- References

- <https://computing.llnl.gov/tutorials/openMP/>
- <http://openmp.org>
- Hager, Wellein: Introduction to High Performance Computing for Scientists and Engineers. CRC Press, ISBN 978-1439811924, 356 pages, July 2010
- <http://icl.cs.utk.edu/papi/>

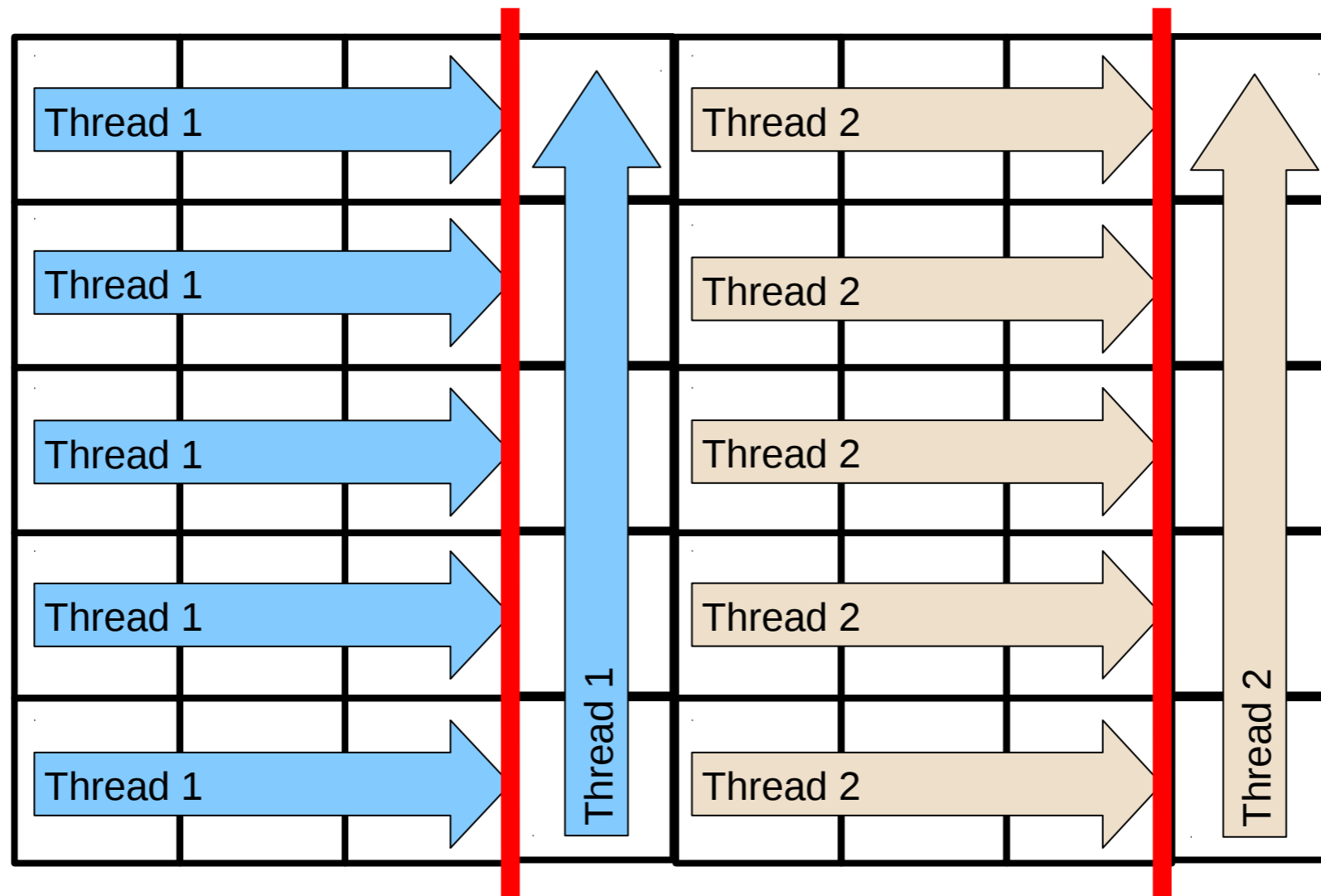
- Make yourself familiar with given hardware and shared memory parallelization
- Parallelize compute intensive parts first
 - Here: Loop for force calculation
- NUMA: Allocate memory in parallel

OpenMP: Linked Cell



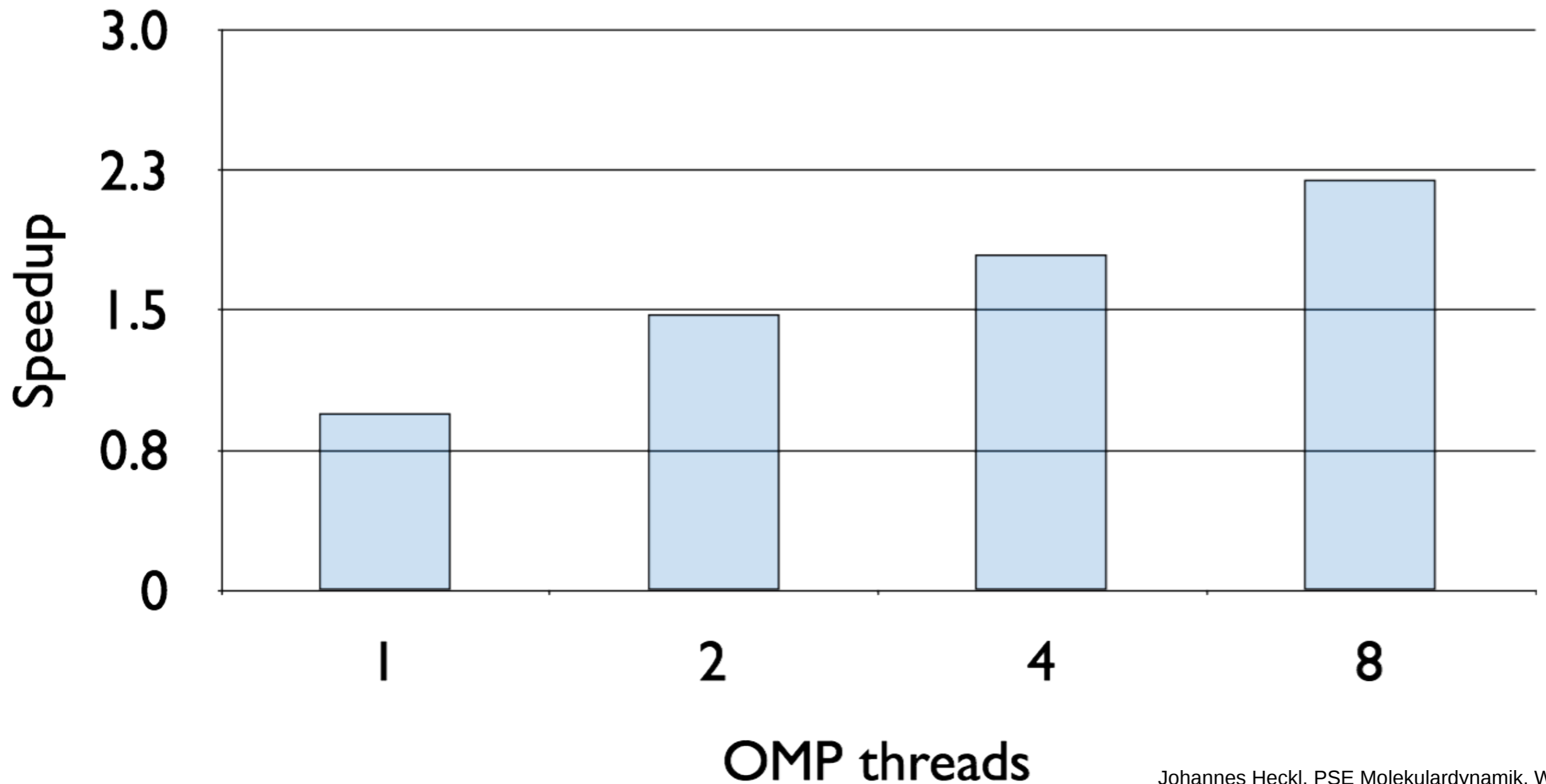
Problem: Synchronisation for boundary cells between Thread 1 and 2, due to Newton 3.

OpenMP: Linked Cell



- Possible solution:
- Compute inner cells
 - Synchronize all threads
 - Compute boundary cells

OpenMP: Molecular Dynamics - 2011/2012



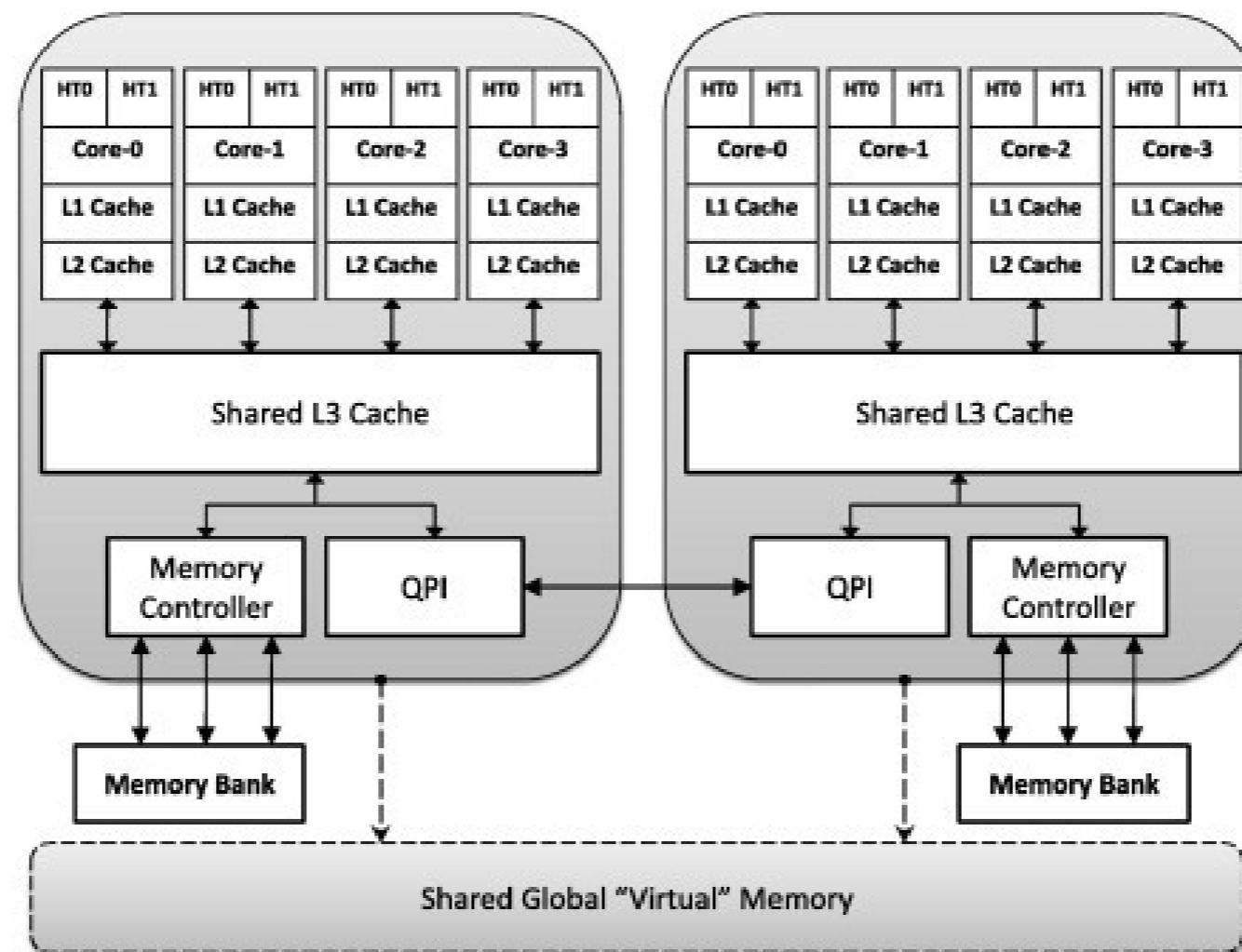
Johannes Heckl, PSE Molekulardynamik, WS11/12

Revision: MAC Cluster

- http://www.mac.tum.de/wiki/index.php/MAC_Cluster
- Read usage instructions carefully!
- Here: MAC-Cluster AMD-BDZ / Intel SNB Partition

	MAC-Cluster SNB Partition	MAC-Cluster BDZ Partition
Architecture	Intel SandyBridge-EP Xeon E5-2670 (2.6 GHz)	AMD Opteron 6274 (2.2 GHz)
#Nodes	28	19
#Processor cores	448	1216
Aggregate peak performance (Tflop/s)	9.3	10.7
Aggregate memory (TByte)	3.5	4.9

Multicore Architectures: Nehalem EP



Çatalyüreka et. al, Graph coloring algorithms for multi-core and massively multithreaded architectures
[Parallel Computing](#)
[Volume 38, Issues 10–11](#), October–November 2012, Pages 576–59

Multicore Architectures: Intel SNB

```
lu32reb2@mac-login-intel:~> salloc --partition=snb --ntasks=1 --cpus-per-task=32 --time=1:00:00
```

```
lu32reb2@mac-login-intel:~> srun papi_component_avail
```

```
Available components and hardware information.
```

```
-----  
PAPI Version           : 5.0.0.0  
Vendor string and code : GenuineIntel (1)  
Model string and code  : Intel(R) Xeon(R) CPU E5-2670 0 @ 2.60GHz (45)  
CPU Revision           : 7.000000  
CPUID Info             : Family: 6  Model: 45  Stepping: 7  
CPU Max Megahertz      : 2601  
CPU Min Megahertz      : 1200  
Hdw Threads per core   : 2  
Cores per Socket       : 8  
NUMA Nodes             : 2  
CPUs per Node          : 16  
Total CPUs             : 32  
Running in a VM        : no  
Number Hardware Counters : 0  
Max Multiplex Counters : 64  
-----
```

```
Compiled-in components:
```

```
Name:  perf_events          Linux perf_event CPU counters
```

```
\-> Disabled: /proc/sys/kernel/perf_event_paranoid prohibits using counters
```

```
Name:  rapl                 Linux SandyBridge RAPL energy measurements
```

Preparation: Worksheet 5