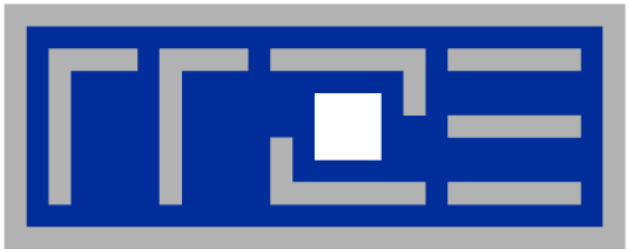
For final slides and example code see:

https://goo.gl/DrGlq5



Node-Level Performance Engineering

Georg Hager, Jan Eitzinger, Gerhard Wellein
Erlangen Regional Computing Center (RRZE)
and Department of Computer Science
University of Erlangen-Nuremberg

SC16 full-day tutorial
November 13, 2016
Salt Lake City, UT, USA


: slide updated from USB version

Agenda

GW

- **Preliminaries** — 08:30
- **Introduction to multicore architecture**
  - Threads, cores, SIMD, caches, chips, sockets, ccNUMA
- **Multicore tools** — 10:00

GH

- **Microbenchmarking for architectural exploration** — 10:30
  - Streaming benchmarks
  - Hardware bottlenecks
- **Node-level performance modeling (part I)**
  - The Roofline Model and dense MVM — 12:00

GW

- **Lunch break**
- **Node-level performance modeling (part II)** — 13:30
  - Case studies: Sparse MVM, Jacobi solver
- **Optimal resource utilization**
  - SIMD parallelism — 15:00

GH

  - ccNUMA — 15:30
  - OpenMP synchronization and multicores
- **Pattern-driven performance engineering** — 17:00

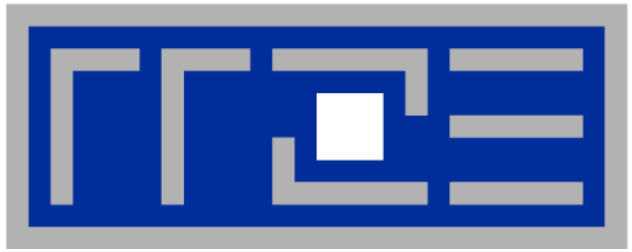
A conversation

From a student seminar on “Efficient programming of modern multi- and manycore processors”

Student: I have implemented this algorithm on the GPGPU, and it solves a system with 26546 unknowns in 0.12 seconds, so it is really fast.

Me: What makes you think that 0.12 seconds is fast?

Student: It is fast because my baseline C++ code on the CPU is about 20 times slower.

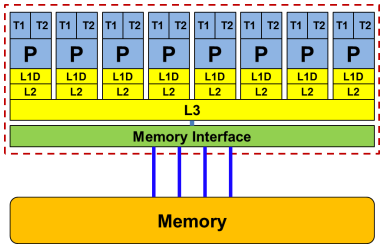


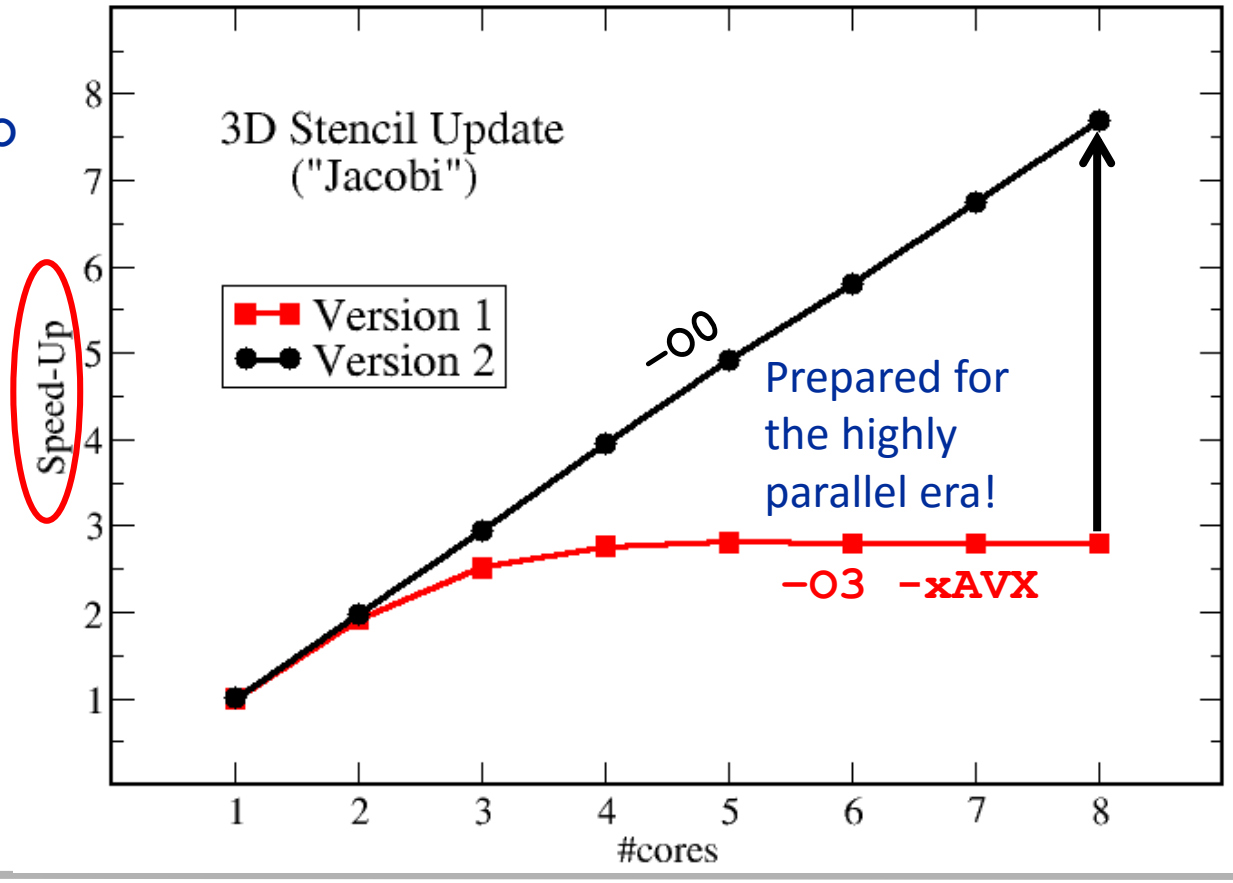
Prelude:
Scalability 4 the win!

Scalability Myth: Code scalability is the key issue

```
!$OMP PARALLEL DO
do k = 1 , Nk
  do j = 1 , Nj; do i = 1 , Ni
     y(i,j,k)= b*(  x(i-1,j,k)+ x(i+1,j,k)+ x(i,j-1,k)+
                    x(i,j+1,k)+ x(i,j,k-1)+ x(i,j,k+1))
    enddo; enddo
enddo
!$OMP END PARALLEL DO
```

Changing only the compile options makes this code scalable on an 8-core chip





Scalability Myth: Code scalability is the key issue

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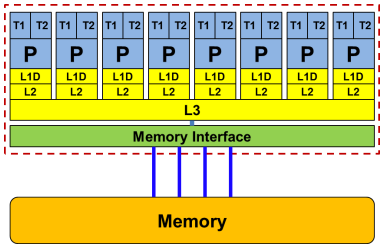
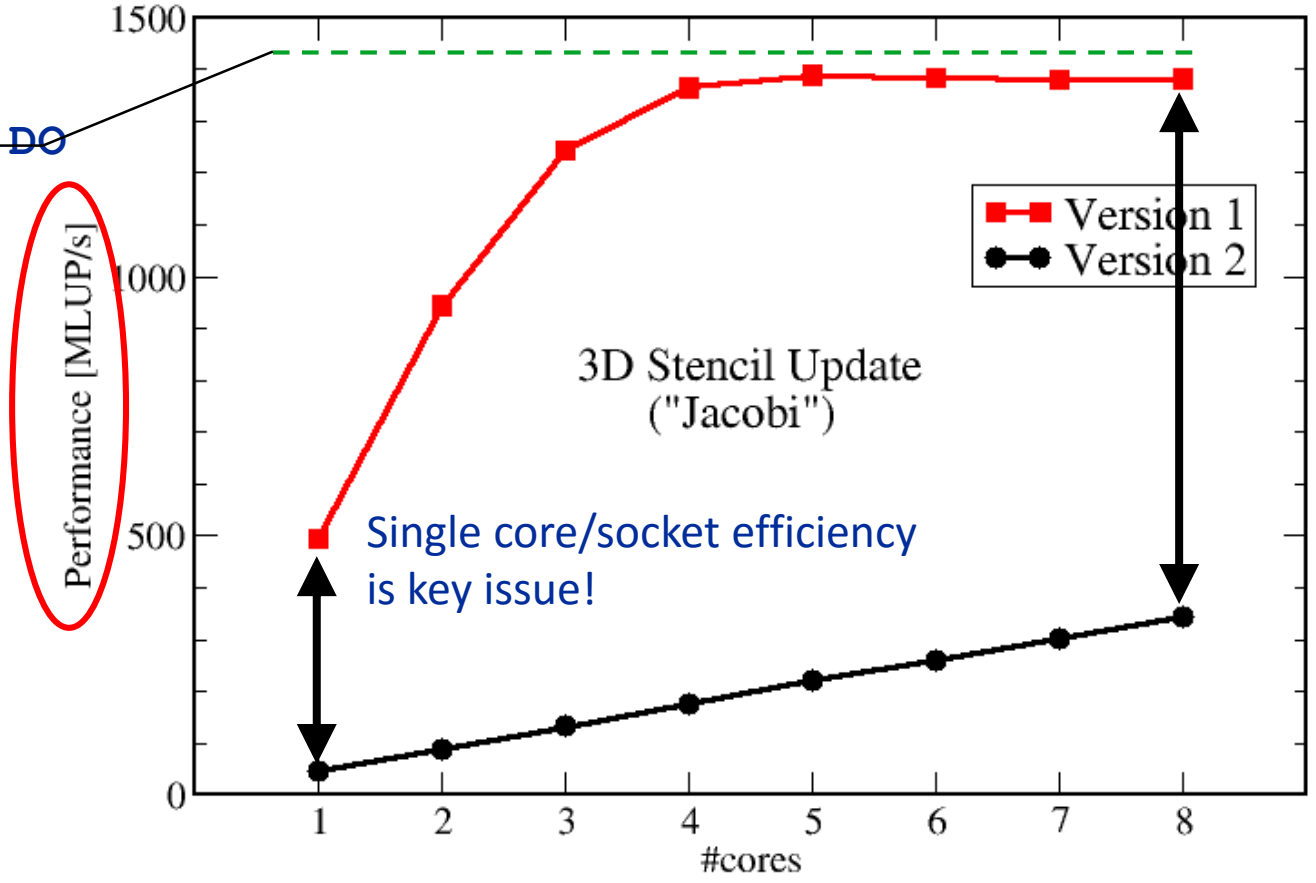
                    x(i,j+1,k)+ x(i,j,k-1)+ x(i,j,k+1))
    enddo; enddo
enddo
```

Upper limit from simple performance model:
35 GB/s & 24 Byte/update





Questions to ask in high performance computing

- **Do I understand the performance behavior of my code?**
  - Does the performance match a model I have made?
- **What is the optimal performance for my code on a given machine?**
  - High Performance Computing == Computing at the bottleneck
- **Can I change my code so that the "optimal performance" gets higher?**
  - Circumventing/ameliorating the impact of the bottleneck
- **My model does not work – what's wrong?**
  - This is the good case, because you learn something
  - Performance monitoring / microbenchmarking may help clear up the situation

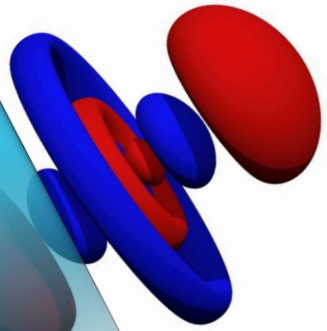
How model-building works: Physics

Newtonian mechanics

$$\vec{F} = m\vec{a}$$

Fails @ small scales!

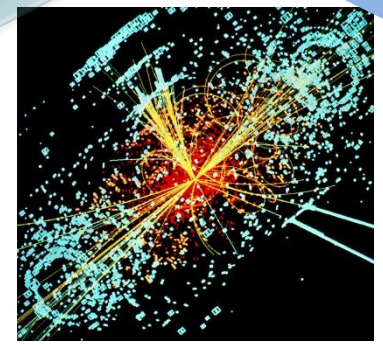
Nonrelativistic quantum mechanics



$$i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$

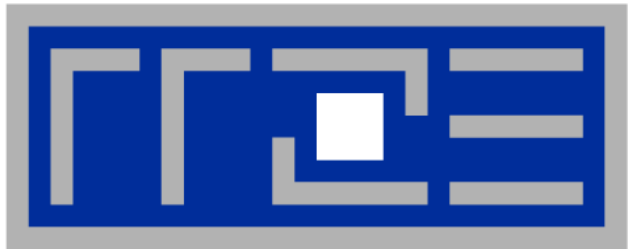
Fails @ even smaller scales!

If a model fails, we learn something!



Relativistic quantum field theory

$$U(1)_Y \otimes SU(2)_L \otimes SU(3)_c$$



Introduction:
Modern node architecture

A glance at basic core features:

pipelining, superscalarity, SMT

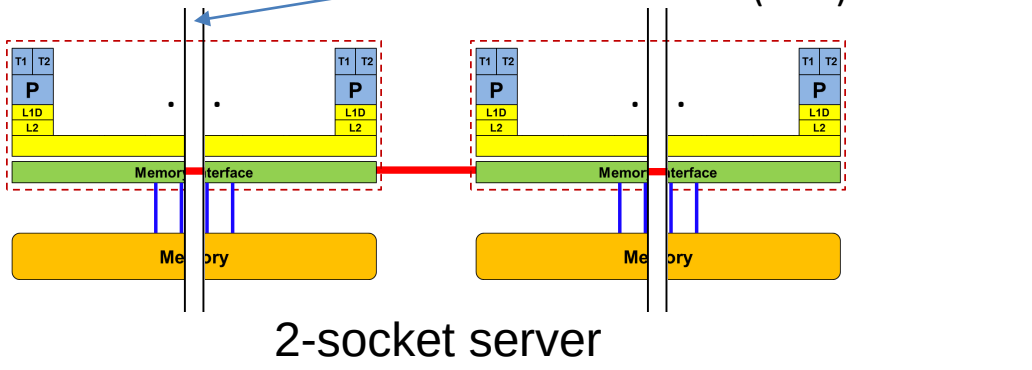
Caches and data transfers through the memory hierarchy

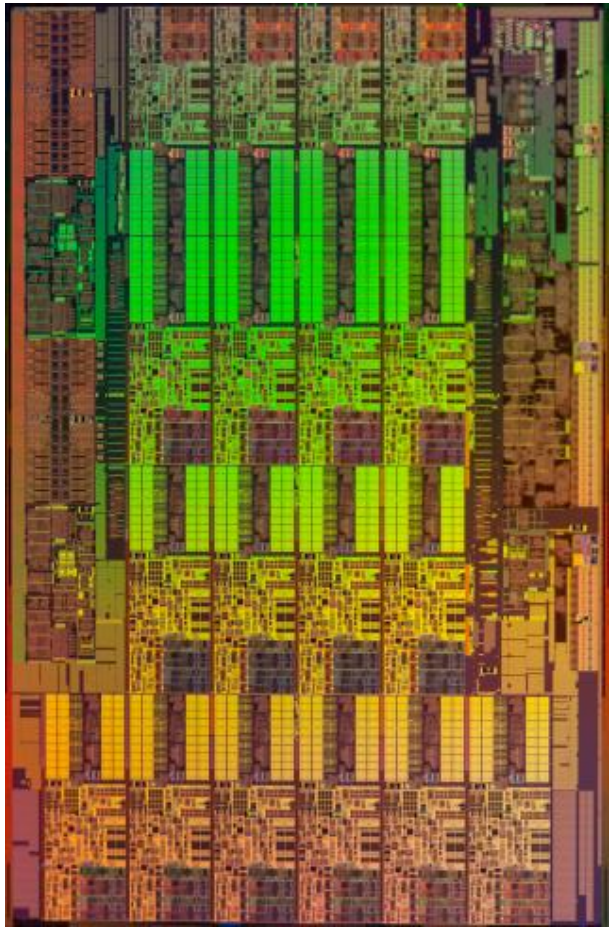
Accelerators

Bottlenecks & hardware-software interaction

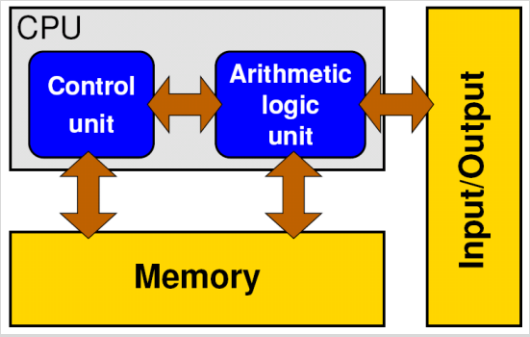
Multi-core today: Intel Xeon 2600v3 (2014)

- **Xeon E5-2600v3 “Haswell EP”:**
  Up to 18 cores running at 2+ GHz (+ “Turbo Mode”: 3.5+ GHz)
- **Simultaneous Multithreading**
  → reports as 36-way chip
- **5.7 Billion Transistors / 22 nm**
- **Die size: 662 mm²**





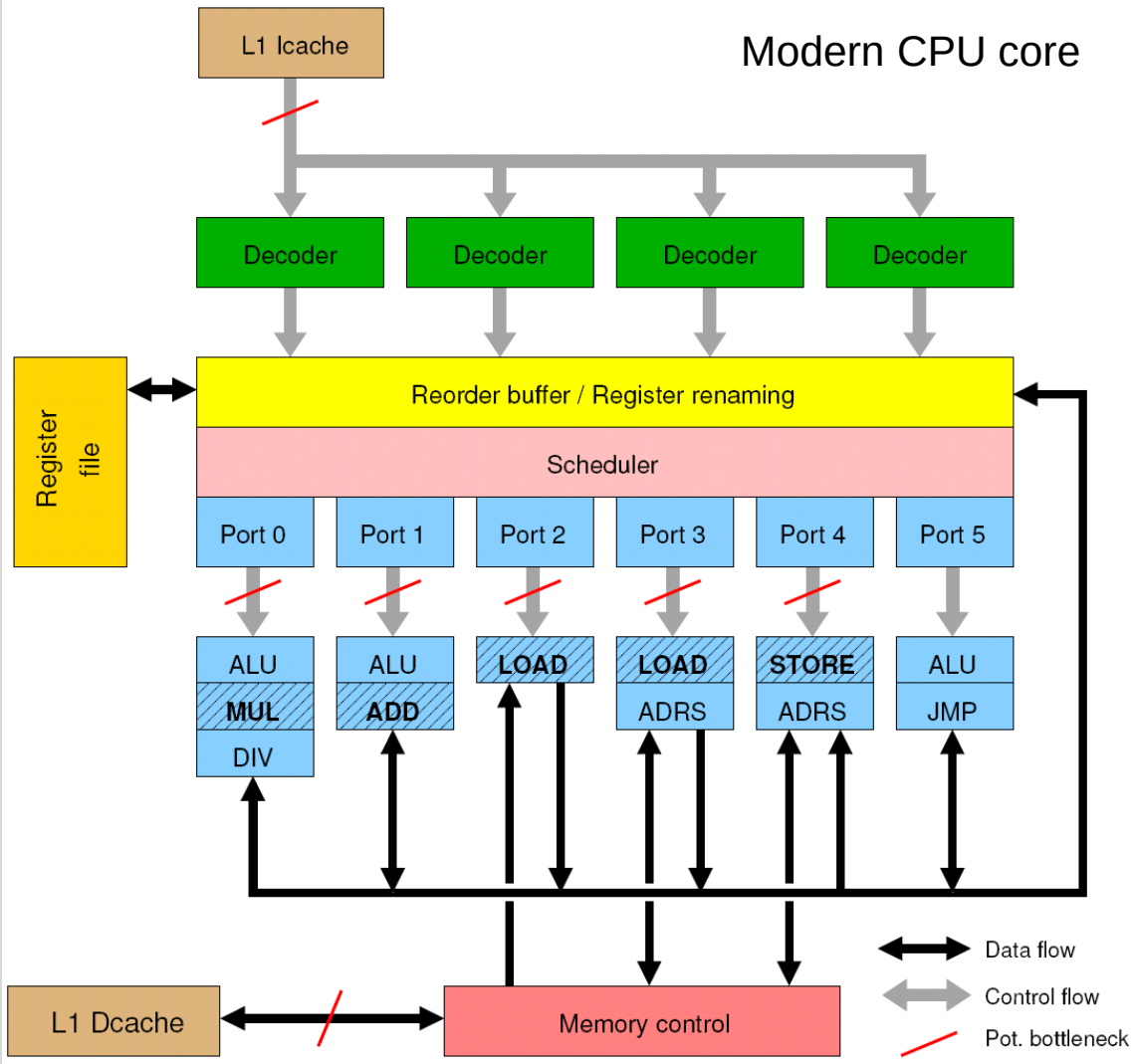
General-purpose cache based microprocessor core



Stored-program computer

- Implements “Stored Program Computer” concept (Turing 1936)
- Similar designs on all modern systems
- (Still) multiple potential bottlenecks

- The clock cycle is the “heartbeat” of the core



Pipelining of arithmetic/functional units

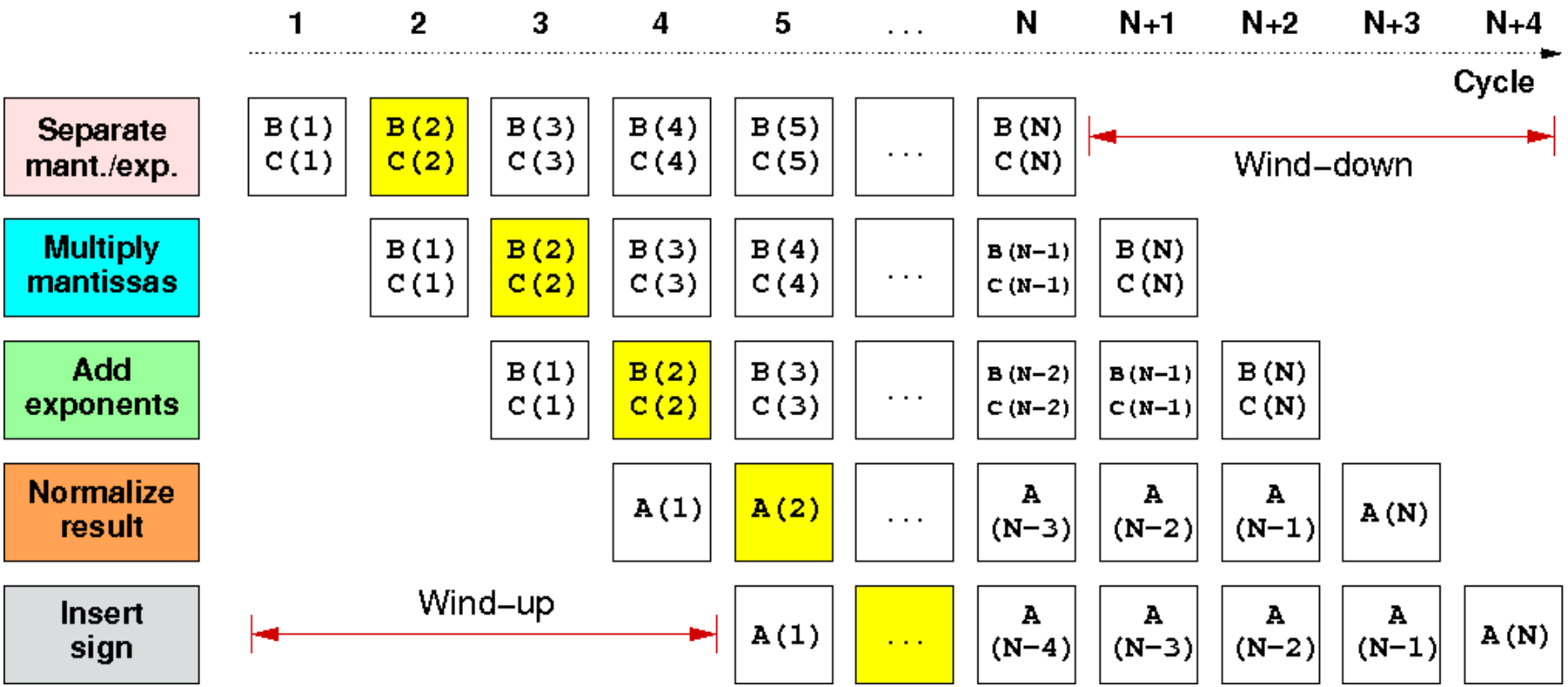
- **Idea:**
  - Split complex instruction into several simple / fast steps (stages)
  - Each step takes the same amount of time, e.g. a single cycle
  - Execute different steps on different instructions at the same time (in parallel)

- **Allows for shorter cycle times (simpler logic circuits), e.g.:**
  - floating point multiplication takes 5 cycles, but
  - processor can work on 5 different multiplications simultaneously
  - one result at each cycle after the pipeline is full

- **Drawback:**
  - Pipeline must be filled - startup times (#Instructions >> pipeline steps)
  - Efficient use of pipelines requires large number of independent instructions → instruction level parallelism
  - Requires complex instruction scheduling by compiler/hardware – software-pipelining / out-of-order

- **Pipelining is widely used in modern computer architectures**

5-stage Multiplication-Pipeline: A(i)=B(i)*C(i) ; i=1,...,N

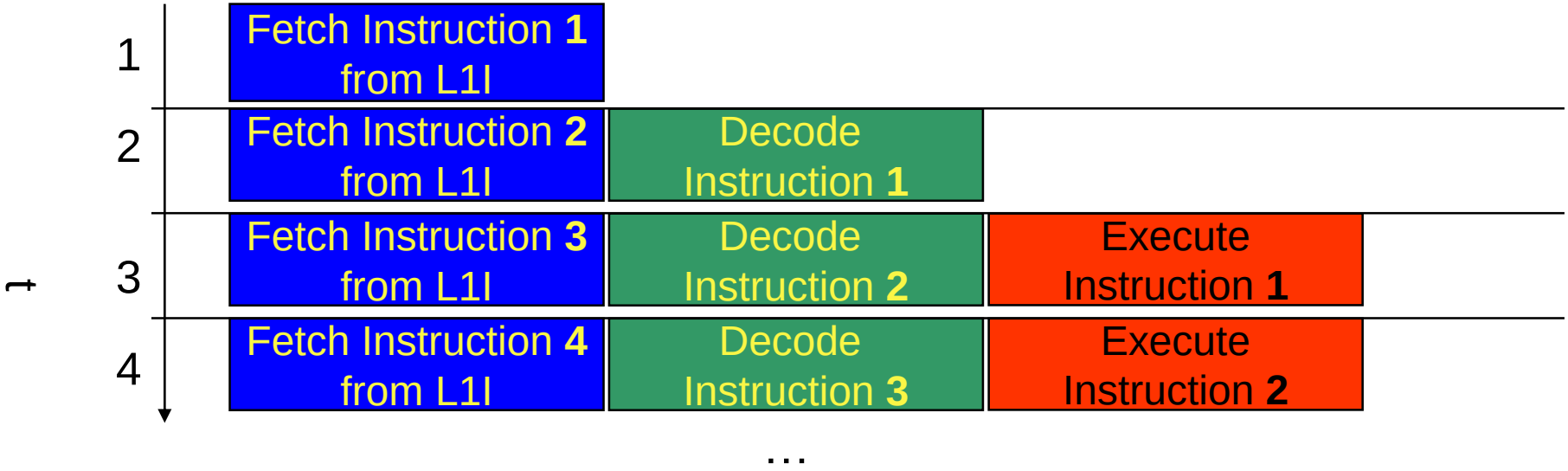


First result is available after 5 cycles (=latency of pipeline)!

Wind-up/-down phases: Empty pipeline stages

- **Besides arithmetic & functional unit, instruction execution itself is pipelined also, e.g.: one instruction performs at least 3 steps:**

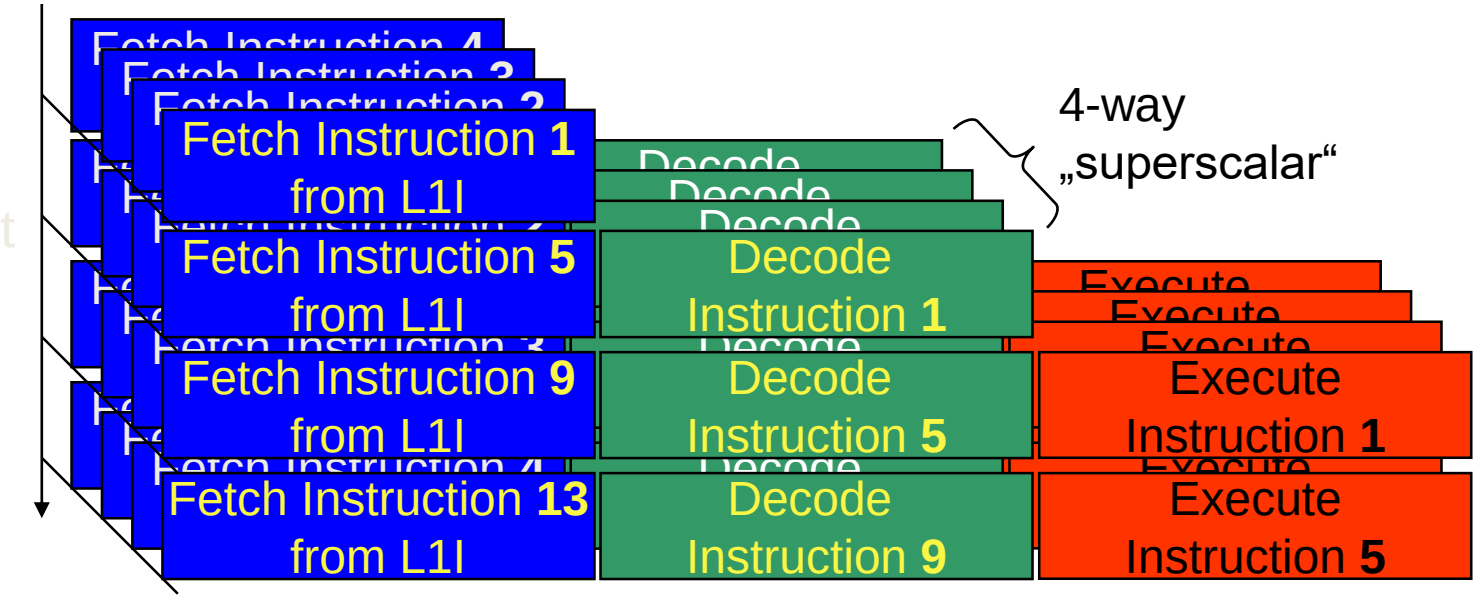
Hardware Pipelining on processor (all units can run concurrently):



…

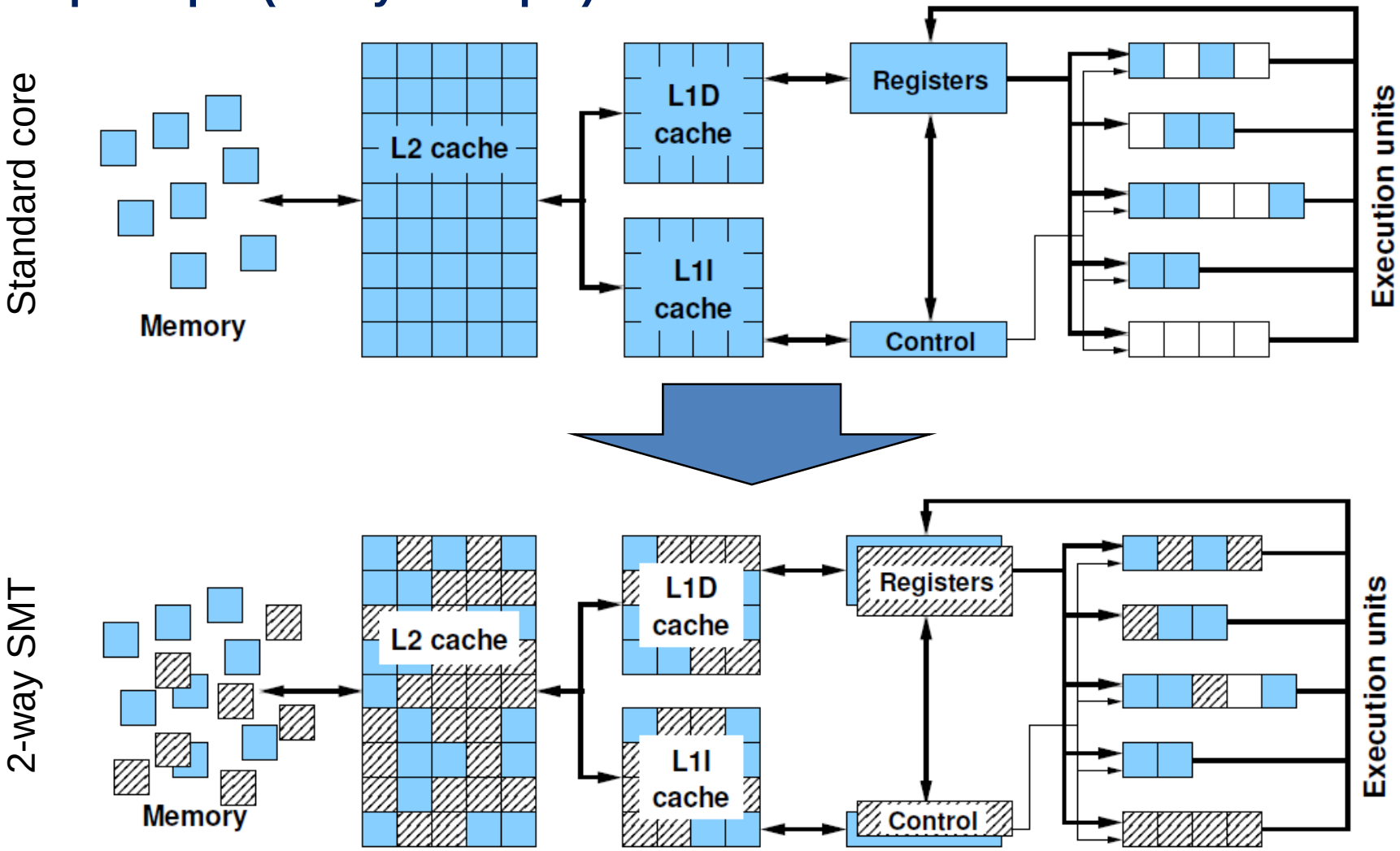
- Branches can stall this pipeline! (Speculative Execution, Predication)
- Each unit is pipelined itself (e.g., Execute = Multiply Pipeline)

- Multiple units enable use of Instrucion Level Parallelism (ILP): Instruction stream is “parallelized” on the fly



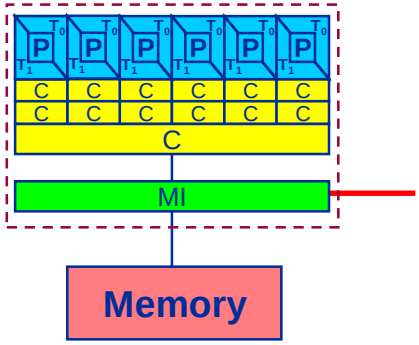
- Issuing m concurrent instructions per cycle: m-way superscalar
- Modern processors are 3- to 6-way superscalar & can perform 2 or 4 floating point operations per cycles

SMT principle (2-way example):



SMT impact

- SMT adds another layer of topology (inside the physical core)
- Caveat: SMT threads share all caches!
- Possible benefit: Better pipeline throughput
  - Filling otherwise unused pipelines
  - Filling pipeline bubbles with other thread's executing instructions:



Thread 0:

```
do i=1,N
  a(i) = a(i-1)*c
enddo
```

Thread 1:

```
do i=1,N
  b(i) = s*b(i-2)+d
enddo
```

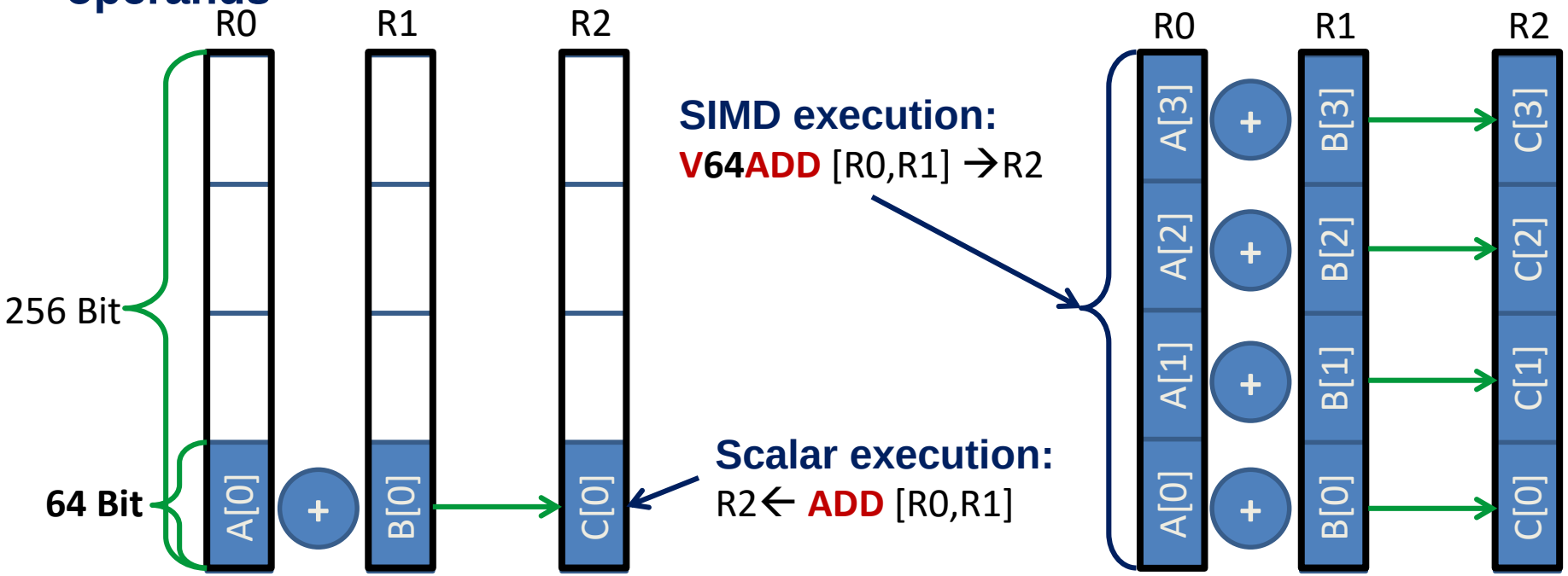
Dependency → pipeline stalls until previous MULT is over

Unrelated work in other thread can fill the pipeline bubbles

- Beware: Executing it all in a single thread (if possible) may achieve the same goal without SMT:

```
do i=1,N
  a(i) = a(i-1)*c
  b(i) = s*b(i-2)+d
enddo
```

- **Single Instruction Multiple Data (SIMD) operations allow the concurrent execution of the same operation on "wide" registers**
- **x86 SIMD instruction sets:**
  - SSE: register width = 128 Bit → 2 double precision floating point operands
  - AVX: register width = 256 Bit → 4 double precision floating point operands
- **Adding two registers holding double precision floating point operands**



- Steps (done by the compiler) for "SIMD processing"

```
for(int i=0; i<n;i++)
        C[i]=A[i]+B[i];
```

"Loop unrolling"

```
for(int i=0; i<n;i+=4){
        C[i]   =A[i]   +B[i];
        C[i+1]=A[i+1]+B[i+1];
        C[i+2]=A[i+2]+B[i+2];
        C[i+3]=A[i+3]+B[i+3];}
//remainder loop handling
```

Load 256 Bits starting from address of `A[i]` to register `R0`

Add the corresponding 64 Bit entries in `R0` and `R1` and store the 4 results to `R2`

Store `R2` (256 Bit) to address starting at `C[i]`

```
LABEL1:
        VLOAD R0 ← A[i]
        VLOAD R1 ← B[i]
        V64ADD[R0,R1] → R2
        VSTORE R2 → C[i]
        i←i+4
        i<(n-4)? JMP LABEL1
//remainder loop handling
```

- **No SIMD vectorization for loops with data dependencies:**

```
for(int i=0; i<n;i++)
        A[i]=A[i-1]*s;
```

- **"Pointer aliasing" may prevent SIMDfication**

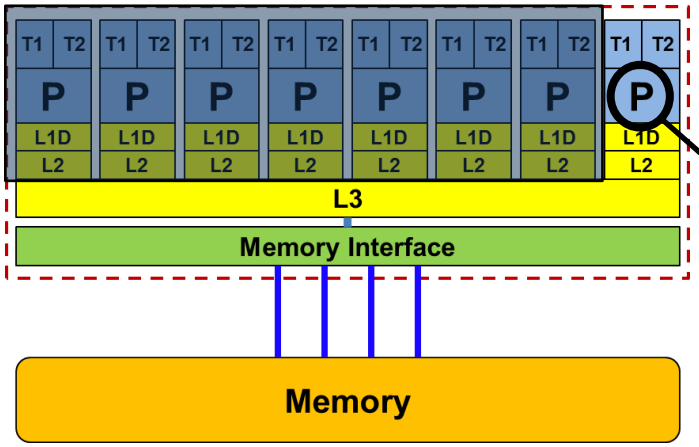
```
void f(double *A, double *B, double *C, int n) {
        for(int i=0; i<n; ++i)
           C[i] = A[i] + B[i];
}
```

  - C/C++ allows that `A → &C[-1]` and `B → &C[-2]`
    → `C[i] = C[i-1] + C[i-2]`: **dependency → No SIMD**

  - **If "pointer aliasing" does not happen, tell it to the compiler:**
    - `-fno-alias` (Intel), `-Msafeptr` (PGI), `-fargument-noalias` (gcc)
    - `restrict` keyword (C only!):

```
void f(double restrict *A, double restrict *B, double restrict *C, int n) {…}
```

There is no single driving force for single core performance!



Maximum floating point (FP) performance:

$$P_{core} = n_{super}^{FP} \cdot n_{FMA} \cdot n_{SIMD} \cdot f$$

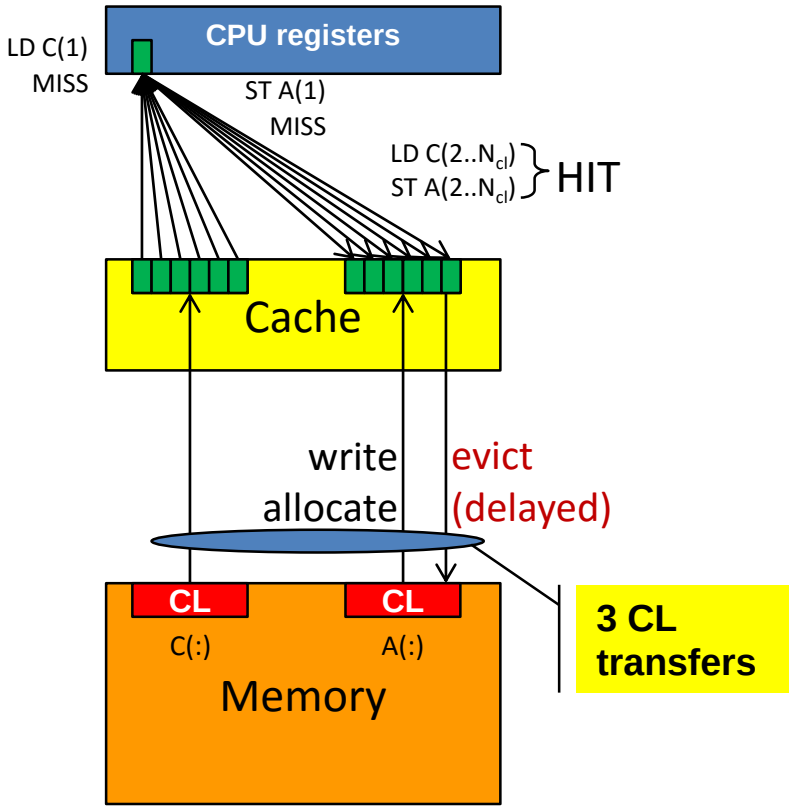
Super-scalarity | FMA factor | SIMD factor | Clock Speed

Typical representatives	n_{super}^{FP} inst./cy	n_{FMA}	n_{SIMD} ops/inst.		Code	f [GHz]	P_{core} [GF/s]
Nehalem	2	1	2	Q1/2009	X5570	2.93	11.7
Westmere	2	1	2	Q1/2010	X5650	2.66	10.6
Sandy Bridge	2	1	4	Q1/2012	E5-2680	2.7	21.6
Ivy Bridge	2	1	4	Q3/2013	E5-2660 v2	2.2	17.6
Haswell	2	2	4	Q3/2014	E5-2695 v3	2.3	36.8
Broadwell	2	2	4	Q1/2016	E5-2699 v4	2.2	35.2
IBM POWER8	2	2	2	Q2/2014	S822LC	2.93	23.4

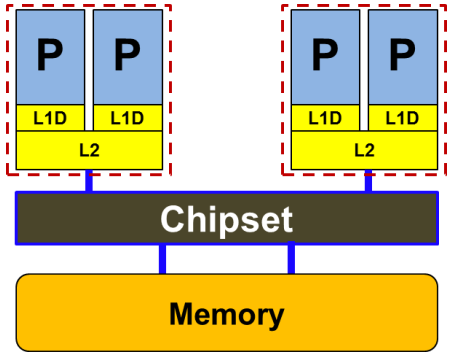
How does data travel from memory to the CPU and back?

- Remember: Caches are organized in cache lines (e.g., 64 bytes)
- Only complete cache lines are transferred between memory hierarchy levels (except registers)
- MISS: Load or store instruction does not find the data in a cache level
  → CL transfer required

- Example: Array copy `A(:)=C(:)`



Yesterday (2006): UMA



2-socket server

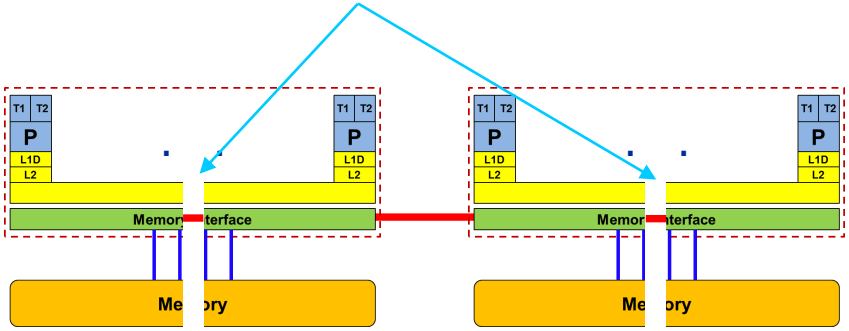
Uniform Memory Architecture (UMA)

Flat memory ; symmetric MPs

But: system “anisotropy”

Today: ccNUMA

Haswell(++): “Cluster on Die” (CoD) mode

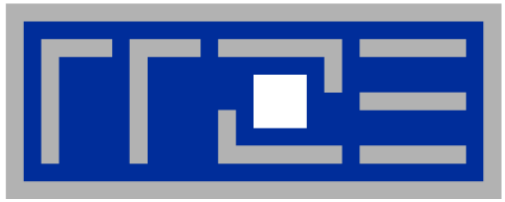


2-socket server

Cache-coherent Non-Uniform Memory Architecture (ccNUMA)

Two or more NUMA domains per node

ccNUMA provides scalable bandwidth but: *Where does my data finally end up?*



Interlude:
A glance at current accelerator technology

NVidia “Pascal” GP100

vs.

Intel Xeon Phi “Knights Landing”

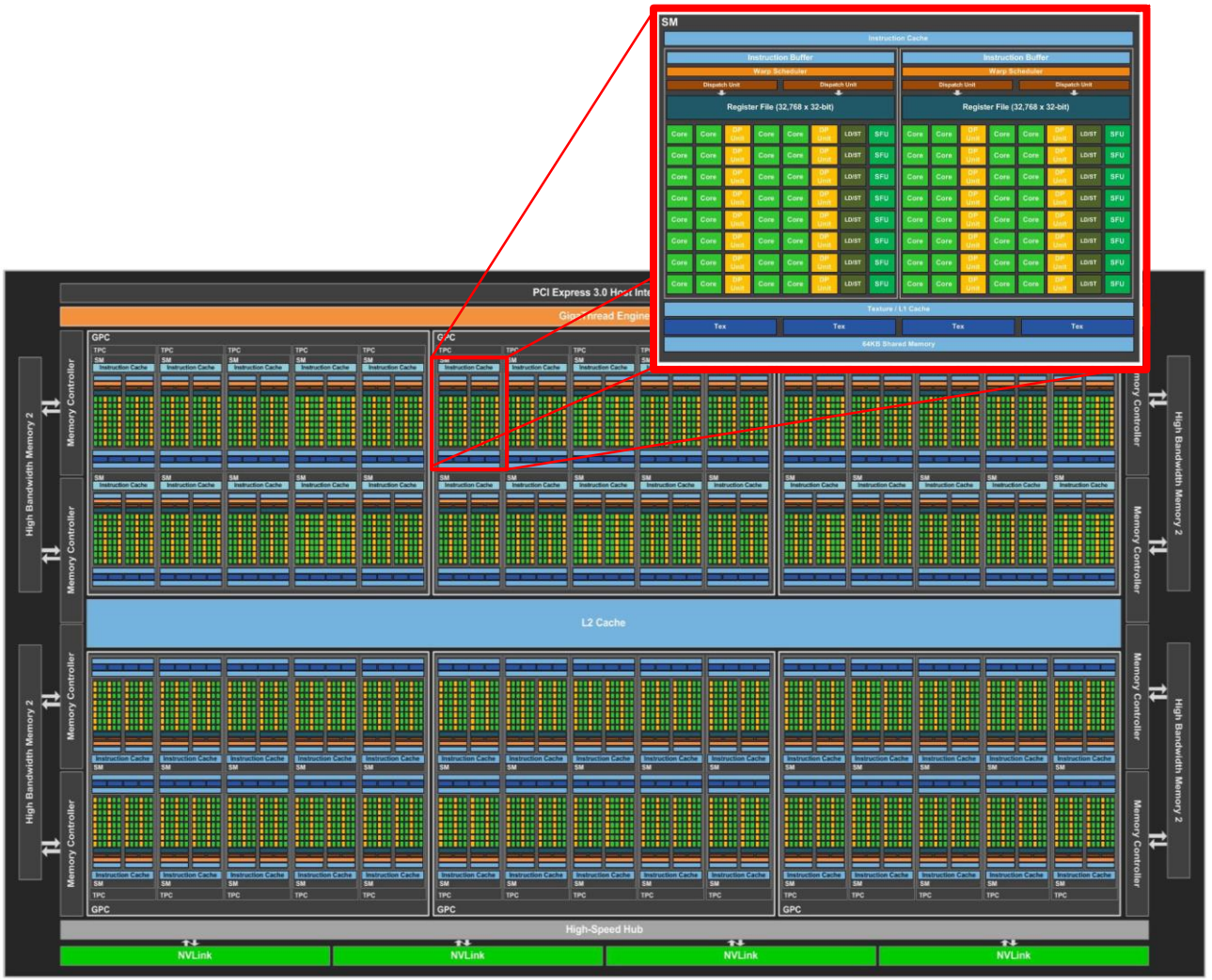
NVidia Pascal GP100 block diagram

updated

Architecture

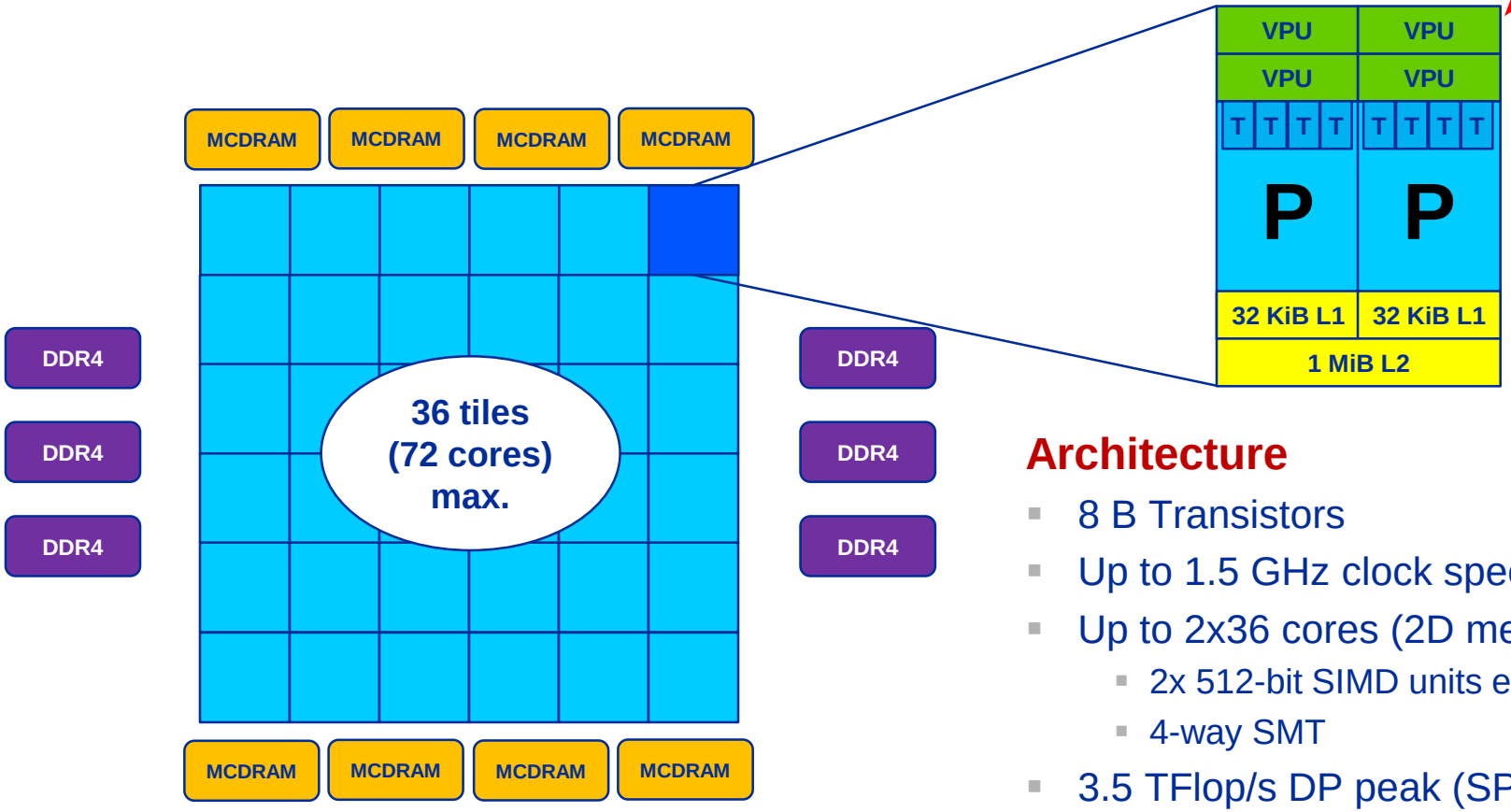
- 15.3 B Transistors
- ~ 1.4 GHz clock speed
- Up to 60 “SM” units
  - 64 (SP) “cores” each
- 5.7 TFlop/s DP peak
- 4 MB L2 Cache
- 4096-bit HBM2
- MemBW ~ 732 GB/s (theoretical)
- MemBW ~ 510 GB/s (measured)

- 2:1 SP:DP performance



© NVIDIA Corp.

Intel Xeon Phi “Knights Landing” block diagram



Architecture

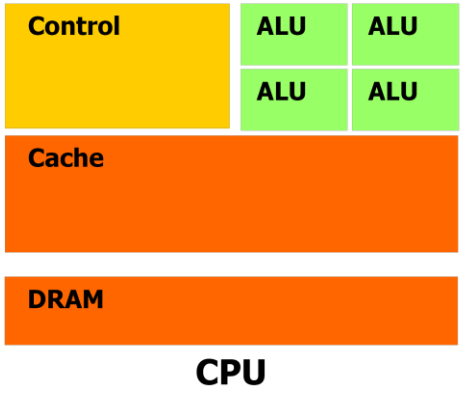
- 8 B Transistors
- Up to 1.5 GHz clock speed
- Up to 2x36 cores (2D mesh)
  - 2x 512-bit SIMD units each
  - 4-way SMT
- 3.5 TFlop/s DP peak (SP 2x)
- 36 MiB L2 Cache
- 16 GiB MCDRAM
  - MemBW ~ 470 GB/s (measured)
- Large DDR4 main memory
  - MemBW ~ 90 GB/s (measured)

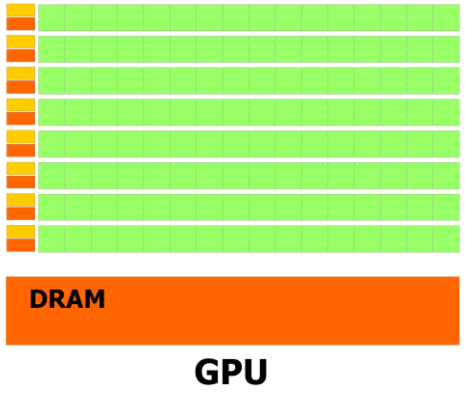
Trading single thread performance for parallelism:
GPGPUs vs. CPUs

updated

GPU vs. CPU
light speed estimate
(per device)

MemBW ~ 5-10x
Peak ~ 6-15x





	2x Intel Xeon E5-2697v4 “Broadwell”	Intel Xeon Phi 7250 “Knights Landing”	NVidia Tesla P100 “Pascal”
Cores@Clock	2 x 18 @ ≥2.3 GHz	68 @ 1.4 GHz	56 SMs @ ~1.3 GHz
SP Performance/core	≥73.6 GFlop/s	89.6 GFlop/s	~166 GFlop/s
Threads@STREAM	~8	~40	>8000?
SP peak	≥2.6 TFlop/s	6.1 TFlop/s	~9.3 TFlop/s
Stream BW (meas.)	2 x 62.5 GB/s	450 GB/s (HBM)	510 GB/s
Transistors / TDP	~2x7 Billion / 2x145 W	8 Billion / 215W	14 Billion/300W

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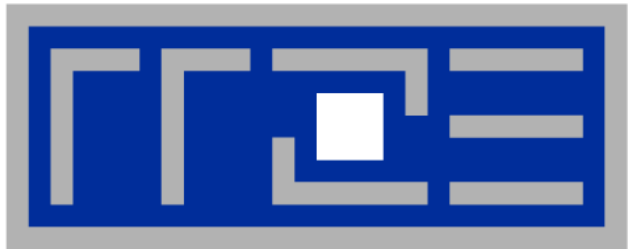
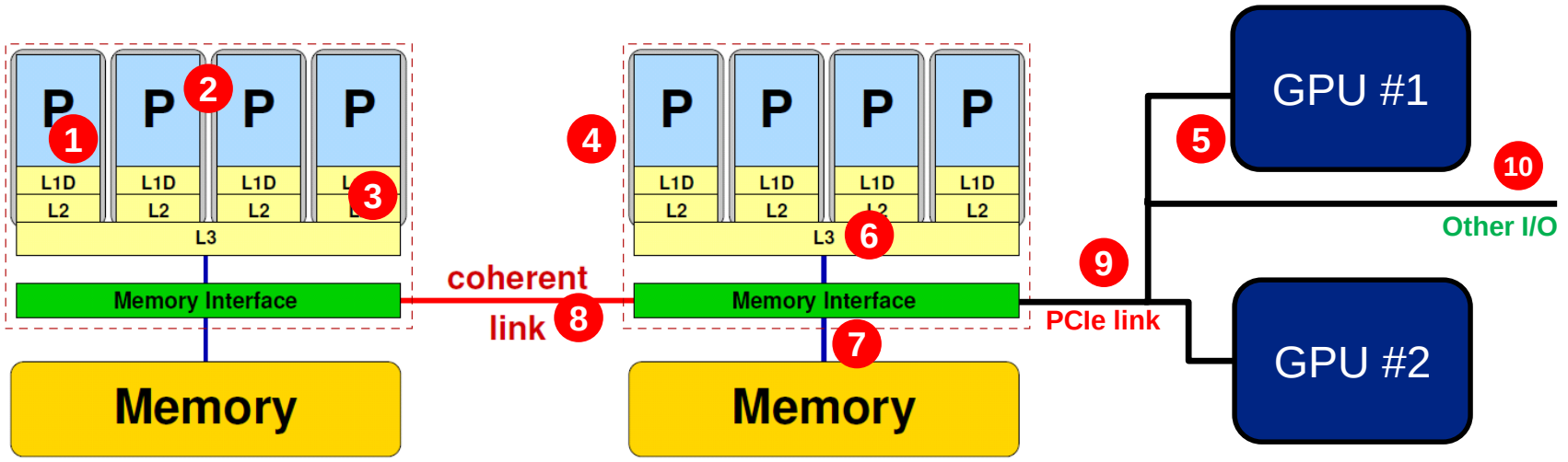


Node topology and programming models

Parallelism in a modern compute node

- **Parallel and shared resources within a shared-memory node**



Parallel resources:

- Execution/SIMD units 1
- Cores 2
- Inner cache levels 3
- Sockets / ccNUMA domains 4
- Multiple accelerators 5

Shared resources:

- Outer cache level per socket 6
- Memory bus per socket 7
- Intersocket link 8
- PCIe bus(es) 9
- Other I/O resources 10

How does your application react to all of those details?

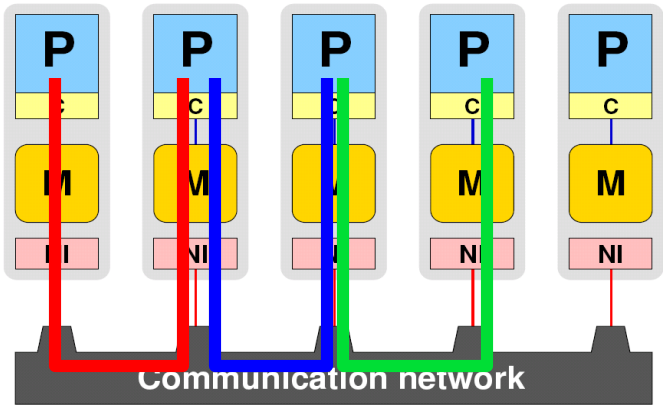
Parallel programming models
on modern compute nodes

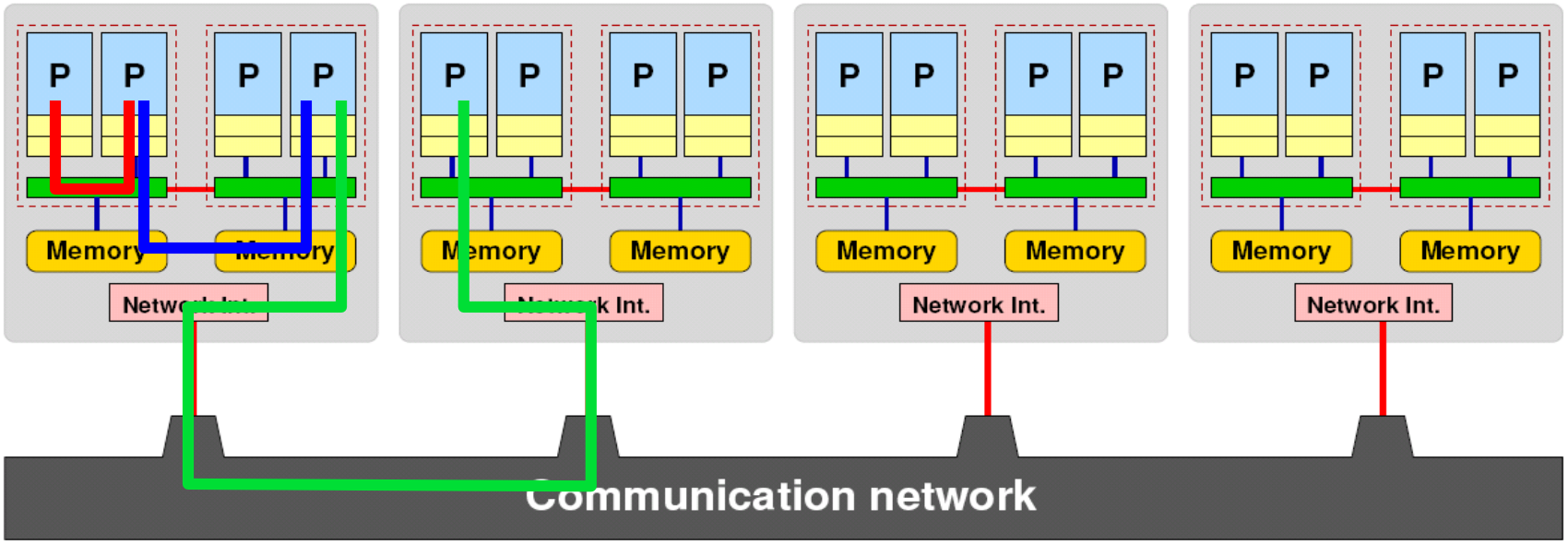
- **Shared-memory (intra-node)**
  - Good old MPI
  - OpenMP
  - POSIX threads
  - Intel Threading Building Blocks (TBB)
  - Cilk+, OpenCL, StarSs,… you name it
- **"Accelerated"**
  - OpenMP 4.0+
  - CUDA
  - OpenCL
  - OpenACC
- **Distributed-memory (inter-node)**
  - MPI
  - PGAS (CAF, UPC, …)
- **Hybrid**
  - Pure MPI + X, X == <you name it>

All models require awareness of *topology* and *affinity* issues for getting best performance out of the machine!

Parallel programming models:
Pure MPI

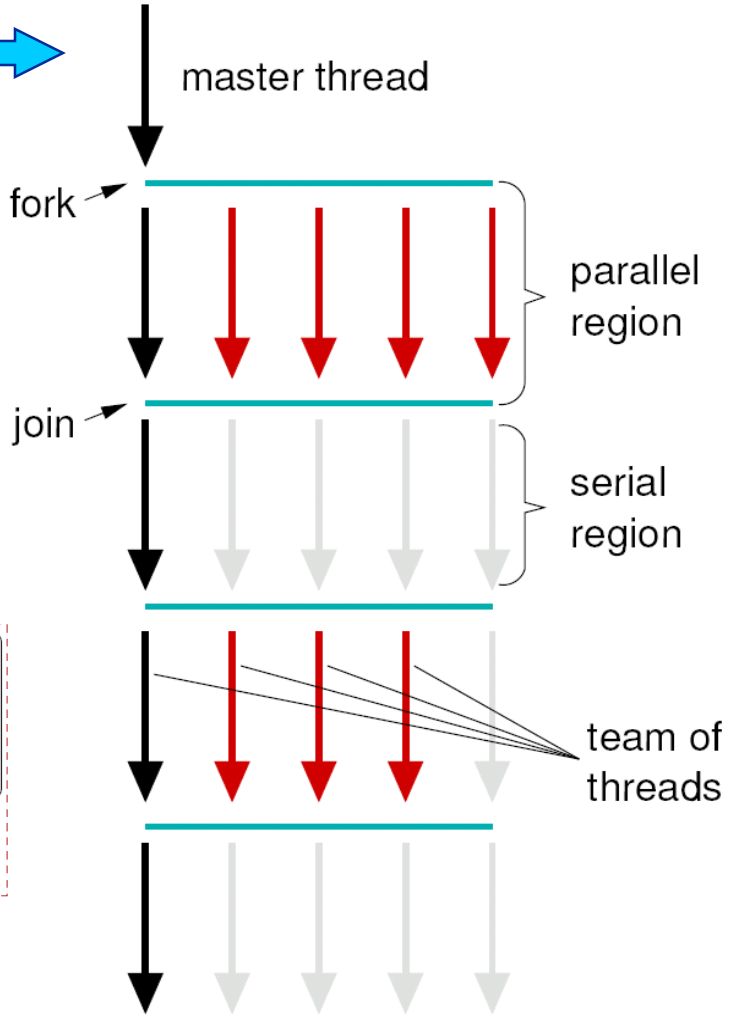
- **Machine structure is invisible to user:**
  - → Very simple programming model
  - → MPI "knows what to do"!?
- **Performance issues**
  - Intranode vs. internode MPI
  - Node/system topology

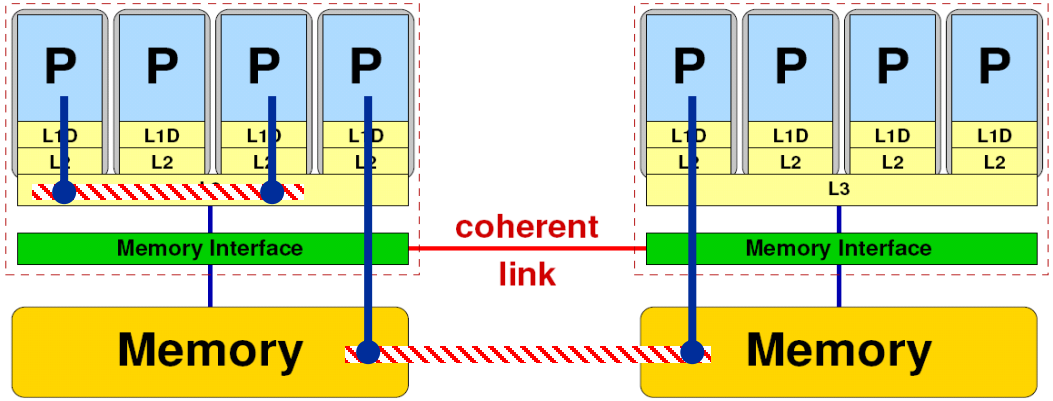




Parallel programming models:
Pure threading on the node

- **Machine structure is invisible to user**
  - → Very simple programming model
  - Threading SW (OpenMP, pthreads, TBB,…) should know about the details
- **Performance issues**
  - Synchronization overhead
  - Memory access
  - Node topology





Parallel programming models: Lots of choices

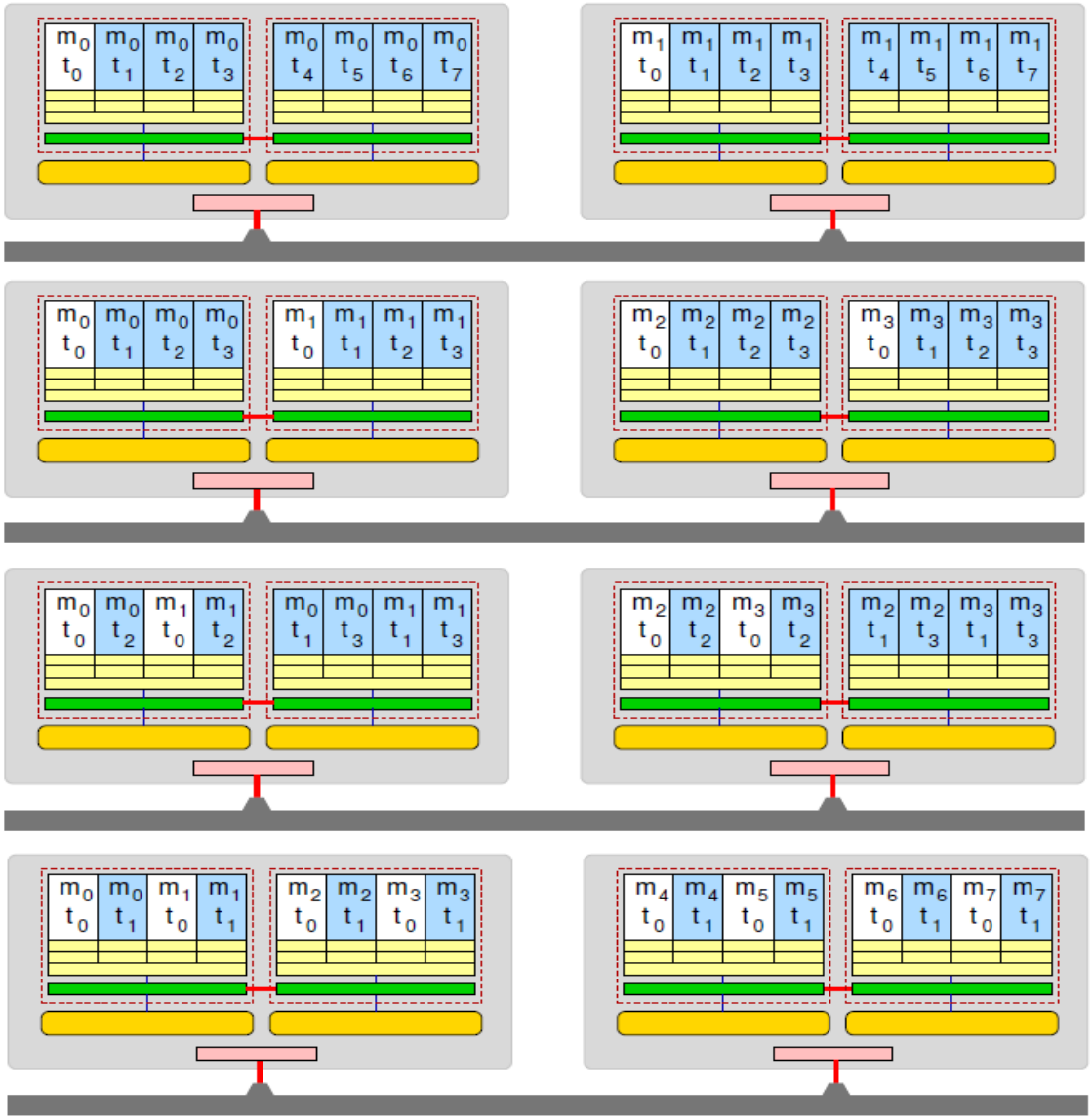
Hybrid MPI+OpenMP on a multicore multisocket cluster

One MPI process / node

One MPI process / socket:
OpenMP threads on same socket: **"blockwise"**

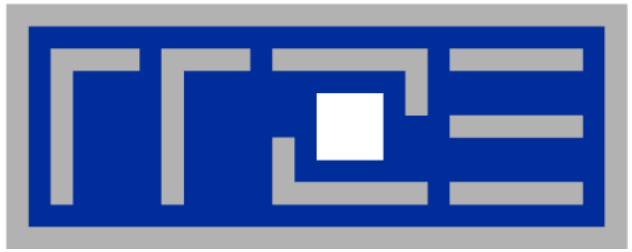
OpenMP threads pinned **"round robin"** across cores in node

Two MPI processes / socket
OpenMP threads on same socket



Conclusions about architecture

- **Modern computer architecture has a rich "topology"**
- **Node-level hardware parallelism takes many forms**
  - Sockets/devices – CPU: 1-8, GPGPU: 1-6
  - Cores – moderate (CPU: 4-16) to massive (GPGPU: 1000's)
  - SIMD – moderate (CPU: 2-8) to massive (GPGPU: 10's-100's)
  - Superscalarity (CPU: 2-6)
- **Exploiting performance: parallelism + bottleneck awareness**
  - **"High Performance Computing" == computing at a bottleneck**
- **Performance of programming models is sensitive to architecture**
  - Topology/affinity influences overheads
  - Standards do not contain (many) topology-aware features
  - Apart from overheads, performance features are largely independent of the programming model



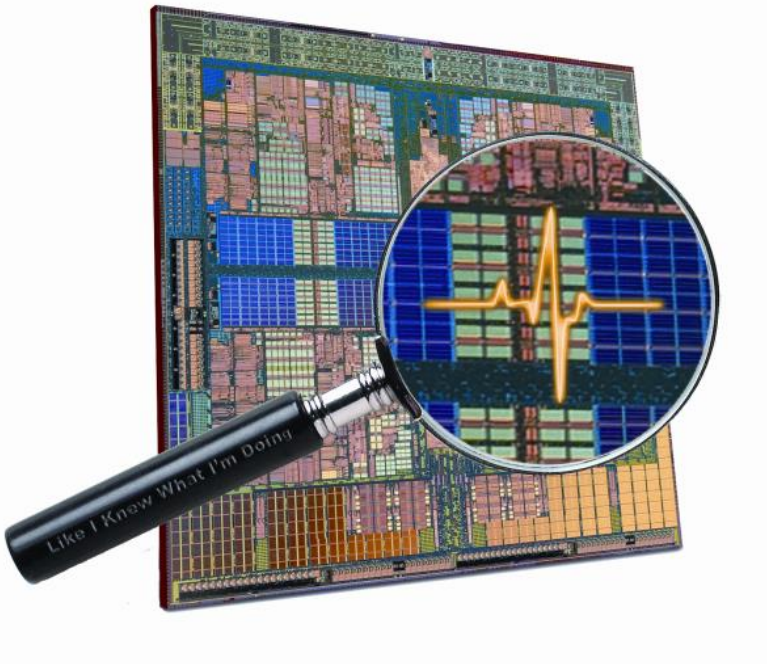
Multicore Performance and Tools

Tools for Node-level Performance Engineering

- Gather **Node Information**
  *hwloc, **likwid-topology**, likwid-powermeter*
- **Affinity control** and data placement
  *OpenMP and MPI runtime environments, hwloc, numactl, **likwid-pin***
- **Runtime Profiling**
  Compilers, gprof, HPC Toolkit, …
- **Performance Profilers**
  *Intel Vtune™, **likwid-perfctr**, PAPI based tools, Linux perf, …*
- **Microbenchmarking**
  *STREAM, **likwid-bench**, lmbench*

LIKWID tool suite:

Like
I
Knew
What
I'm
Doing



Open source tool collection (developed at RRZE):
https://github.com/RRZE-HPC/likwid

J. Treibig, G. Hager, G. Wellein: *LIKWID: A lightweight performance-oriented tool suite for x86 multicore environments.* PSTI2010, Sep 13-16, 2010, San Diego, CA http://arxiv.org/abs/1004.4431

Likwid Tool Suite

- **Command line tools for Linux:**
  - easy to install
  - works with standard linux kernel
  - simple and clear to use
  - supports Intel and AMD CPUs

- **Current tools:**
  - **likwid-topology**: Print thread and cache topology
  - **likwid-powermeter**: Measure energy consumption
  - **likwid-pin**: Pin threaded application without touching code
  - **likwid-perfctr:** Measure performance counters
  - **likwid-bench**: Microbenchmarking tool and environment
  - … some more

Output of `likwid-topology -g`

on one node of Intel Haswell-EP

```
--------------------------------------------------------------------------------
CPU name:       Intel(R) Xeon(R) CPU E5-2695 v3 @ 2.30GHz
CPU type:       Intel Xeon Haswell EN/EP/EX processor
CPU stepping:   2
********************************************************************************
Hardware Thread Topology
********************************************************************************
Sockets:                        2
Cores per socket:               14
Threads per core:               2
--------------------------------------------------------------------------------
HWThread        Thread          Core            Socket          Available
0               0               0               0               *
1                 0             1               0               *

...
43               1              1               1               *
44               1              2               1               *
--------------------------------------------------------------------------------
Socket 0:       ( 0 28 1 29 2 30 3 31 4 32 5 33 6 34 7 35 8 36 9 37 10 38 11 39 12 40 13 41 )
Socket 1:       ( 14 42 15 43 16 44 17 45 18 46 19 47 20 48 21 49 22 50 23 51 24 52 25 53 26 54 27 55 )
--------------------------------------------------------------------------------
********************************************************************************
Cache Topology
********************************************************************************
Level:                          1
Size:                           32 kB
Cache groups:   ( 0 28 ) ( 1 29 ) ( 2 30 ) ( 3 31 ) ( 4 32 ) ( 5 33 ) ( 6 34 ) ( 7 35 ) ( 8 36 ) ( 9 37 ) ( 10 38 ) ( 11 39 ) ( 12 40 ) ( 13 41
) ( 14 42 ) ( 15 43 ) ( 16 44 ) ( 17 45 ) ( 18 46 ) ( 19 47 ) ( 20 48 ) ( 21 49 ) ( 22 50 ) ( 23 51 ) ( 24 52 ) ( 25 53 ) ( 26 54 ) ( 27 55 )
--------------------------------------------------------------------------------
Level:                          2
Size:                           256 kB
Cache groups:   ( 0 28 ) ( 1 29 ) ( 2 30 ) ( 3 31 ) ( 4 32 ) ( 5 33 ) ( 6 34 ) ( 7 35 ) ( 8 36 ) ( 9 37 ) ( 10 38 ) ( 11 39 ) ( 12 40 ) ( 13 41
) ( 14 42 ) ( 15 43 ) ( 16 44 ) ( 17 45 ) ( 18 46 ) ( 19 47 ) ( 20 48 ) ( 21 49 ) ( 22 50 ) ( 23 51 ) ( 24 52 ) ( 25 53 ) ( 26 54 ) ( 27 55 )
--------------------------------------------------------------------------------
Level:                          3
Size:                           17 MB
Cache groups:   ( 0 28 1 29 2 30 3 31 4 32 5 33 6 34 ) ( 7 35 8 36 9 37 10 38 11 39 12 40 13 41 ) ( 14 42 15 43 16 44 17 45 18 46 19 47 20 48 )
( 21 49 22 50 23 51 24 52 25 53 26 54 27 55 )
--------------------------------------------------------------------------------
```

All physical processor IDs

Output of likwid-topology continued

```
********************************************************************************
NUMA Topology
********************************************************************************
NUMA domains:                   4
--------------------------------------------------------------------------------
Domain:                         0
Processors:             ( 0 28 1 29 2 30 3 31 4 32 5 33 6 34 )
Distances:                      10 21 31 31
Free memory:                    13292.9 MB
Total memory:                   15941.7 MB
--------------------------------------------------------------------------------
Domain:                         1
Processors:             ( 7 35 8 36 9 37 10 38 11 39 12 40 13 41 )
Distances:                      21 10 31 31
Free memory:                    13514 MB
Total memory:                   16126.4 MB
--------------------------------------------------------------------------------
Domain:                         2
Processors:             ( 14 42 15 43 16 44 17 45 18 46 19 47 20 48 )
Distances:                      31 31 10 21
Free memory:                    15025.6 MB
Total memory:                   16126.4 MB
--------------------------------------------------------------------------------
Domain:                         3
Processors:             ( 21 49 22 50 23 51 24 52 25 53 26 54 27 55 )
Distances:                      31 31 21 10
Free memory:                    15488.9 MB
Total memory:                   16126 MB
--------------------------------------------------------------------------------
```

Output of likwid-topology continued

Cluster on die mode and SMT enabled!

```
********************************************************************************
Graphical Topology
********************************************************************************
Socket 0:
+-----------------------------------------------------------------------------------------------------------------------------------------------------------------------+
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| |  0 28   | |  1 29   | |  2 30   | |  3 31   | |  4 32   | |  5 33   | |  6 34   | |  7 35   | |  8 36   | |  9 37   | | 10 38   | | 11 39   | | 12 40   | | 13 41   | |
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| | +-------------------------------------------------------------------------+ | +-------------------------------------------------------------------------------------+ | |
| | |                                   17MB                                  | | |                                   17MB                                              | | |
| | +-------------------------------------------------------------------------+ | +-------------------------------------------------------------------------------------+ | |
+-----------------------------------------------------------------------------------------------------------------------------------------------------------------------+
Socket 1:
+-----------------------------------------------------------------------------------------------------------------------------------------------------------------------+
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| | 14 42   | | 15 43   | | 16 44   | | 17 45   | | 18 46   | | 19 47   | | 20 48   | | 21 49   | | 22 50   | | 23 51   | | 24 52   | | 25 53   | | 26 54   | | 27 55   | |
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |  32kB   | |
| +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ +---------+ |
| |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |  256kB  | |
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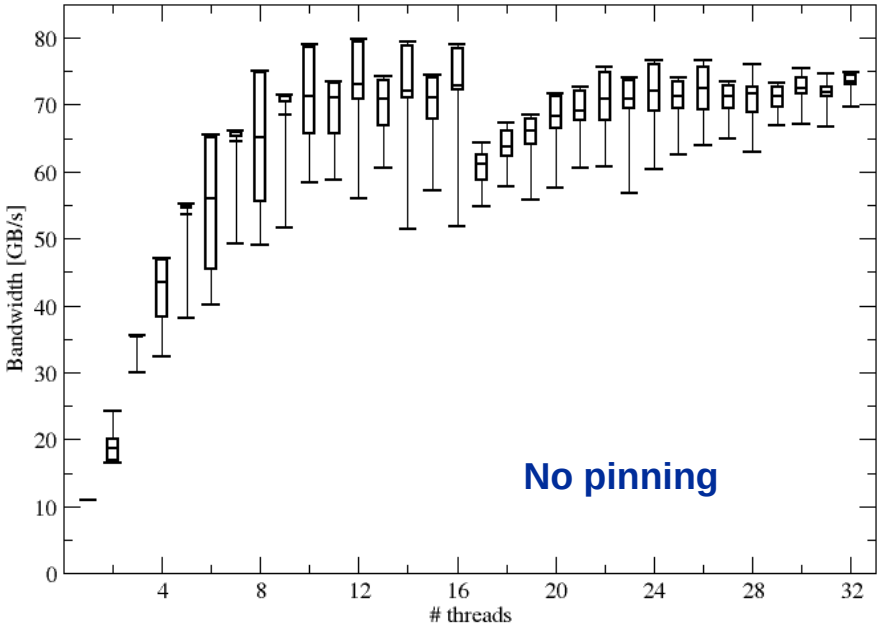
| | +-------------------------------------------------------------------------+ | +-------------------------------------------------------------------------------------+ | |
| | |                                   17MB                                  | | |                                   17MB                                              | | |
| | +-------------------------------------------------------------------------+ | +-------------------------------------------------------------------------------------+ | |
+-----------------------------------------------------------------------------------------------------------------------------------------------------------------------+
```

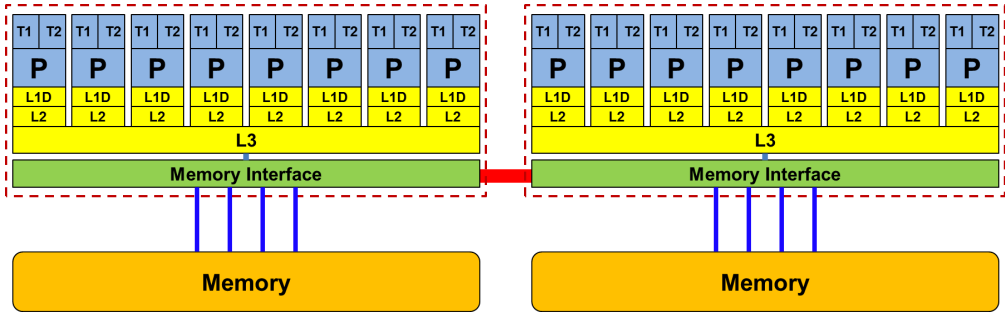
Enforcing thread/process-core affinity under the Linux OS

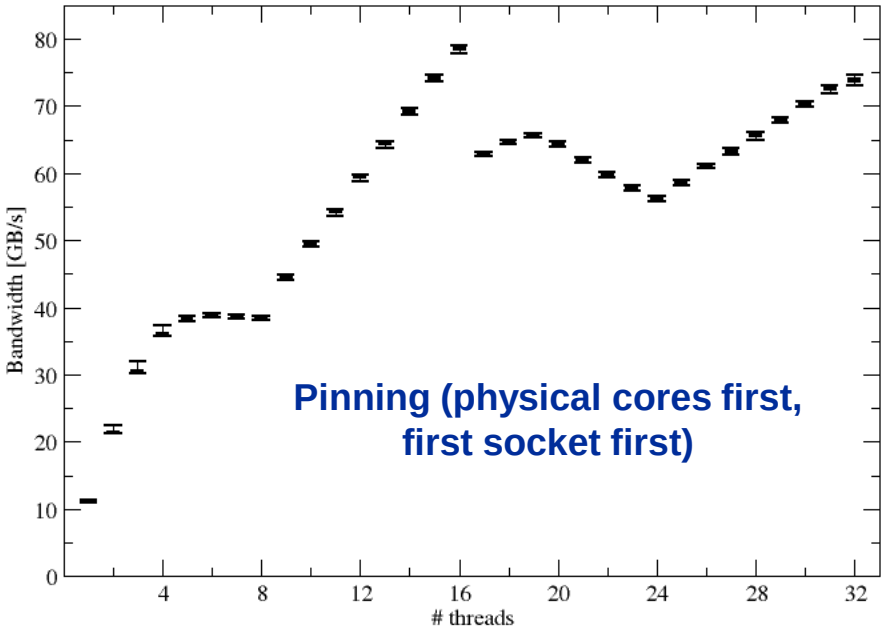
Standard tools and OS affinity facilities under program control

likwid-pin

Example: STREAM benchmark on 16-core Sandy Bridge:
Anarchy vs. thread pinning







There are several reasons for caring about affinity:

- **Eliminating performance variation**
- **Making use of architectural features**
- **Avoiding resource contention**

More thread/Process-core affinity ("pinning") options

- **Highly OS-dependent system calls**
  - But available on all systems

    Linux: `sched_setaffinity()`
    Windows: `SetThreadAffinityMask()`

- **Hwloc project** (http://www.open-mpi.de/projects/hwloc/)
- **Support for "semi-automatic" pinning in some compilers/environments**
  - All modern compilers with OpenMP support
  - Generic Linux: `taskset`, `numactl`, `likwid-pin` (see below)
  - OpenMP 4.0 (see OpenMP tutorial)
- **Affinity awareness in MPI libraries**
  - SGI MPT
  - OpenMPI
  - Intel MPI
  - …

Likwid-pin

Overview

- Pins processes and threads to specific cores without touching code
- Directly supports pthreads, gcc OpenMP, Intel OpenMP
- Based on combination of wrapper tool together with overloaded pthread library → binary must be dynamically linked!
- Can be used as a superior replacement for taskset
- Supports logical core numbering within a node

- Usage examples:
  - `likwid-pin -c 0-3,4,6  ./myApp parameters`
  - `likwid-pin -c S0:0-7  ./myApp parameters`
  - `likwid-pin -c N:0-15 ./myApp parameters`

- `OMP_NUM_THREADS` is set by the tool if not set explicitly

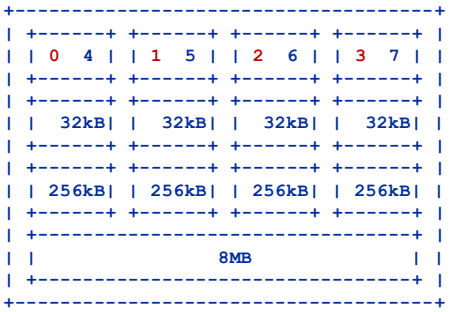
LIKWID terminology

Thread group syntax

- The OS numbers all processors (hardware threads) on a node
- The numbering is enforced at boot time by the BIOS and may have nothing to do with topological entities
- LIKWID concept: **thread group** consisting of HW threads sharing a topological entity (e.g., socket, shared cache,…)
- A thread group is defined by a single **character + index**

- Example:
  likwid-pin -c S1:0-3,6,7 ./a.out
- Group expression chaining with @:
  likwid-pin -c S0:0-3@S1:0-3 ./a.out

numbering across physical cores first within the group

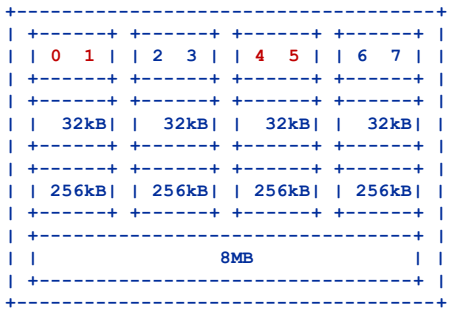


- Alternative expression based syntax:
  likwid-pin -c E:S0:4:2:4 ./a.out

E:<thread domain>:<num threads>:<chunk size>:<stride>

- Expression syntax is convenient for Xeon Phi:
  likwid-pin -c E:N:120:2:4 ./a.out

compact numbering within the group



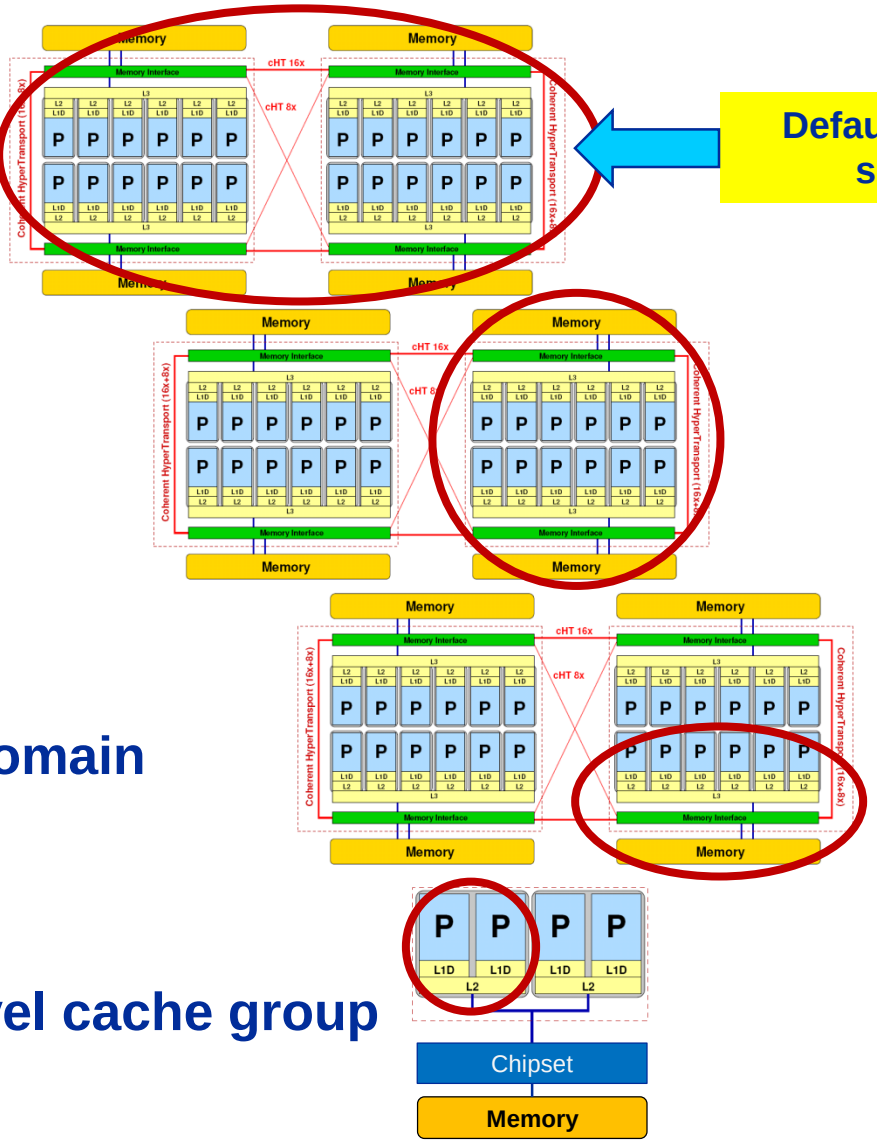
- **Possible unit prefixes**

N **node**

S **socket**

M **NUMA domain**

C **outer level cache group**



Default if –c is not specified!

- **Running the STREAM benchmark with likwid-pin:**

```
$ likwid-pin -c S0:0-3 ./stream
-------------------------------------------------
 Double precision appears to have 16 digits of accuracy
 Assuming 8 bytes per DOUBLE PRECISION word
-------------------------------------------------
 Array size =   20000000
 Offset     =         32
 The total memory requirement is  457 MB
 You are running each test  10 times
 --
 The *best* time for each test is used
 *EXCLUDING* the first and last iterations
[pthread wrapper] MAIN -> 0
[pthread wrapper] PIN_MASK: 0->1  1->2  2->3
[pthread wrapper] SKIP MASK: 0x1
        threadid 140668624234240 -> SKIP
        threadid 140668598843264 -> core 1 - OK
        threadid 140668594644992 -> core 2 - OK
        threadid 140668590446720 -> core 3 - OK

  [... rest of STREAM output omitted ...]
```

Main PID always pinned

Skip shepherd thread if necessary

Pin all spawned threads in turn

Intel KMP_AFFINITY environment variable

- **KMP_AFFINITY=[<*modifier*>,...]<*type*>[,<*permute*>][,<*offset*>]**

- **modifier**
  - granularity=<*specifier*> takes the following specifiers: fine, thread, and core
  - norespect
  - noverbose
  - proclist={<*proc-list*>}
  - respect
  - verbose

- **type (required)**
  - compact
  - disabled
  - explicit (**GOMP_CPU_AFFINITY**)
  - none
  - scatter

OS processor IDs

Respect an OS affinity mask in place

- **Default:**
  noverbose,respect,granularity=core

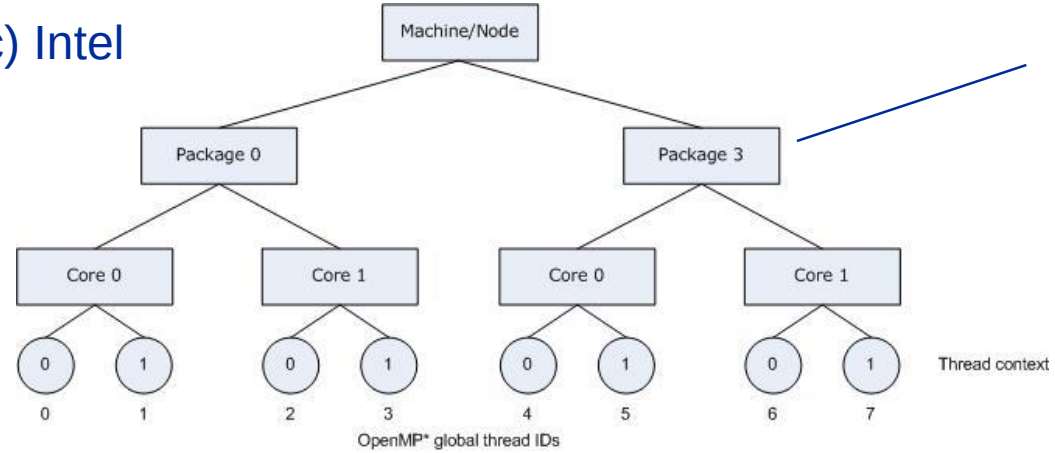
- **KMP_AFFINITY=verbose,none** to list machine topology map

Intel KMP_AFFINITY examples

optional

- **KMP_AFFINITY=granularity=fine,compact**

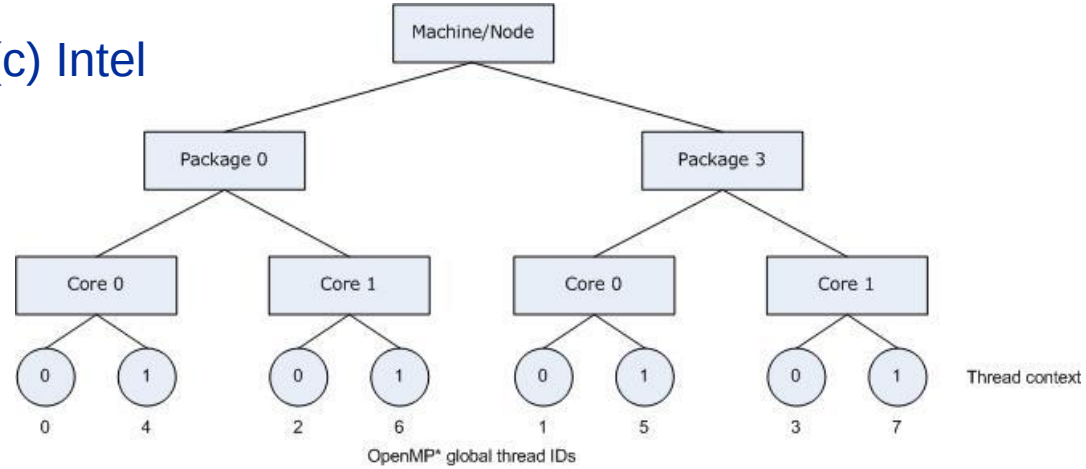
(c) Intel



Package means chip/socket

- **KMP_AFFINITY=granularity=fine,scatter**

(c) Intel

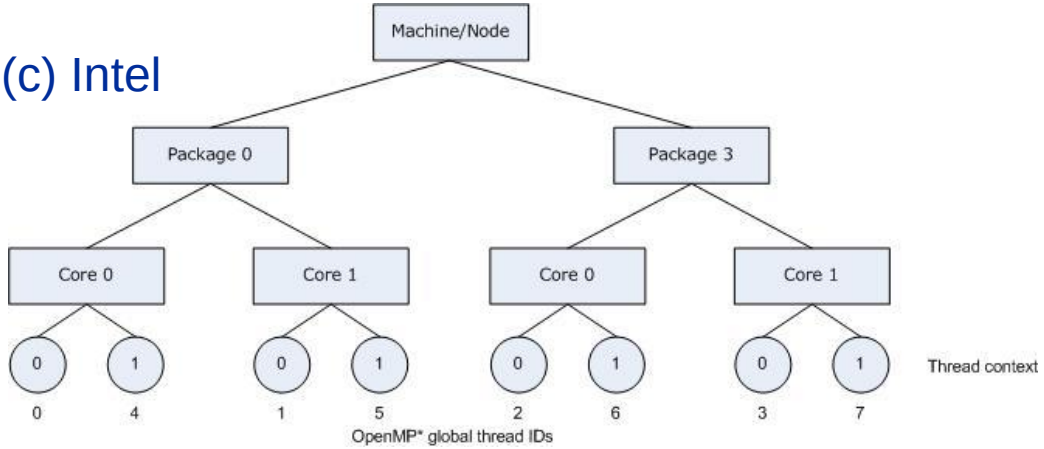


Intel KMP_AFFINITY permute example

optional

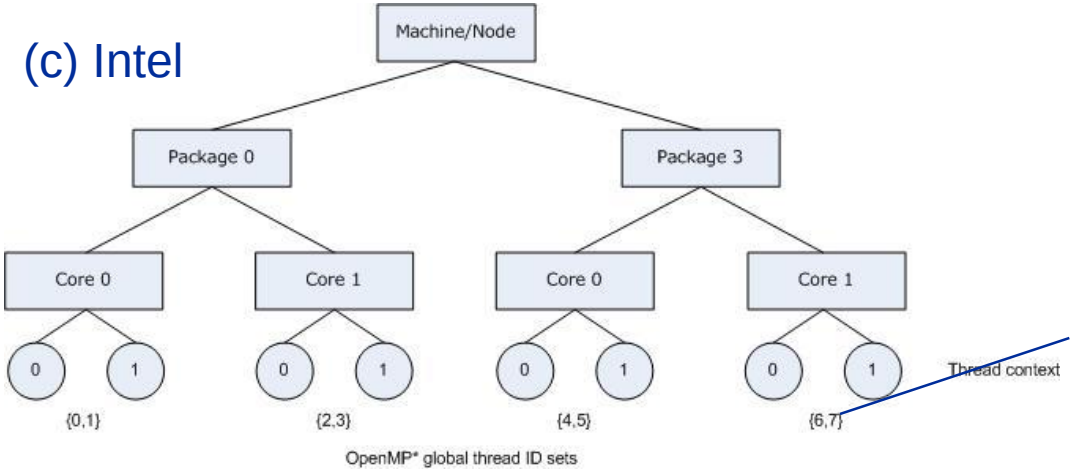
- **KMP_AFFINITY=granularity=fine,compact,1,0**

(c) Intel



- **KMP_AFFINITY=granularity=core,compact**

(c) Intel



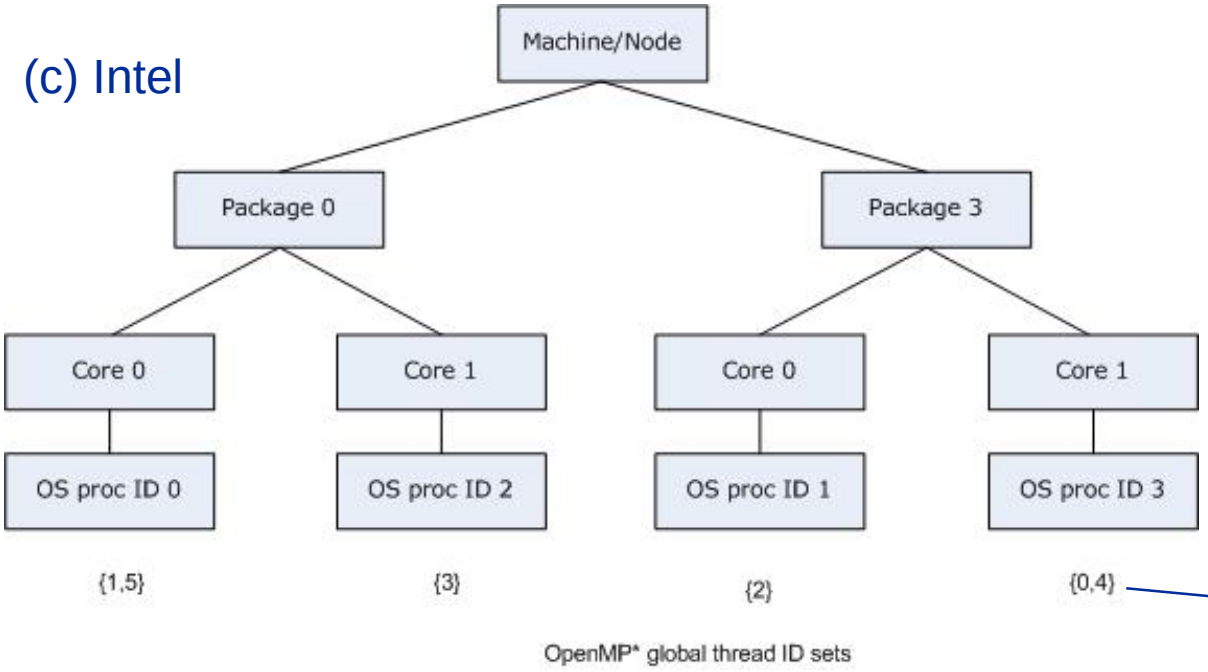
Threads may float within core

GNU GOMP_AFFINITY

optional

- **GOMP_AFFINITY=3,0-2 used with 6 threads**

(c) Intel



Round robin oversubscription

- **Always operates with OS processor IDs**

Multicore performance tools: Probing performance behavior

likwid-perfctr

1. Runtime profile / Call graph (gprof): Where are the hot spots?
2. Instrument hot spots (prepare for detailed measurement)
3. Find performance signatures

Possible signatures:

- Bandwidth saturation
- Instruction throughput limitation (real or language-induced)
- Latency impact (irregular data access, high branch ratio)
- Load imbalance
- ccNUMA issues (data access across ccNUMA domains)
- Pathologic cases (false cacheline sharing, expensive operations)

likwid-perfctr can help here

Goal: Come up with educated guess about a performance-limiting motif (Performance Pattern)

Probing performance behavior

- **How do we find out about the performance properties and requirements of a parallel code?**
  - Profiling via advanced tools is often overkill
- **A coarse overview is often sufficient**
  - likwid-perfctr (similar to “perfex” on IRIX, “hpmcount” on AIX, “lipfpm” on Linux/Altix)
  - Simple end-to-end measurement of hardware performance metrics
  - “Marker” API for starting/stopping counters
  - Multiple measurement region support
  - Preconfigured and extensible metric groups, list with **`likwid-perfctr -a`**

```
BRANCH: Branch prediction miss rate/ratio
CACHE: Data cache miss rate/ratio
CLOCK: Clock of cores
DATA: Load to store ratio
FLOPS_DP: Double Precision MFlops/s
FLOPS_SP: Single Precision MFlops/s
FLOPS_X87: X87 MFlops/s
L2: L2 cache bandwidth in MBytes/s
L2CACHE: L2 cache miss rate/ratio
L3: L3 cache bandwidth in MBytes/s
L3CACHE: L3 cache miss rate/ratio
MEM: Main memory bandwidth in MBytes/s
TLB: TLB miss rate/ratio
```

likwid-perfctr

Example usage with preconfigured metric group (shortened)

```
$ likwid-perfctr -C N:0-3 -g FLOPS_DP  ./stream.exe
--------------------------------------------------------------------------------
CPU name:       Intel(R) Xeon(R) CPU E5-2660 v2 @ 2.20GHz
CPU type:       Intel Xeon IvyBridge EN/EP/EX processor
CPU clock:      2.20 GHz
--------------------------------------------------------------------------------
[... YOUR PROGRAM OUTPUT ...]
--------------------------------------------------------------------------------
Group 1: FLOPS_DP
+-------------------------------------+---------+------------+------------+------------+-------
|                Event                | Counter |   Core 0   |   Core 1   |   Core 2   |  Core
+-------------------------------------+---------+------------+------------+------------+-------
|          INSTR_RETIRED_ANY          |  FIXC0  |  521332883 |  523904122 |  519696583 |  519193
|        CPU_CLK_UNHALTED_CORE        |  FIXC1  | 1379625927 | 1381900036 | 1378355460 | 1376447
|        CPU_CLK_UNHALTED_REF         |  FIXC2  | 1389460886 | 1393031508 | 1387504228 | 1385276
| FP_COMP_OPS_EXE_SSE_FP_PACKED_DOUBLE|   PMC0  |  176216849 |  176176025 |  177432054 |  176367
| FP_COMP_OPS_EXE_SSE_FP_SCALAR_DOUBLE|   PMC1  |    1554    |     599    |     72     |    27
|       SIMD_FP_256_PACKED_DOUBLE     |   PMC2  |      0     |       0    |      0     |     0
+-------------------------------------+---------+------------+------------+------------+-------

+----------------------+-----------+-----------+-----------+--------------+
|        Metric        |   Core 0  |   Core 1  |   Core 2  |    Core 3    |
+----------------------+-----------+-----------+-----------+--------------+
|  Runtime (RDTSC) [s] |   0.6856  |   0.6856  |   0.6856  |    0.6856    |
| Runtime unhalted [s] |   0.6270  |   0.6281  |   0.6265  |    0.6256    |
|      Clock [MHz]     | 2184.6742 | 2182.6664 | 2185.7404 |   2186.2243  |
|          CPI         |   2.6463  |   2.6377  |   2.6522  |    2.6511    |
|        MFLOP/s       |  514.0890 |  513.9685 |  517.6320 |   514.5273   |
|      AVX MFLOP/s     |      0    |      0    |      0    |       0      |
|    Packed MUOPS/s    |  257.0434 |  256.9838 |  258.8160 |   257.2636   |
|    Scalar MUOPS/s    |   0.0023  |   0.0009  |   0.0001  | 3.938426e-05 |
+----------------------+-----------+-----------+-----------+--------------+
```

Always measured

Configured metrics (this group)

Derived metrics

likwid-perfctr

Marker API (C/C++ and Fortran)

- A **marker API** is available to restrict measurements to code regions
- The API only turns counters on/off. The configuration of the counters is still done by **`likwid-perfctr`**
- Multiple named region support, accumulation over multiple calls
- Inclusive and overlapping regions allowed

```
#include <likwid.h>
. . .
LIKWID_MARKER_INIT;                    // must be called from serial region
#pragma omp parallel
{
  LIKWID_MARKER_THREADINIT;            // only reqd. if measuring multiple threads
}
. . .
LIKWID_MARKER_START("Compute");
. . .
LIKWID_MARKER_STOP("Compute");
. . .
LIKWID_MARKER_START("Postprocess");
. . .
LIKWID_MARKER_STOP("Postprocess");
. . .
LIKWID_MARKER_CLOSE;                   // must be called from serial region
```

- **Activate macros with `-DLIKWID_PERFMON`**
- **Run `likwid-perfctr` with `-m` option to activate markers**

Things to look at (in roughly this order)

- Excess work
- Load balance (flops, instructions, BW)
- In-socket memory BW saturation
- Flop/s, loads and stores per flop metrics
- SIMD vectorization
- CPI metric
- # of instructions,
  branches, mispredicted branches

Caveats

- Load imbalance may not show in CPI or # of instructions
  - Spin loops in OpenMP barriers/MPI blocking calls
  - Looking at “top” or the Windows Task Manager does not tell you anything useful
- In-socket performance saturation may have various reasons
- Cache miss metrics are sometimes misleading

Measuring energy consumption with LIKWID

Measuring energy consumption

likwid-powermeter and likwid-perfctr -g ENERGY

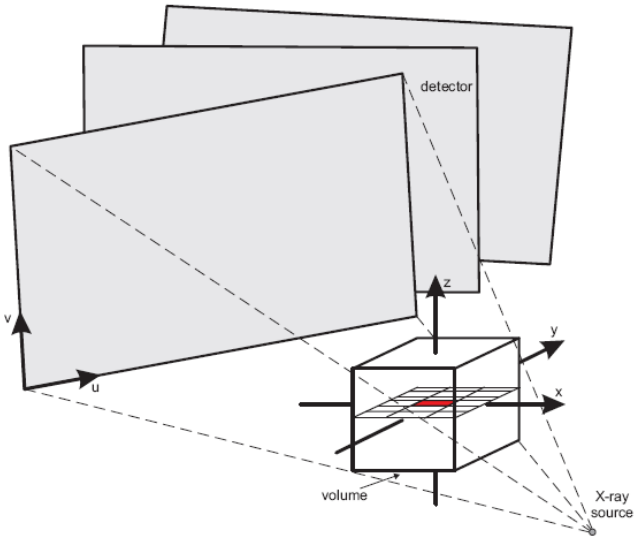
- **Implements Intel RAPL interface (Sandy Bridge)**
- **RAPL = “Running average power limit”**

```
-------------------------------------------------------------
CPU name:       Intel Core SandyBridge processor
CPU clock:      3.49 GHz
-------------------------------------------------------------
Base clock:     3500.00 MHz
Minimal clock:  1600.00 MHz
Turbo Boost Steps:
C1 3900.00 MHz
C2 3800.00 MHz
C3 3700.00 MHz
C4 3600.00 MHz
-------------------------------------------------------------
Thermal Spec Power: 95 Watts
Minimum  Power: 20 Watts
Maximum  Power: 95 Watts
Maximum  Time Window: 0.15625 micro sec
-------------------------------------------------------------
```

Example:

A medical image reconstruction code on Sandy Bridge

optional



Sandy Bridge EP (8 cores, 2.7 GHz base freq.)

Test case	Runtime [s]	Power [W]	Energy [J]
8 cores, plain C	**90.43**	90	8110
8 cores, SSE	29.63	93	2750
8 cores (SMT), SSE	22.61	102	2300
8 cores (SMT), AVX	**18.42**	111	2040

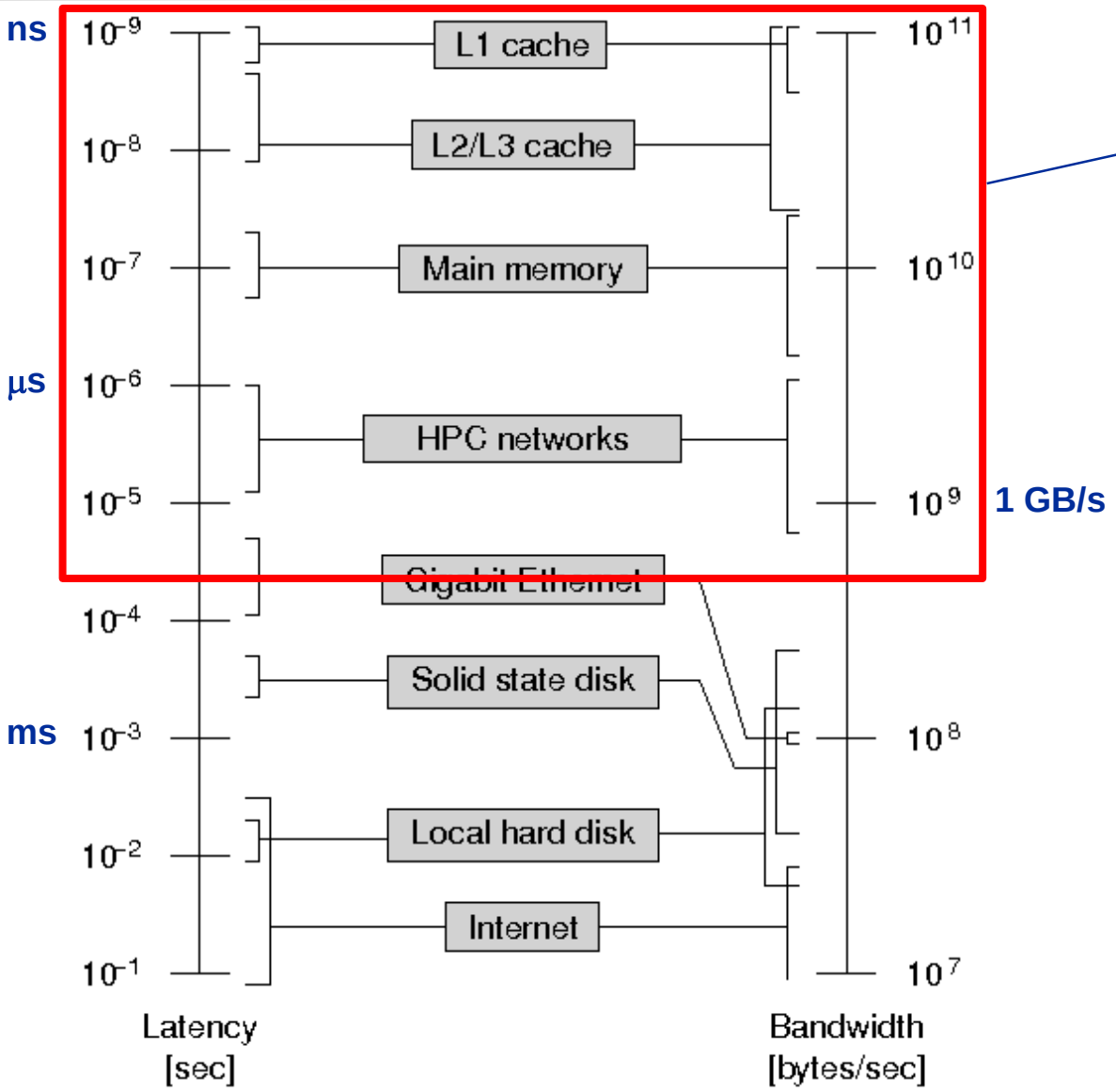
Faster code ➘ less energy

Microbenchmarking for architectural exploration (and more)

Probing of the memory hierarchy

Saturation effects in cache and memory

Latency and bandwidth in modern computer environments

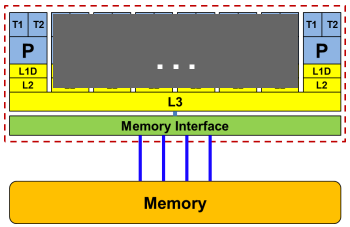


HPC plays here

Avoiding slow data paths is the key to most performance optimizations!

Intel Xeon E5 multicore processors

Microarchitecture	SandyBridge-EP	IvyBridge-EP	Haswell-EP
Shorthand	SNB	IVB	HSW
Xeon Model	E5-2680	E5-2690 v2	E5-2695 v3
Year	03/2012	09/2013	09/2014
Clock speed (fixed)	2.7 GHz	2.2 GHz	2.3 GHz
Cores/Threads	8/16	10/20	14/28
Load/Store throughput per cycle			
AVX(2)	1 LD & 1/2 ST	1 LD & 1/2 ST	2 LD & 1 ST
SSE/scalar	2 LD ‖ 1 LD & 1 ST	2 LD ‖ 1 LD & 1 ST	2 LD & 1 ST
L1 port width	2×16+1×16 B	2×16+1×16 B	2×32+1×32 B
ADD throughput	1 / cy	1 / cy	1 / cy
MUL throughput	1 / cy	1 / cy	2 / cy
FMA throughput	n/a	n/a	2 / cy
L2-L1 data bus	32 B	32 B	64 B
L3-L2 data bus	32 B	32 B	32 B
LLC size	20 MiB	25 MiB	35 MiB
Main memory	4×DDR3-1600	4×DDR3-1866	4×DDR4-2133
Peak memory BW	51.2 GB/s	51.2 GB/s	68.3 GB/s
Load-only BW	43.6 GB/s (85%)	46.1 GB/s (90%)	60.6 GB/s (89%)
T_{L3Mem} per CL	3.96 cy	3.05 cy	2.43 cy



FP instructions throughput per core

Max. data transfer per cycle between caches

Peak main memory bandwidth

Simple streaming benchmark:

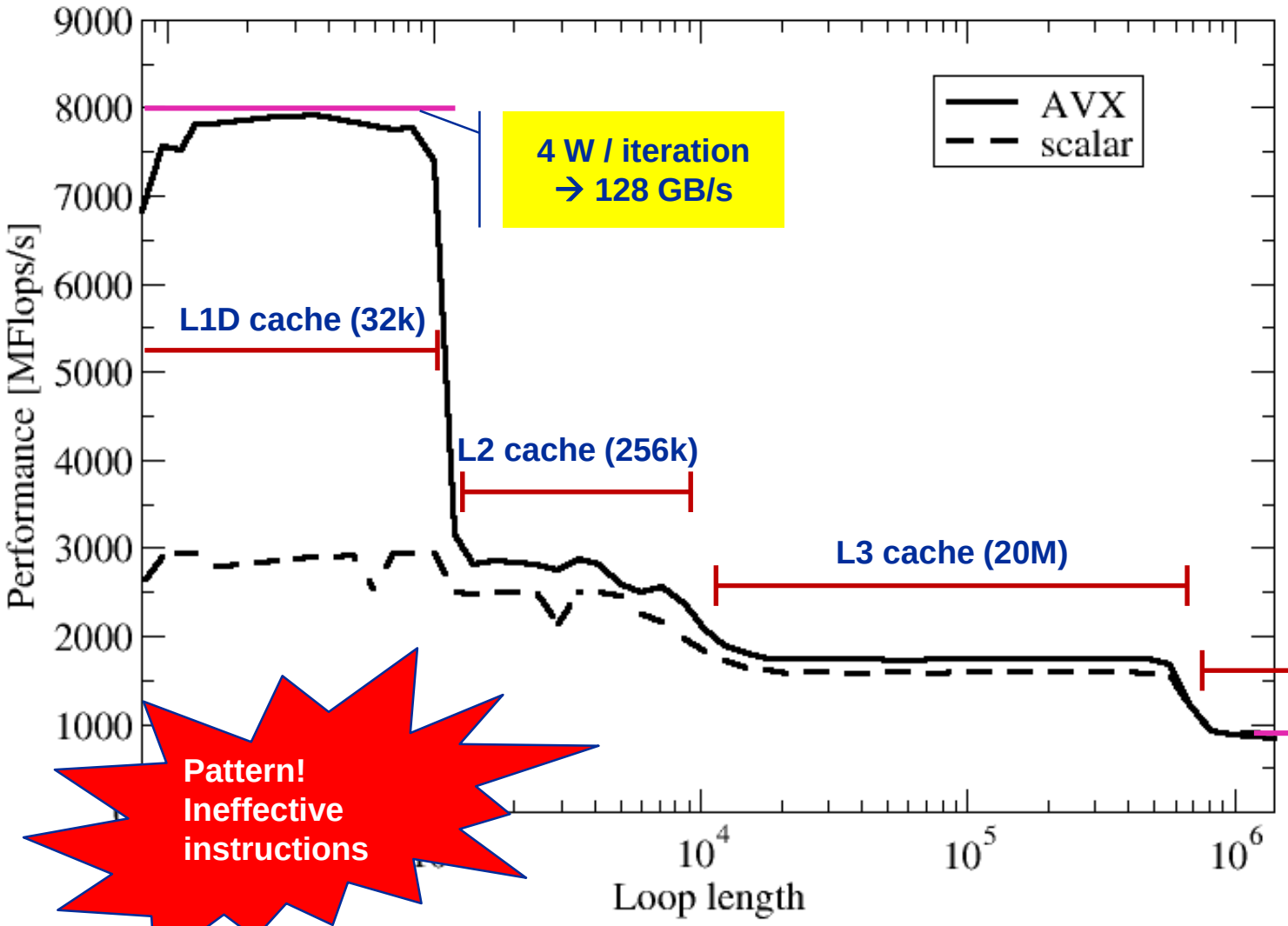
```
double precision, dimension(N) :: A,B,C,D
A=1.d0; B=A; C=A; D=A

do j=1,NITER
  do i=1,N
    A(i) = B(i) + C(i) * D(i)
  enddo
  if(.something.that.is.never.true.) then
    call dummy(A,B,C,D)
  endif
enddo
```

Prevents smarty-pants compilers from doing "clever" stuff

- Report performance for different N
- Choose NITER so that accurate time measurement is possible
- This kernel is limited by data transfer performance for all memory levels on all current architectures!

A(:)=B(:)+C(:)*D(:) on one Sandy Bridge core (3 GHz)



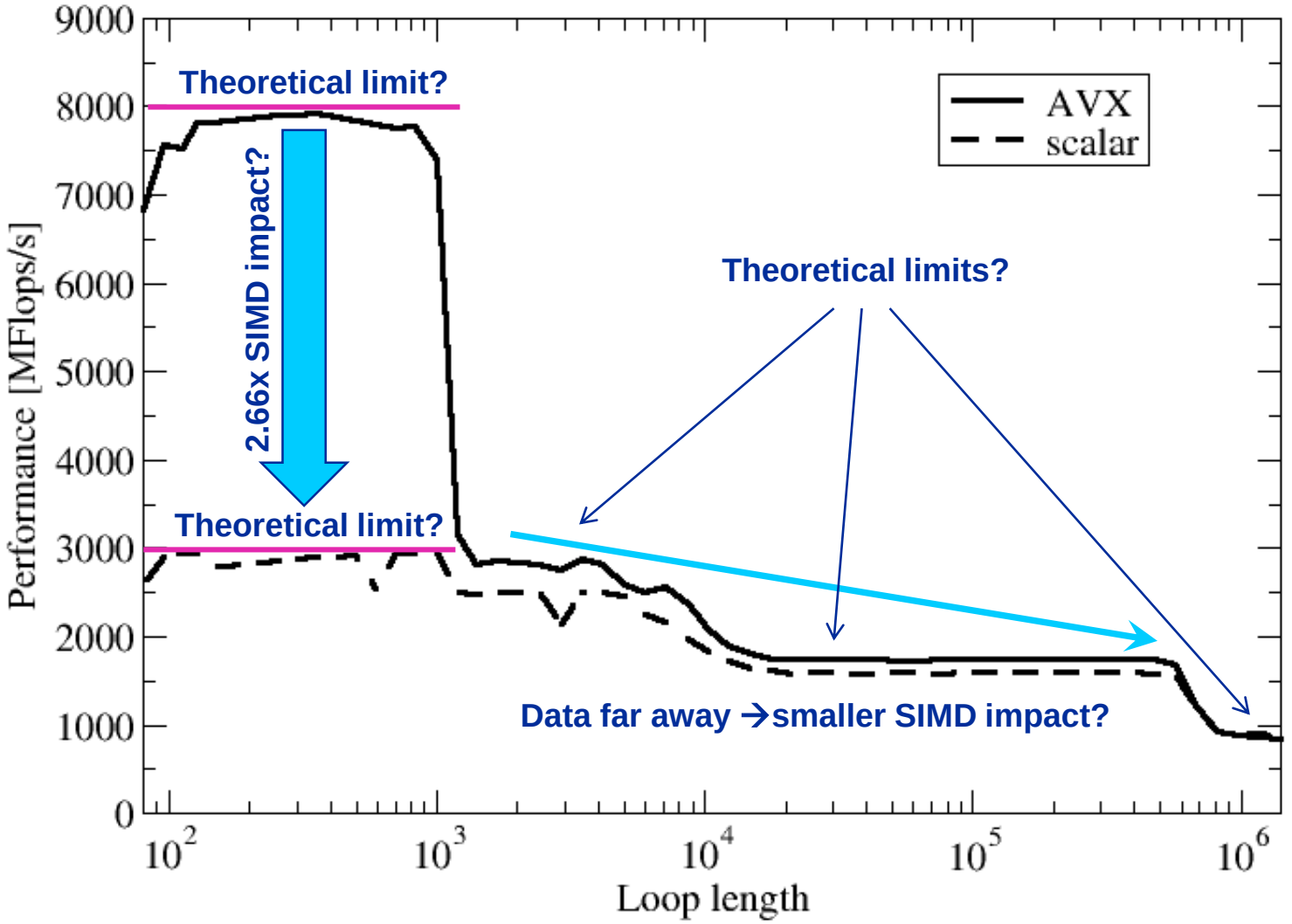
Are the performance levels plausible?

What about multiple cores?

Do the bandwidths scale?

`A(:)=B(:)+C(:)*D(:)` on one Sandy Bridge core (3 GHz):

Observations and further questions



See later for answers!

The throughput-parallel vector triad benchmark

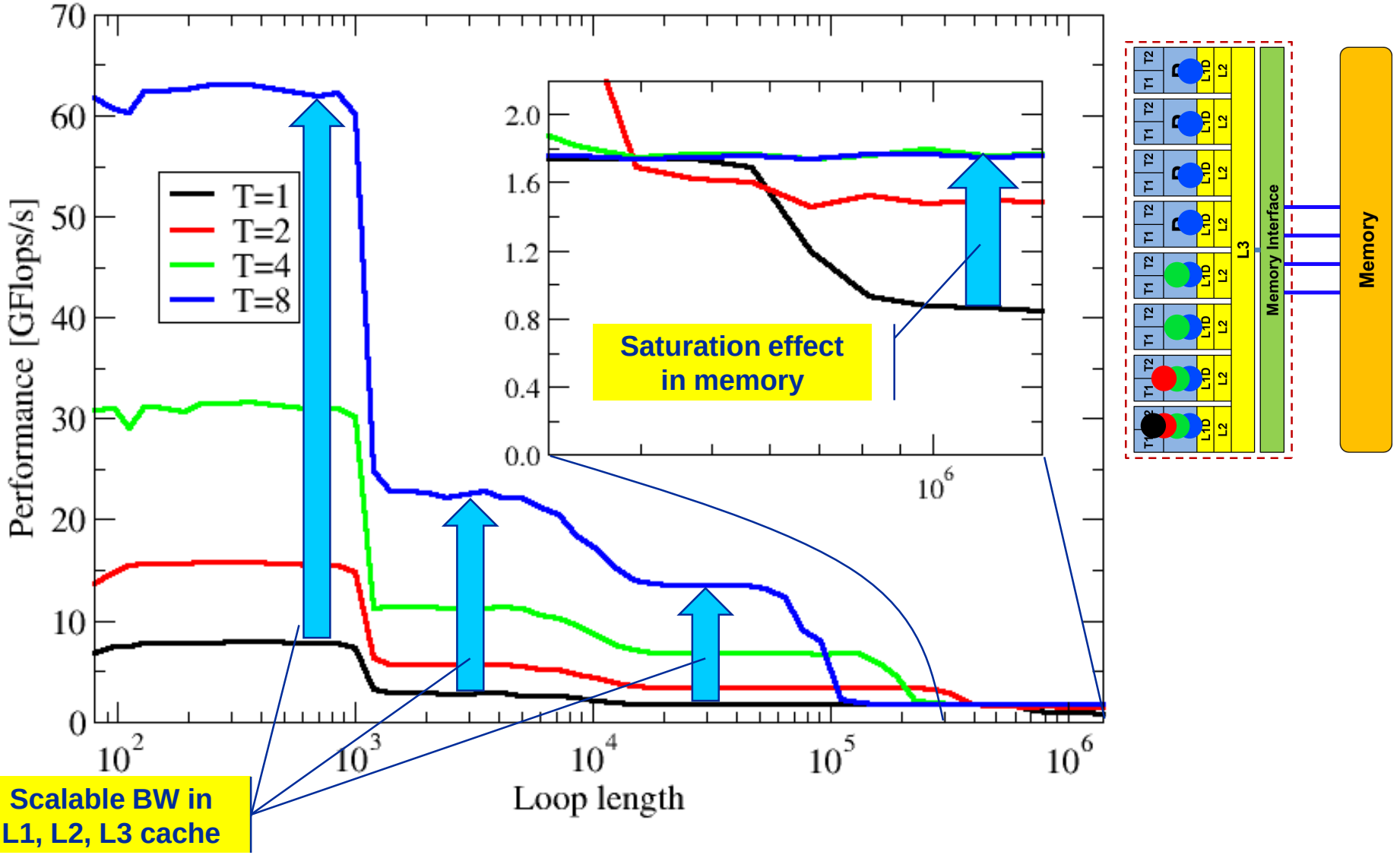
Every core runs its own, independent triad benchmark

```
double precision, dimension(:), allocatable :: A,B,C,D

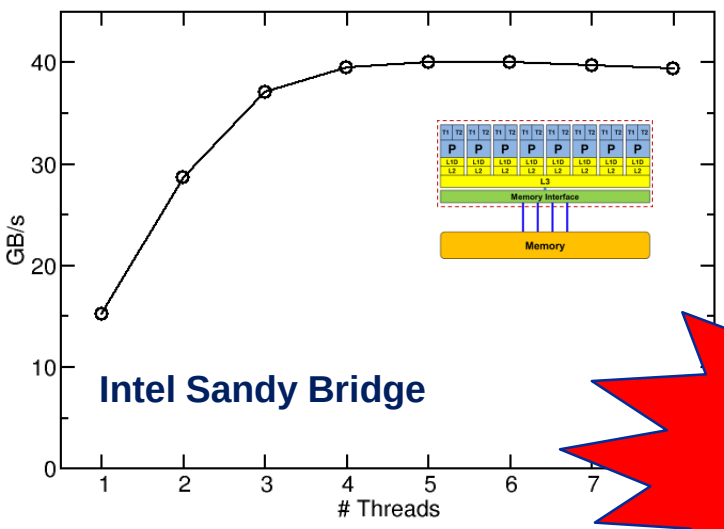
!$OMP PARALLEL private(i,j,A,B,C,D)
allocate(A(1:N),B(1:N),C(1:N),D(1:N))
A=1.d0; B=A; C=A; D=A
do j=1,NITER
  do i=1,N
    A(i) = B(i) + C(i) * D(i)
  enddo
  if(.something.that.is.never.true.) then
    call dummy(A,B,C,D)
  endif
enddo
!$OMP END PARALLEL
```

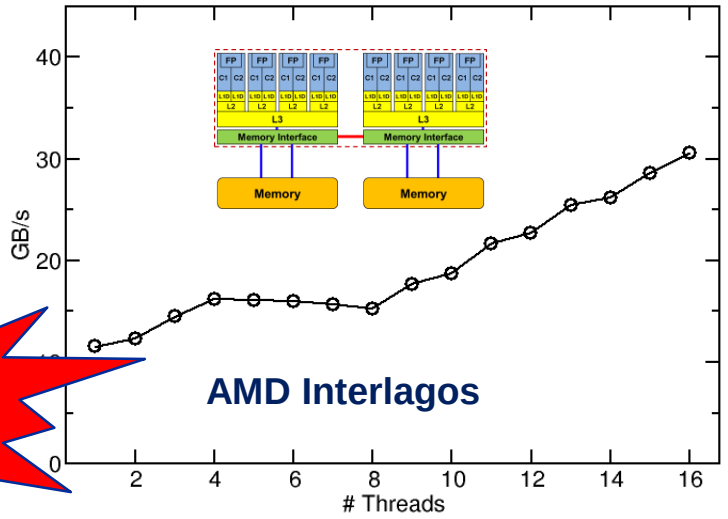
→ pure hardware probing, no impact from OpenMP overhead

Throughput vector triad on Sandy Bridge socket (3 GHz)

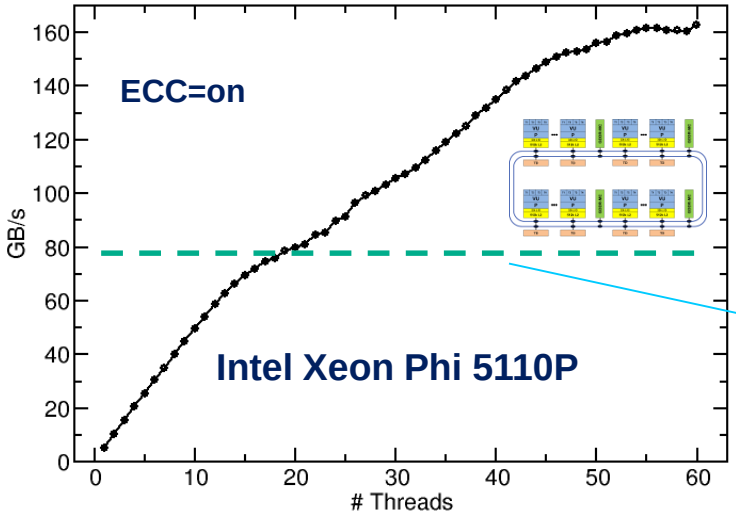


Attainable memory bandwidth: Comparing architectures

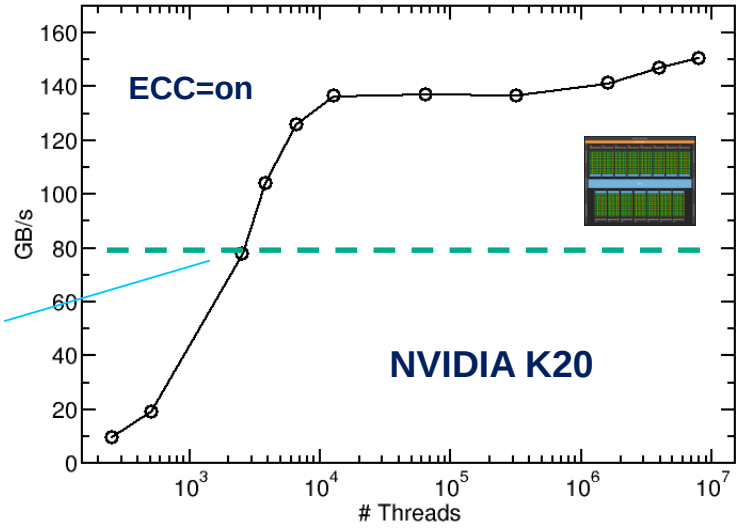




Pattern! Bandwidth saturation



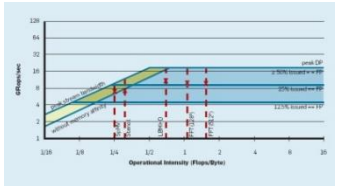
2-socket CPU node



Conclusions from the microbenchmarks

- **Affinity matters!**
  - Almost all performance properties depend on the position of
    - Data
    - Threads/processes
  - Consequences
    - Know where your threads are running
    - Know where your data is

- **Bandwidth bottlenecks are ubiquitous**



“Simple” performance modeling: The Roofline Model

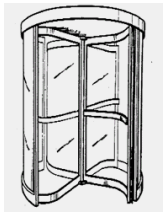
Loop-based performance modeling: Execution vs. data transfer
Example: array summation
Example: dense & sparse matrix-vector multiplication
Example: a 3D Jacobi solver
Model-guided optimization

R.W. Hockney and I.J. Curington: $f_{1/2}$: A parameter to characterize memory and communication bottlenecks. Parallel Computing 10, 277-286 (1989). DOI: 10.1016/0167-8191(89)90100-2

W. Schönauer: Scientific Supercomputing: Architecture and Use of Shared and Distributed Memory Parallel Computers. Self-edition (2000)
S. Williams: Auto-tuning Performance on Multicore Computers.
UCB Technical Report No. UCB/EECS-2008-164. PhD thesis (2008)

Prelude: Modeling customer dispatch in a bank

Revolving door throughput:
b_S [customers/sec]



Processing capability:
P_{max} [tasks/sec]

Intensity:
I [tasks/customer]

How fast can tasks be processed? P [tasks/sec]

The bottleneck is either

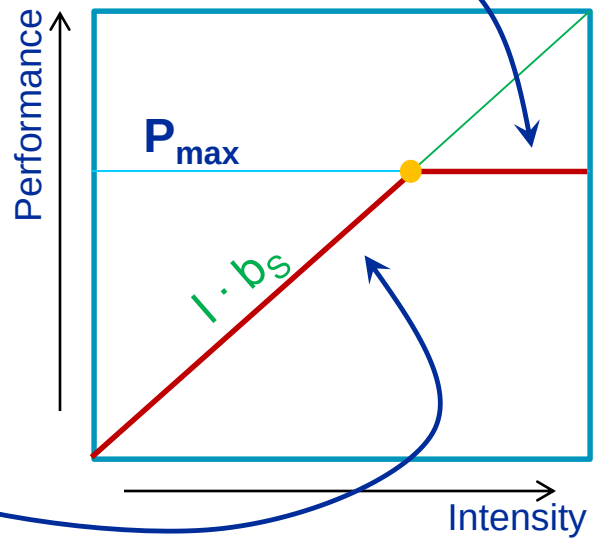
- The service desks (max. tasks/sec): $P_{\max}$
- The revolving door (max. customers/sec): $I \cdot b_S$

$$P = \min(P_{\max}, I \cdot b_S)$$

This is the "Roofline Model"

- High intensity: P limited by "execution"
- Low intensity: P limited by "bottleneck"
- "Knee" at $P_{max} = I \cdot b_S$:
  Best use of resources

- **Roofline is an "optimistic" model: ("light speed")**



The Roofline Model

1. P_{max} = Applicable peak performance of a loop, assuming that data comes from the level 1 cache (this is not necessarily P_{peak})
   → e.g., P_{max} = 176 GFlop/s

2. I = Computational intensity ("work" per byte transferred) over the slowest data path utilized (code balance $B_C = I^{-1}$)
   → e.g., I = 0.167 Flop/Byte → B_C = 6 Byte/Flop

3. b_S = Applicable peak bandwidth of the slowest data path utilized
   → e.g., b_S = 56 GByte/s

Expected performance:

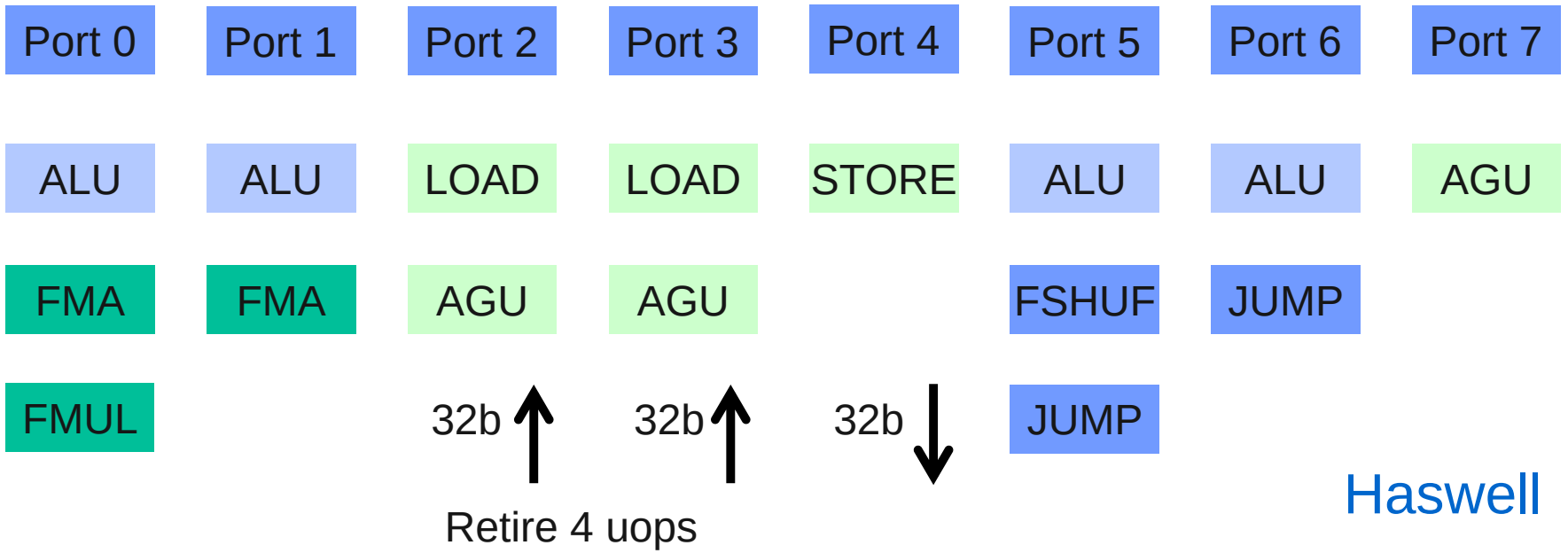
$$P = \min(P_{\max}, I \cdot b_S) = \min\left(P_{\max}, \frac{b_S}{B_C}\right)$$

[Byte/s]

[Byte/Flop]

Preliminary: Estimating P_{max}

Every new CPU generation provides incremental improvements.



Example: Estimate P_{max} of vector triad on Haswell

```
double  *A, *B, *C, *D;
for (int i=0; i<N; i++) {
   A[i] = B[i] + C[i] * D[i];
}
```

Minimum number of cycles to process one AVX-vectorized iteration (one core)?

→ Equivalent to 4 scalar iterations

Cycle 1: LOAD + LOAD + STORE
Cycle 2: LOAD + LOAD + FMA + FMA
Cycle 3: LOAD + LOAD + STORE

Answer: 1.5 cycles

Example: Estimate P_{max} of vector triad on Haswell (2.3 GHz)

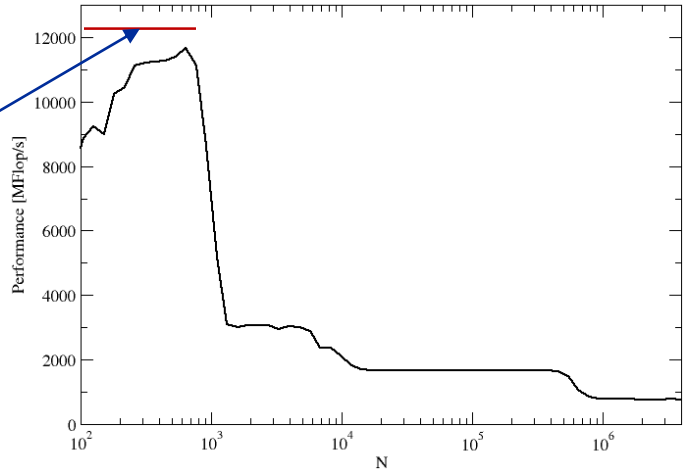
```
double  *A, *B, *C, *D;
for (int i=0; i<N; i++) {
   A[i] = B[i] + C[i] * D[i];
}
```

What is the performance in GFlops/s per core and the bandwidth in GBytes/s?

One AVX iteration (1.5 cycles) does 4 x 2 = 8 flops:

$$\frac{2.3 \cdot 10^9 \text{ cy/s}}{1.5 \text{ cy}} \cdot 4 \text{ updates} \cdot \frac{2 \text{ flops}}{\text{update}} = \mathbf{12.27} \frac{\mathbf{Gflops}}{\mathbf{s}}$$

$$6.13 \cdot 10^9 \frac{\text{updates}}{\text{s}} \cdot 32 \frac{\text{bytes}}{\text{update}} = 196 \frac{\text{Gbyte}}{\text{s}}$$



P_{max} + bandwidth limitations: The vector triad

Vector triad `A(:)=B(:)+C(:)*D(:)` on a 2.3 GHz 14-core Haswell chip

Consider full chip (14 cores):

Memory bandwidth: b_S = **50 GB/s**

Code balance (incl. write allocate):
B_c = (4+1) Words / 2 Flops = 20 B/F → ***I* = 0.05 F/B**

→ $I \cdot b_S$ **= 2.5 GF/s** (0.5% of peak performance)

P_{peak} / core = 36.8 Gflop/s ((8+8) Flops/cy x 2.3 GHz)
P_{max} / core = 12.27 Gflop/s (see prev. slide)

→ P_{max} **= 14 * 12.27 Gflop/s =172 Gflop/s** (33% peak)

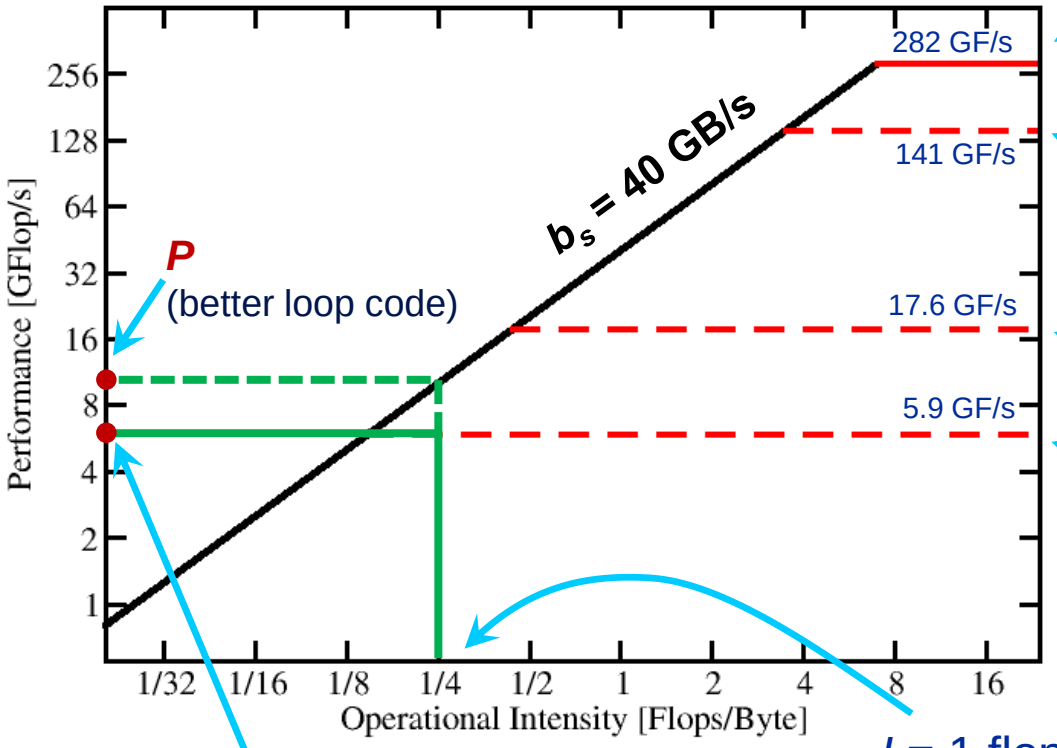
$$P = \min(P_{\max}, I \cdot b_S) = \min(172, 2.5)\ \mathrm{GFlop/s} = 2.5\ \mathrm{GFlop/s}$$

A not so simple Roofline example

Example: `do i=1,N; s=s+a(i); enddo`

in single precision on a 2.2 GHz Sandy Bridge socket @ "large" N

$$P = \min(P_{\max}, I \cdot b_S)$$



Machine peak (ADD+MULT) Out of reach for this code

ADD peak (best possible code)

no SIMD

3-cycle latency per ADD if not pipelined

How do we get these? → See next!

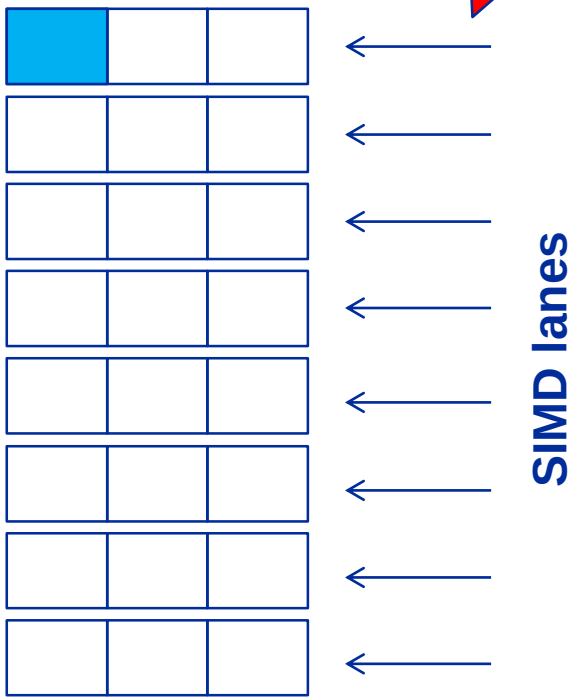
I = 1 flop / 4 byte (SP!)

Applicable peak for the summation loop

Plain scalar code, no SIMD

```
LOAD r1.0 ← 0
i ← 1
loop:
  LOAD r2.0 ← a(i)
  ADD r1.0 ← r1.0+r2.0
  ++i →? loop
result ← r1.0
```

ADD pipes utilization:



→ 1/24 of ADD peak

Applicable peak for the summation loop

Scalar code, 3-way unrolling

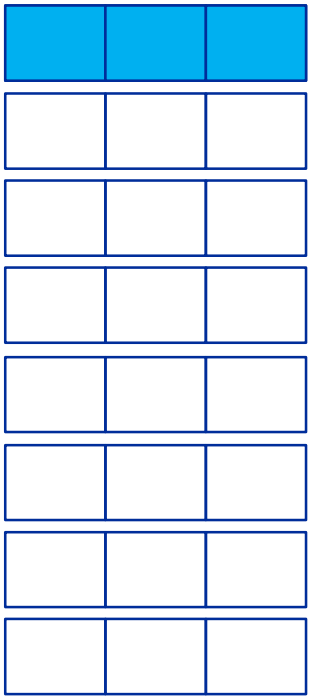
```
LOAD r1.0 ← 0
LOAD r2.0 ← 0
LOAD r3.0 ← 0
i ← 1

loop:
  LOAD r4.0 ← a(i)
  LOAD r5.0 ← a(i+1)
  LOAD r6.0 ← a(i+2)

  ADD r1.0 ← r1.0 + r4.0
  ADD r2.0 ← r2.0 + r5.0
  ADD r3.0 ← r3.0 + r6.0

  i+=3 →? loop
result ← r1.0+r2.0+r3.0
```

ADD pipes utilization:



→ 1/8 of ADD peak

Applicable peak for the summation loop

SIMD-vectorized, 3-way unrolled

```
LOAD [r1.0,…,r1.7] ← [0,…,0]
LOAD [r2.0,…,r2.7] ← [0,…,0]
LOAD [r3.0,…,r3.7] ← [0,…,0]
i ← 1

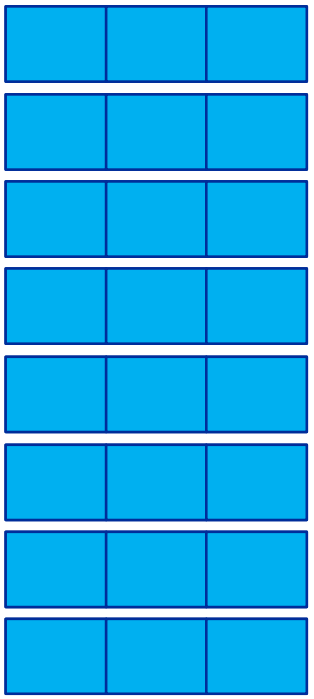
loop:
  LOAD [r4.0,…,r4.7] ← [a(i),…,a(i+7)]
  LOAD [r5.0,…,r5.7] ← [a(i+8),…,a(i+15)]
  LOAD [r6.0,…,r6.7] ← [a(i+16),…,a(i+23)]

  ADD r1 ← r1 + r4
  ADD r2 ← r2 + r5
  ADD r3 ← r3 + r6

  i+=24 →? loop
result ← r1.0+r1.1+...+r3.6+r3.7
```

Pattern! ALU saturation

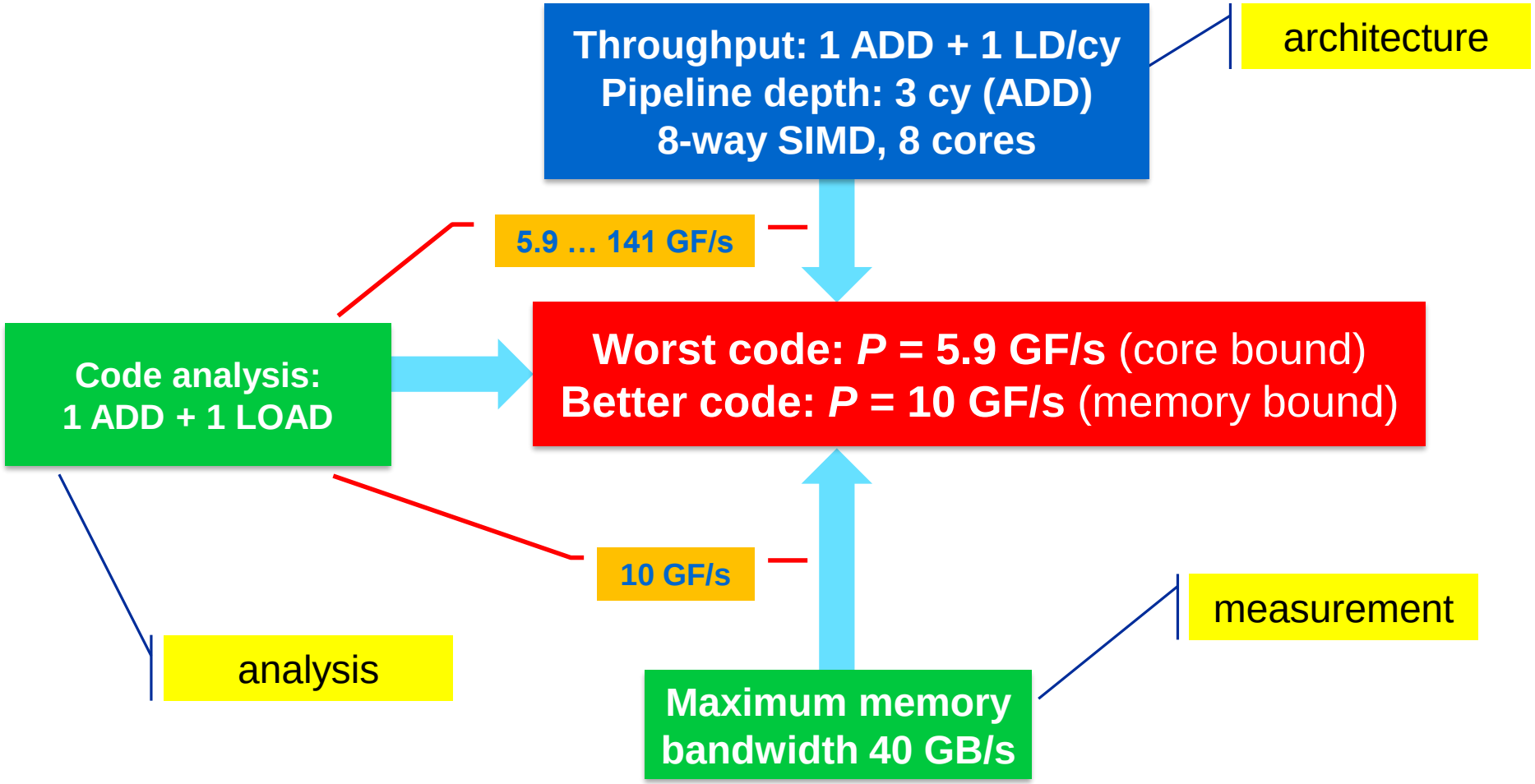
ADD pipes utilization:



→ ADD peak

Input to the roofline model

… on the example of `do i=1,N; s=s+a(i); enddo`
in single precision



Prerequisites for the Roofline Model

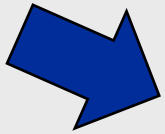
- **The roofline formalism is based on some (crucial) assumptions:**
  - There is a clear concept of "work" vs. "traffic"
    - "work" = flops, updates, iterations…
    - "traffic" = required data to do "work"
  - Attainable bandwidth of code = input parameter! Determine effective bandwidth via simple streaming benchmarks to model more complex kernels and applications
  - Data transfer and core execution overlap perfectly!
    - **Either** the limit is core execution **or** it is data transfer
  - Slowest limiting factor "wins"; all others are assumed to have no impact
  - Latency effects are ignored: perfect data streaming, "steady-state" execution, no start-up effects

Case study:
Dense Matrix Vector Multiplication

Where does the data come from?

Example: Dense matrix-vector multiplication in DP (AVX)

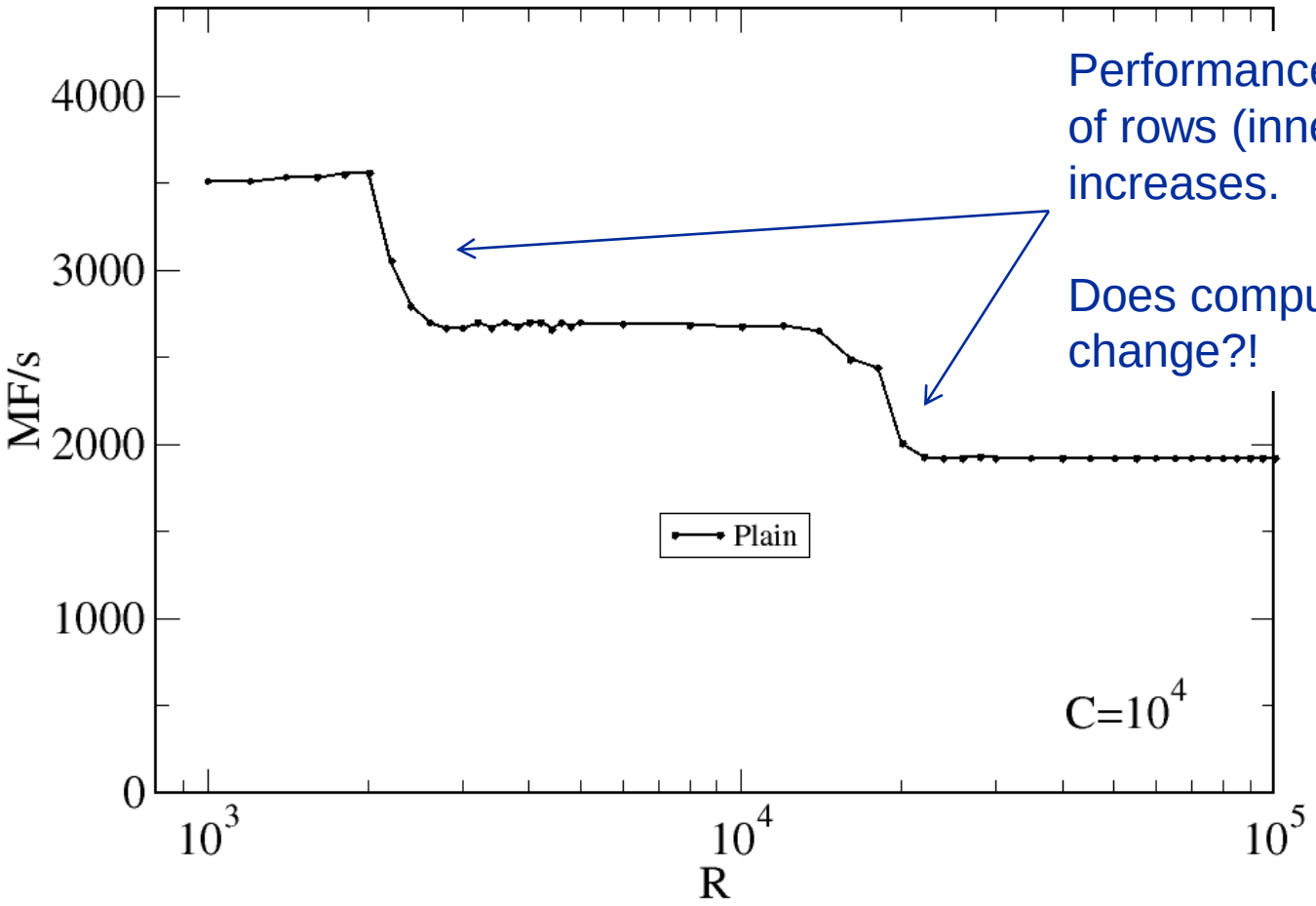
```
do c = 1 , C
 do r = 1 , R
     y(r)=y(r) + A(r,c)* x(c)
 enddo
enddo
```



```
do c = 1 , C
   tmp=x(c)
   do r = 1 , R
      y(r)=y(r) + A(r,c)* tmp
   enddo
enddo
```

- Assume C = R ≈ 10,000
- Applicable peak performance?
- Relevant data path?
- Computational Intensity?

DMVM (DP) – Single core performance vs. column height



Performance drops as number of rows (inner loop length) increases.

Does computational intensity change?!

Intel Xeon E5 2695 v3 (Haswell-EP), 2.3 GHz, CoD mode, Core P_{peak}=18.4 GF/s, Caches: 32 KB / 256 KB / 35 MB, PageSize: 2 MB; ifort V15.0.1.133; b_S = 32 Gbyte/s

DMVM data traffic analysis

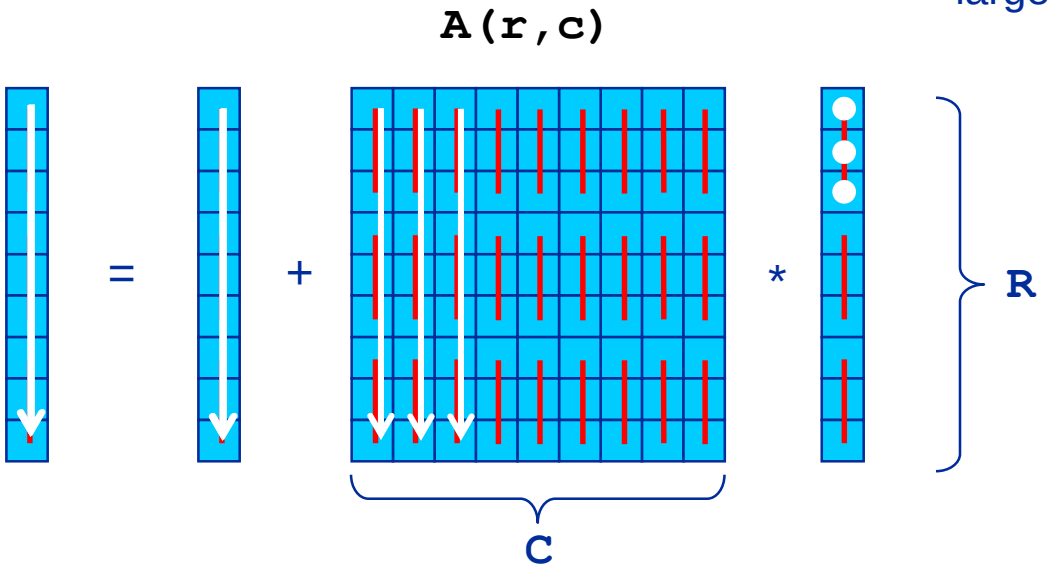
```
do c = 1 , C
  tmp=x(c)
  do r = 1 , R
     y(r)=y(r) + A(r,c)* tmp
  enddo
enddo
```

`tmp` stays in a register during inner loop

`A(:,:)` is loaded from memory – no data reuse

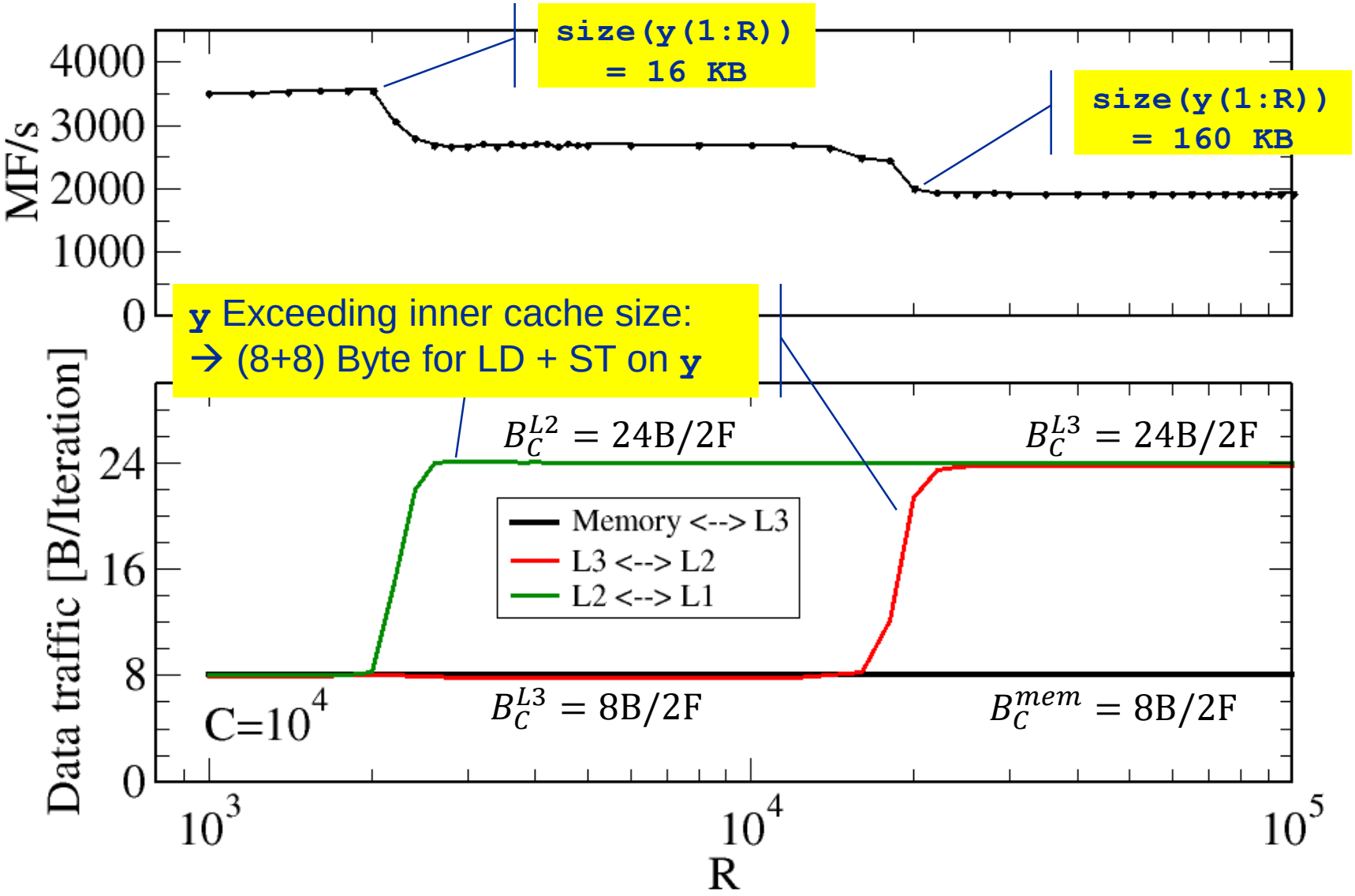
`y(:)` is loaded and stored in each outer iteration → for c>1 update `y(:)` in cache

`y(:)` may not fit in innermost cache → more traffic from lower level caches for larger `R`

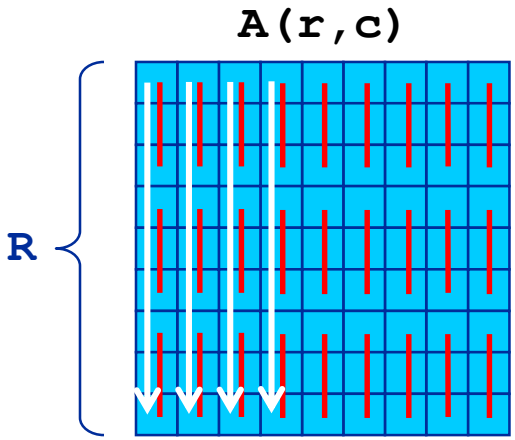


Roofline analysis: Distinguish code balance in memory (B_C^{mem}) from code balance in relevant cache level(s) (B_C^{L3}, B_C^{L2},…)!

DMVM (DP) – Single core data traffic analysis

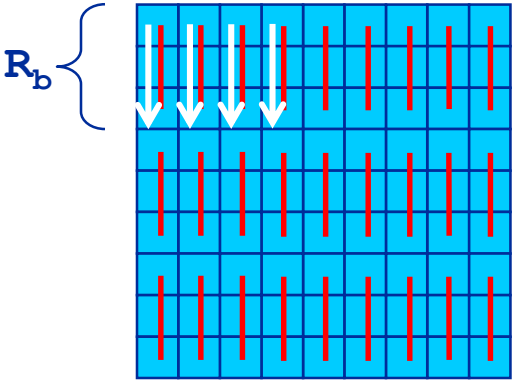


Reducing traffic by blocking




```
do c = 1 , C
  tmp=x(c)
  do r = 1 , R
     y(r)=y(r) + A(r,c)* tmp
  enddo
enddo
```

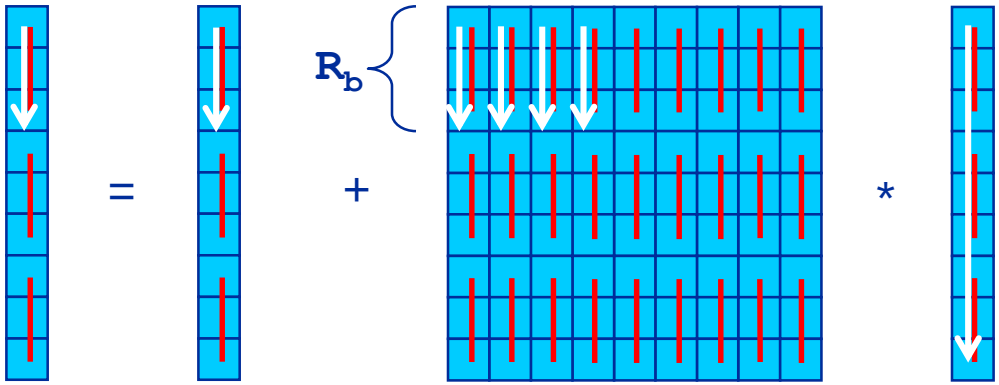
`y(:)` may not fit into some cache → more traffic for lower level




```
do rb = 1 , R , Rb
 rbS = rb
 rbE = min((rb+Rb-1), R)
 do c = 1 , C
   do r = rbS , rbE
      y(r)=y(r) + A(r,c)*x(c)
   enddo
 enddo
enddo
```

`y(rbS:rbE)` may fit into some cache if R_b is small enough → traffic reduction

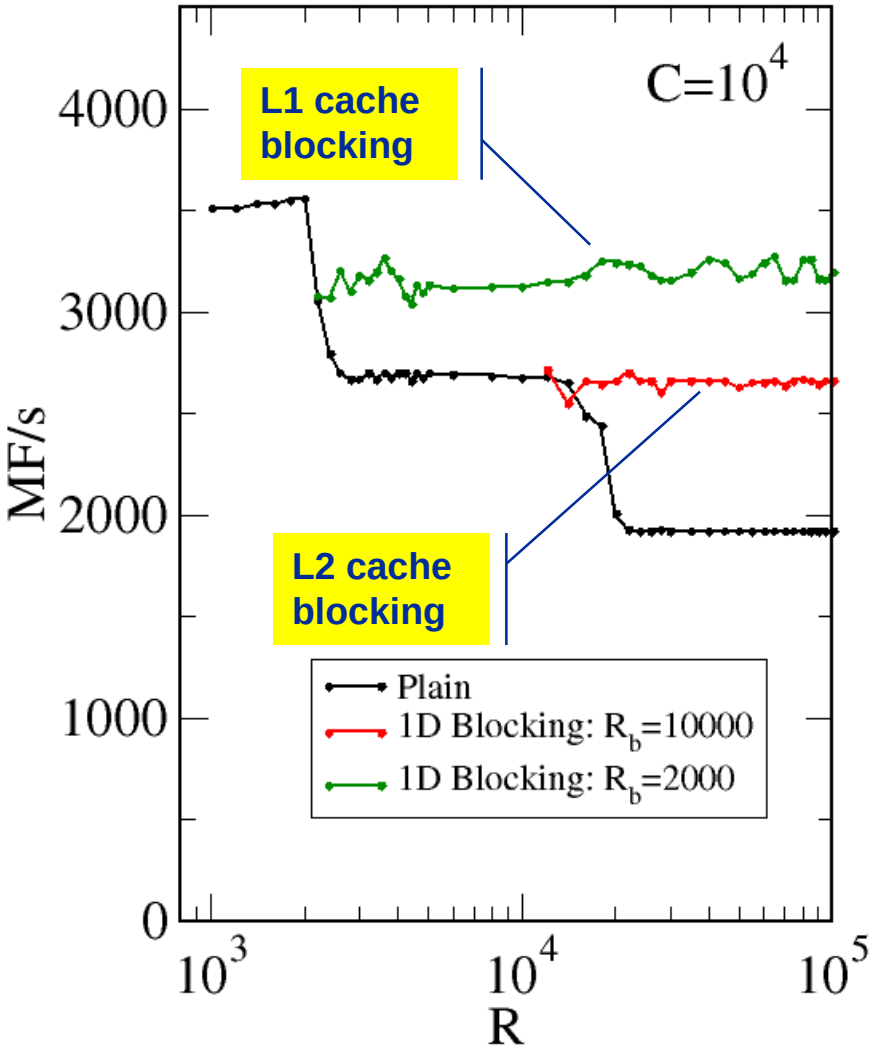
Reducing traffic by blocking



- **LHS only updated once in some cache level if blocking is applied**
- **Price: RHS is loaded multiple times instead of once!**
  - How often? → R / R_b times
- **Consequence: For R=C, traffic reduction of LHS & RHS by a factor of R / (1+R/[2R_b])**
  - Still a large reduction if block size can be made larger than about 10

DMVM (DP) – Reducing traffic by inner loop blocking

optional



- "1D blocking" for inner loop
- Blocking factor R_b ←→ cache level

```
do rb = 1 , R , Rb

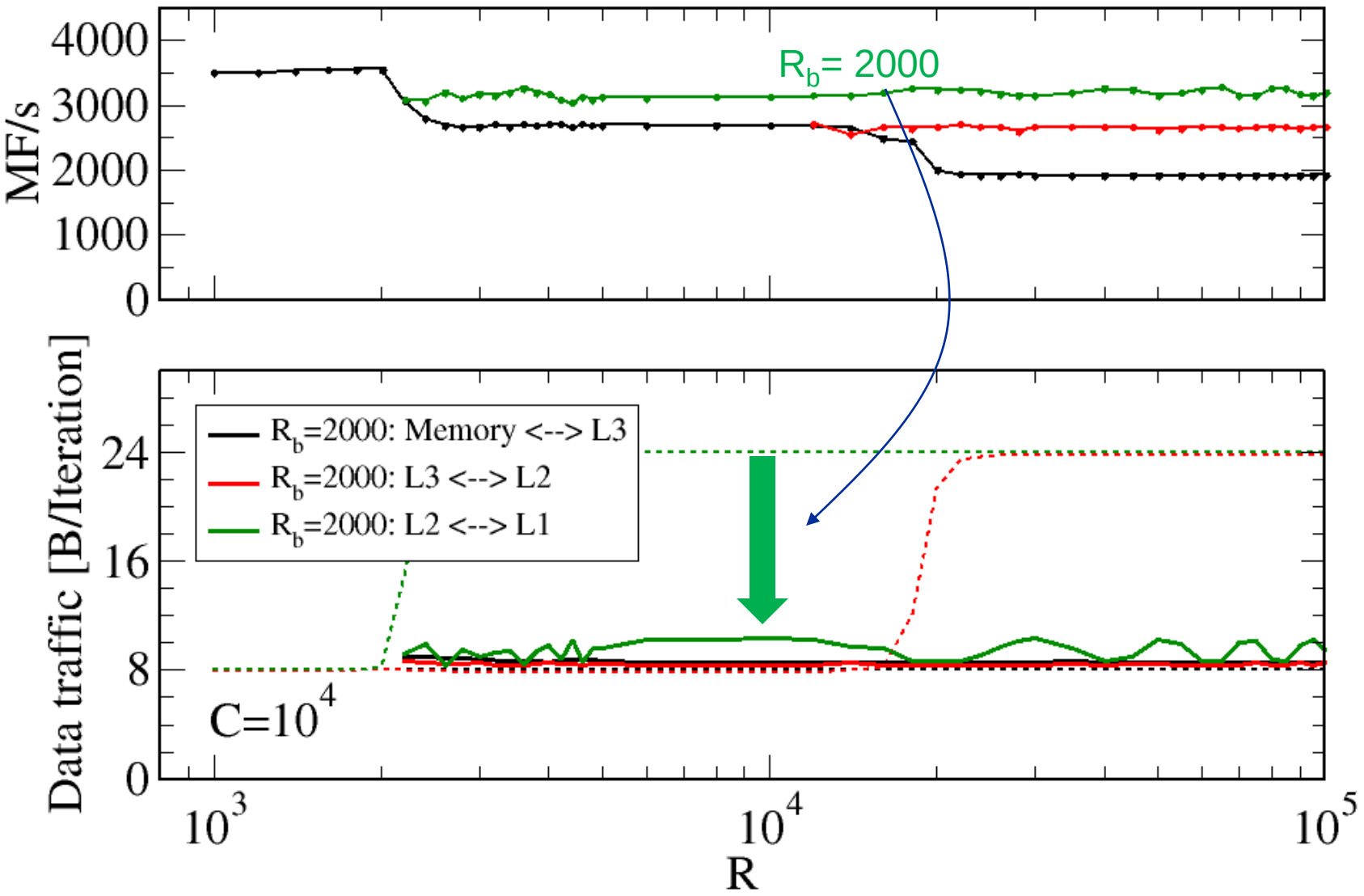
 rbS = rb
 rbE = min((rb+Rb-1), R)

 do c = 1 , C
   do r = rbS , rbE
      y(r)=y(r) + A(r,c)*x(c)
   enddo
 enddo

enddo
```

→ Fully reuse subset of `y(rbS:rbE)` from L1/L2 cache

DMVM (DP) – Validation of blocking optimization



DMVM (DP) – OpenMP parallelization

```
!$omp parallel do reduction(+:y)
do c = 1 , C
  do r = 1 , R
     y(r) = y(r) + A(r,c) * x(c)
enddo ; enddo
!$omp end parallel do
```

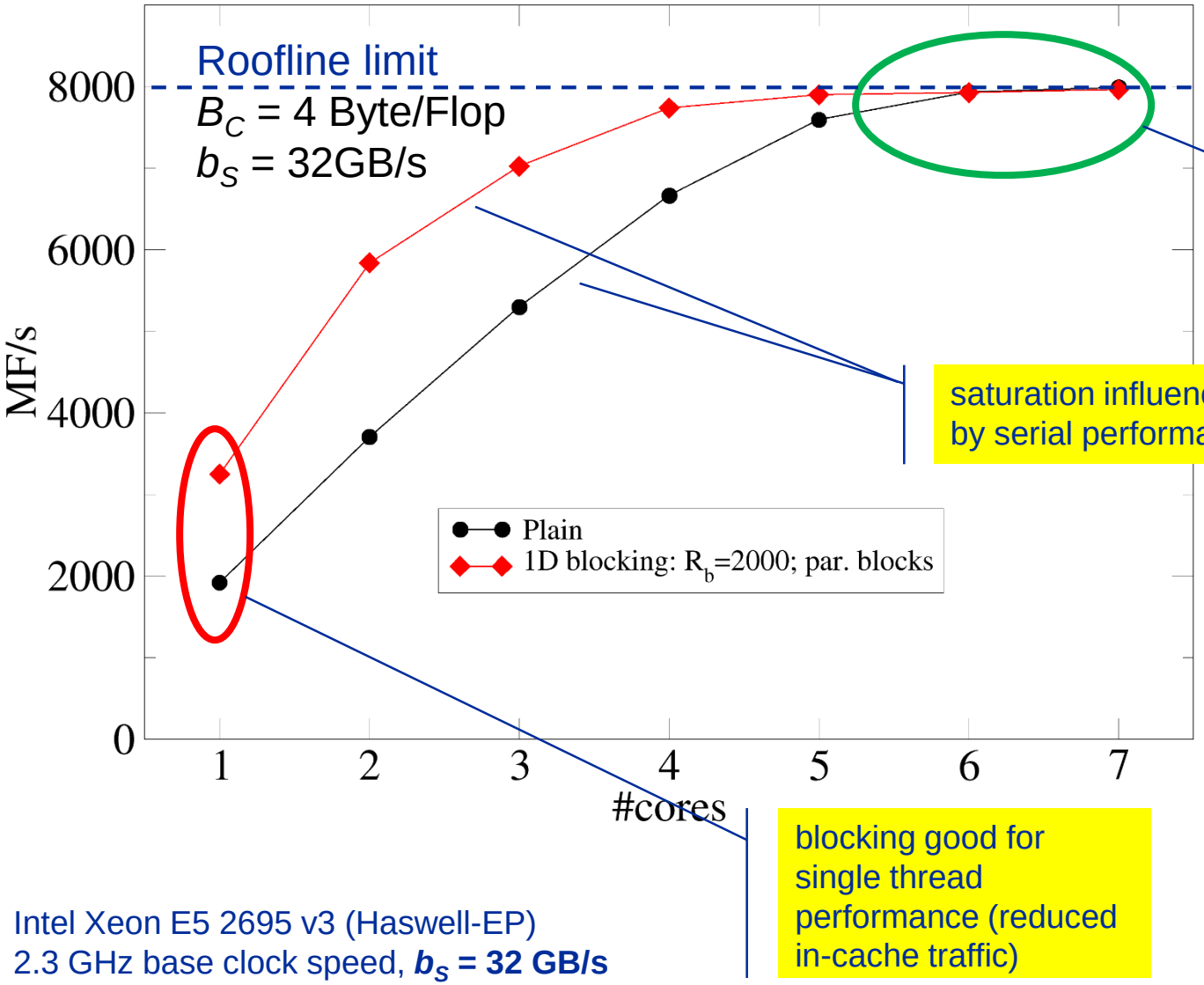
plain code

```
!$omp parallel do private(rbS,rbE)
do rb = 1 , R , Rb
 rbS = rb
 rbE = min((rb+Rb-1), R)
 do c = 1 , C
   do r = rbS , rbE
      y(r) = y(r) + A(r,c) * x(c)
enddo ; enddo ; enddo
!$omp end parallel do
```

blocked code

DMVM (DP) – OpenMP parallelization & saturation

"Using more cores can heal bad single-core performance"



Pattern! Bandwidth saturation

memory traffic unchanged → saturation unchanged!

saturation influenced by serial performance

So, is blocking useless?
→ NO (see later)

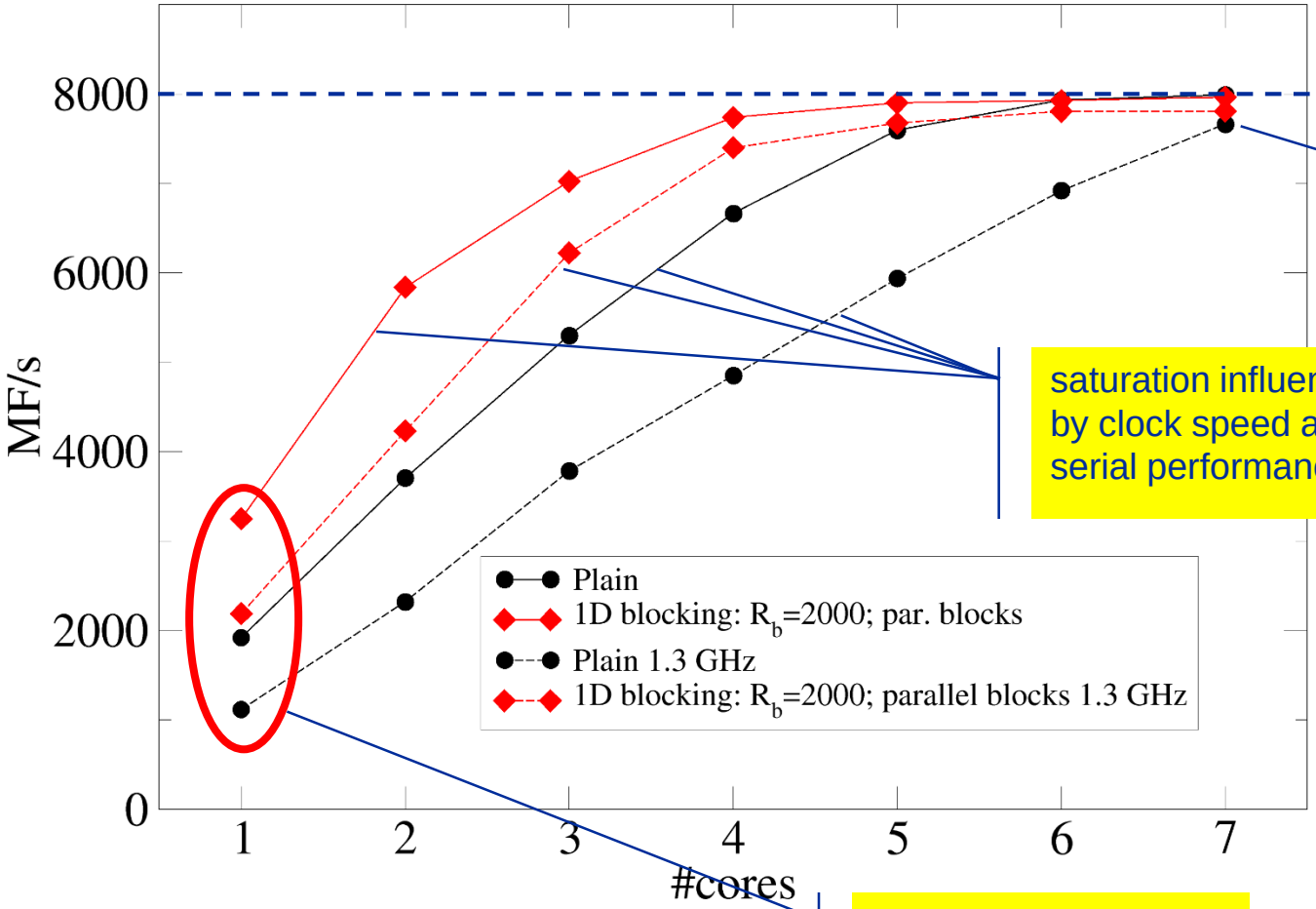
Can we do anything to improve B_C^{mem}?
→ NO, not here

blocking good for single thread performance (reduced in-cache traffic)

Intel Xeon E5 2695 v3 (Haswell-EP)
2.3 GHz base clock speed, ***b_S* = 32 GB/s**

DMVM (DP) – saturation & clock speed

optional



Even the worst code almost saturates the bandwidth @1.3 GHz

saturation influenced by clock speed and serial performance

Clock speed has high impact on single thread performance

Clock speed or parallelism can "heal" slow code!

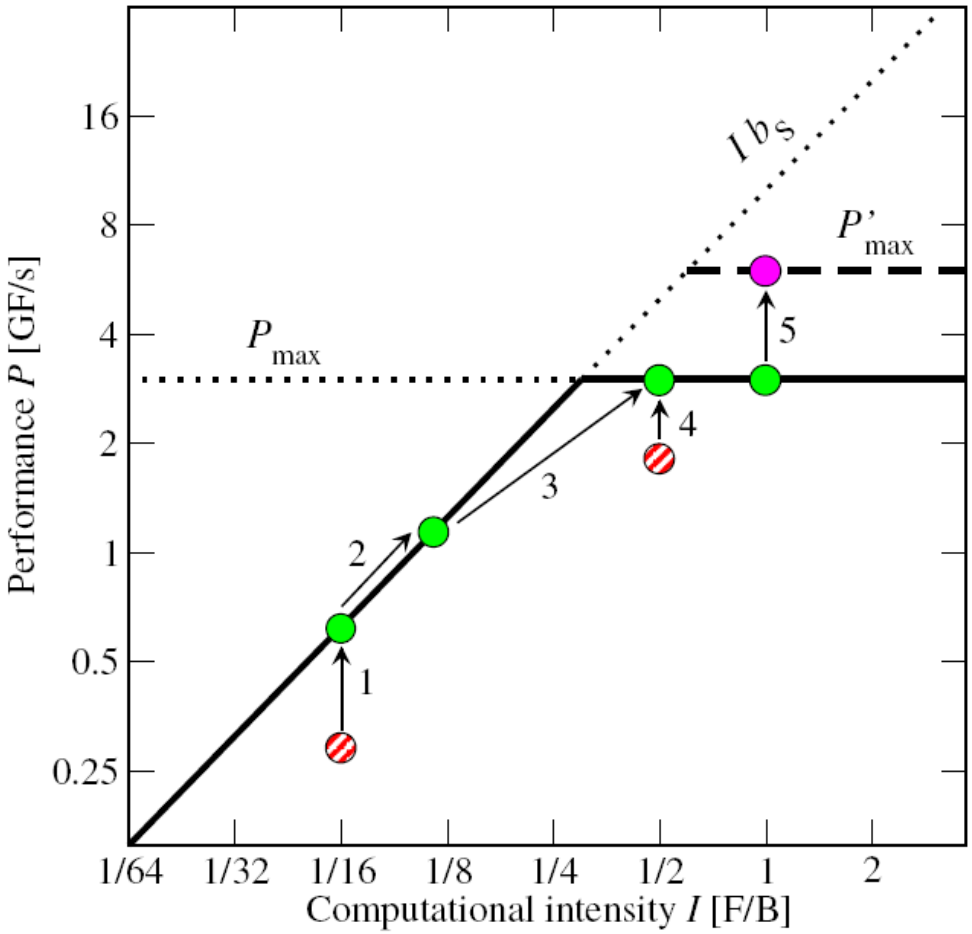
Intel Xeon E5 2695 v3 (Haswell-EP)
2.3 GHz base clock speed, b_S = 32 GB/s

Conclusions from the dMVM example

- **We have found the reasons for the breakdown of single-core performance with growing number of matrix rows**
  - LHS vector fitting in different levels of the cache hierarchy
  - Validated theory by performance counter measurements
- **Inner loop blocking was employed to improve code balance in L3 and/or L2**
  - Validated by performance counter measurements
- **Blocking led to better single-threaded performance**
- **Saturated performance unchanged (as predicted by Roofline)**
  - Because the problem is still small enough to fit the LHS at least into the L3 cache

Typical code optimizations in the Roofline Model

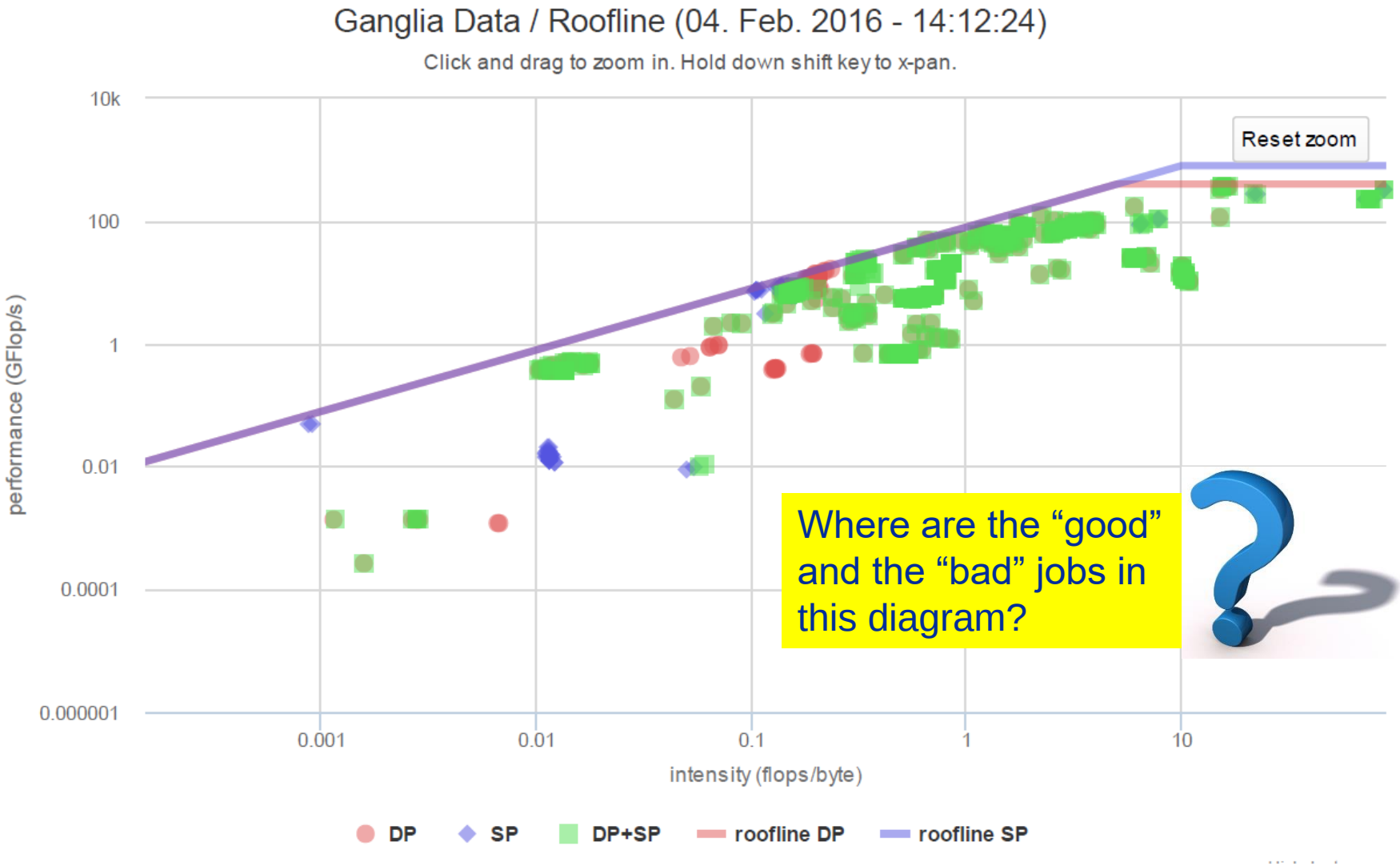
1. Hit the BW bottleneck by good serial code
   (e.g., Perl → Fortran)
2. Increase intensity to make better use of BW bottleneck
   (e.g., loop blocking → see later)
3. Increase intensity and go from memory-bound to core-bound
   (e.g., temporal blocking)
4. Hit the core bottleneck by good serial code
   (e.g., `-fno-alias` → see later)
5. Shift P_{max} by accessing additional hardware features or using a different algorithm/implementation
   (e.g., scalar → SIMD)



Using Roofline for monitoring “live” jobs on a cluster

Based on measured BW and Flop/s data via likwid-perfctr

optional



Case study: A Jacobi smoother

The basic performance properties in 2D

Layer conditions

Optimization by spatial blocking

Stencil schemes

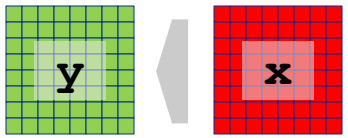
- Stencil schemes frequently occur in PDE solvers on regular lattice structures
- Basically it is a sparse matrix vector multiply (spMVM) embedded in an iterative scheme (outer loop)
- but the regular access structure allows for matrix free coding

```
do iter = 1, max_iterations

  Perform sweep over regular grid: y(:) ← x(:)

  Swap y ←→ x

enddo
```



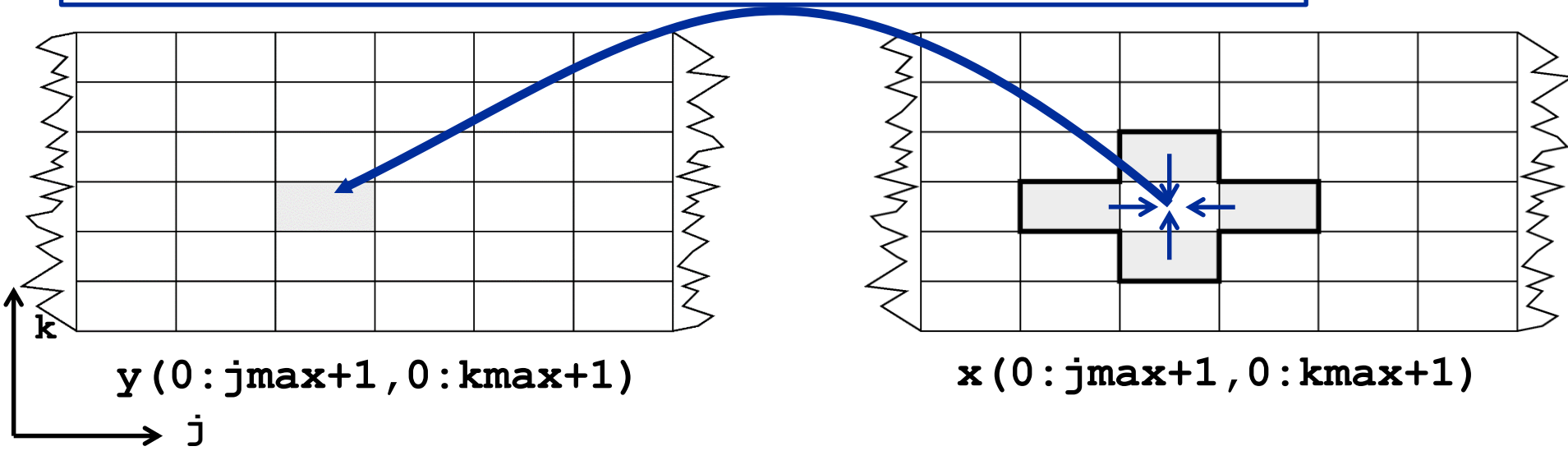
- Complexity of implementation and performance depends on
  - stencil operator, e.g. Jacobi-type, Gauss-Seidel-type, …
  - spatial extent, e.g. 7-pt or 25-pt in 3D,…

Jacobi-type 5-pt stencil in 2D

sweep

```
do k=1,kmax
  do j=1,jmax
    y(j,k) = const * (  x(j-1,k) + x(j+1,k) &
                      +    x(j,k-1) + x(j,k+1) )
  enddo
enddo
```

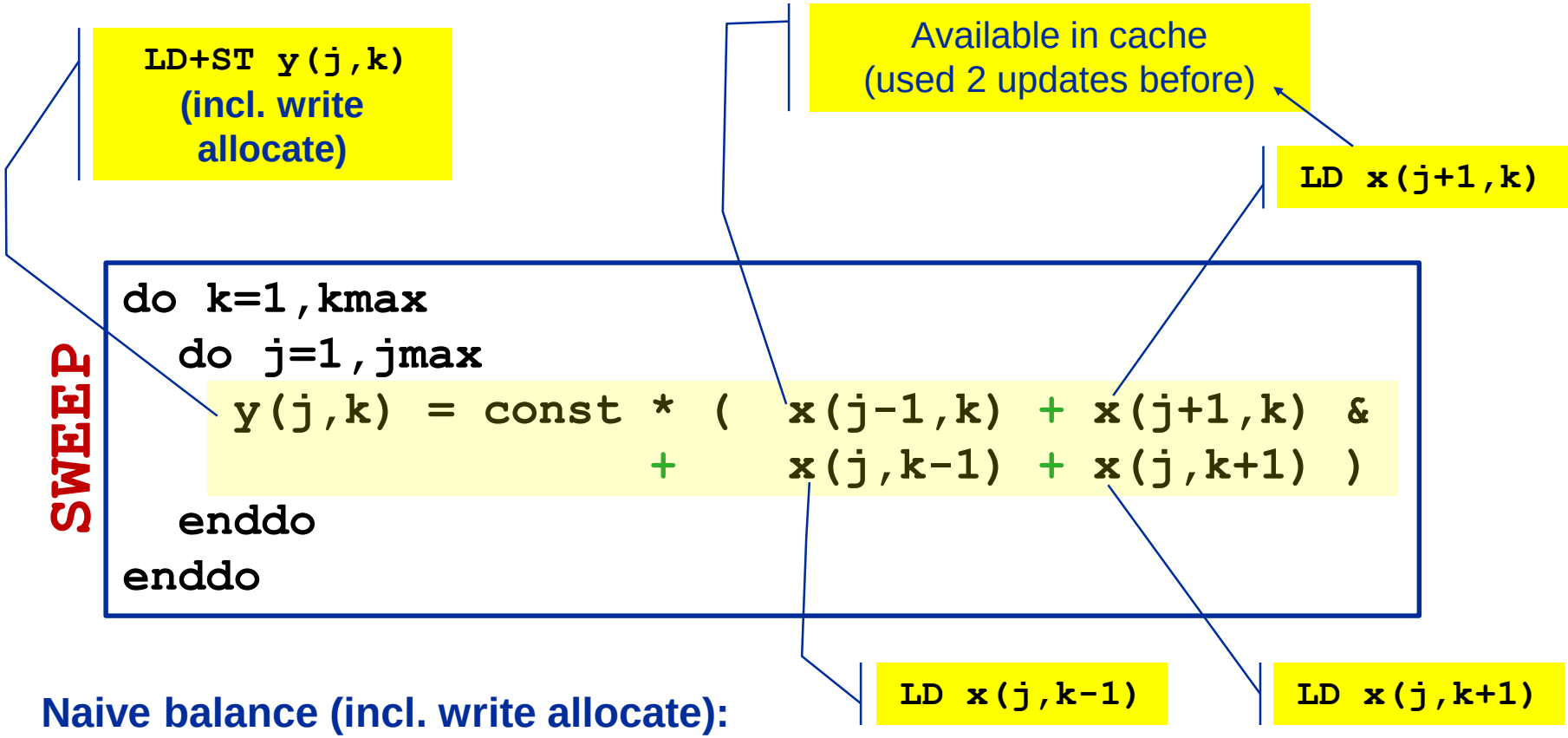
Lattice Update (LUP)



Appropriate performance metric: "**Lattice Updates per second**" [**LUP/s**]

(here: Multiply by 4 FLOP/LUP to get FLOP/s rate)

Jacobi 5-pt stencil in 2D: data transfer analysis

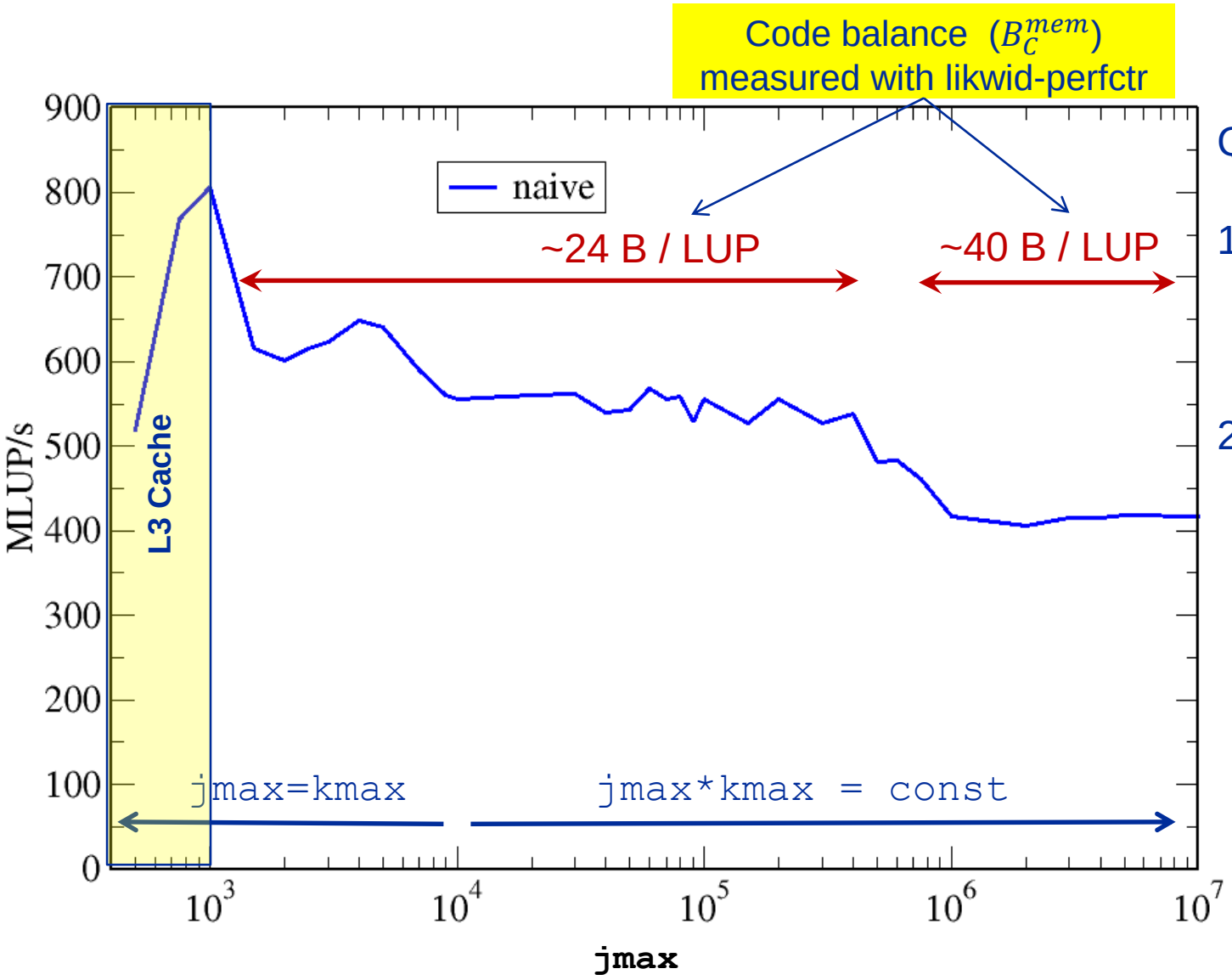


Naive balance (incl. write allocate):

`x( :, :)` : 3 LD +
`y( :, :)` : 1 ST+ 1LD

→ B_C = 5 Words / LUP = 40 B / LUP (assuming double precision)

Jacobi 5-pt stencil in 2D: Single core performance



Questions:

1. How to achieve 24 B/LUP also for large **jmax**?
2. How to sustain >600 MLUP/s for **jmax > 10^4** ?

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Intel Xeon E5-2690 v2
("IvyBridge"@3 GHz)

Interchanged with SpMVM example

Case study: A Jacobi smoother

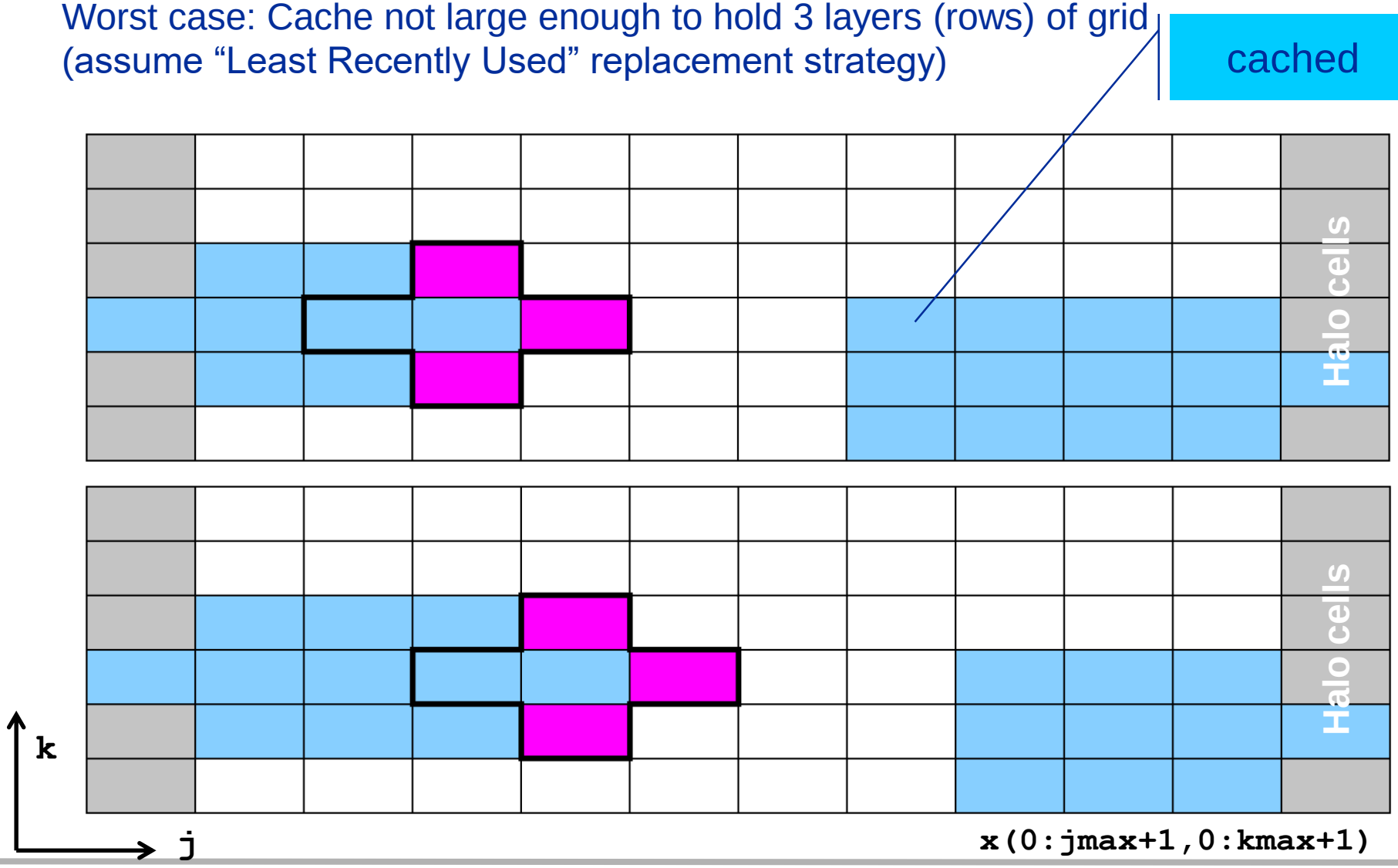
The basics in two dimensions

Layer conditions

Optimization by spatial blocking

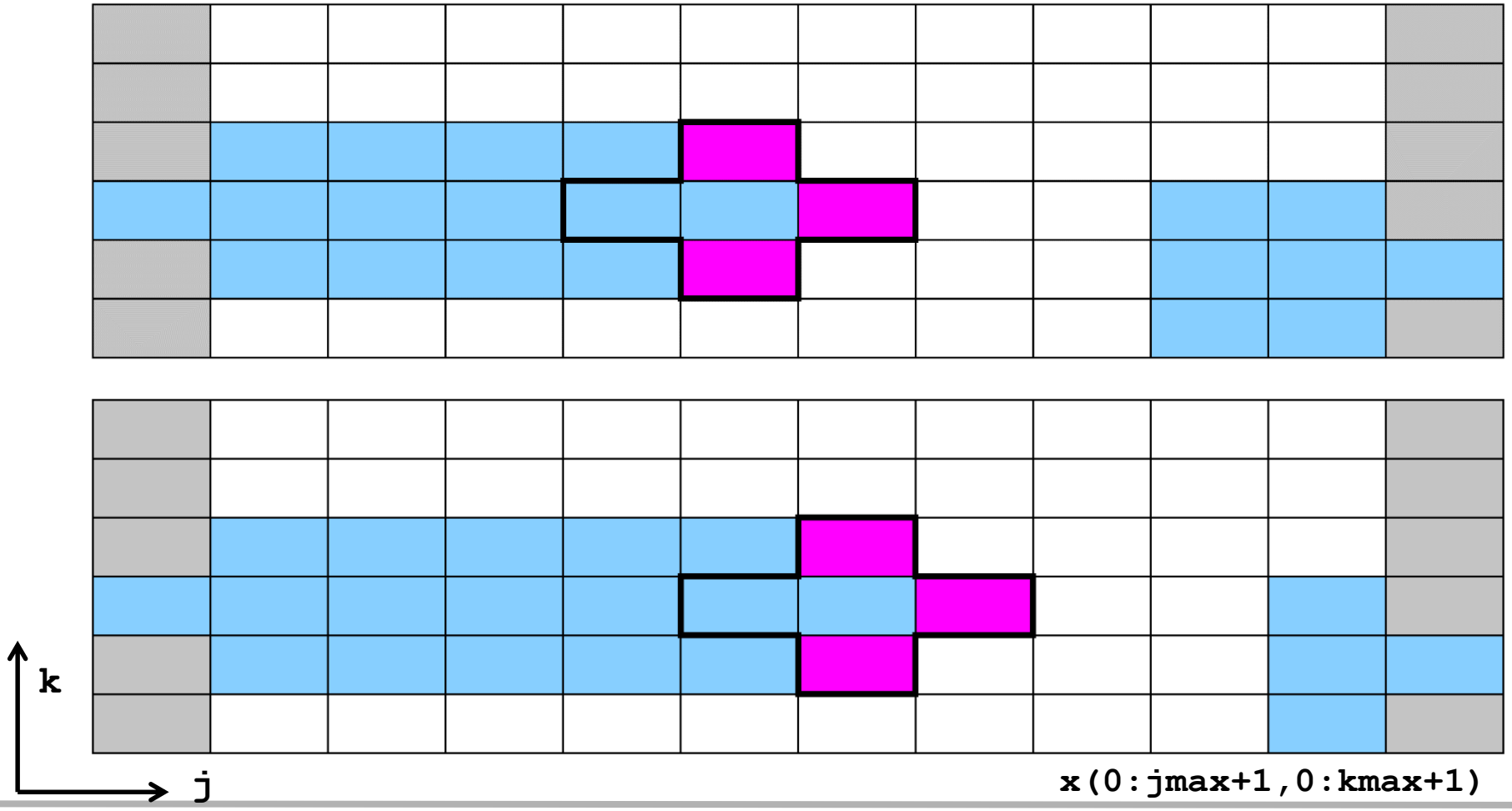
Analyzing the data flow

Worst case: Cache not large enough to hold 3 layers (rows) of grid (assume “Least Recently Used” replacement strategy)



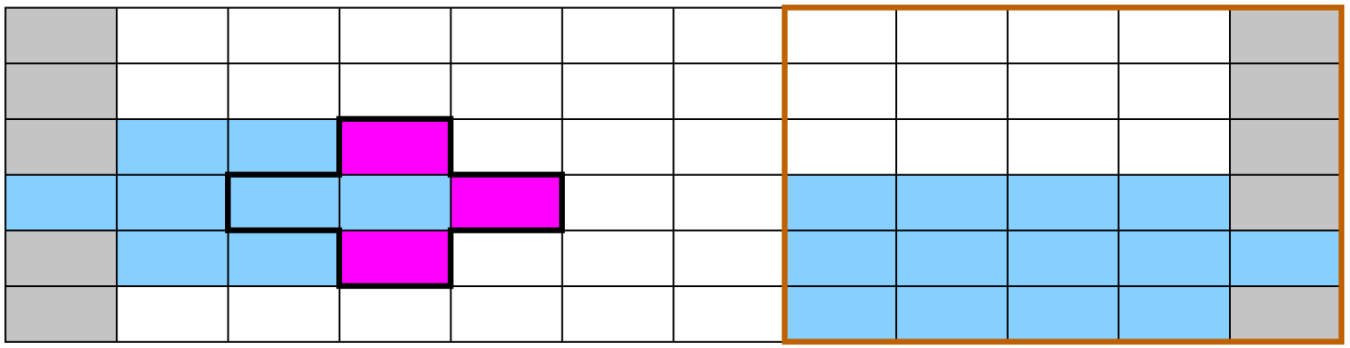
Analyzing the data flow

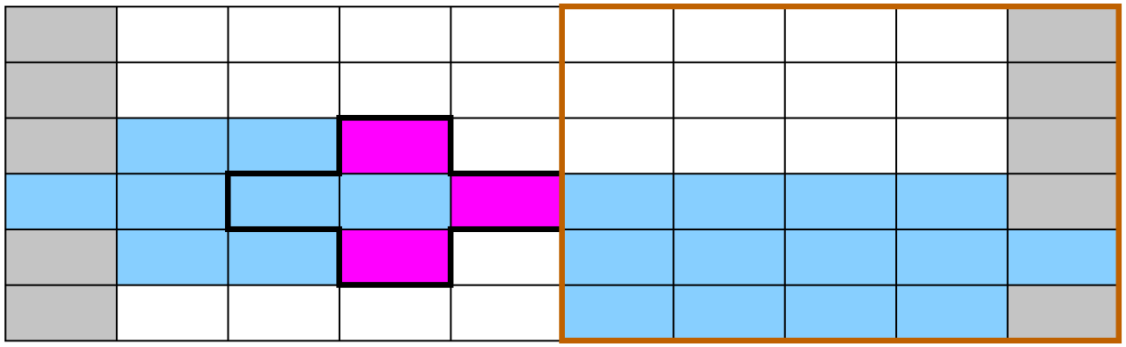
Worst case: Cache not large enough to hold 3 layers (rows) of grid
(+assume „Least Recently Used“ replacement strategy)



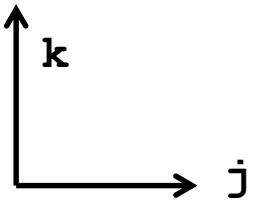
Analyzing the data flow

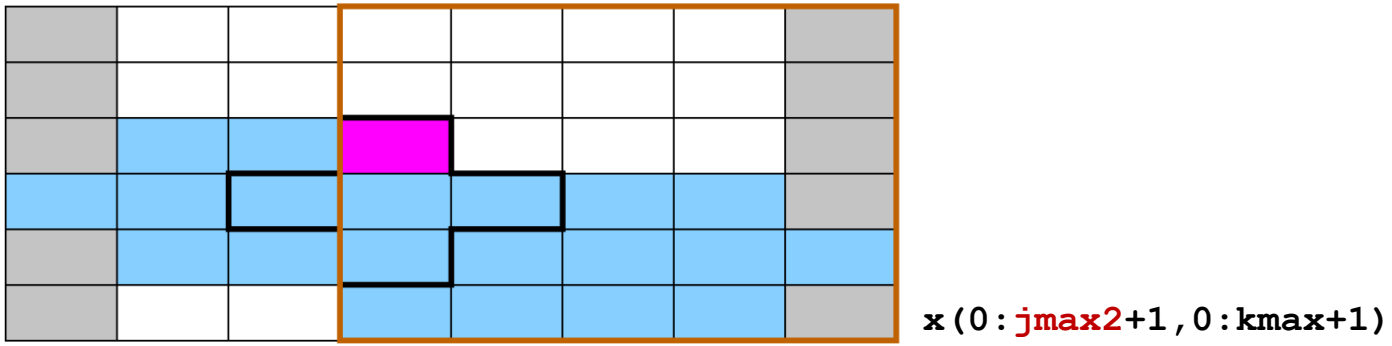
Reduce inner (j-) loop dimension successively





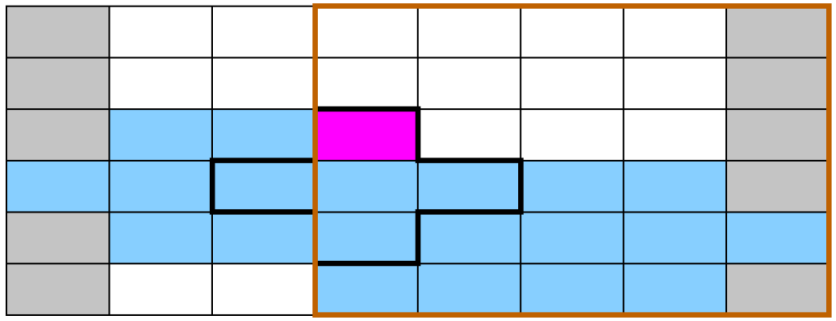
Best case: 3 „layers“ of grid fit into the cache!





Analyzing the data flow: Layer condition

2D 5-pt Jacobi-type stencil



```
do k=1,kmax
  do j=1,jmax
    y(j,k) = const * (x(j-1,k) + x(j+1,k) &
                    +  x(j,k-1) + x(j,k+1) )
  enddo
enddo
```

3 * jmax * 8B < CacheSize/2

"Layer condition"

3 rows of jmax

double precision

Safety margin (Rule of thumb)

Layer condition:

- Does not depend on outer loop length (**kmax**)
- No strict guideline (cache associativity – data traffic for y not included)
- Needs to be adapted for other stencils (e.g., 3D 7-pt stencil)

Analyzing the data flow: Layer condition (2D 5-pt Jacobi)

y: (1 LD + 1 ST) / LUP

x: 1 LD / LUP

```
do k=1,kmax
  do j=1,jmax
    y(j,k) = const * (x(j-1,k) + x(j+1,k) &
                    +  x(j,k-1) + x(j,k+1) )
  enddo
enddo
```

B_C = 24 B / LUP

YES

3 * jmax * 8B < CacheSize/2

Layer condition fulfilled?

NO

y: (1 LD + 1 ST) / LUP

```
do k=1,kmax
  do j=1,jmax
    y(j,k) = const * (x(j-1,k) + x(j+1,k) &
                    +  x(j,k-1) + x(j,k+1) )
  enddo
enddo
```

x: 3 LD / LUP

B_C = 40 B / LUP

Analyzing the data flow: Layer condition (2D 5-pt Jacobi)

- **Establish layer condition for all domain sizes**
- **Idea: Spatial blocking**
  - Reuse elements of `x()` as long as they stay in cache
  - Sweep can be executed in any order, e.g. compute blocks in j-direction

→ **"Spatial Blocking" of j-loop:**

```
do jb=1,jmax,jblock !      Assume jmax is multiple of jblock
  do k=1,kmax
    do j= jb, (jb+jblock-1) ! Length of inner loop: jblock
      y(j,k) = const * (x(j-1,k) + x(j+1,k) &
                      +  x(j,k-1) + x(j,k+1) )
    enddo
  enddo
enddo
```

New layer condition (blocking)
3 * jblock * 8B < CacheSize/2

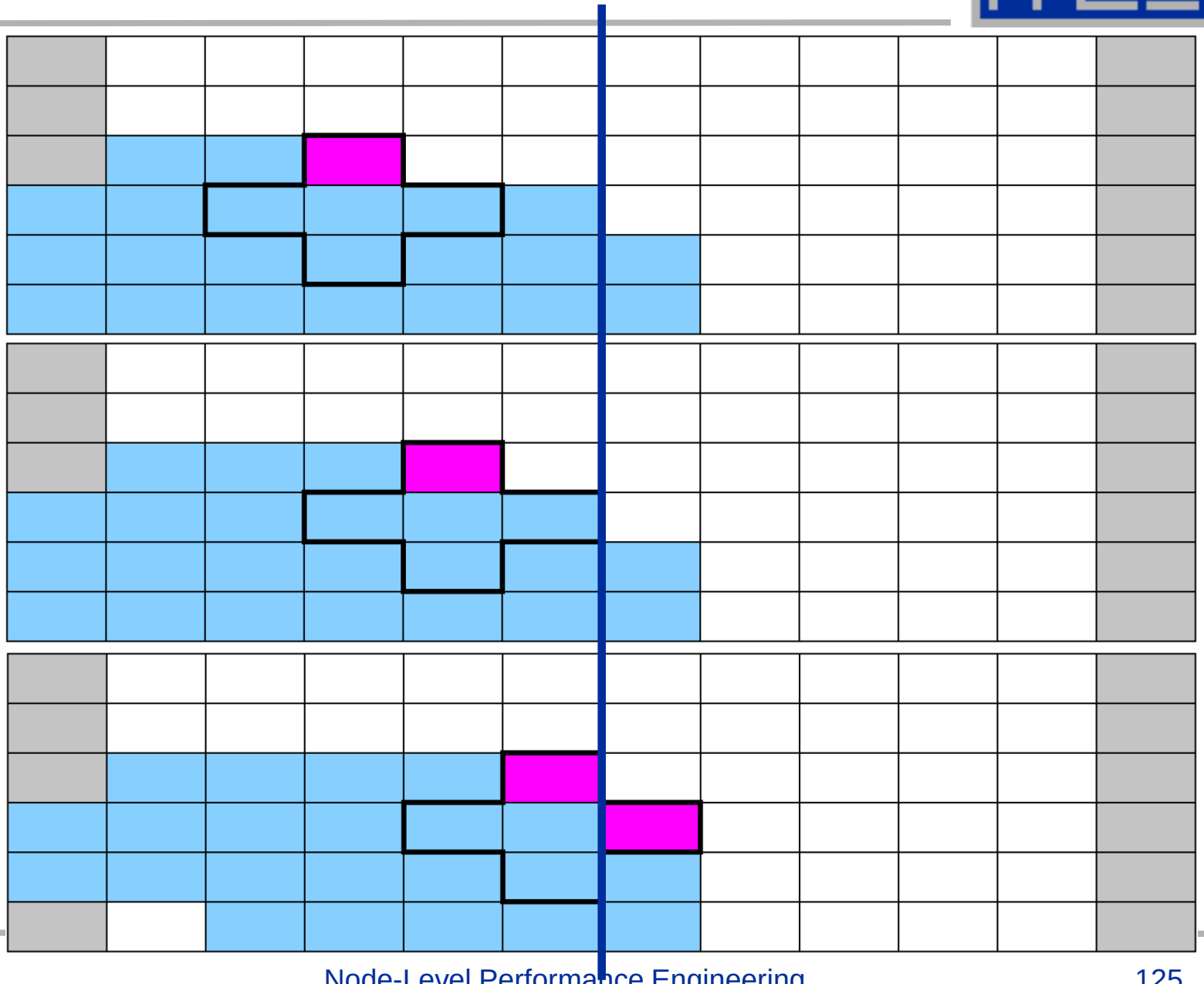
→ **Determine for given `CacheSize` an appropriate `jblock` value:**

jblock < CacheSize / 48 B

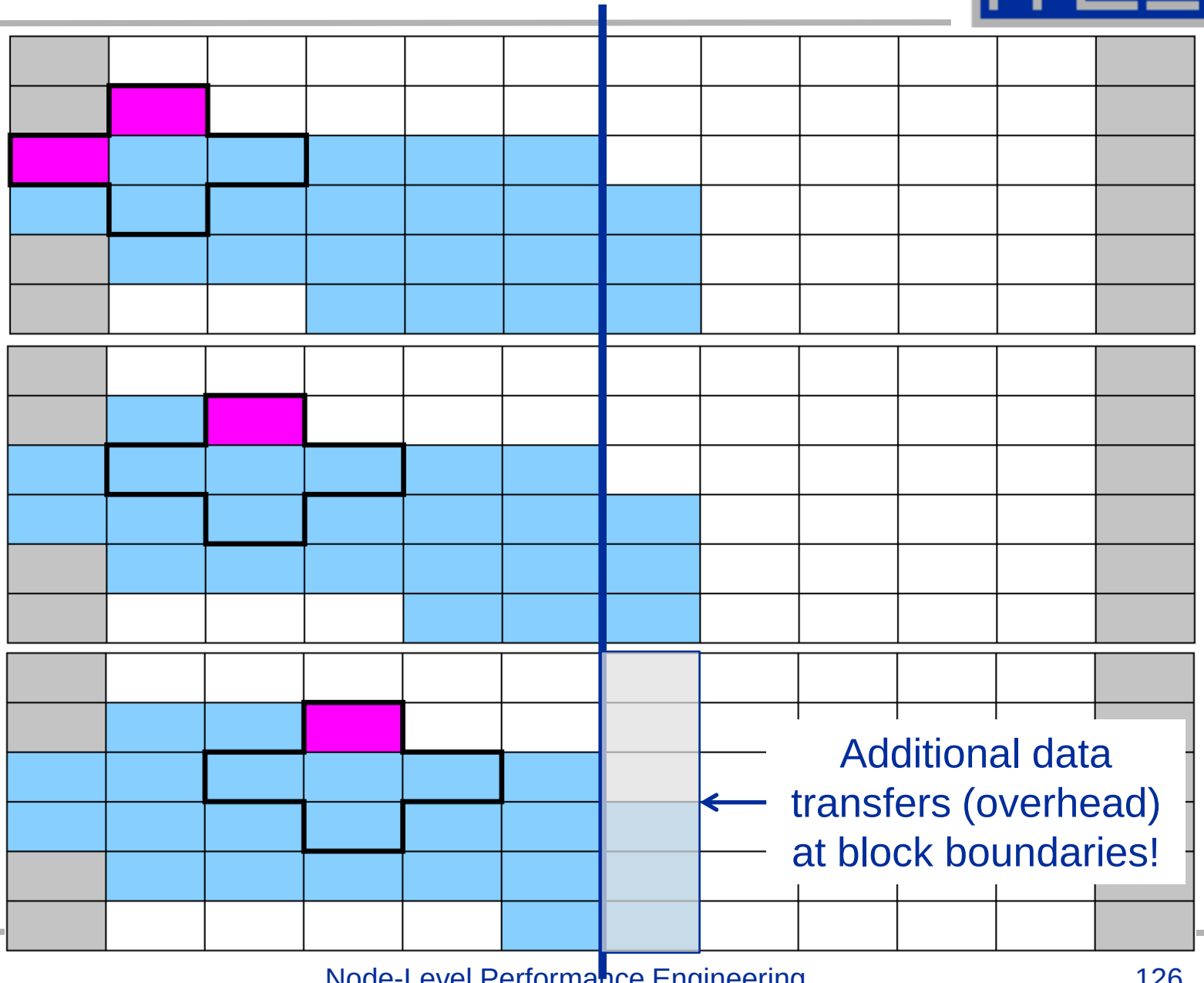
Establish the layer condition by blocking

Split up domain into subblocks:

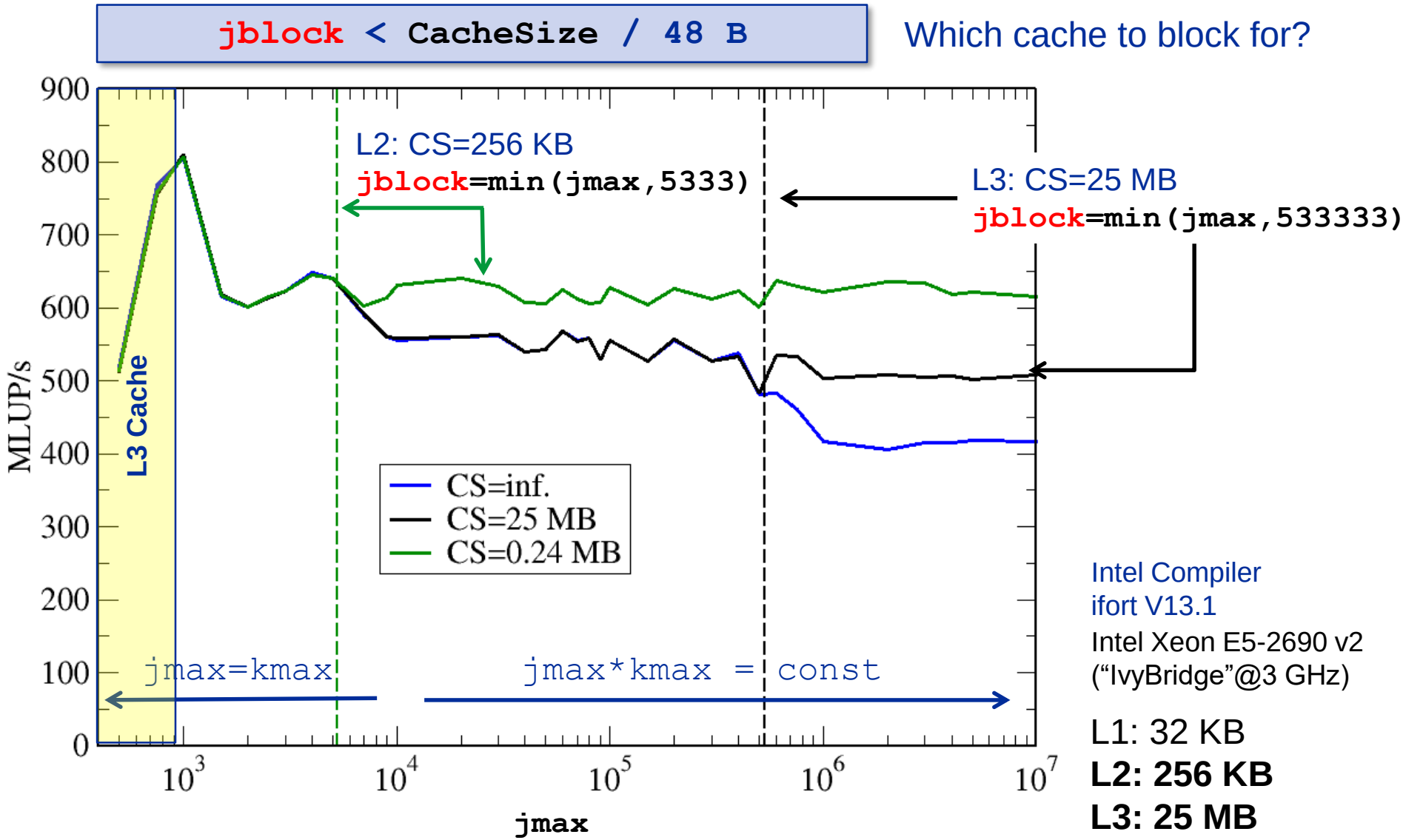
e.g. block size = 5



Establish the layer condition by blocking



Establish layer condition by spatial blocking



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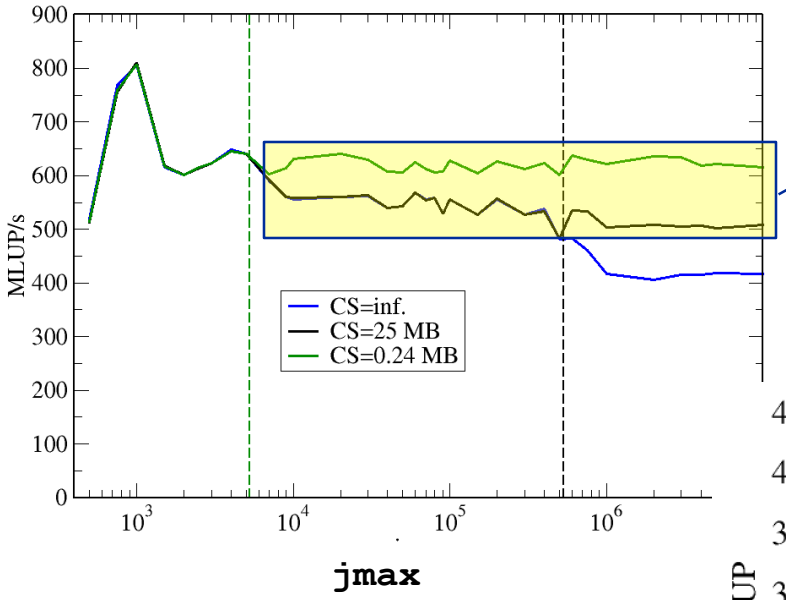
("IvyBridge"@3 GHz)

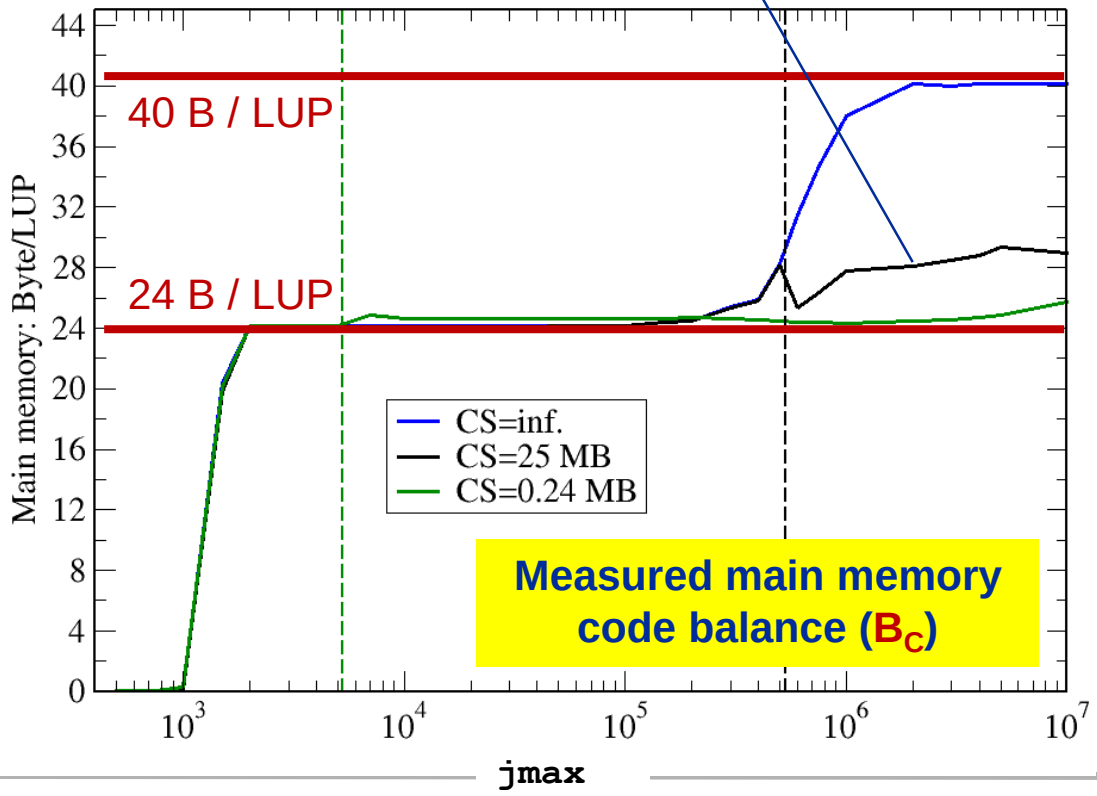
L1: 32 KB
L2: 256 KB
L3: 25 MB

Layer condition & spatial blocking: Memory code balance



Main memory access is not reason for different performance (but L3 access is!)

Blocking factor (CS=25 MB) still a little too large



Measured main memory code balance (B_C)

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ifort V13.1
Intel Xeon E5-2690 v2
("IvyBridge"@3 GHz)

Jacobi Stencil – OpenMP parallelization

```
!$OMP PARALLEL DO SCHEDULE(STATIC)
do k=1,kmax
  do j=1,jmax
    y(j,k) = 1/4.*(x(j-1,k)    +x(j+1,k) &
                 + x(j,k-1)    +x(j,k+1) )
  enddo
enddo
```

Basic guideline:
Parallelize outermost loop

Equally large chunks in k-direction
→ "Layer condition" for each thread

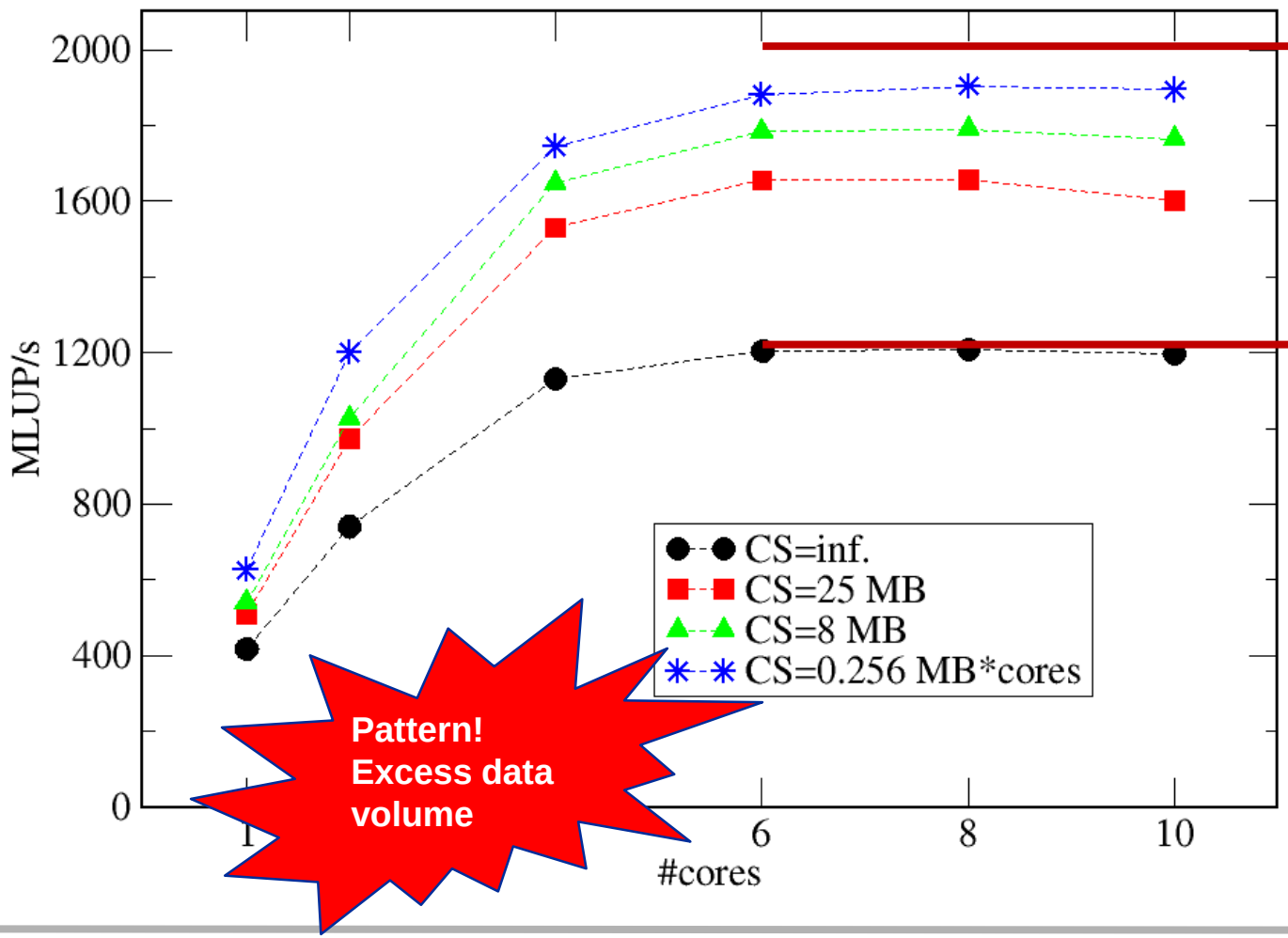
"Layer condition" for shared cache:
`nthreads * 3 *imax * 8B < CS/2`

Homework: what about if the cache to block for is not shared among the threads?

Socket scaling – validate Roofline model

$$P = \min(P_{\max}, b_S / B_C)$$

What is $P_{\max}$ here? → homework!



B_C= 24 B/LUP

B_C= 40 B/LUP

Intel Compiler
ifort V13.1
OpenMP Parallel

Intel Xeon E5-2690 v2
("IvyBridge"@3 GHz)

b_S = 48 GB/s

Conclusions from the Jacobi example

- **We have made sense of the memory-bound performance vs. problem size**
  - "Layer conditions" lead to predictions of code balance
  - "What part of the data comes from where" is a crucial question
  - The model works only if the bandwidth is "saturated"
    - In-cache modeling is more involved
- **Avoiding slow data paths == re-establishing the most favorable layer condition**
- **Improved code showed the speedup predicted by the model**
- **Optimal blocking factor can be estimated**
  - Be guided by the cache size the layer condition
  - No need for exhaustive scan of "optimization space"
- **Food for thought**
  - Multi-dimensional loop blocking – would it make sense?
  - Can we choose a "better" OpenMP loop schedule?
  - What would change if we parallelized inner loops?

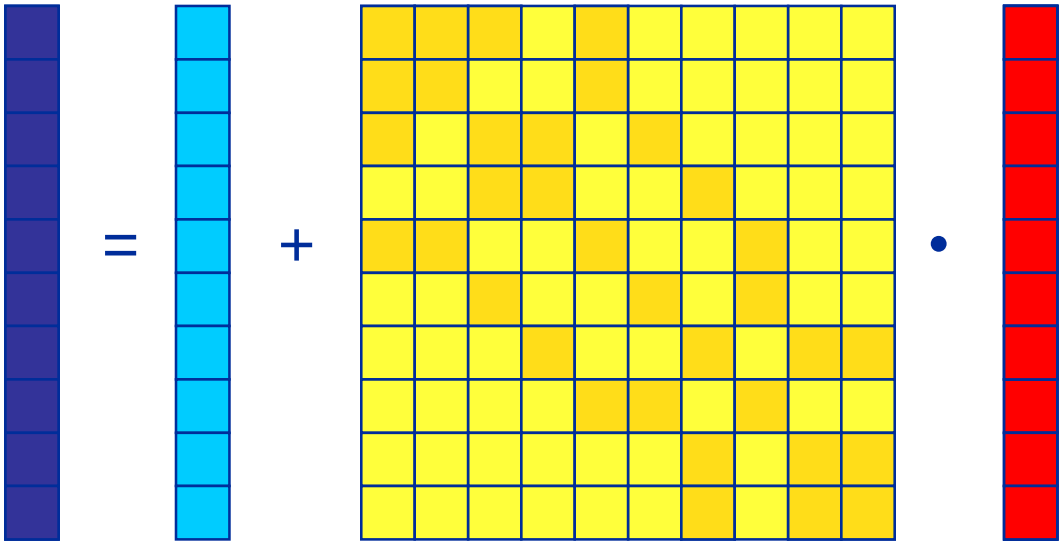
Case study:
Sparse Matrix Vector Multiplication

An example for what to do if the Roofline model isn't quite so predictive

Sparse Matrix Vector Multiplication (spMVM)

- **Key ingredient in some matrix diagonalization algorithms**
  - Lanczos, Davidson, Jacobi-Davidson

- **Store only N_{nz} nonzero elements of matrix and RHS, LHS vectors with N_r (number of matrix rows) entries**
- **"Sparse": $N_{nz} \sim N_r$**

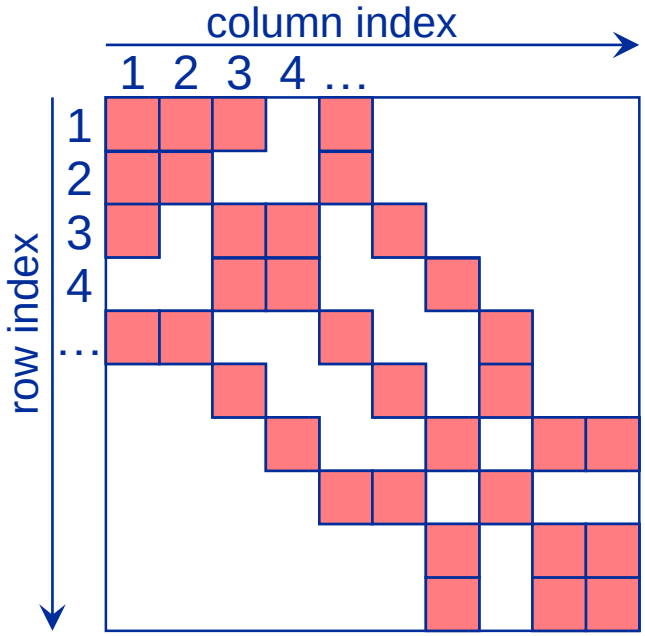


General case: some indirect addressing required!

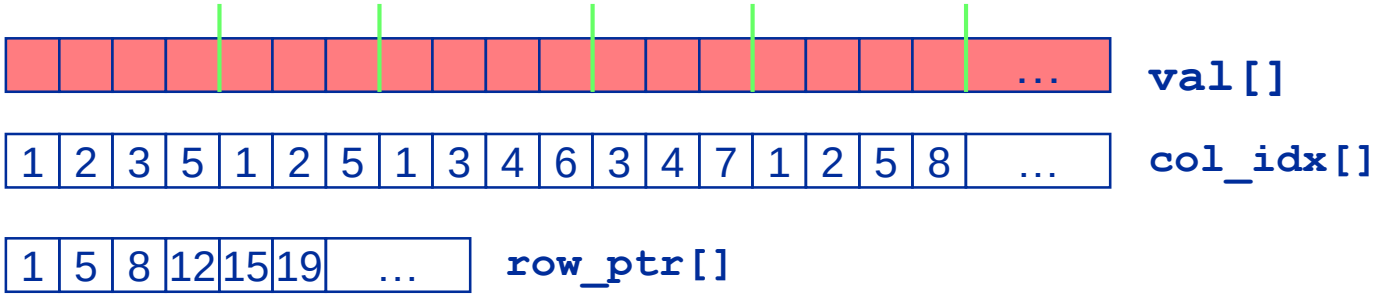
SpMVM characteristics

- **For large problems, spMVM is inevitably memory-bound**
  - Intra-socket saturation effect on modern multicores
- **SpMVM is easily parallelizable in shared and distributed memory**
- **Data storage format is crucial for performance properties**
  - Most useful general format on CPUs: Compressed Row Storage (CRS)
  - Depending on compute architecture

CRS matrix storage scheme



- **`val[]`** stores all the nonzeros (length N_{nz})
- **`col_idx[]`** stores the column index of each nonzero (length N_{nz})
- **`row_ptr[]`** stores the starting index of each new row in **`val[]`** (length: N_r)



Case study: Sparse matrix-vector multiply

- **Strongly memory-bound for large data sets**
  - Streaming, with partially indirect access:

```
!$OMP parallel do
do i = 1,N_r
 do j = row_ptr(i), row_ptr(i+1) - 1
  c(i) = c(i) + val(j) * b(col_idx(j))
 enddo
enddo
!$OMP end parallel do
```

  - Usually many spMVMs required to solve a problem

- **Now let's look at some performance measurements…**

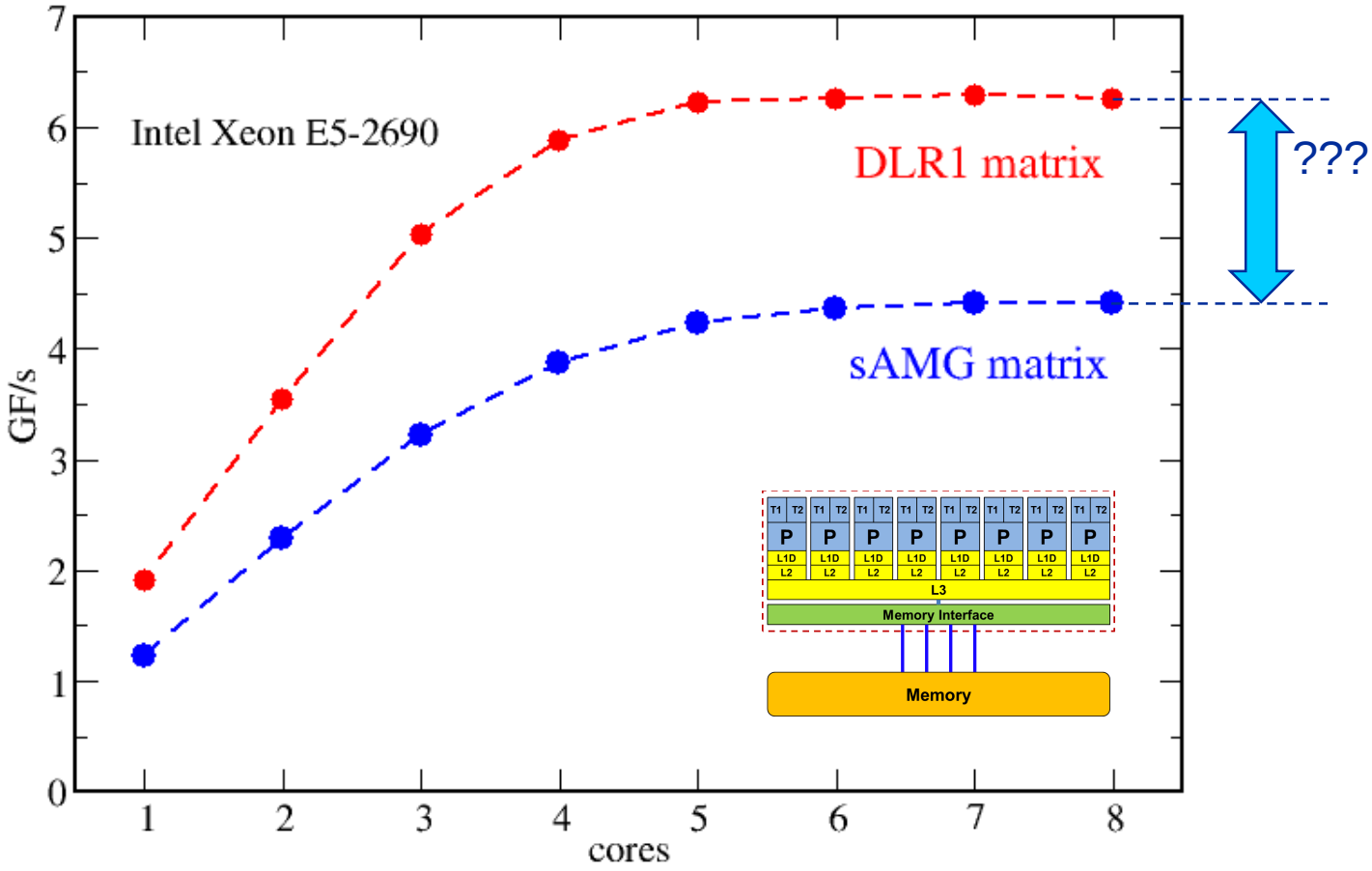
Performance characteristics

- Strongly memory-bound for large data sets → saturating performance across cores on the chip
- Performance seems to depend on the matrix

- Can we explain this?

- Is there a "light speed" for spMVM?

- Optimization?



Example: SpMVM node performance model

- Sparse MVM in double precision w/ CRS data storage:

```
do i = 1,Nr
  do j = row_ptr(i), row_ptr(i+1) - 1
    C(i) = C(i) + val(j) * B(col_idx(j))
  enddo
enddo
```

- DP CRS comp. intensity

$$I_{CRS}^{DP} = \frac{2}{8 + 4 + 8\alpha + 16/N_{nzr}} \frac{\text{flops}}{\text{byte}}$$

  - α quantifies traffic for loading RHS
    - $\alpha = 0$ → RHS is in cache
    - $\alpha = 1/N_{nzr}$ → RHS loaded once
    - $\alpha = 1$ → no cache
    - $\alpha > 1$ → Houston, we have a problem!
  - "Expected" performance = b_S x I_{CRS}
  - Determine α by measuring performance and actual memory traffic
    - Maximum memory BW may not be achieved with spMVM

"best" in-memory intensity: $I = \frac{1}{6}\,\text{F/B}$, or $B_C^{mem} = 6\,\text{B/F}$

Determine RHS traffic

$$I_{CRS}^{DP} = \frac{2}{8+4+8\alpha+16/N_{nzr}} \frac{\text{flops}}{\text{byte}} = \frac{N_{nz} \cdot 2 \text{ flops}}{V_{meas}}$$

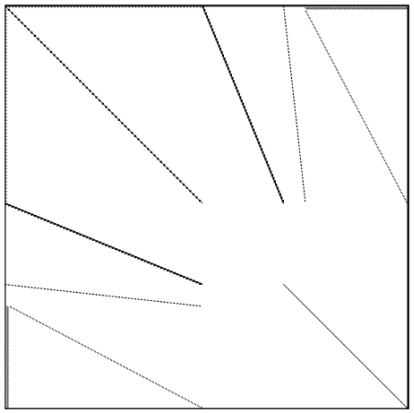
- V_{meas} is the measured overall memory data traffic (using, e.g., likwid-perfctr)
- Solve for α:

$$\alpha = \frac{1}{4}\left(\frac{V_{meas}}{N_{nz} \cdot 2 \text{ bytes}} - 6 - \frac{8}{N_{nzr}}\right)$$

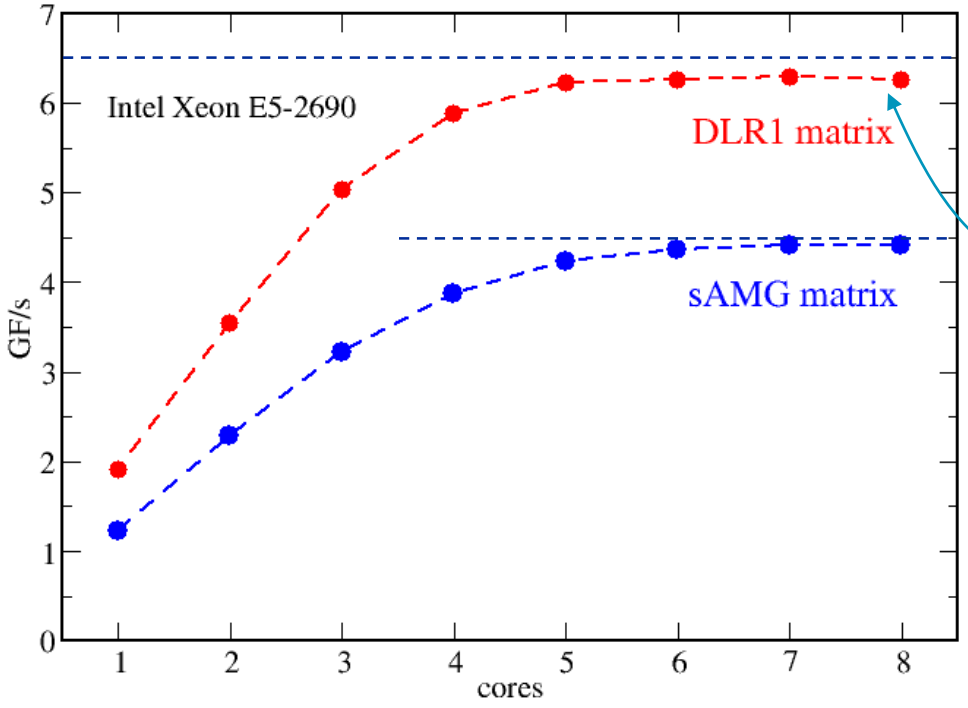
- Example: kkt_power matrix from the UoF collection on one Intel SNB socket
  - $N_{nz} = 14.6 \cdot 10^6, N_{nzr} = 7.1$
  - $V_{meas} \approx 258 \text{ MB}$
  - → $\alpha = 0.43$, $\alpha N_{nzr} = 3.1$
  - → RHS is loaded 3.1 times from memory
  - and:

$$\frac{I_{CRS}^{DP}(1/N_{nzr})}{I_{CRS}^{DP}(\alpha)} = 1.15$$

15% extra traffic → optimization potential!



Now back to the start…



- $b_S = 39\ \mathrm{GB/s}$
- $B_c^{min} = 6\ \mathrm{B/F}$
- Maximum spMVM performance:

$$P_{max} = 6.5\ \mathrm{GF/s}$$

- → DLR1 causes minimum code balance!

- sAMG matrix code balance:

$$B_c \leq \frac{b_S}{4.5\ \mathrm{GF/s}} = 8.7\ \mathrm{B/F}$$

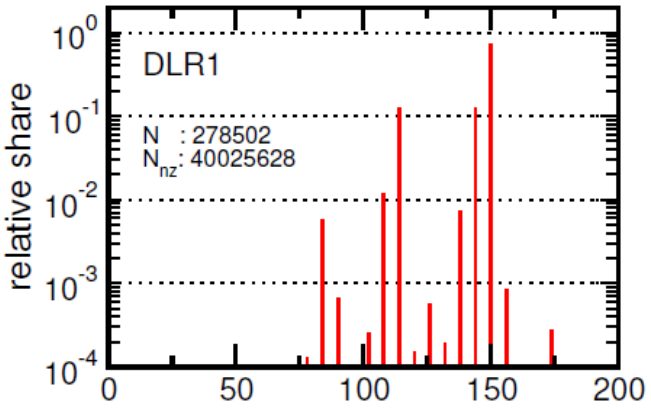
- Why is this only an upper limit?
- What is the next step?
- Could we have predicted this qualitative difference?

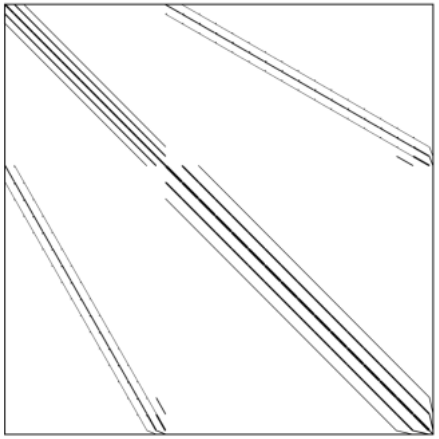
Sparse matrix testcases

optional

“DLR1” (A. Basermann, DLR)

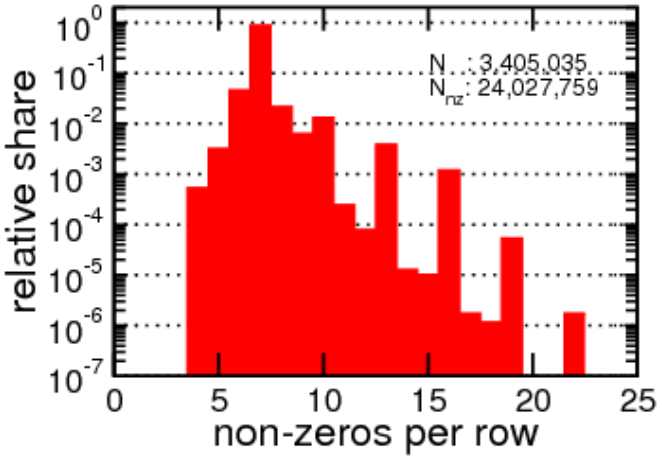
Adjoint problem computation (turbulent transonic flow over a wing) with the TAU CFD system of the German Aerospace Center (DLR)
Avg. non-zeros/row ~150

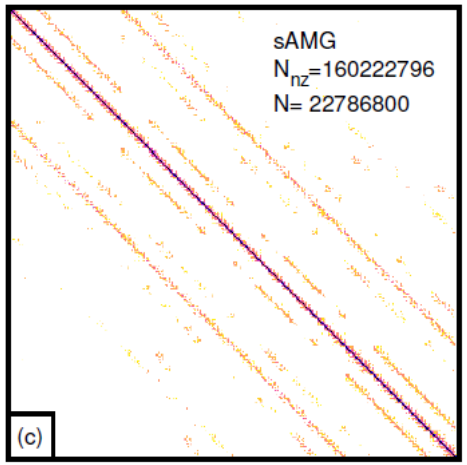




“sAMG” (K. Stüben, FhG-SCAI)

Matrix from FhG’s adaptive multigrid code sAMG for the irregular discretization of a Poisson problem on a car geometry.
Avg. non-zeros/row ~ 7





Roofline analysis for spMVM

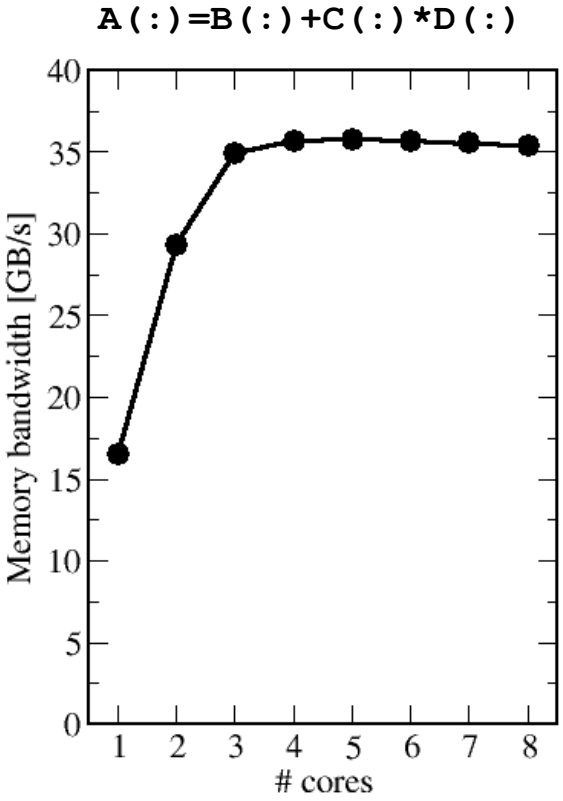
- **Conclusion from Roofline analysis**
  - The roofline model does not “work” for spMVM due to the RHS traffic uncertainties
  - We have “turned the model around” and measured the actual memory traffic to determine the RHS overhead
  - Result indicates:
    1. how much actual traffic the RHS generates
    2. how efficient the RHS access is (compare BW with max. BW)
    3. how much optimization potential we have with matrix reordering

- **Consequence: Modeling is not always 100% predictive. It‘s all about *learning more* about performance properties!**

Shortcomings of the roofline model

- **Saturation effects in multicore chips are not explained**
  - Reason: "saturation assumption"
  - Cache line transfers and core execution do sometimes not overlap perfectly
  - It is not sufficient to measure single-core STREAM to make it work
  - Only increased "pressure" on the memory interface can saturate the bus
    → need more cores!
- **In-cache performance is not correctly predicted**
- **The ECM performance model gives more insight:**

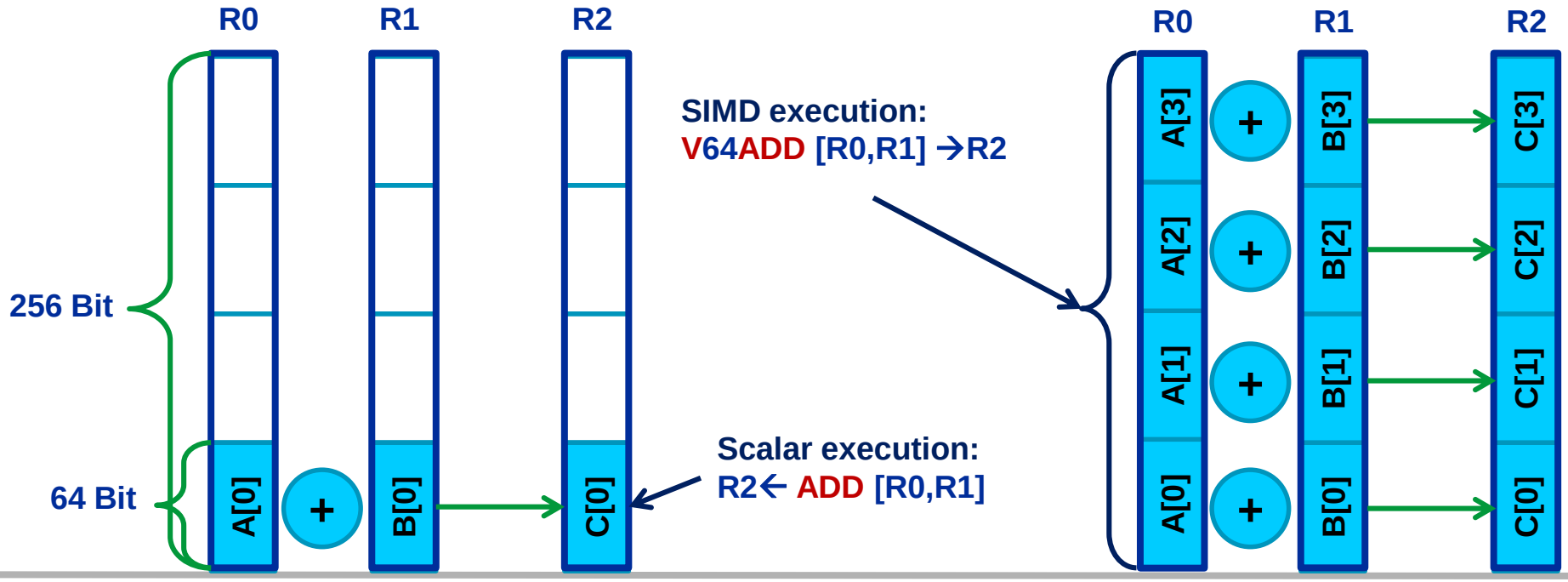
H. Stengel, J. Treibig, G. Hager, and G. Wellein: *Quantifying performance bottlenecks of stencil computations using the Execution-Cache-Memory model*. Proc. ICS15, the 29th International Conference on Supercomputing, June 8-11, 2015, Newport Beach, CA. DOI: 10.1145/2751205.2751240. Preprint: arXiv:1410.5010



Coding for SingleInstructionMultipleData processing

SIMD processing – Basics

- **Single Instruction Multiple Data (SIMD) operations allow the concurrent execution of the same operation on "wide" registers.**
- **x86 SIMD instruction sets:**
  - SSE: register width = 128 Bit → 2 double precision floating point operands
  - AVX: register width = 256 Bit → 4 double precision floating point operands
- **Adding two registers holding double precision floating point operands**



Vectorization compiler options (Intel)

- **The compiler will vectorize starting with –O2.**
- **To enable specific SIMD extensions use the –x option:**
  - **`-xSSE2`** vectorize for SSE2 capable machines

  Available SIMD extensions:

  `SSE2, SSE3, SSSE3, SSE4.1, SSE4.2, AVX`

  - **`-xAVX(2)`** on Sandy Bridge (Haswell) processors

  Recommended option:
  - **`-xHost`** will optimize for the architecture you compile on

  On AMD Opteron: use plain **`–O3`** as the **`-x`** options may involve CPU type checks.

Vectorization compiler options

- **Controlling non-temporal stores (part of the SIMD extensions)**
  - `-opt-streaming-stores always|auto|never`

`always`	use NT stores, assume application is memory bound (use with caution!)
`auto`	compiler decides when to use NT stores
`never`	do not use NT stores unless activated by source code directive

Vectorization source code directives

- Fine-grained control of loop vectorization
- Use `!DEC$` (Fortran) or `#pragma` (C/C++) sentinel to start a compiler directive

- `#pragma vector always`
  vectorize even if it seems inefficient (hint!)

- `#pragma novector`
  do not vectorize even if possible

- `#pragma vector nontemporal`
  use NT stores when allowed (i.e. alignment conditions are met)

- `#pragma vector aligned`
  specifies that all array accesses are aligned to 16-byte boundaries (DANGEROUS! You must not lie about this!)

User mandated vectorization

- Since Intel Compiler 12.0 the `simd` pragma is available
- `#pragma simd` enforces vectorization where the other pragmas fail
- Prerequesites:
  - Countable loop
  - Innermost loop
  - Must conform to for-loop style of OpenMP worksharing constructs
- There are additional clauses: `reduction, vectorlength, private`
- Refer to the compiler manual for further details

```
#pragma simd reduction(+:x)
  for (int i=0; i<n; i++) {
     x = x + A[i];
  }
```

- NOTE: Using the #pragma simd the compiler may generate incorrect code if the loop violates the vectorization rules!

- **Alignment issues**
  - Alignment of arrays with SSE (AVX) should be on 16-byte (32-byte) boundaries to allow packed aligned loads and NT stores **(for Intel processors)**
    - **AMD has a scalar nontemporal store instruction**
  - Otherwise the compiler will revert to unaligned loads and not use NT stores – even if you say **`vector nontemporal`**
  - Modern x86 CPUs have less (not zero) impact for misaligned LD/ST, but **Xeon Phi (KNC) relies heavily on it!**
  - How is manual alignment accomplished?
- **Dynamic allocation of aligned memory (`align` = alignment boundary):**

```
#define _XOPEN_SOURCE 600
#include <stdlib.h>

int posix_memalign(void **ptr,
                   size_t align,
                   size_t size);
```

Reading x86 assembly code and exploiting SIMD parallelism

- Understanding SIMD execution by inspecting assembly code
- SIMD vectorization how-to
- Intel compiler options and features for SIMD

Why check the assembly code?

- **Sometimes the only way to make sure the compiler "did the right thing"**
  - Example: "LOOP WAS VECTORIZED" message is printed, but Loads & Stores may still be scalar!

- **Get the assembler code (Intel compiler):**

```
icc -S -masm=intel -O3  -xHost  triad.c  -o a.out
```

- **Disassemble Executable:**

```
objdump -d  ./a.out | less
```

The x86 ISA is documented in:

Intel Software Development Manual (SDM) 2A and 2B
AMD64 Architecture Programmer's Manual Vol. 1-5

Basics of the x86-64 ISA

- Instructions have 0 to 4 operands
- Operands can be registers, memory references or immediates
- Opcodes (binary representation of instructions) vary from 1 to 17 bytes
- There are two syntax forms: Intel (left) and AT&T (right)
- Addressing Mode: BASE + INDEX * SCALE + DISPLACEMENT
- C: `A[i]` equivalent to `*(A+i)` (a pointer has a type: `A+i*8`)

```
movaps [rdi + rax*8+48], xmm3
add rax, 8
js 1b
```

```
movaps    %xmm4, 48(%rdi,%rax,8)
addq      $8, %rax
js        ..B1.4
```

```
401b9f: 0f 29 5c c7 30      movaps %xmm3,0x30(%rdi,%rax,8)
401ba4: 48 83 c0 08         add    $0x8,%rax
401ba8: 78 a6               js     401b50 <triad_asm+0x4b>
```

16 general Purpose Registers (64bit):

`rax, rbx, rcx, rdx, rsi, rdi, rsp, rbp, r8-r15`

alias with eight 32 bit register set:

`eax, ebx, ecx, edx, esi, edi, esp, ebp`

Floating Point SIMD Registers:

`xmm0-xmm15` SSE (128bit) alias with 256-bit registers

`ymm0-ymm15` AVX (256bit)

SIMD instructions are distinguished by:

AVX (VEX) prefix:	`v`
Operation:	`mul, add, mov`
Modifier:	nontemporal (`nt`), unaligned (`u`), aligned (`a`), high (`h`)
Width:	scalar (`s`), packed (`p`)
Data type:	single (`s`), double (`d`)

Case Study: Vector Triad (DP) on IvyBridge-EP

```
for (int i = 0; i < length; i++) {
    A[i] = B[i] + D[i] * C[i];
}
```

To get object code use `objdump -d` on object file or executable or compile with `-S`

Assembly code (-O1):

CLANG

```
LBB0_3
movsd   xmm0, [rdx]
mulsd   xmm0, [rcx]
addsd   xmm0, [rsi]
movsd   [rax], xmm0
add     rsi, 8
add     rdx, 8
add     rcx, 8
add     rax, 8
dec     edi
jne     LBB0_3
```

ICC

```
..B1.6:
movsd   xmm0, [r12+rax*8]
mulsd   xmm0, [r13+rax*8]
addsd   xmm0, [r14+rax*8]
movsd   [r15+rax*8], xmm0
inc     rax
cmp     rax, rbx
jl      ..B1.6
```

GCC

```
.L4:
movsd xmm0,[rbx+rax]
mulsd xmm0,[r12+rax]
addsd xmm0,[r13+0+rax]
movsd [rbp+0+rax],xmm0
add rax, 8
cmp rax, r14
jne .L4
```

7 instructions per loop iteration

Case Study: Vector Triad (DP) –O3 –xHost + #pragma vector aligned

AVX

```
..B1.7:
vmovupd    ymm0, [r15+rcx*8]
vmovupd    ymm4, [32+r15+rcx*8]
vmovupd    ymm7, [64+r15+rcx*8]
vmovupd    ymm10,[96+r15+rcx*8]
vmulpd     ymm2, ymm0, [rdx+rcx*8]
vmulpd     ymm5, ymm4, [32+rdx+rcx*8]
vmulpd     ymm8, ymm7, [64+rdx+rcx*8]
vmulpd     ymm11, ymm10, [96+rdx+rcx*8]
vaddpd     ymm3, ymm2, [r14+rcx*8]
vaddpd     ymm6, ymm5, [32+r14+rcx*8]
vaddpd     ymm9, ymm8, [64+r14+rcx*8]
vaddpd     ymm12, ymm11, [96+r14+rcx*8]
vmovupd    [r13+rcx*8], ymm3
vmovupd    [32+r13+rcx*8], ymm6
vmovupd    [64+r13+rcx*8], ymm9
vmovupd    [96+r13+rcx*8], ymm12
add        rcx, 16
cmp        rcx, rsi
jb         ..B1.7
```

1.19 instructions per loop iteration

Case Study: Vector Triad (DP) –O3 –xHost
`#pragma vector aligned` on Haswell-EP

optional

AVX + FMA3

```
..B1.7:
vmovupd    ymm2, [r15+rcx*8]
vmovupd    ymm4, [32+r15+rcx*8]
vmovupd    ymm6, [64+r15+rcx*8]
vmovupd    ymm8, [96+r15+rcx*8]
vmovupd    ymm0, [rdx+rcx*8]
vmovupd    ymm3, [32+rdx+rcx*8]
vmovupd    ymm5, [64+rdx+rcx*8]
vmovupd    ymm7, [96+rdx+rcx*8]
vfmadd213pd ymm2, ymm0, [r14+rcx*8]
vfmadd213pd ymm4, ymm3, [32+r14+rcx*8]
vfmadd213pd ymm6, ymm5, [64+r14+rcx*8]
vfmadd213pd ymm8, ymm7, [96+r14+rcx*8]
vmovupd    [r13+rcx*8], ymm2
vmovupd    [32+r13+rcx*8], ymm4
vmovupd    [64+r13+rcx*8], ymm6
vmovupd    [96+r13+rcx*8], ymm8
add        rcx, 16
cmp        rcx, rsi
jb         ..B1.7
```

1.19 instructions per loop iteration

On X86 ISA instruction are converted to so-called µops (elementary ops like load, add, mult). For performance the number of µops is important.

23 uops vs. 27 µops (AVX)

SIMD processing – The whole picture

SIMD influences instruction execution in the core – other runtime contributions stay the same!

AVX example (Haswell-EP):

See P_{max} analysis

Execution — **3 cy**

Caches — **15 cy**

Memory — **21 cy**

Per-cacheline (8 iterations) cycle counts

Comparing total execution time (cycles):

	Execution	Cache	Memory
Scalar	12	15	21
SSE	6	15	21
AVX	3	15	21

Total runtime with data loaded from memory:

Scalar	48 cy
SSE	42 cy
AVX	39 cy

SIMD is only effective if runtime is dominated by instruction execution!

How to leverage SIMD: your options

Alternatives:

- The compiler does it for you (but: aliasing, alignment, language)
- Compiler directives (pragmas)
- Alternative programming models for compute kernels (OpenCL, ispc)
- Intrinsics (restricted to C/C++)
- Implement directly in assembler

To use intrinsics the following headers are available:

- **xmmintrin.h (SSE)**
- **pmmintrin.h (SSE2)**
- **immintrin.h (AVX)**
- **x86intrin.h (all extensions)**

```
for (int j=0; j<size; j+=16){
    t0 = _mm_loadu_ps(data+j);
    t1 = _mm_loadu_ps(data+j+4);
    t2 = _mm_loadu_ps(data+j+8);
    t3 = _mm_loadu_ps(data+j+12);
    sum0 = _mm_add_ps(sum0, t0);
    sum1 = _mm_add_ps(sum1, t1);
    sum2 = _mm_add_ps(sum2, t2);
    sum3 = _mm_add_ps(sum3, t3);
}
```

Rules for vectorizable loops

1. Inner loop
2. Countable (loop length can be determined at loop entry)
3. Single entry and single exit
4. Straight line code (no conditionals)
5. No (unresolvable) read-after-write data dependencies
6. No function calls (exception intrinsic math functions)

Better performance with:

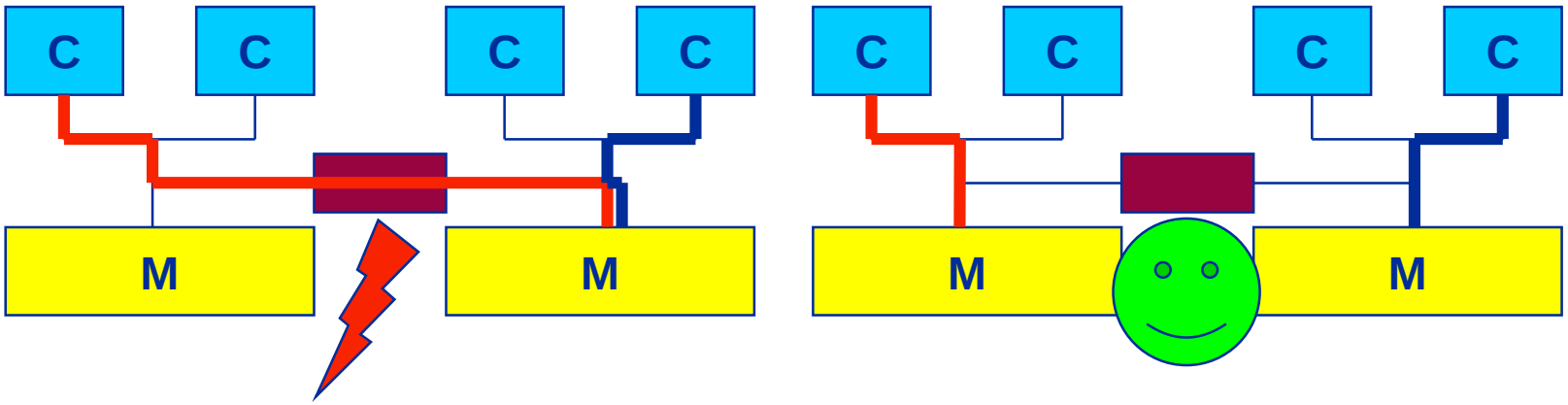
1. Simple inner loops with unit stride (contiguous data access)
2. Minimize indirect addressing
3. Align data structures to SIMD width boundary
4. In C use the **`restrict`** keyword and/or **`const`** qualifiers and/or compiler options to rule out array/pointer aliasing

Efficient parallel programming on ccNUMA nodes

Performance characteristics of ccNUMA nodes

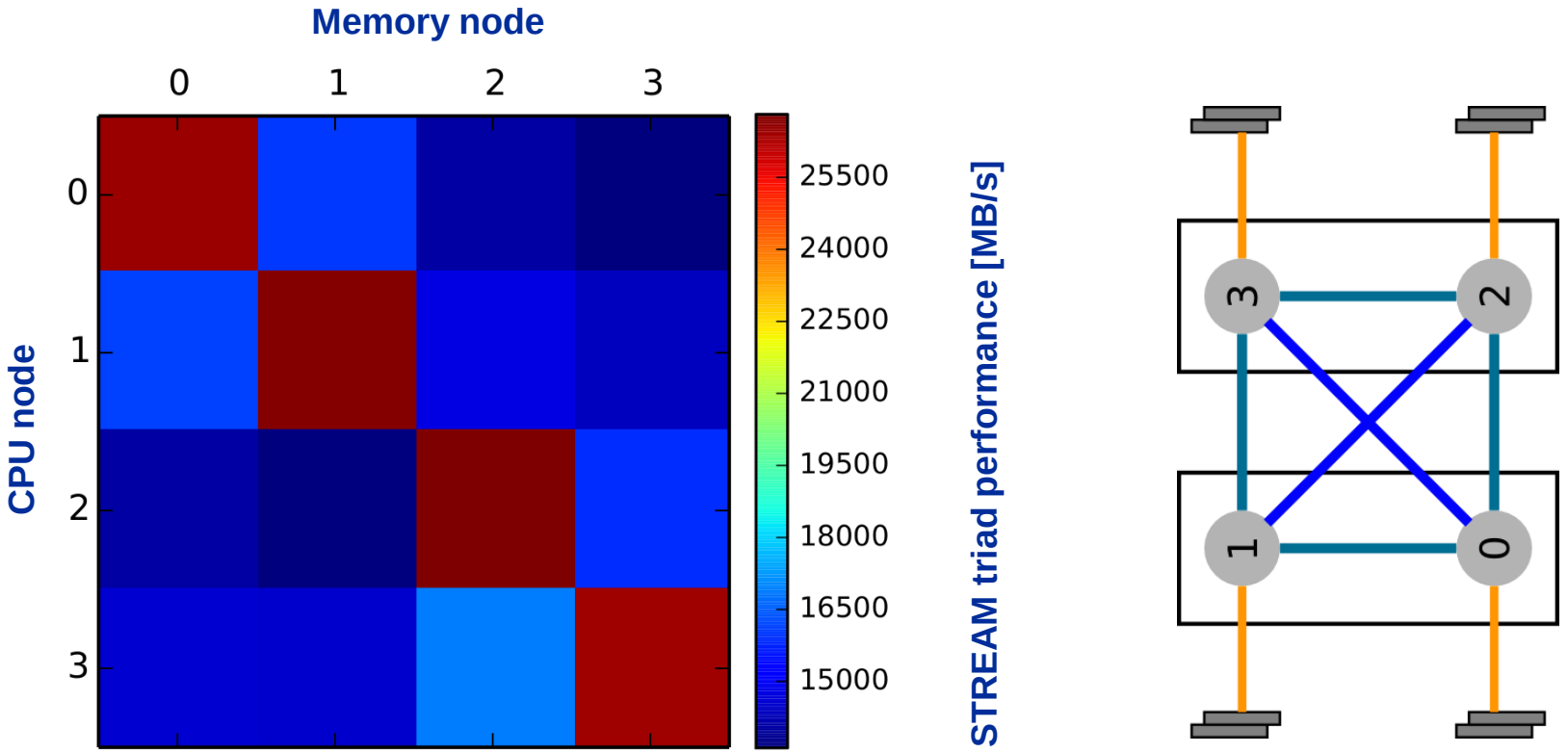
First touch placement policy

- **ccNUMA:**
  - Whole memory is transparently accessible by all processors
  - but physically distributed
  - with varying bandwidth and latency
  - and potential contention (shared memory paths)
- **How do we make sure that memory access is always as "local" and "distributed" as possible?**



  - Page placement is implemented in units of OS pages (often 4kB, possibly more)

- **ccNUMA map: Bandwidth penalties for remote access**
  - Run 11 threads per ccNUMA domain (half chip)
  - Place memory in different domain → 4x4 combinations
  - STREAM copy benchmark using standard stores



numactl as a simple ccNUMA locality tool :

How do we enforce some locality of access?

- **`numactl` can influence the way a binary maps its memory pages:**

```
numactl --membind=<nodes> a.out     # map pages only on <nodes>
        --preferred=<node>  a.out   # map pages on <node>
                                    # and others if <node> is full
        --interleave=<nodes> a.out  # map pages round robin across
                                    # all <nodes>
```

- **Examples:**

```
for m in `seq 0 3`; do
  for c in `seq 0 3`; do
    env OMP_NUM_THREADS=8 \
        numactl --membind=$m --cpunodebind=$c ./stream
  enddo
enddo
```

ccNUMA map scan

```
env OMP_NUM_THREADS=4 numactl --interleave=0-3 \
                              likwid-pin -c N:0,4,8,12 ./stream
```

- **But what is the default without `numactl`?**

ccNUMA default memory locality

- **"Golden Rule" of ccNUMA:**

  A memory page gets mapped into the local memory of the processor that first touches it!

  - Except if there is not enough local memory available
  - This might be a problem, see later
- **Caveat: "touch" means "write", not "allocate"**
- **Example:**

```
double *huge = (double*)malloc(N*sizeof(double));

for(i=0; i<N; i++) // or i+=PAGE_SIZE
   huge[i] = 0.0;
```

Memory not mapped here yet

Mapping takes place here

- **It is sufficient to touch a single item to map the entire page**

Coding for ccNUMA data locality

- **Most simple case: explicit initialization**

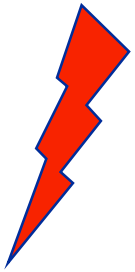
```
integer,parameter :: N=10000000
double precision A(N), B(N)



A=0.d0



!$OMP parallel do
do i = 1, N
  B(i) = function ( A(i) )
end do
!$OMP end parallel do
```



```
integer,parameter :: N=10000000
double precision A(N),B(N)
!$OMP parallel
!$OMP do schedule(static)
do i = 1, N
  A(i)=0.d0
end do
!$OMP end do
...
!$OMP do schedule(static)
do i = 1, N
  B(i) = function ( A(i) )
end do
!$OMP end do
!$OMP end parallel
```

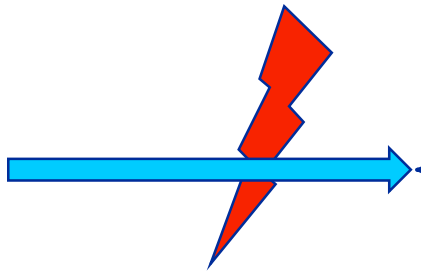
Coding for ccNUMA data locality

- Sometimes initialization is not so obvious: I/O cannot be easily parallelized, so “localize” arrays before I/O

```
integer,parameter :: N=10000000
double precision A(N), B(N)

READ(1000) A

!$OMP parallel do
do i = 1, N
  B(i) = function ( A(i) )
end do
!$OMP end parallel do
```



```
integer,parameter :: N=10000000
double precision A(N),B(N)
!$OMP parallel
!$OMP do schedule(static)
do i = 1, N
  A(i)=0.d0
end do
!$OMP end do
!$OMP single
READ(1000) A
!$OMP end single
!$OMP do schedule(static)
do i = 1, N
  B(i) = function ( A(i) )
end do
!$OMP end do
!$OMP end parallel
```

Coding for Data Locality

- **Required condition: OpenMP loop schedule of initialization must be the same as in all computational loops**
  - Only choice: `static`! Specify explicitly on all NUMA-sensitive loops, just to be sure…
  - Imposes some constraints on possible optimizations (e.g. load balancing)
  - If dynamic scheduling/tasking is unavoidable, more advanced methods may be in order

- **How about global objects?**
  - Better not use them
  - If communication vs. computation is favorable, might consider properly placed copies of global data
- **C++: Arrays of objects and `std::vector<>` are by default initialized sequentially**
  - STL allocators provide an elegant solution

Coding for Data Locality:
Placement of static arrays or arrays of objects

- **Don't forget that constructors tend to touch the data members of an object. Example:**

```
class D {
  double d;
public:
  D(double _d=0.0) throw() : d(_d) {}
  inline D operator+(const D& o) throw() {
    return D(d+o.d);
  }
  inline D operator*(const D& o) throw() {
    return D(d*o.d);
  }
...
};
```

→ **placement problem with**

```
D* array = new D[1000000];
```

Coding for Data Locality:
Parallel first touch for arrays of objects

- **Solution: Provide overloaded `D::operator new[]`**

```
void* D::operator new[](size_t n) {
  char *p = new char[n];    // allocate

  size_t i,j;
#pragma omp parallel for private(j) schedule(...)
  for(i=0; i<n; i += sizeof(D))
    for(j=0; j<sizeof(D); ++j)
      p[i+j] = 0;
  return p;
}

void D::operator delete[](void* p) throw() {
  delete [] static_cast<char*>p;
}
```

parallel first touch

- **Placement of objects is then done automatically by the C++ runtime via "placement new"**

Coding for Data Locality:
NUMA allocator for parallel first touch in `std::vector<>`


```
template <class T> class NUMA_Allocator {
public:
  T* allocate(size_type numObjects, const void
              *localityHint=0) {
    size_type ofs,len = numObjects * sizeof(T);
    void *m = malloc(len);
    char *p = static_cast<char*>(m);
    int i,pages = len >> PAGE_BITS;
#pragma omp parallel for schedule(static) private(ofs)
    for(i=0; i<pages; ++i) {
      ofs = static_cast<size_t>(i) << PAGE_BITS;
      p[ofs]=0;
    }
    return static_cast<pointer>(m);
  }
...
};
```

Application:

```
vector<double,NUMA_Allocator<double> > x(10000000)
```

Diagnosing Bad Locality

- **If your code is cache bound, you might not notice any locality problems**
- **Otherwise, bad locality limits scalability at very low CPU numbers (whenever a node boundary is crossed)**
  - If the code makes good use of the memory interface
- **Running with `numactl --interleave` might give you a hint**
  - See later
- **Consider using performance counters**
  - LIKWID-perfctr can be used to measure nonlocal memory accesses
  - Example for Intel Westmere dual-socket system (Core i7, hex-core):

```
env OMP_NUM_THREADS=12 likwid-perfctr -g MEM -C N:0-11 ./a.out
```

Using performance counters for diagnosing bad ccNUMA access locality

- **Intel Westmere EP node (2x6 cores):**

Only one memory BW per socket ("Uncore")

Metric	core 0	core 1	...	core 6	core 7	...
Runtime [s]	0.730168	0.733754		0.732808	0.732943	
CPI	10.4164	10.2654		10.5002	10.7641	
Memory bandwidth [MBytes/s]	11880.9	0		11732.4	0	
Remote Read BW [MBytes/s]	4219	0		4163.45	0	
Remote Write BW [MBytes/s]	1706.19	0		1705.09	0	
Remote BW [MBytes/s]	5925.19	0		5868.54	0	

Half of BW comes from other socket!

If all fails…

- **Even if all placement rules have been carefully observed, you may still see nonlocal memory traffic. Reasons?**
  - Program has erratic access patters → may still achieve some access parallelism (see later)
  - OS has filled memory with buffer cache data:

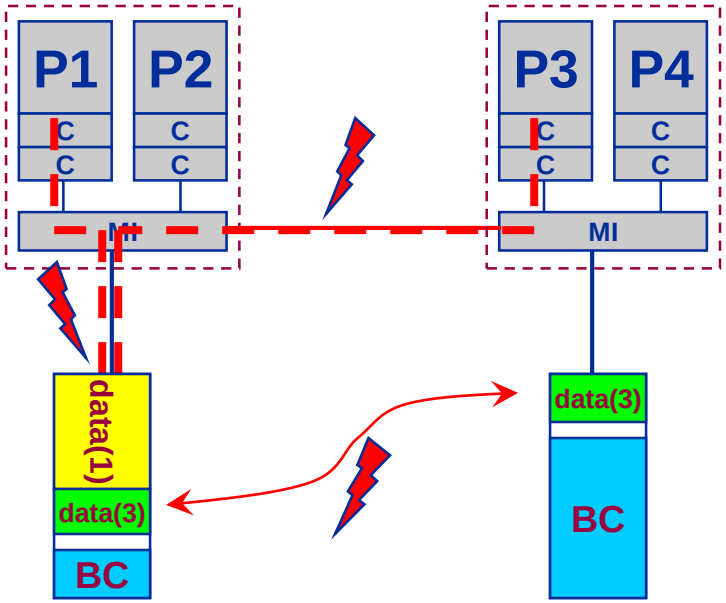
```
# numactl --hardware    # idle node!
available: 2 nodes (0-1)
node 0 size: 2047 MB
node 0 free: 906 MB
node 1 size: 1935 MB
node 1 free: 1798 MB
```

```
top - 14:18:25 up 92 days,  6:07,  2 users,  load average: 0.00, 0.02, 0.00
Mem:   4065564k total,  1149400k used,  2716164k free,    43388k buffers
Swap:  2104504k total,     2656k used,  2101848k free,  1038412k cached
```

ccNUMA problems beyond first touch:
Buffer cache

optional

- **OS uses part of main memory for disk buffer (FS) cache**
  - If FS cache fills part of memory, apps will probably allocate from foreign domains
  - → non-local access!
  - "sync" is not sufficient to drop buffer cache blocks



- **Remedies**
  - Drop FS cache pages after user job has run (admin's job)
    - seems to be automatic after aprun has finished on Crays
  - User can run "sweeper" code that allocates and touches all physical memory before starting the real application
  - **`numactl`** tool or **`aprun`** can force local allocation (where applicable)
  - Linux: There is no way to limit the buffer cache size in standard kernels

ccNUMA problems beyond first touch:
Buffer cache

optional

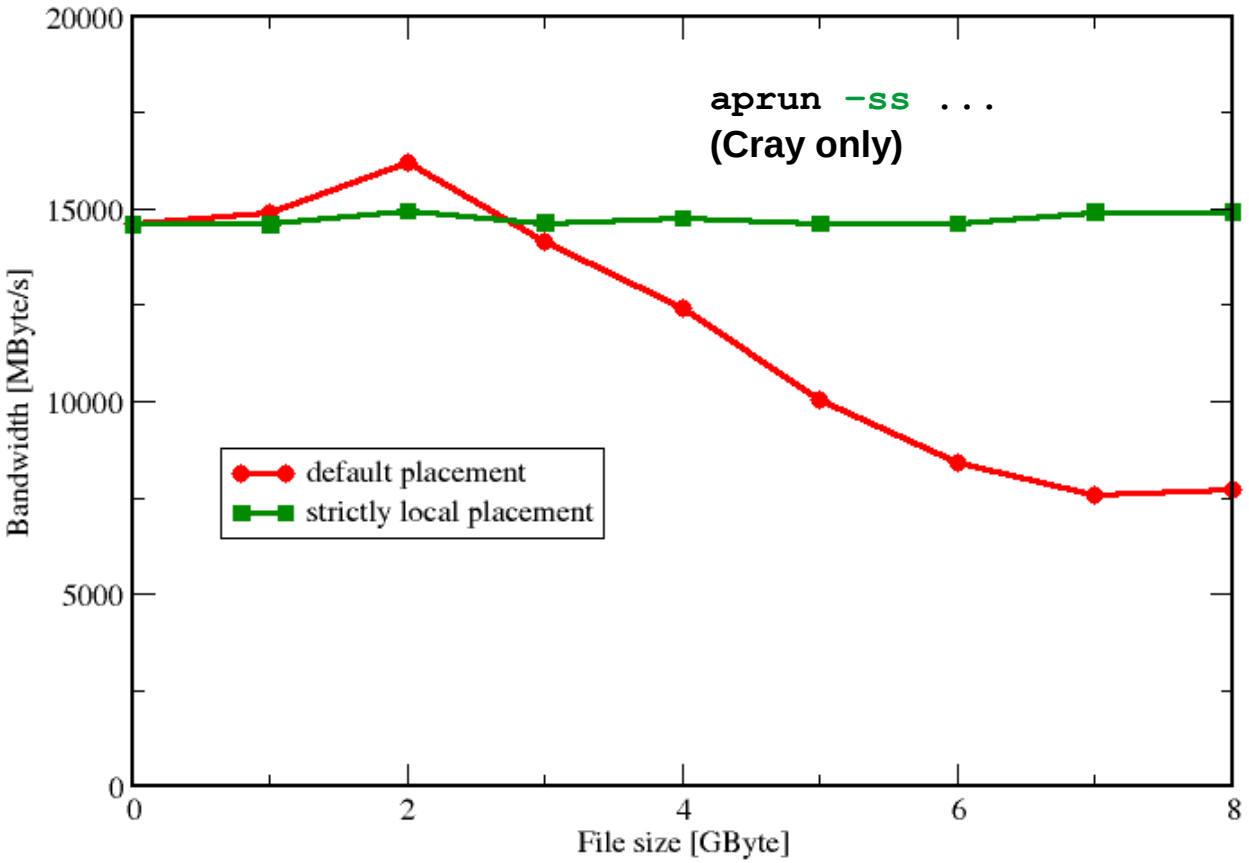
Real-world example: ccNUMA and the Linux buffer cache

Benchmark:

1. Write a file of some size from LD0 to disk
2. Perform bandwidth benchmark using all cores in LD0 and maximum memory installed in LD0

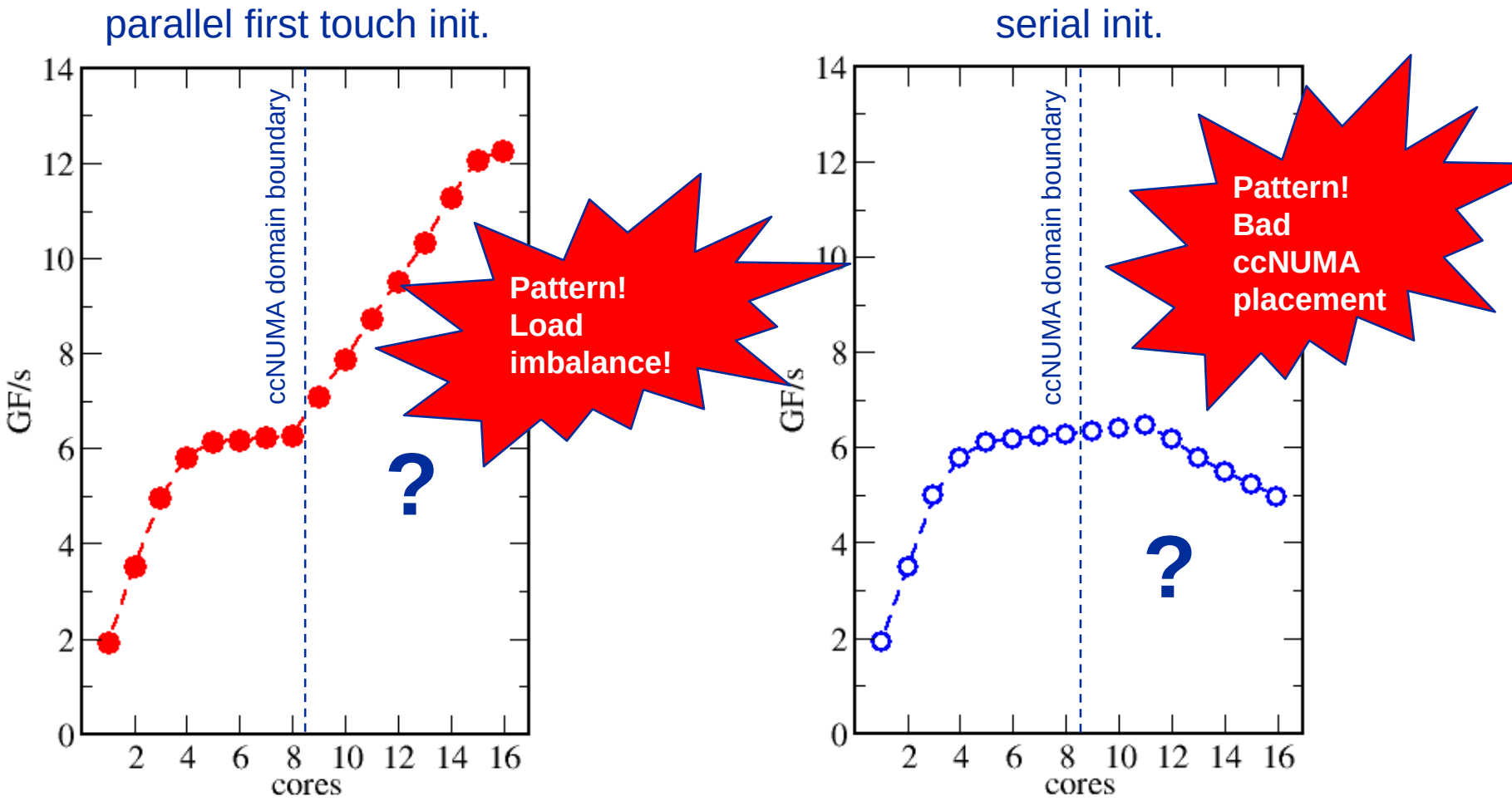
Result: By default, Buffer cache is given priority over local page placement

→ restrict to local domain if possible!

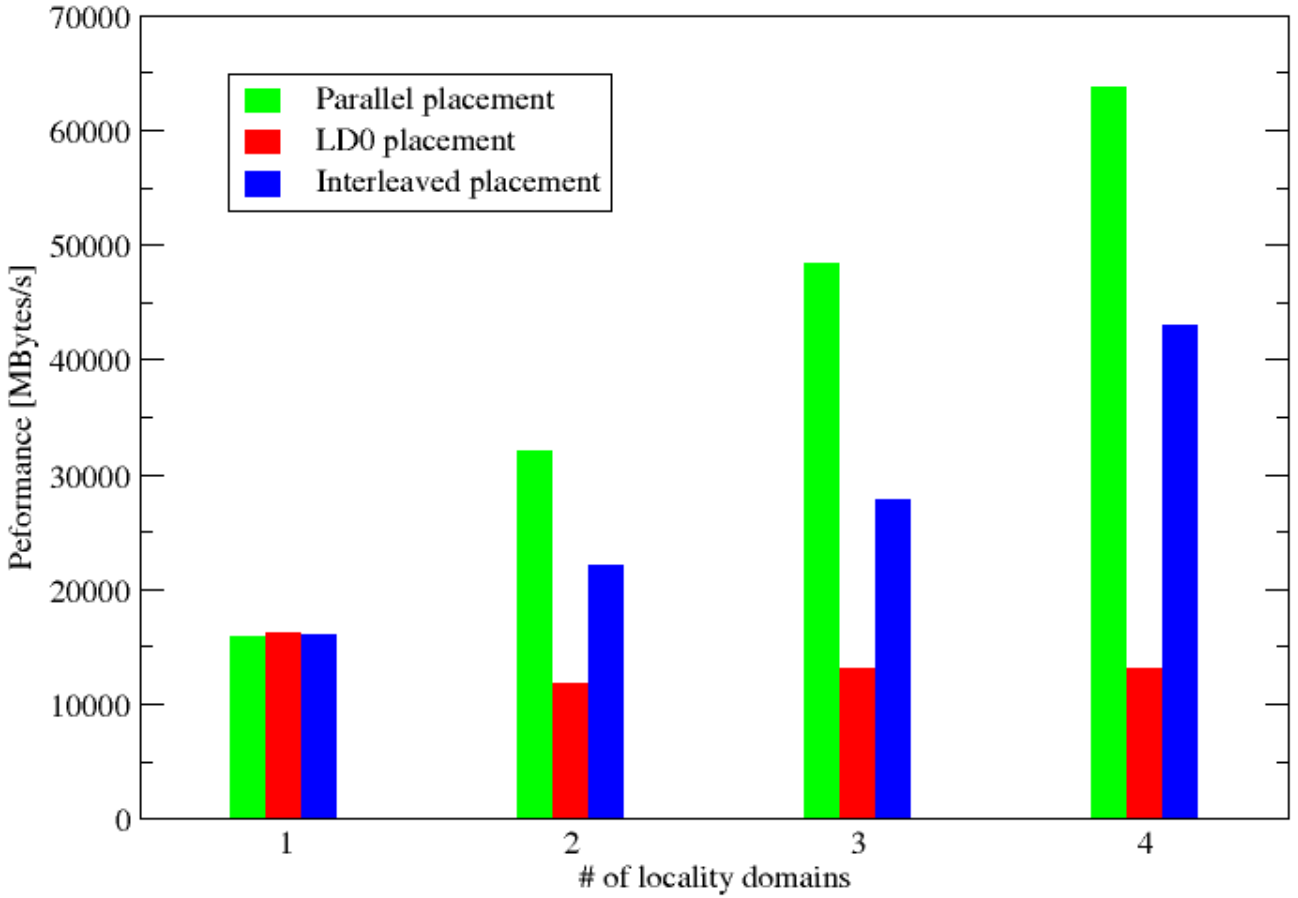


Back to the spMVM code: a little riddle

DLR1 matrix on 2x 8-core Sandy Bridge node



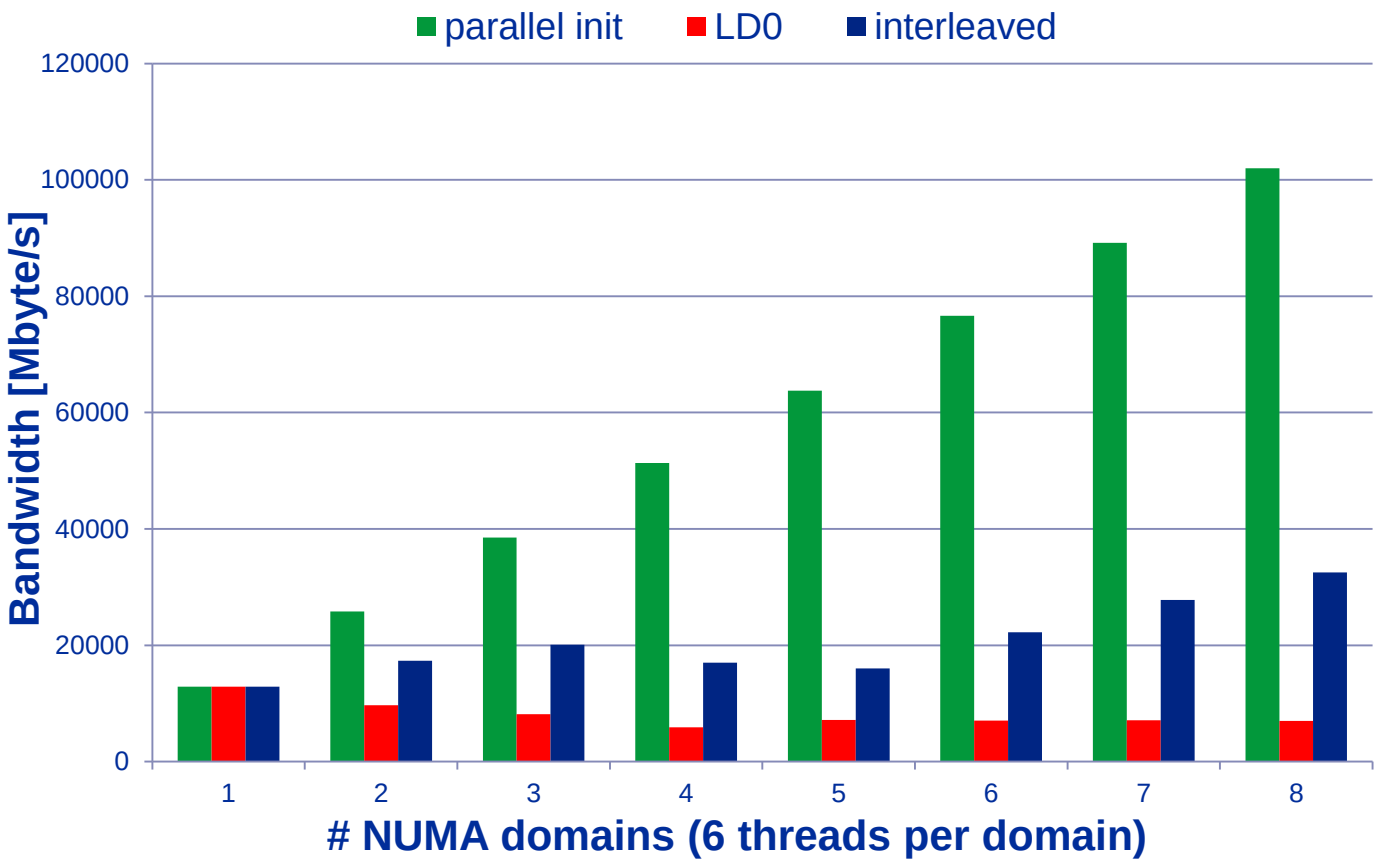
- **Parallel init: Correct parallel initialization**
- **LD0: Force data into LD0 via `numactl -m 0`**
- **Interleaved: `numactl --interleave <LD range>`**



The curse and blessing of interleaved placement:
OpenMP STREAM triad on 4-socket (48 core) Magny Cours node

optional

- **Parallel init: Correct parallel initialization**
- **LD0: Force data into LD0 via `numactl -m 0`**
- **Interleaved: `numactl --interleave <LD range>`**



Summary on ccNUMA issues

- **Identify the problem**
  - Is ccNUMA an issue in your code?
  - Simple test: run with **`numactl --interleave`**
- **Apply first-touch placement**
  - Look at initialization loops
  - Consider loop lengths and static scheduling
  - C++ and global/static objects may require special care
- **If dynamic scheduling cannot be avoided**
  - Distribute the data anyway, just do not use sequential placement!
- **OS file buffer cache may impact proper placement**

OpenMP performance issues on multicore

Barrier synchronization overhead

Topology dependence

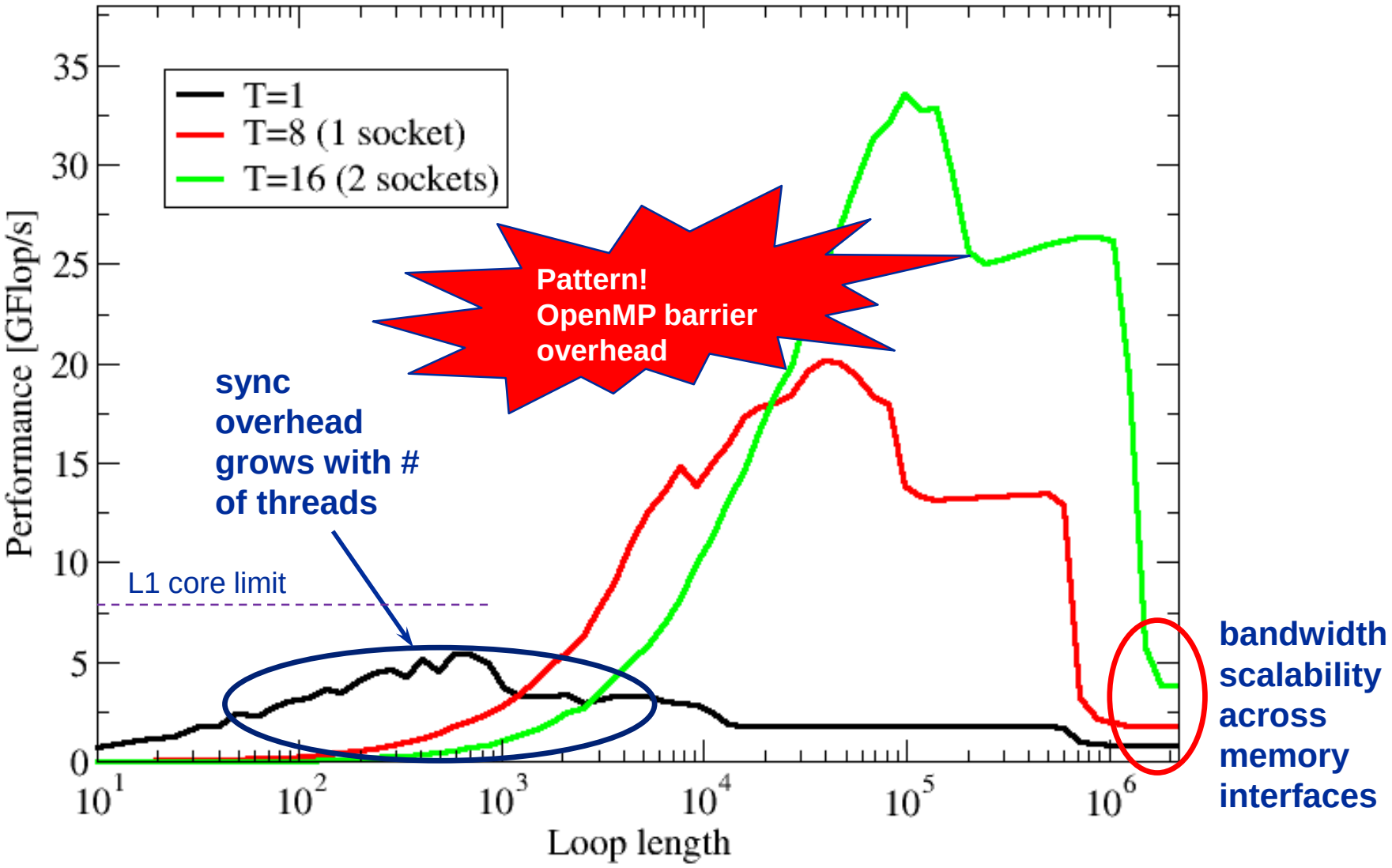
OpenMP work sharing in the benchmark loop

```
double precision, dimension(:), allocatable :: A,B,C,D

allocate(A(1:N),B(1:N),C(1:N),D(1:N))
A=1.d0; B=A; C=A; D=A
!$OMP PARALLEL private(i,j)
do j=1,NITER
!$OMP DO
  do i=1,N
    A(i) = B(i) + C(i) * D(i)
  enddo
!$OMP END DO
  if(.something.that.is.never.true.) then
    call dummy(A,B,C,D)
  endif
enddo
!$OMP END PARALLEL
```

Implicit barrier

OpenMP vector triad on Sandy Bridge sockets (3 GHz)



Welcome to the multi-/many-core era

Synchronization of threads may be expensive!

```
!$OMP PARALLEL …
…
!$OMP BARRIER
!$OMP DO
…
!$OMP ENDDO
!$OMP END PARALLEL
```

Threads are synchronized at **explicit** AND **implicit** barriers. These are a main source of overhead in OpenMP progams.

Determine costs via modified OpenMP Microbenchmarks testcase (epcc)

On x86 systems there is no hardware support for synchronization!

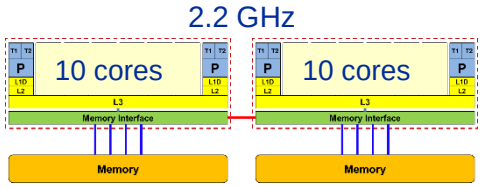
- **Next slides: Test OpenMP Barrier performance…**
- **for different compilers**
- **and different topologies:**
  - **shared cache**
  - **shared socket**
  - **between sockets**
- **and different thread counts**
  - **2 threads**
  - **full domain (chip, socket, node)**

Thread synchronization overhead on IvyBridge-EP

Barrier overhead in CPU cycles

2 Threads	Intel 16.0	GCC 5.3.0
Shared L3	**599**	**425**
SMT threads	**612**	**423**
Other socket	**1486**	**1067**

Strong topology dependence!



Full domain	Intel 16.0	GCC 5.3.0
Socket (10 cores)	1934	1301
Node (20 cores)	**4999**	**7783**
Node +SMT	5981	9897

Overhead grows with thread count

- **Strong dependence on compiler, CPU and system environment!**
- `OMP_WAIT_POLICY=ACTIVE` **can make a big difference**

Thread synchronization overhead on Xeon Phi 7210 (64-core)

Barrier overhead in CPU cycles (Intel C compiler 16.03)

2 threads on distinct cores: 730

	SMT1	SMT2	SMT3	SMT4
One core	n/a	**963**	1580	2240
Full chip	5720	8100	9900	**11400**

Still the pain may be much larger, as more work can be done in one cycle on Phi compared to a full Ivy Bridge node

3.2x cores (20 vs 64) on Phi

4x more operations per cycle per core on Phi

→ 4 · 3.2 = 12.8x more work done on Xeon Phi per cycle

1.9x more barrier penalty (cycles) on Phi (11400 vs. 6000)

→ One barrier causes 1.9 · 12.8 ≈ 24x more pain ☺.

Pattern-driven Performance Engineering

Basics of Benchmarking

Performance Patterns

Signatures

Basics of optimization

1. Define relevant test cases
2. Establish a sensible performance metric
3. Acquire a runtime profile (sequential)
4. Identify hot kernels (Hopefully there are any!)
5. Carry out optimization process for each kernel

Motivation:

- Understand observed performance
- Learn about code characteristics and machine capabilities
- Deliberately decide on optimizations

Best practices for benchmarking

- **Preparation**
  - Reliable timing (minimum time which can be measured?)
  - Document code generation (flags, compiler version)
  - Get access to an exclusive system
  - System state (clock speed, turbo mode, memory, caches)
  - Consider to automate runs with a script (shell, python, perl)

- **Doing**
  - Affinity control
  - Check: Is the result reasonable?
  - Is result deterministic and reproducible?
  - Statistics: Mean, Best ?
  - Basic variants: Thread count, affinity, working set size

Thinking in bottlenecks

- A bottleneck is a performance limiting setting
- Microarchitectures expose numerous bottlenecks

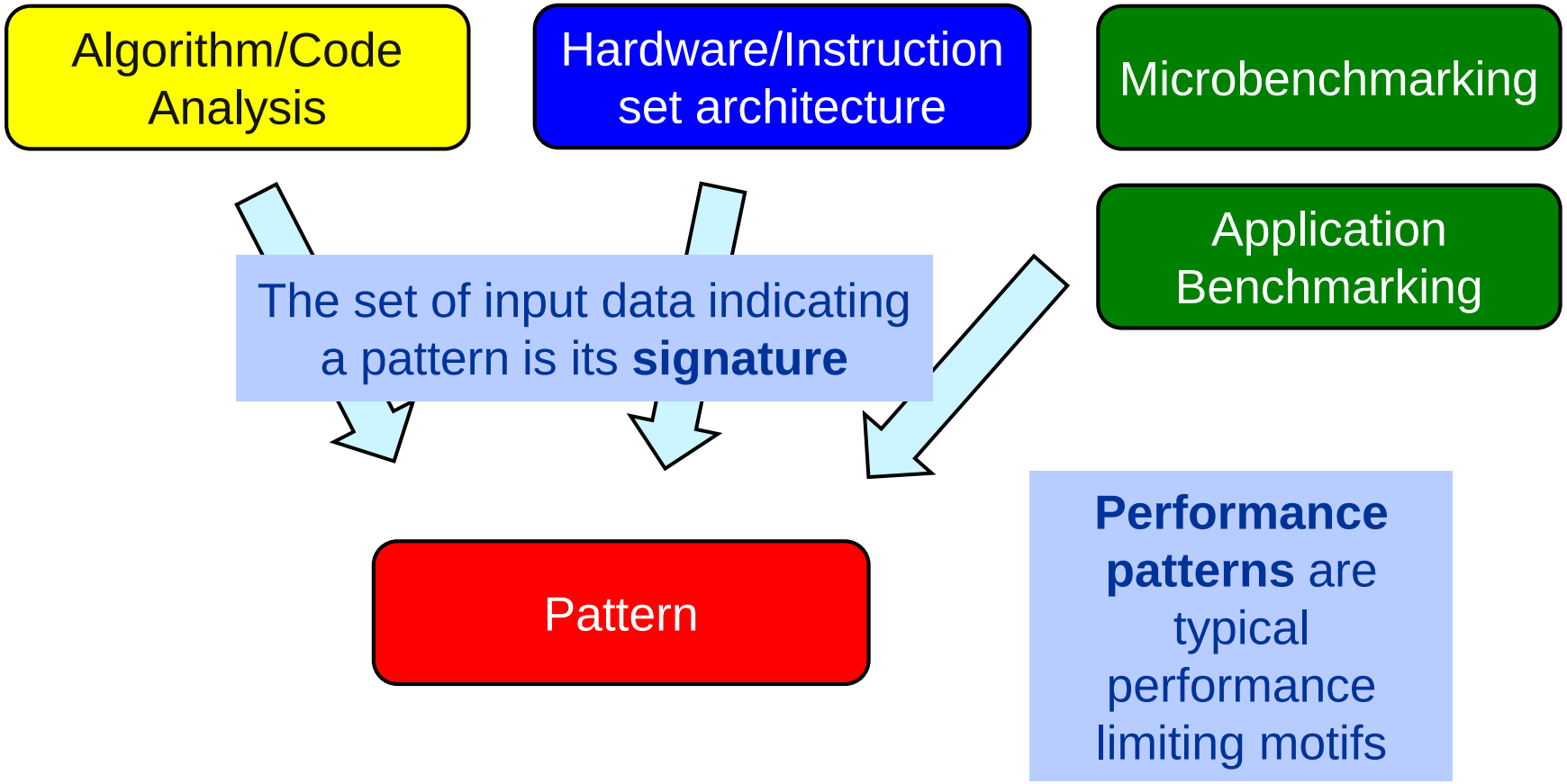
Observation 1:

Most applications face a single bottleneck at a time!

Observation 2:

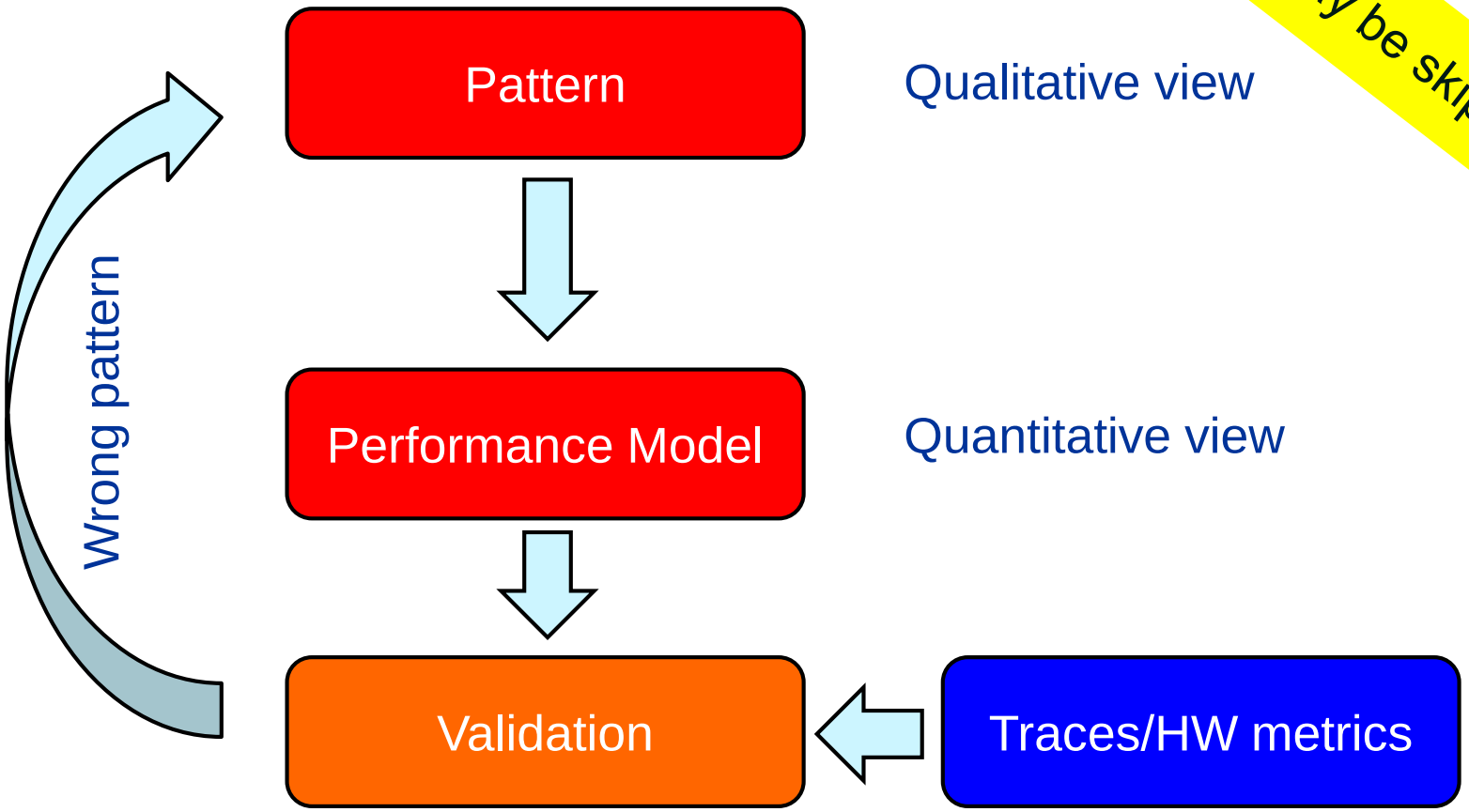
There is a limited number of relevant bottlenecks!

Performance Engineering Process: Analysis



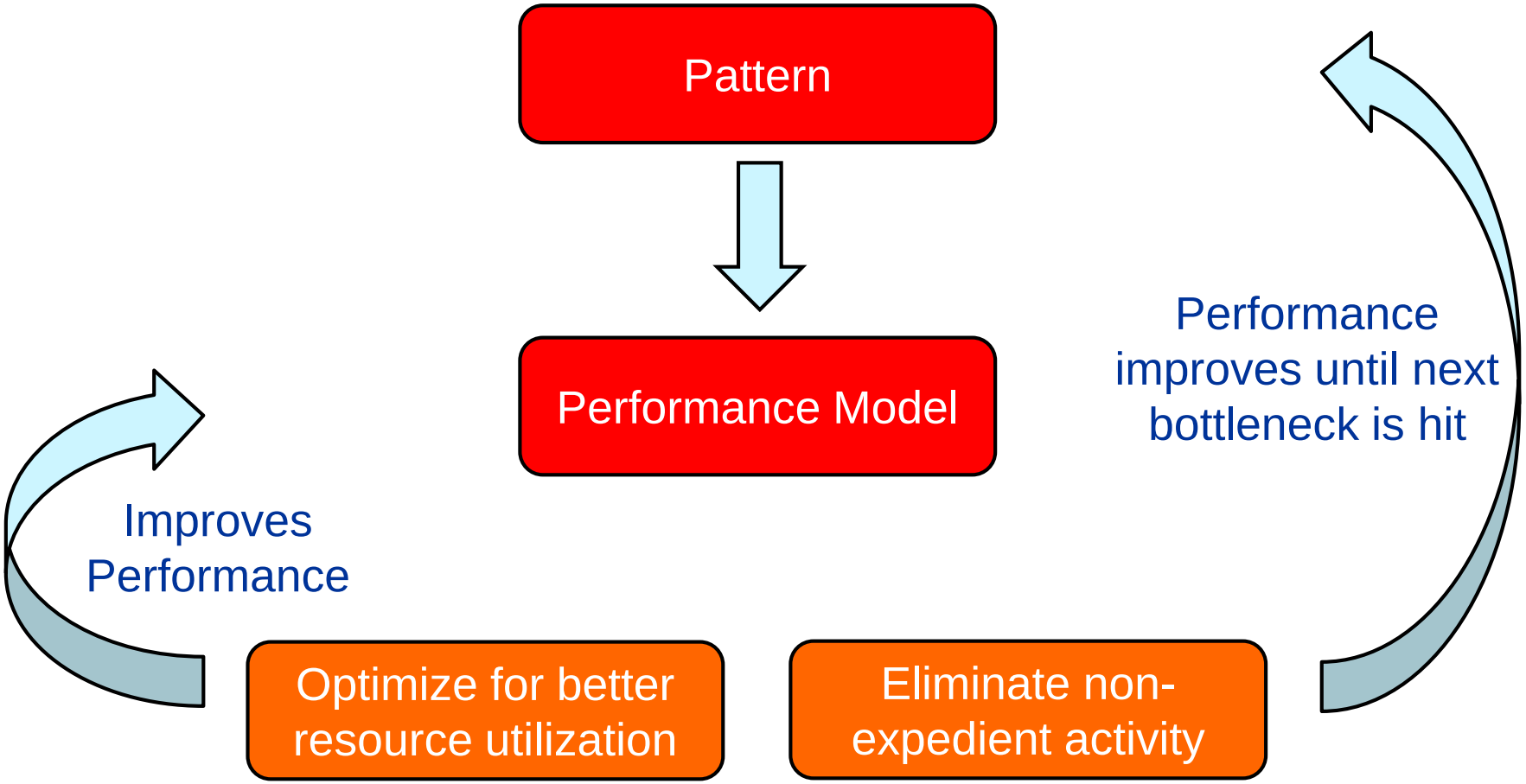
Step 1 **Analysis:** Understanding observed performance

Performance Engineering Process: Modeling



Step 2 **Formulate Model:** Validate pattern and get quantitative insight

Performance Engineering Process: Optimization



Step 3 **Optimization:** Improve utilization of available resources

Performance pattern classification

1. **Maximum resource utilization (computing at a bottleneck)**

2. **Hazards (something “goes wrong”)**

3. **Work related (too much work or too inefficiently done)**

Patterns (I): Bottlenecks & hazards

optional

Pattern		Performance behavior	Metric signature, LIKWID performance group(s)
Bandwidth saturation (Jacobi)		Saturating speedup across cores sharing a data path	Bandwidth meets BW of suitable streaming benchmark (MEM, L3)
ALU saturation (In-L1 sum optimal code)		Throughput at design limit(s)	Good (low) CPI, integral ratio of cycles to specific instruction count(s) (FLOPS_*, DATA, CPI)
Inefficient data access	**Excess data volume**	(spMVM RHS access) Simple bandwidth performance model much too optimistic	Low BW utilization / Low cache hit ratio, frequent CL evicts or replacements (CACHE, DATA, MEM)
	Latency-bound access		
Micro-architectural anomalies		Large discrepancy from simple performance model based on LD/ST and arithmetic throughput	Relevant events are very hardware-specific, e.g., memory aliasing stalls, conflict misses, unaligned LD/ST, requeue events

Patterns (II): Hazards

Pattern	Performance behavior	Metric signature, LIKWID performance group(s)
False sharing of cache lines	Large discrepancy from performance model in parallel case, bad scalability	Frequent (remote) CL evicts (CACHE)
Bad ccNUMA page placement (No parallel initialization)	Bad or no scaling across NUMA domains, performance improves with interleaved page placement	Unbalanced bandwidth on memory interfaces / High remote traffic (MEM)
Pipelining issues (In-L1 sum w/o unrolling)	In-core throughput far from design limit, performance insensitive to data set size	(Large) integral ratio of cycles to specific instruction count(s), bad (high) CPI (FLOPS_*, DATA, CPI)
Control flow issues	See above	High branch rate and branch miss ratio (BRANCH)

Patterns (III): Work-related

optional

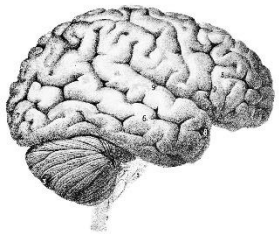
Pattern		Performance behavior	Metric signature, LIKWID performance group(s)
Load imbalance / serial fraction (SpMVM scaling)		Saturating/sub-linear speedup	Different amount of “work” on the cores (FLOPS_*); note that instruction count is not reliable!
Synchronization overhead (L1 OpenMP vector triad)		Speedup going down as more cores are added / No speedup with small problem sizes / Cores busy but low FP performance	Large non-FP instruction count (growing with number of cores used) / Low CPI (FLOPS_*, CPI)
Instruction overhead		Low application performance, good scaling across cores, performance insensitive to problem size	Low CPI near theoretical limit / Large non-FP instruction count (constant vs. number of cores) (FLOPS_*, DATA, CPI)
Code composition	**Expensive instructions**	Similar to instruction overhead (C/C++ aliasing problem)	Many cycles per instruction (CPI) if the problem is large-latency arithmetic
	Ineffective instructions		Scalar instructions dominating in data-parallel loops (FLOPS_*, CPI)

Patterns conclusion

- **Pattern signature = performance behavior + hardware metrics**
- **Patterns are applies hotspot (loop) by hotspot**
- **Patterns map to typical execution bottlenecks**
- **Patterns are extremely helpful in classifying performance issues**
  - The first pattern is always a hypothesis
  - Validation by tanking data (more performance behavior, HW metrics)
  - Refinement or change of pattern
- **Performance models are crucial for most patterns**
  - Model follows from pattern

Tutorial conclusion

- **Multicore architecture == multiple complexities**
  - Affinity matters → pinning/binding is essential
  - Bandwidth bottlenecks → inefficiency is often made on the chip level
  - Topology dependence of performance features → know your hardware!
- **Put cores to good use**
  - Bandwidth bottlenecks → surplus cores → functional parallelism!?
  - Shared caches → fast communication/synchronization → better implementations/algorithms?
- **Simple modeling techniques and patterns help us**
  - … understand the limits of our code on the given hardware
  - … identify optimization opportunities
  - … learn more, especially when they do not work!
- **Simple tools get you 95% of the way**
  - e.g., with the LIKWID tool suite



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THANK YOU.

Presenter Biographies

Georg Hager holds a PhD in computational physics from the University of Greifswald. He is a senior research scientist in the HPC group at Erlangen Regional Computing Center (RRZE). Recent research includes architecture-specific optimization for current microprocessors, performance modeling on processor and system levels, and the efficient use of hybrid parallel systems. His textbook “Introduction to High Performance Computing for Scientists and Engineers” is required or recommended reading in many HPC-related courses around the world. See his blog at http://blogs.fau.de/hager for current activities, publications, and talks.

Jan Eitzinger (formerly Treibig) holds a PhD in Computer Science from the University of Erlangen. He is now a postdoctoral researcher in the HPC Services group at Erlangen Regional Computing Center (RRZE). His current research revolves around architecture-specific and low-level optimization for current processor architectures, performance modeling on processor and system levels, and programming tools. He is the developer of LIKWID, a collection of lightweight performance tools. In his daily work he is involved in all aspects of user support in High Performance Computing: training, code parallelization, profiling and optimization, and the evaluation of novel computer architectures.

Gerhard Wellein holds a PhD in solid state physics from the University of Bayreuth and is a professor at the Department for Computer Science at the University of Erlangen. He leads the HPC group at Erlangen Regional Computing Center (RRZE) and has more than ten years of experience in teaching HPC techniques to students and scientists from computational science and engineering programs. His research interests include solving large sparse eigenvalue problems, novel parallelization approaches, performance modeling, and architecture-specific optimization.

Abstract

- **SC16 tutorial: Node-Level Performance Engineering**
- **Presenter(s): Georg Hager, (Jan Eitzinger), Gerhard Wellein**

- **ABSTRACT:**

The advent of multi- and manycore chips has led to a further opening of the gap between peak and application performance for many scientific codes. This trend is accelerating as we move from petascale to exascale. Paradoxically, bad node-level performance helps to "efficiently" scale to massive parallelism, but at the price of increased overall time to solution. If the user cares about time to solution on any scale, optimal performance on the node level is often the key factor. We convey the architectural features of current processor chips, multiprocessor nodes, and accelerators, as far as they are relevant for the practitioner. Peculiarities like SIMD vectorization, shared vs. separate caches, bandwidth bottlenecks, and ccNUMA characteristics are introduced, and the influence of system topology and affinity on the performance of typical parallel programming constructs is demonstrated. *Performance engineering* and *performance patterns* are suggested as powerful tools that help the user understand the bottlenecks at hand and to assess the impact of possible code optimizations. A cornerstone of these concepts is the roofline model, which is described in detail, including useful case studies, limits of its applicability, and possible refinements.

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