

# **Performance Engineering on Multi- and Manycores**

**Georg Hager, Gerhard Wellein**

HPC Services, Erlangen Regional Computing Center (RRZE)

**Tutorial @ SAHPC 2012**

**December 1-3, 2012**

**KAUST, Thuwal**

**Saudi Arabia**

- Where can I find those *gorgeous* slides?

<http://goo.gl/cTSKL>

or:

<http://blogs.fau.de/hager/tutorials/sahpc-2012/>



- Is there a book or anything?

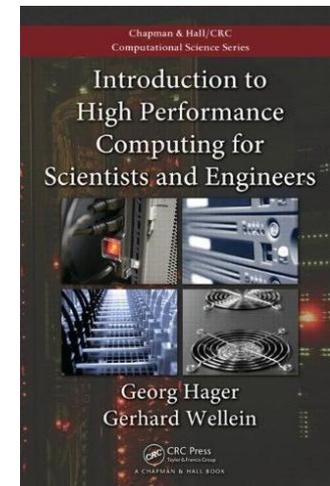
Georg Hager and Gerhard Wellein:

*Introduction to High Performance Computing for Scientists and Engineers*

CRC Press, 2010

ISBN 978-1439811924

356 pages



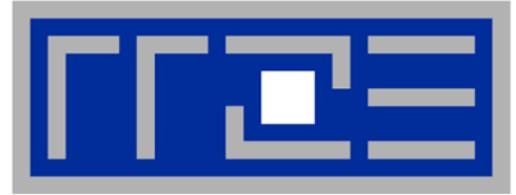
- Fun and facts for HPC: <http://blogs.fau.de/hager/>



- **Motivation**
- **Performance Engineering**
  - Performance modeling
  - The Performance Engineering process
- **Modern architectures**
  - Multicore
  - Accelerators
  - Programming models
- **Data access**
- **Performance properties of multicore systems**
  - Saturation
  - Scalability
  - Synchronization
- **Case study: OpenMP-parallel sparse MVM**
- **Basic performance modeling: Roofline**
  - Theory
  - Case study: 3D Jacobi solver and guided optimizations
  - Modeling erratic access
- **Some more architecture**
  - Simultaneous multithreading (SMT)
  - ccNUMA
- **Putting cores to good use**
  - Asynchronous communication in spMVM
- **A simple power model for multicore**
  - Power-efficient code execution
- **Conclusions**



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**Motivation 1:  
Scalability 4 the win!**



## **Lore 1**

**In a world of highly parallel computer architectures only highly scalable codes will survive**

## **Lore 2**

**Single core performance no longer matters since we have so many of them and use scalable codes**

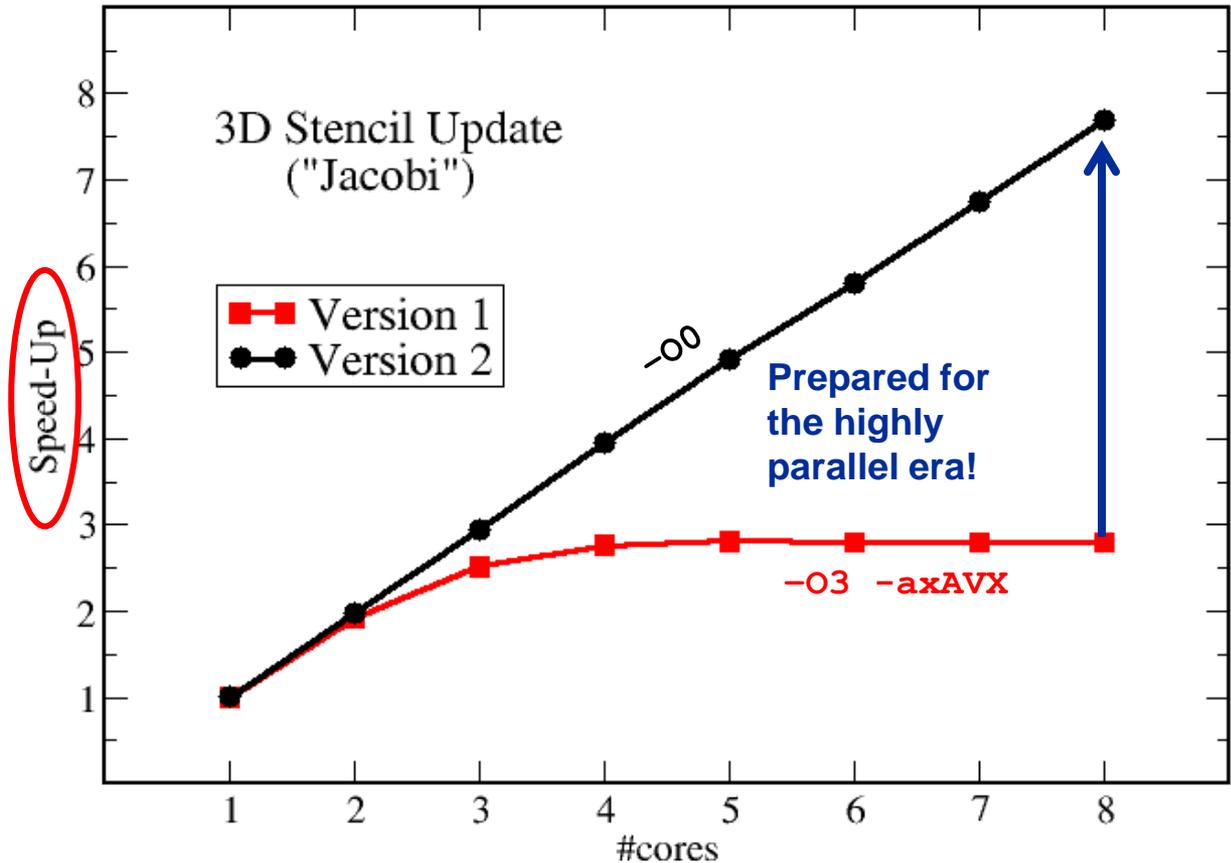
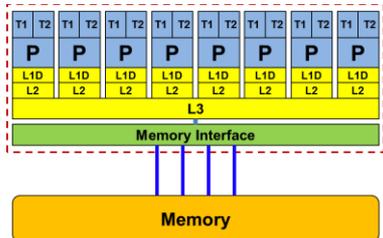
# Scalability Myth: Code scalability is the key issue



```

!$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
    
```

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



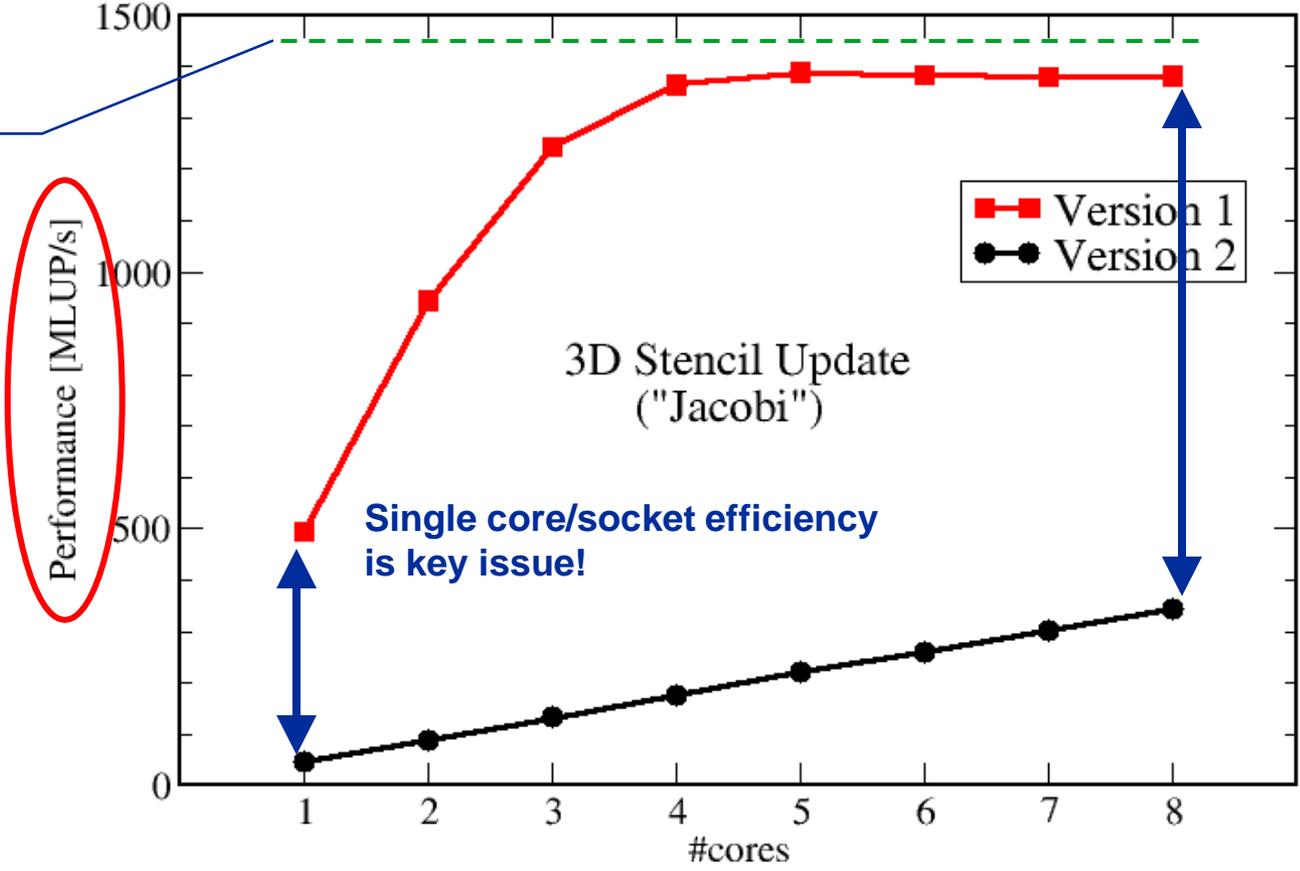
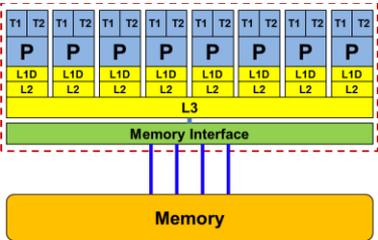
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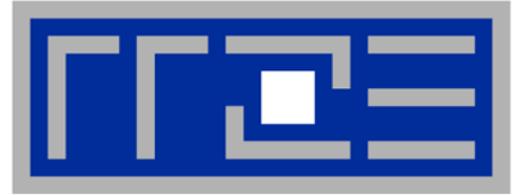


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      x(i,j+1,k) + x(i,j,k-1) + x(i,j,k+1))
  enddo; enddo
enddo
    
```

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





**Motivation 2:  
The 200x GPGPU speedup story**

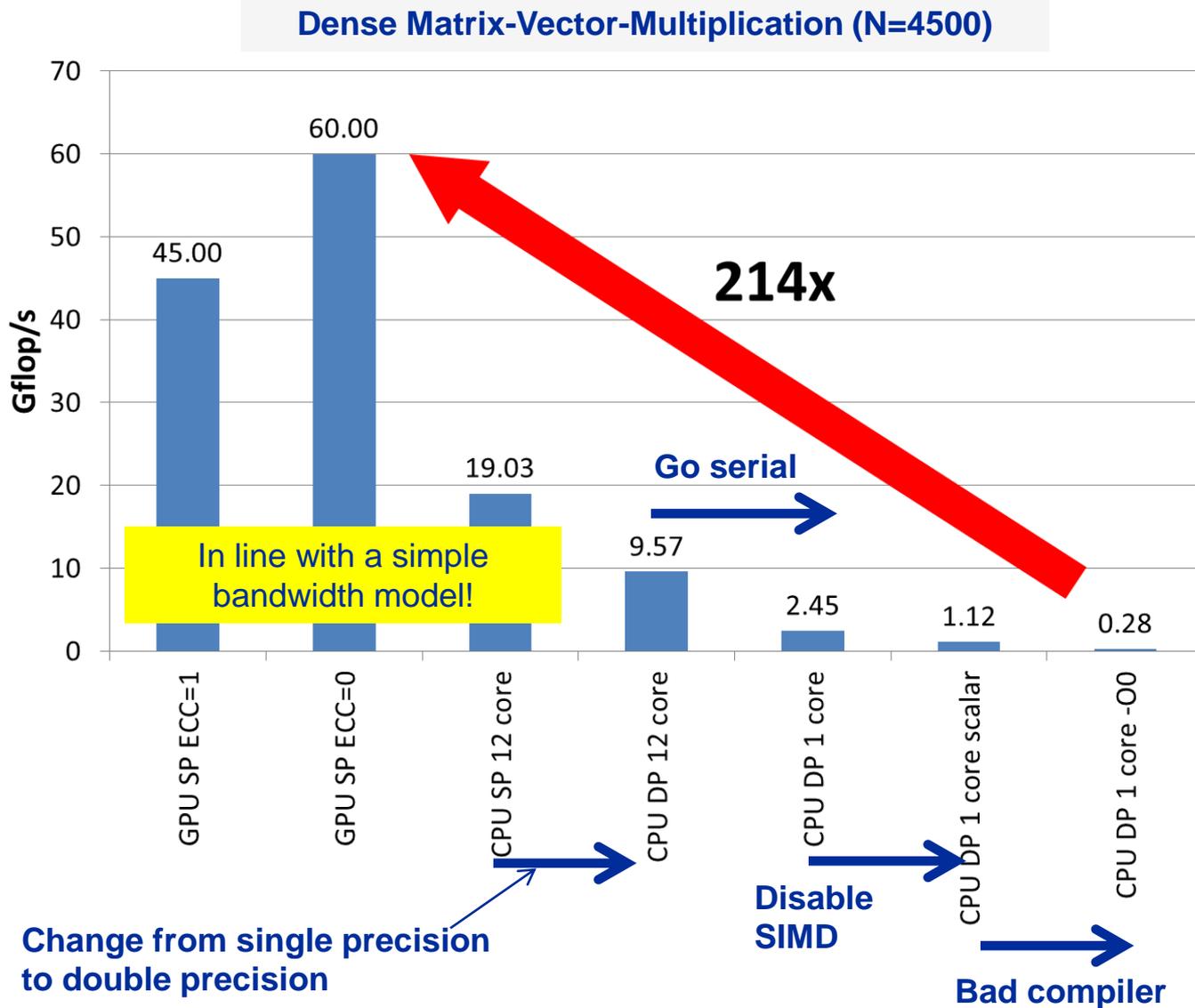
# Accelerator myth: The 200x speedup story...



NVIDIA Tesla C2050

vs.

2x Intel Xeon 5650  
(6-core)



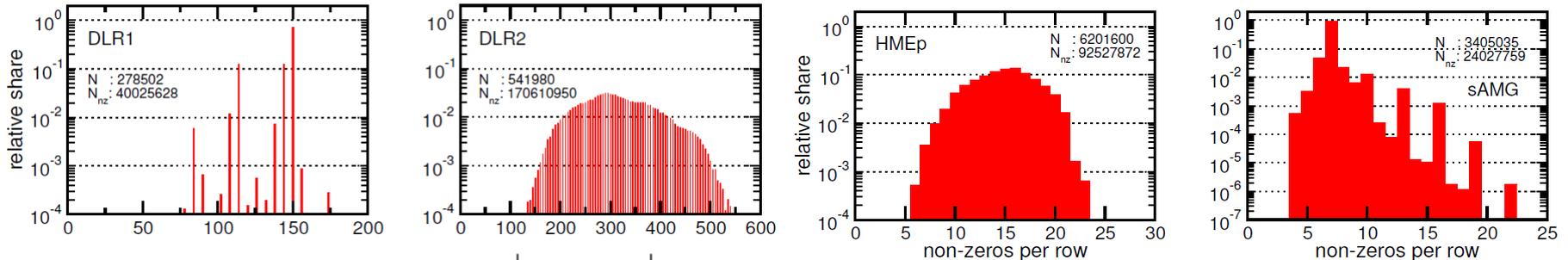


## Sparse matrix-vector multiply

M. Kreutzer et al., LSP12

[DOI: 10.1109/IPDPSW.2012.211](https://doi.org/10.1109/IPDPSW.2012.211)

Matrix structure of test cases



		DLR1	DLR2	HMEp	sAMG
data reduction [%]		17.5	48.0	36.0	68.4
SP ECC=0	ELLPACK-R	22.1	15.2	15.8	14.6
	pJDS	27.6	18.7	18.9	19.5
SP ECC=1	ELLPACK-R	18.0	13.2	12.1	11.6
	pJDS	19.1	12.1	11.6	12.6
DP ECC=0	ELLPACK-R	18.7	11.7	12.3	11.1
	pJDS	18.3	14.6	12.2	13.0
DP ECC=1	ELLPACK-R	12.9	9.6	7.9	7.8
	pJDS	12.9	9.5	7.5	8.5
Westmere EP	CRS (DP)	5.7	5.8	3.9	4.1

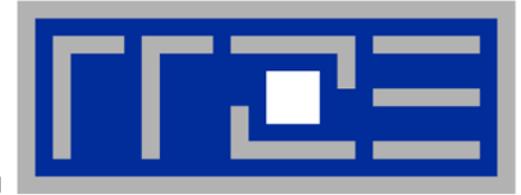
NVIDIA Tesla C2070  
performance in GF/s

2-way Intel Xeon 5650 node

- **GPGPU speedup: 1.6x,...,2.1x (no PCIe data transfer!)**



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# **The Performance Engineering process**

**Model building**

**Our definition**



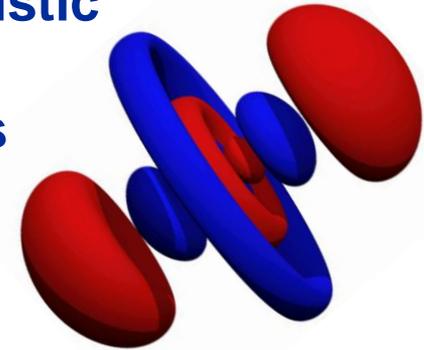
## Newtonian mechanics



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

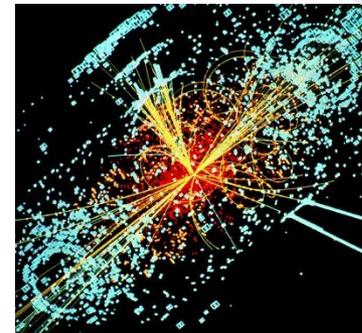
**Fails @ small scales!**

## Nonrelativistic quantum mechanics



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

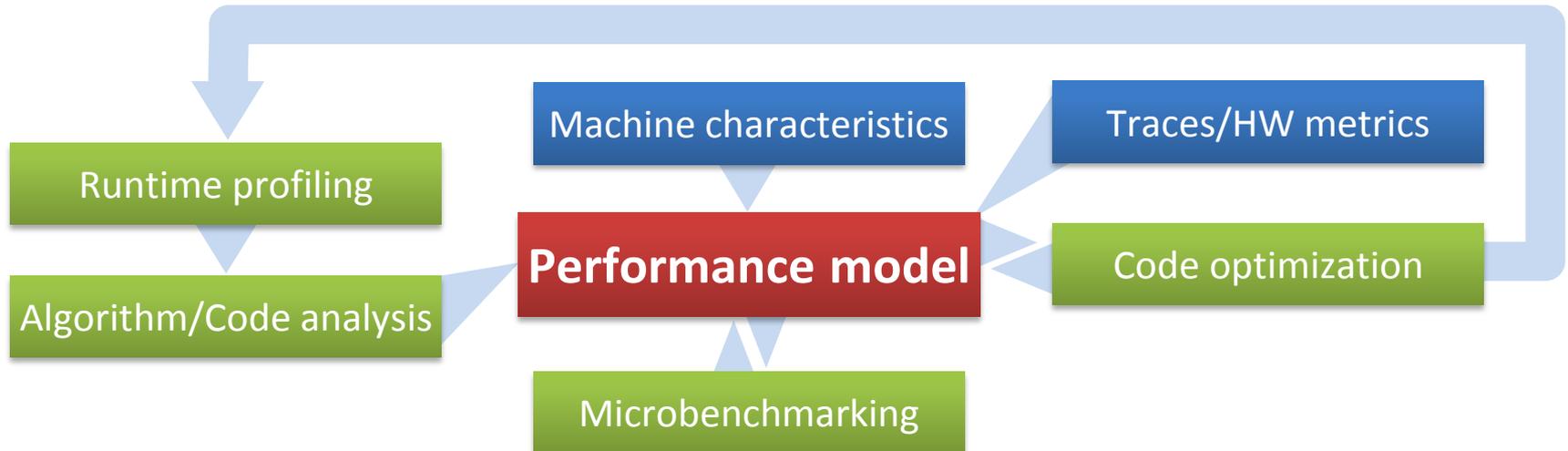
**Fails @ even smaller scales!**



## Relativistic quantum field theory

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

## The Performance Engineering (PE) process:

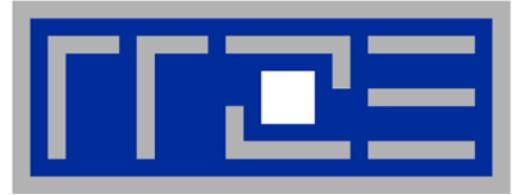


**The performance model is the central component – if the model fails to predict the measurement, you learn something!**

**The analysis has to be done for every loop / basic block!**

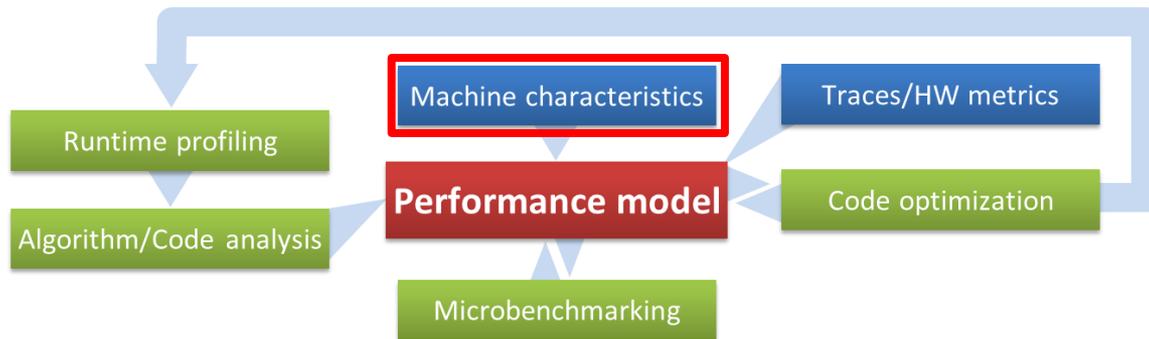


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# Multicore processor and system architecture

## Basics of machine characteristics

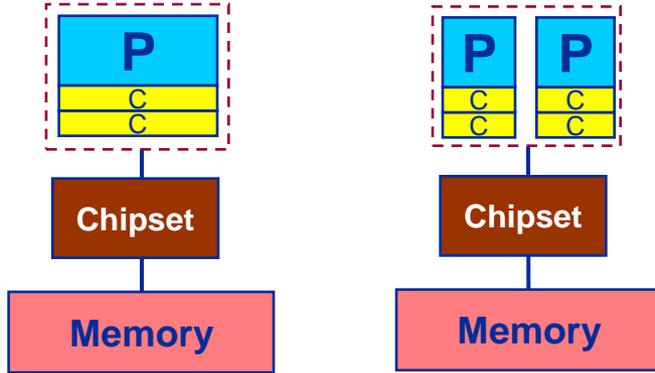


# The x86 multicore evolution so far

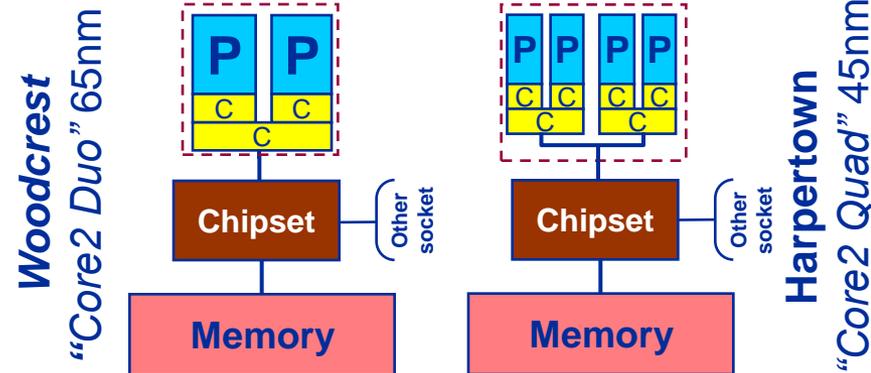
Intel Single-/Dual-/.../Octo-Cores (one-socket view)



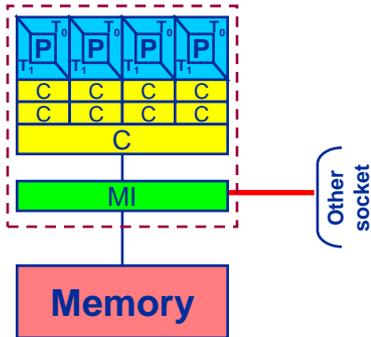
2005: "Fake" dual-core



2006: True dual-core

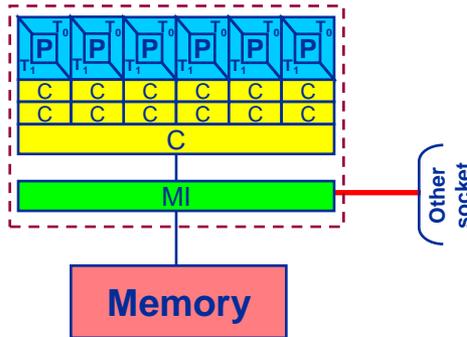


2008: Simultaneous Multi Threading (SMT)



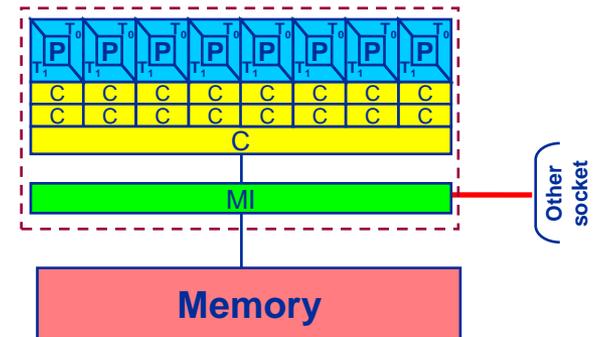
Nehalem EP  
"Core i7"  
45nm

2010: 6-core chip



Westmere EP  
"Core i7"  
32nm

2012: Wider SIMD units  
AVX: 256 Bit



Sandy Bridge EP  
"Core i7"  
32nm

# There is no single driving force for chip performance!



## Floating Point (FP) Performance:

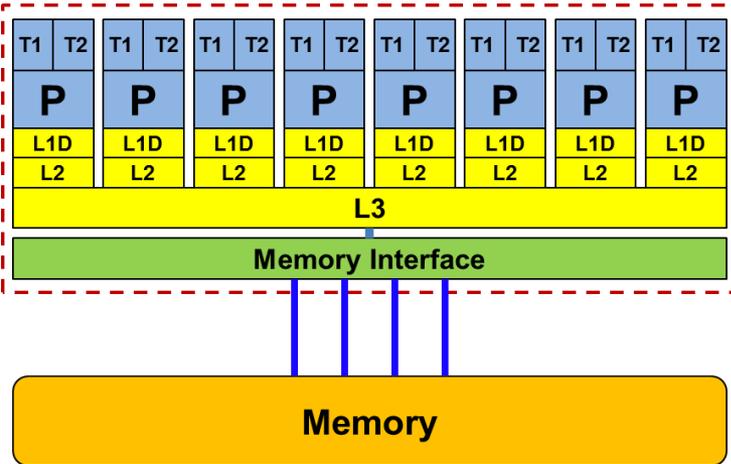
$$P = n_{\text{core}} * F * S * v$$

$n_{\text{core}}$  number of cores: 8

$F$  FP instructions per cycle: 2  
(1 MULT and 1 ADD)

$S$  FP ops / instruction: 4 (dp) / 8 (sp)  
(256 Bit SIMD registers – “AVX”)

$v$  Clock speed : ~2.7 GHz



Intel Xeon  
“Sandy Bridge EP” socket  
4,6,8 core variants available

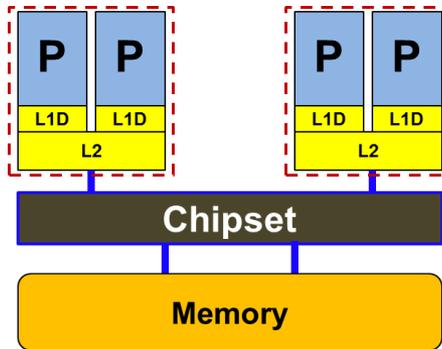
TOP500 rank 1 (1995)

$$P = 173 \text{ GF/s (dp)} / 346 \text{ GF/s (sp)}$$

**But: P=5.4 GF/s (dp) for serial, non-SIMD code**



### Yesterday (2006): Dual-socket Intel “Core2” node:

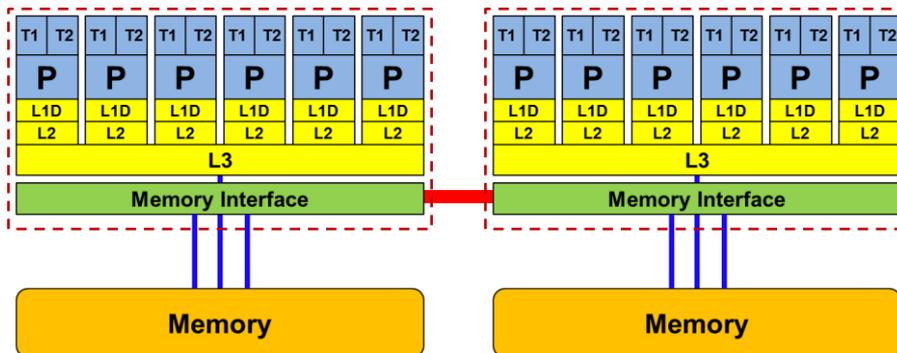


Uniform Memory Architecture (UMA)

Flat memory ; symmetric MPs

But: system “anisotropy”

### Today: Dual-socket Intel (Westmere) node:



Cache-coherent Non-Uniform Memory Architecture (**ccNUMA**)

**HT / QPI** provide scalable bandwidth at the price of ccNUMA architectures:  
*Where does my data finally end up?*

**On AMD it is even more complicated → ccNUMA within a socket!**

# Another flavor of "SMT"

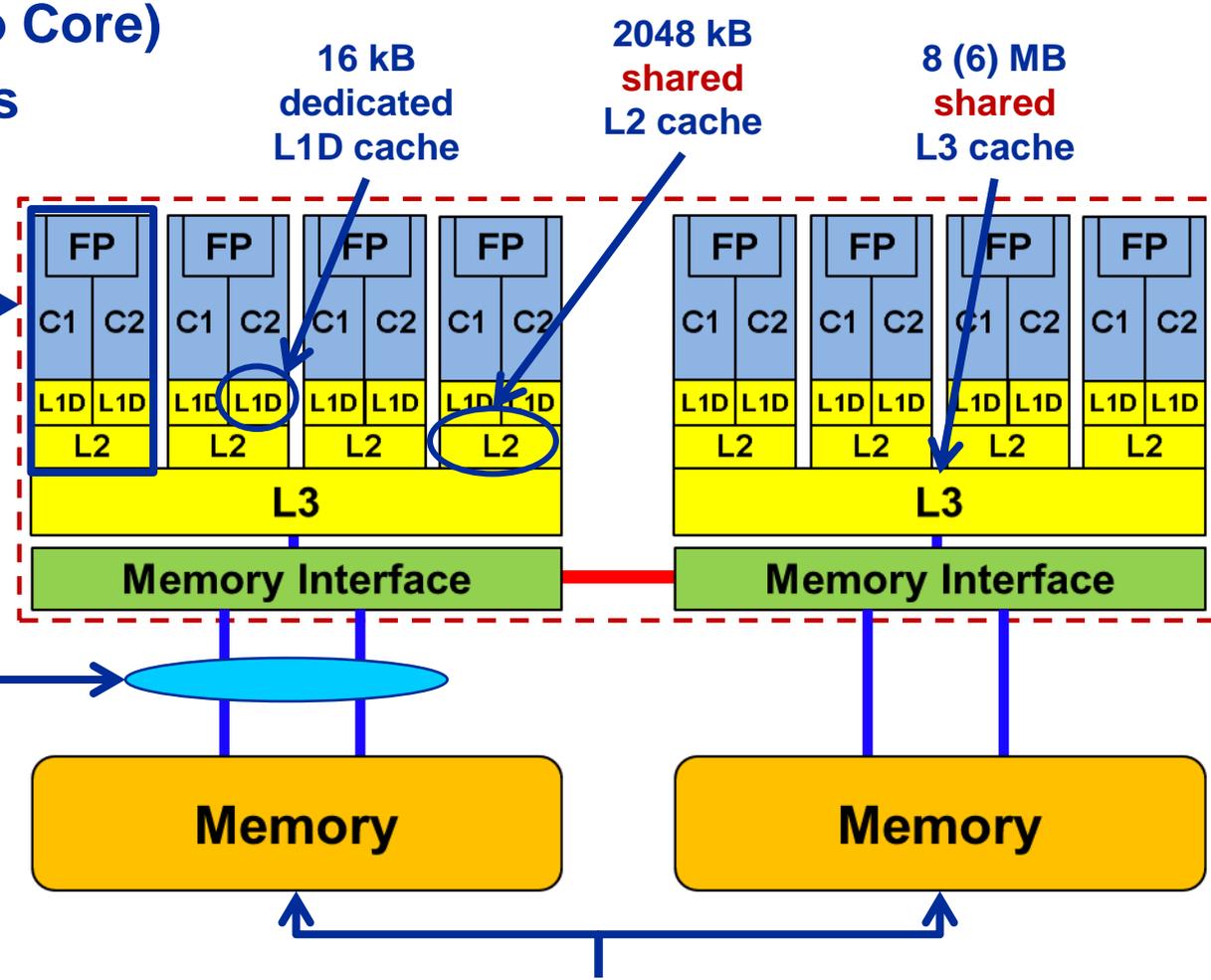
## AMD Interlagos / Bulldozer



- Up to 16 cores (8 Bulldozer modules) in a single socket
- Max. 2.6 GHz (+ Turbo Core)
- $P_{max} = (2.6 \times 8 \times 8) \text{ GF/s} = 166.4 \text{ GF/s}$

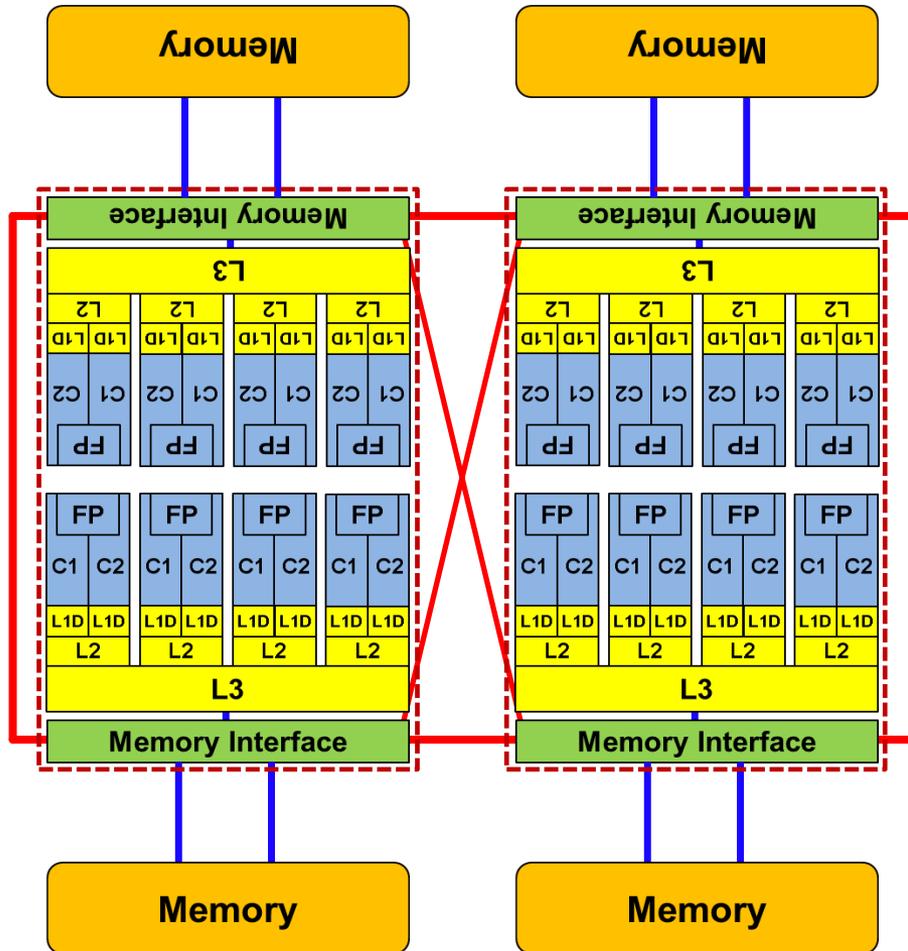
### Each Bulldozer module:

- 2 "lightweight" cores
- 1 FPU: 4 MULT & 4 ADD (double precision) / cycle
- Supports AVX
- Supports FMA4

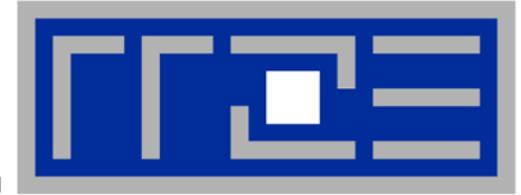


2 DDR3 (shared) memory channel > 15 GB/s

2 NUMA domains per socket



- **Two 8- (integer-) core chips per socket @ 2.3 GHz (3.3 @ turbo)**
- **Separate DDR3 memory interface per chip**
  - ccNUMA on the socket!
- **Shared FP unit per pair of integer cores (“module”)**
  - “256-bit” FP unit
  - SSE4.2, AVX, FMA4
- **16 kB L1 data cache per core**
- **2 MB L2 cache per module**
- **8 MB L3 cache per chip (6 MB usable)**



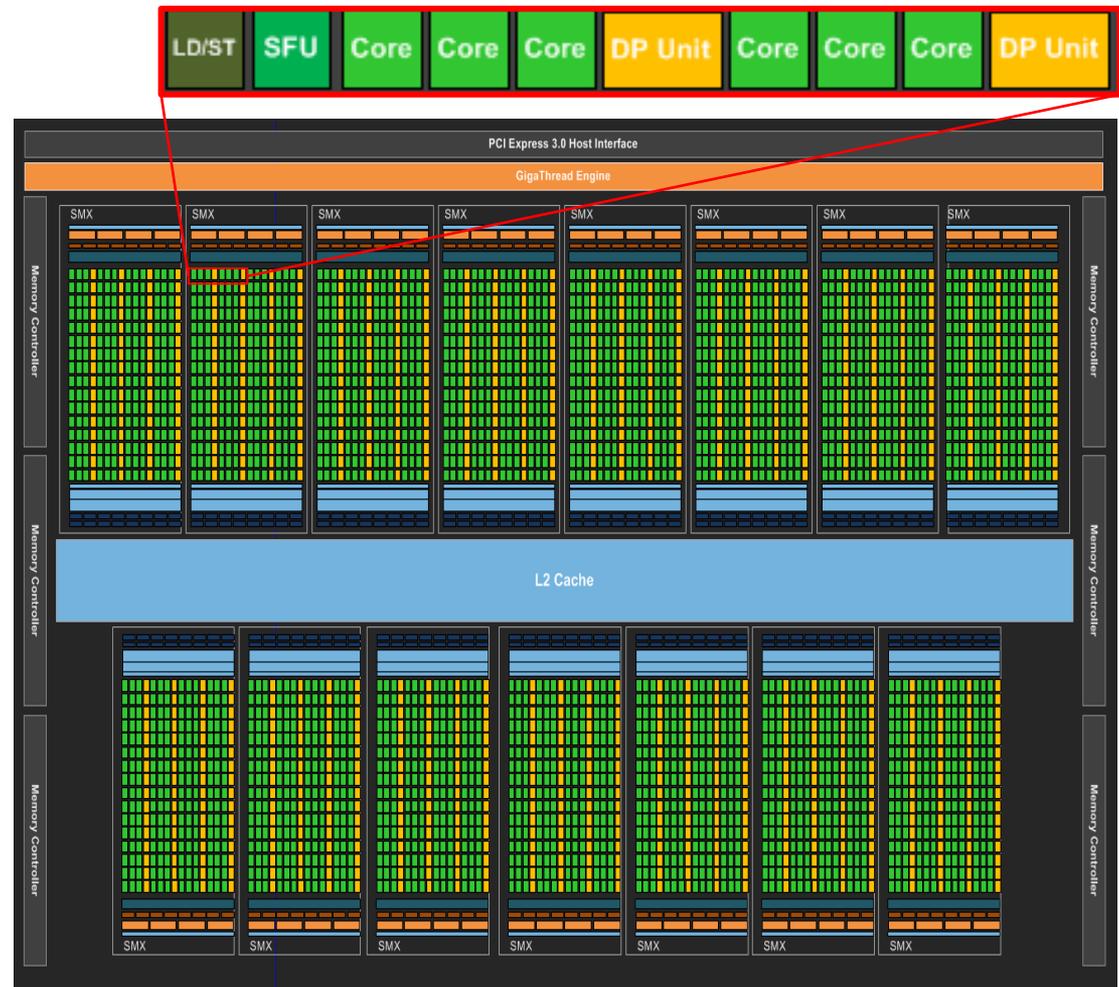
**Interlude:**  
**A glance at current accelerator technology**

# NVIDIA Kepler GK110 Block Diagram



## Architecture

- 7.1B Transistors
- 15 SMX units
- > 1 TFLOP DP peak
- 1.5 MB L2 Cache
- 384-bit GDDR5
- PCI Express Gen3
- 3:1 SP:DP performance**

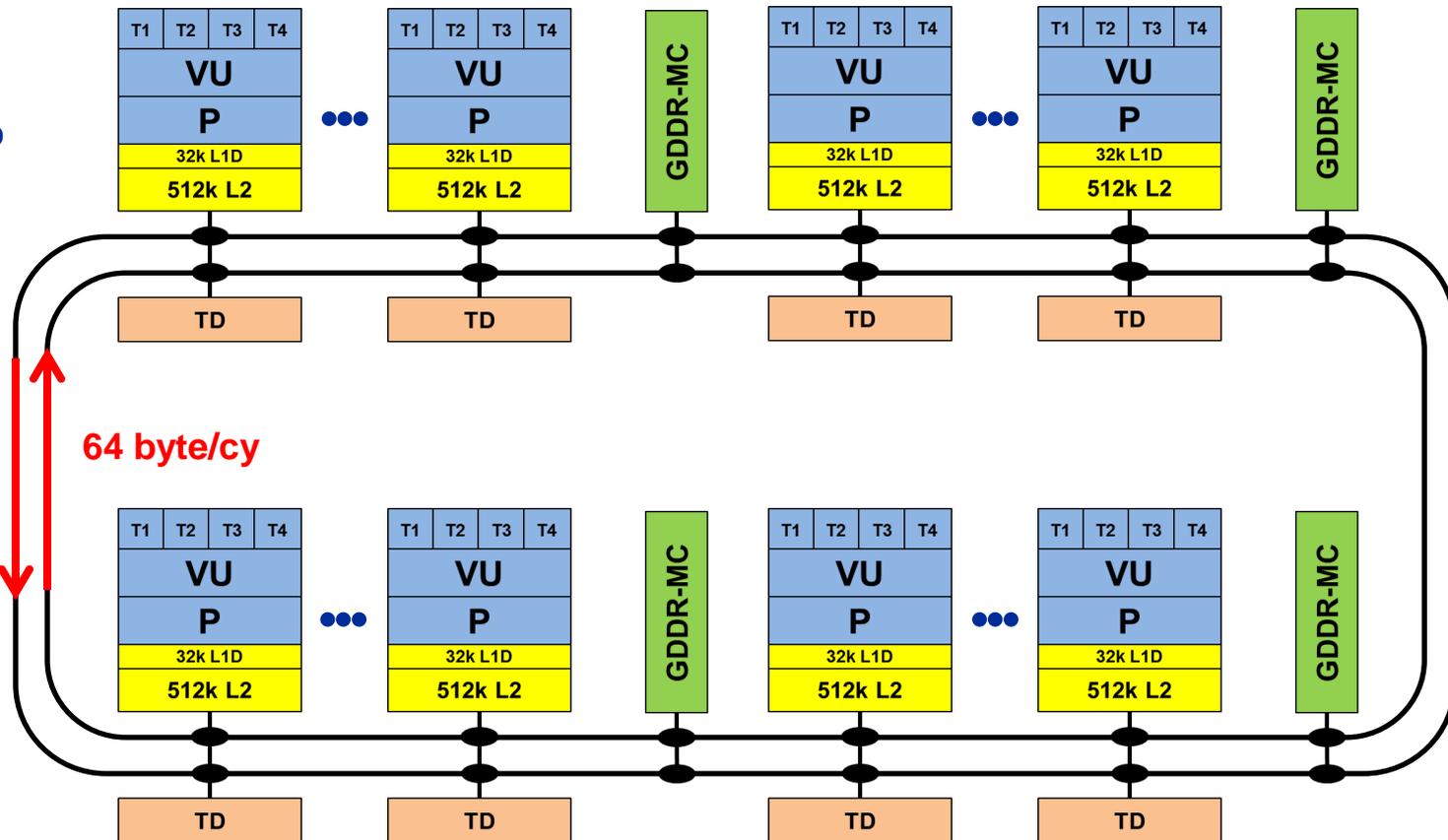


© NVIDIA Corp. Used with permission.



## Architecture

- 3B Transistors
- 60+ cores
- 512 bit SIMD
- $\approx 1$  TFLOP DP peak
- 0.5 MB L2/core
- GDDR5
- 2:1 SP:DP performance





## Intel Xeon Phi

- 60+ IA32 cores each with 512 Bit SIMD FMA unit → 480/960 SIMD DP/SP tracks

- Clock Speed: ~1000 MHz
- Transistor count: ~3 B (22nm)
- Power consumption: ~250 W



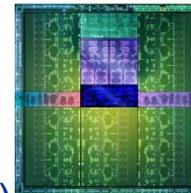
- Peak Performance (DP): ~ 1 TF/s
- Memory BW: ~250 GB/s (GDDR5)

- Threads to execute: 60-240+
- Programming:  
Fortran/C/C++ +OpenMP + SIMD

## NVIDIA Kepler K20

- 15 SMX units each with 192 “cores” → 960/2880 DP/SP “cores” in total

- Clock Speed: ~700 MHz
- Transistor count: 7.1 B (28nm)
- Power consumption: ~250 W



- Peak Performance (DP): ~ 1.3 TF/s
- Memory BW: ~ 250 GB/s (GDDR5)

- Threads to execute: 10.000+
- Programming:  
CUDA, OpenCL, (OpenACC)

- TOP7: “Stampede” at Texas Center for Advanced Computing

**TOP500**  
**rankings**

- TOP1: “Titan” at Oak Ridge National Laboratory

# Trading single thread performance for parallelism:

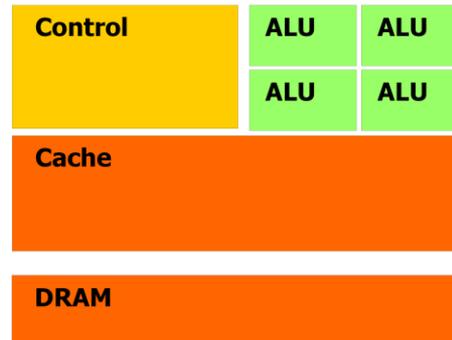
## GPGPUs vs. CPUs



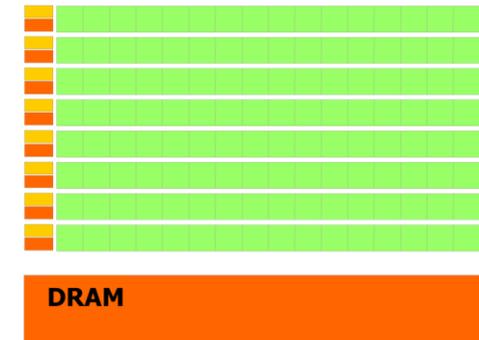
### GPU vs. CPU

light speed estimate:

1. **Compute bound:** 2-10x
2. **Memory Bandwidth:** 1-5x



CPU



GPU

	Intel Core i5 – 2500 ("Sandy Bridge")	Intel Xeon E5-2680 DP node ("Sandy Bridge")	NVIDIA K20x ("Kepler")
Cores@Clock	4 @ 3.3 GHz	2 x 8 @ 2.7 GHz	2880 @ 0.7 GHz
Performance <sup>+</sup> /core	52.8 GFlop/s	43.2 GFlop/s	1.4 GFlop/s
Threads@STREAM	<4	<16	>8000?
Total performance <sup>+</sup>	210 GFlop/s	691 GFlop/s	4,000 GFlop/s
Stream BW	18 GB/s	2 x 40 GB/s	168 GB/s (ECC=1)
Transistors / TDP	1 Billion* / 95 W	2 x (2.27 Billion/130W)	7.1 Billion/250W

<sup>+</sup> Single Precision

\* Includes on-chip GPU and PCI-Express

**Complete compute device**



- **Shared-memory (intra-node)**
  - **Good old MPI** (current standard: 2.2)
  - **OpenMP** (current standard: 3.0)
  - POSIX threads
  - Intel Threading Building Blocks (TBB)
  - Cilk+, OpenCL, StarSs,... you name it
  
- **Distributed-memory (inter-node)**
  - **MPI** (current standard: 2.2)
  - PVM (gone)
  
- **Hybrid**
  - **Pure MPI**
  - MPI+OpenMP
  - MPI + any shared-memory model
  - MPI (+OpenMP) + CUDA/OpenCL/...

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

# Parallel programming models:

## Pure MPI



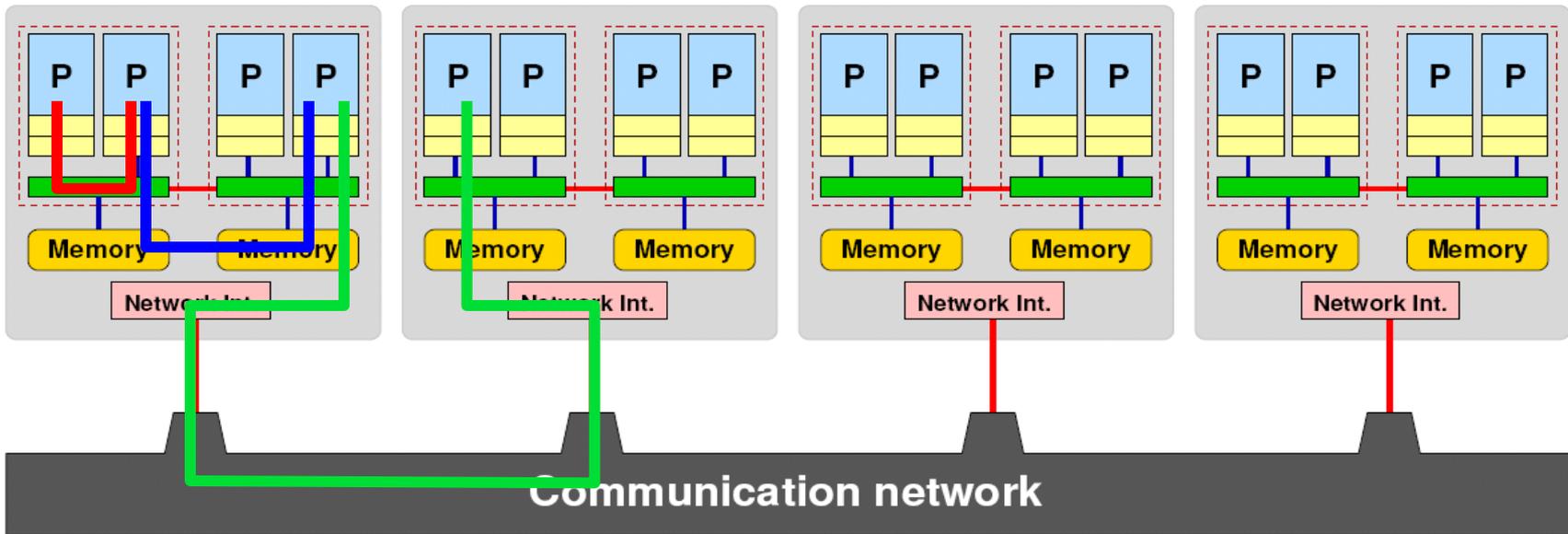
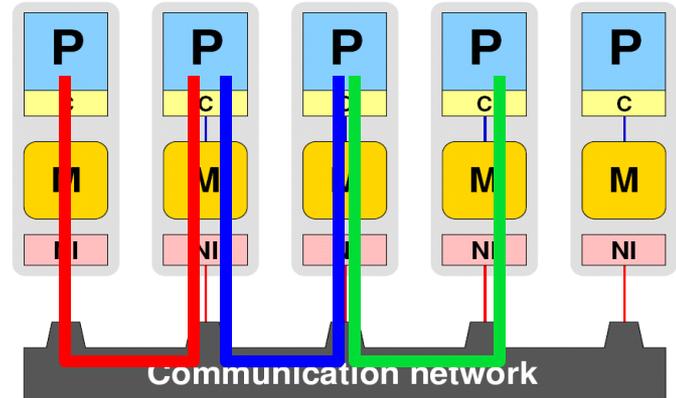
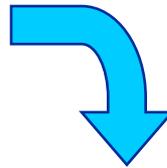
- Machine structure is invisible to user:

- 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

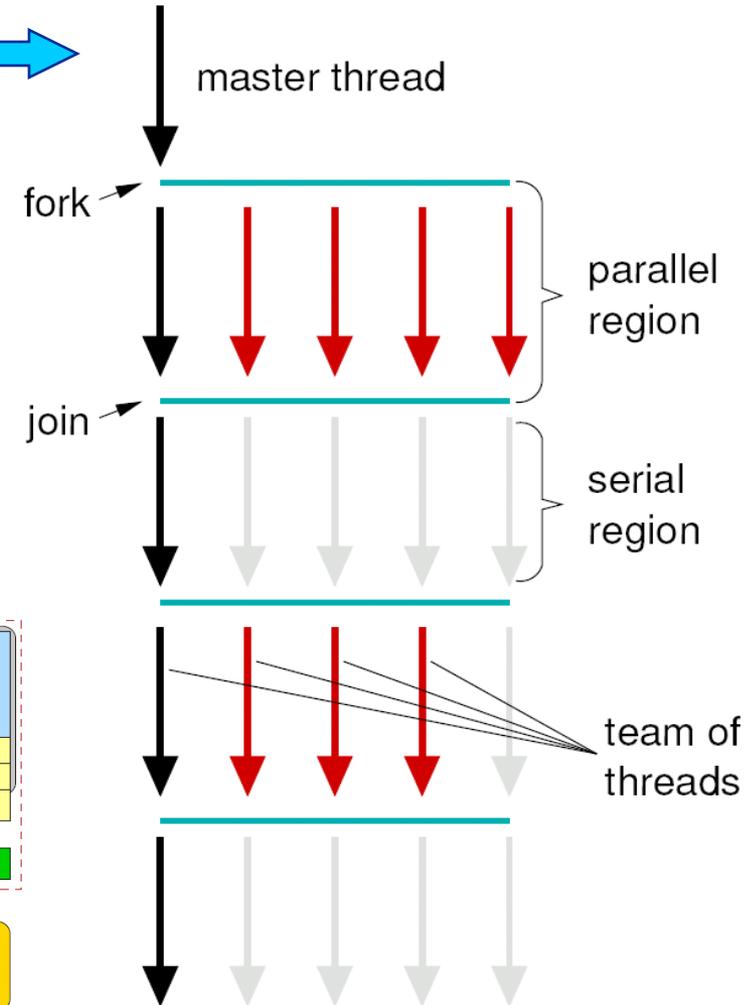
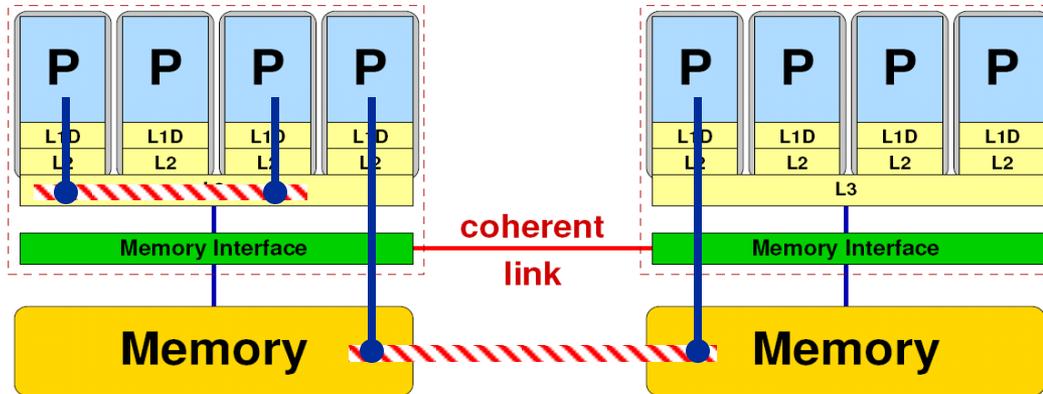


- Machine structure is invisible to user

- Very simple programming model
- Threading SW (OpenMP, pthreads, TBB,...) should know about the details

- Performance issues

- Synchronization overhead
- Memory access
- Node topology

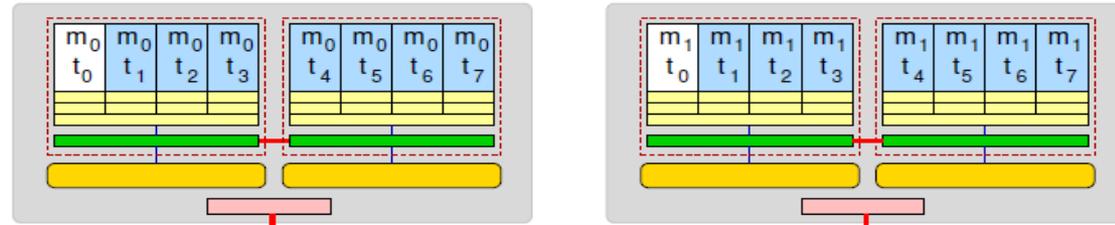


# Parallel programming models:

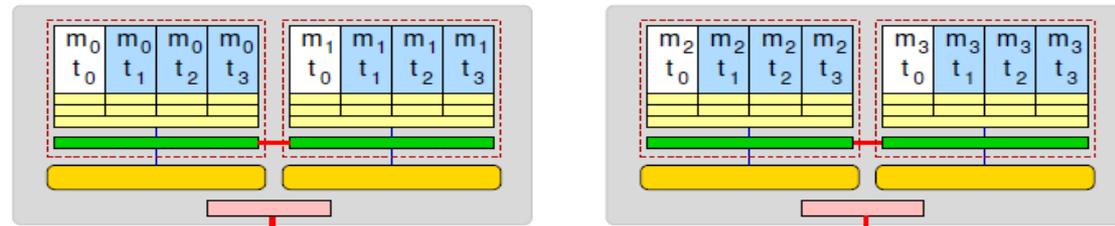
Hybrid MPI+OpenMP on a multicore multisocket cluster



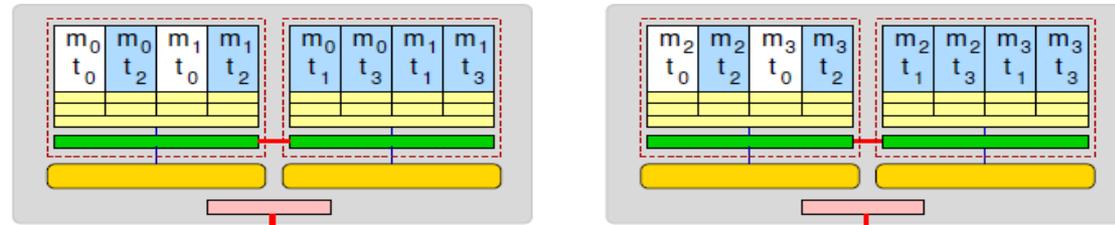
One MPI process / node



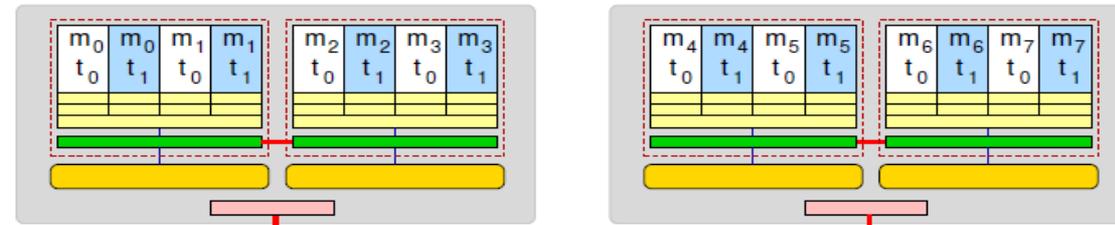
One MPI process / socket:  
OpenMP threads on same  
socket: “**blockwise**”



OpenMP threads pinned  
“**round robin**” across  
cores in node

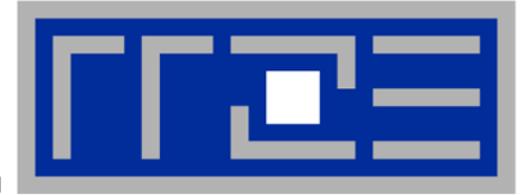


Two MPI processes / socket  
OpenMP threads  
on same socket





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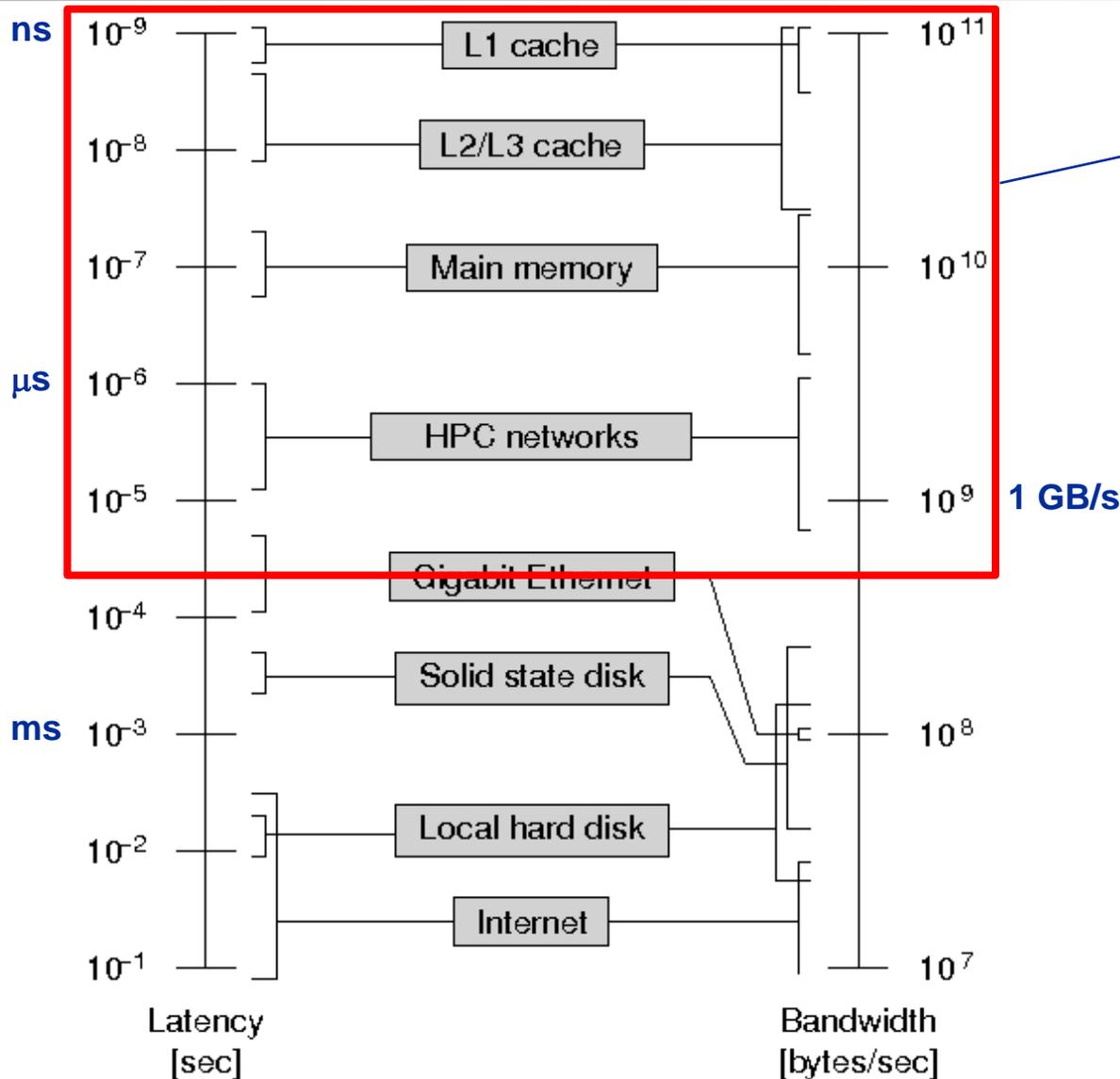


## **Data access on modern processors**

**Characterization of memory hierarchies**

**General performance properties of multicore processors**

# Latency and bandwidth in modern computer environments



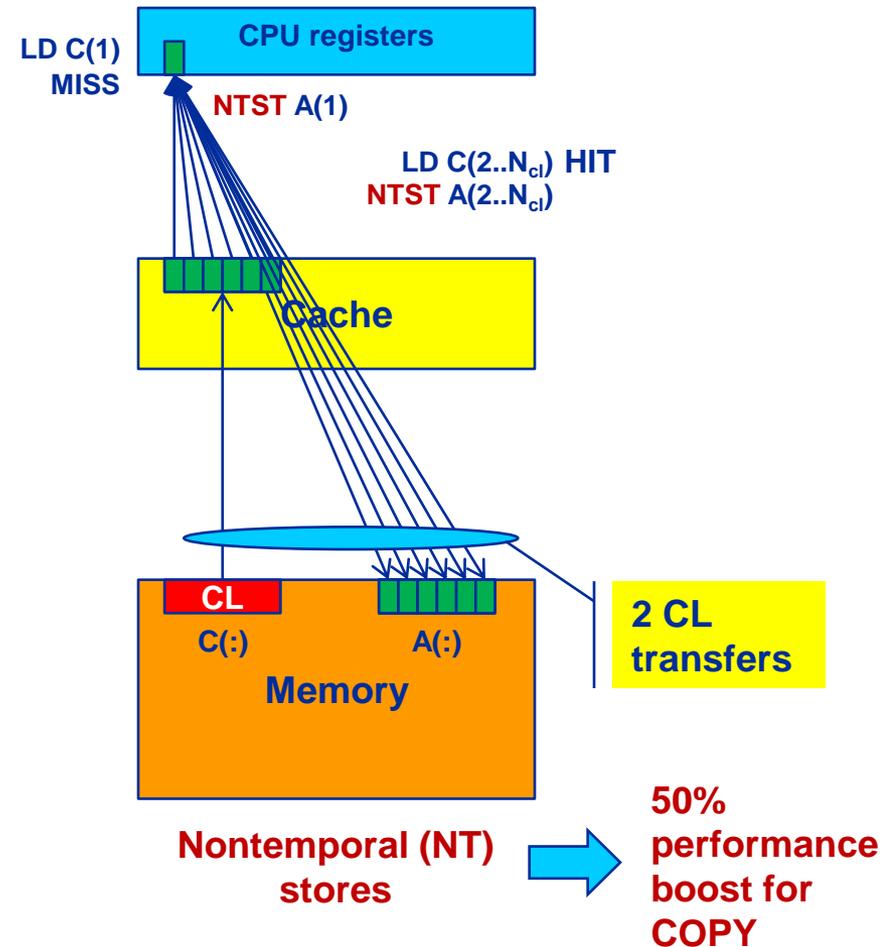
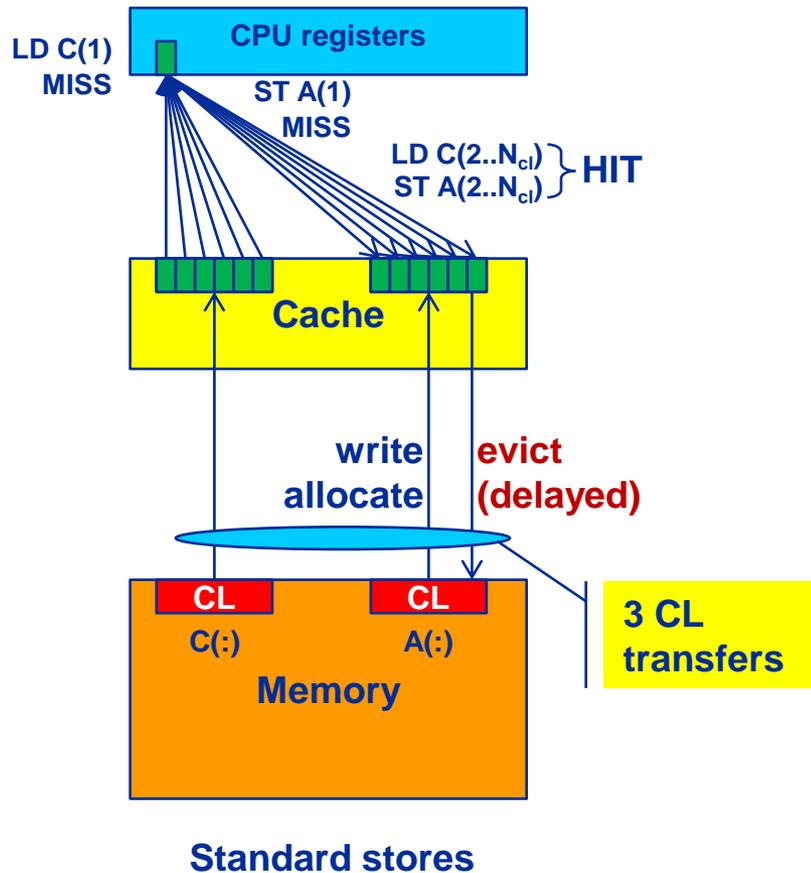
HPC plays here

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

# Interlude: Data transfers in a memory hierarchy



- How does data travel from memory to the CPU and back?
- Example: Array copy  $A(:) = C(:)$



# The parallel vector triad benchmark

A “swiss army knife” for microbenchmarking



## Simple streaming benchmark:

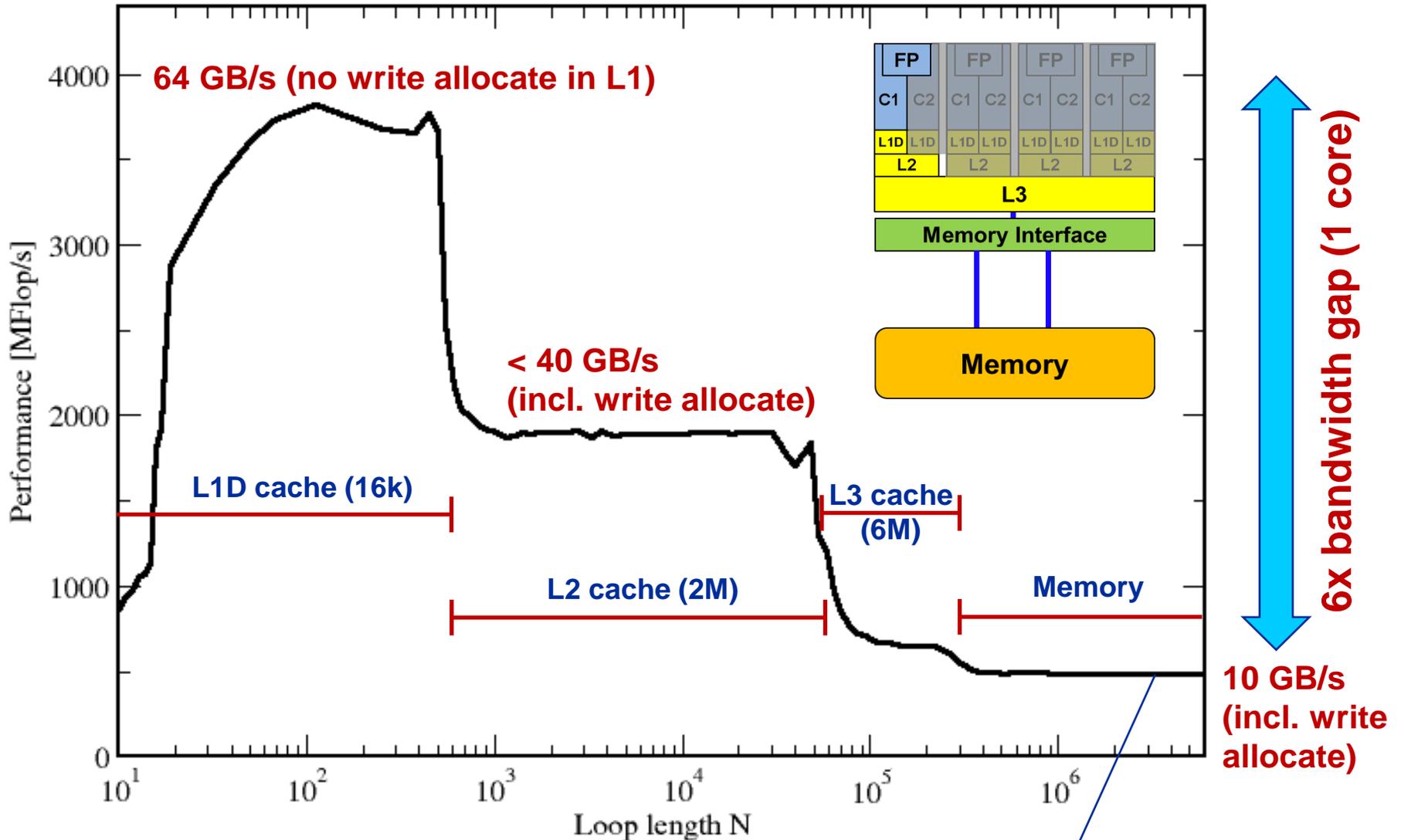
```
double precision, dimension(N) :: A,B,C,D
A=1.d0; B=A; C=A; D=A
```

```
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!**

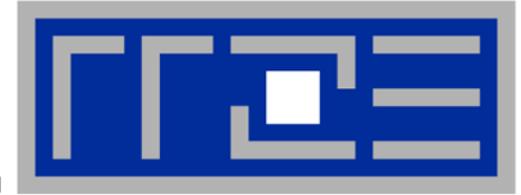
# A(:)=B(:)+C(:)\*D(:) on one Interlagos core



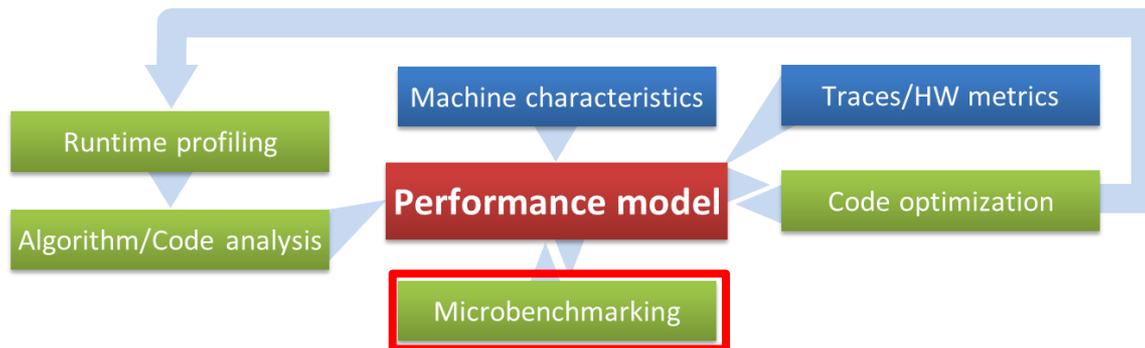
Is this the limit???



- Motivation
- Performance Engineering
  - Performance modeling
  - The Performance Engineering process
- Modern architectures
  - Multicore
  - Accelerators
  - Programming models
- Data access
- **Performance properties of multicore systems**
  - Saturation
  - Scalability
  - Synchronization
- Case study: OpenMP-parallel sparse MVM
- Basic performance modeling: Roofline
  - Theory
  - Case study: 3D Jacobi solver and guided optimizations
  - Modeling erratic access
- **Some more architecture**
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  - ccNUMA
- **Putting cores to good use**
  - Asynchronous communication in spMVM
- **A simple power model for multicore**
  - Power-efficient code execution
- Conclusions

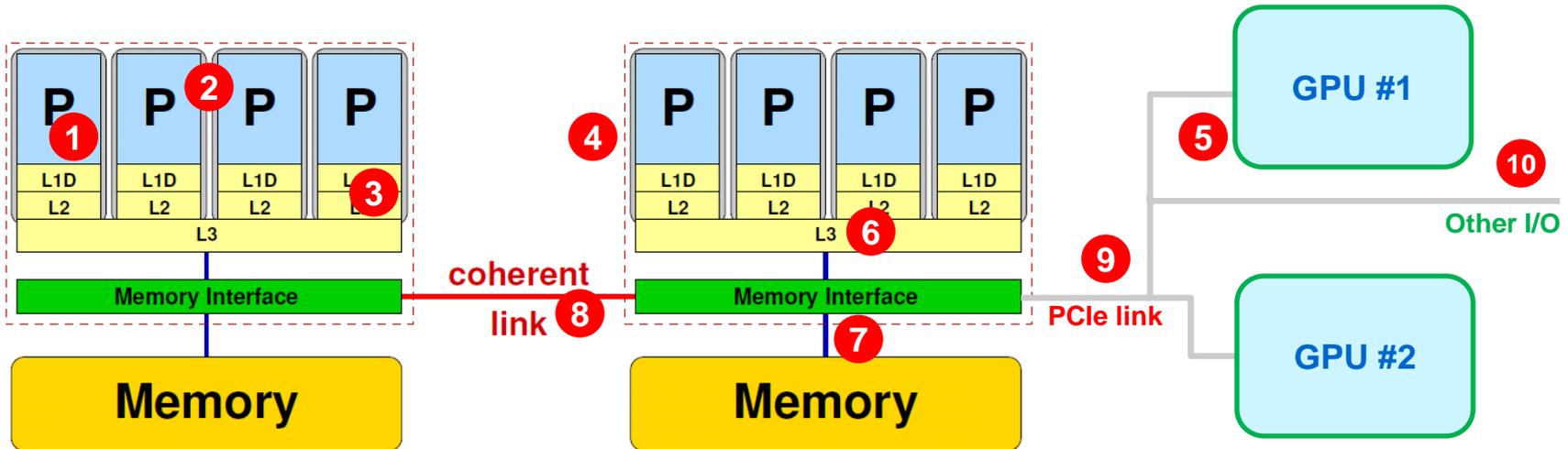


## General remarks on the performance properties of multicore multi-socket systems





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



### Parallel resources:

- Execution/SIMD units 1
- Cores 2
- Inner cache levels 3
- Sockets / memory 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?**

# The parallel vector triad benchmark

(Near-)Optimal code on (Cray) x86 machines



```
call get_walltime(S)
!$OMP parallel private(j)
do j=1,R
  if(N.ge.CACHE_LIMIT) then
!DIR$ LOOP_INFO cache_nt(A)
!$OMP parallel do
  do i=1,N
    A(i) = B(i) + C(i) * D(i)
  enddo
!$OMP end parallel do
  else
!DIR$ LOOP_INFO cache(A)
!$OMP parallel do
  do i=1,N
    A(i) = B(i) + C(i) * D(i)
  enddo
!$OMP end parallel do
  endif
  ! prevent loop interchange
  if(A(N2).lt.0) call dummy(A,B,C,D)
enddo
!$OMP end parallel

call get_walltime(E)
```

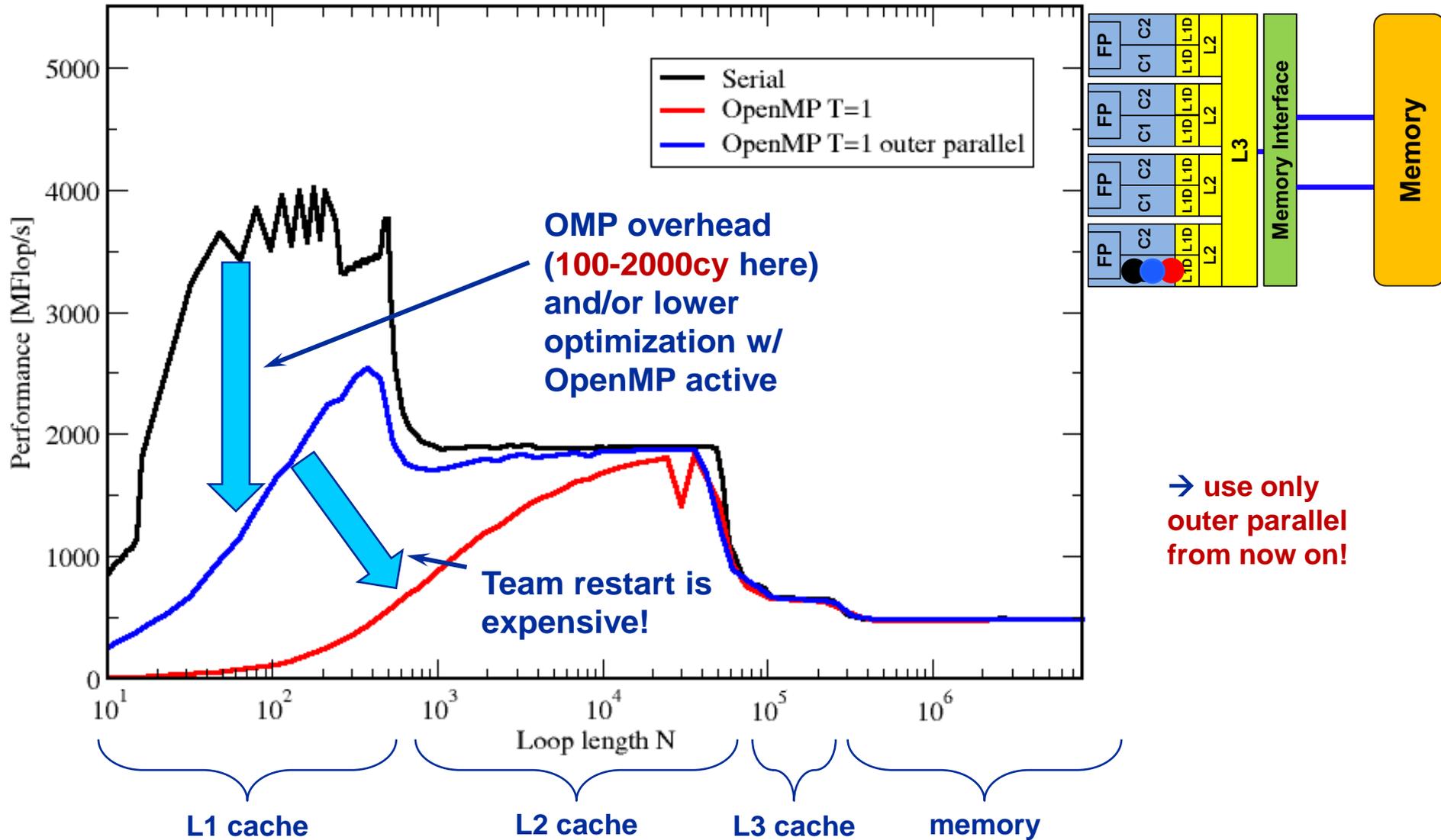
“outer parallel”: Avoid thread team restart at every workshared loop

Large-N version  
(nontemporal stores)

Small-N version  
(standard stores)

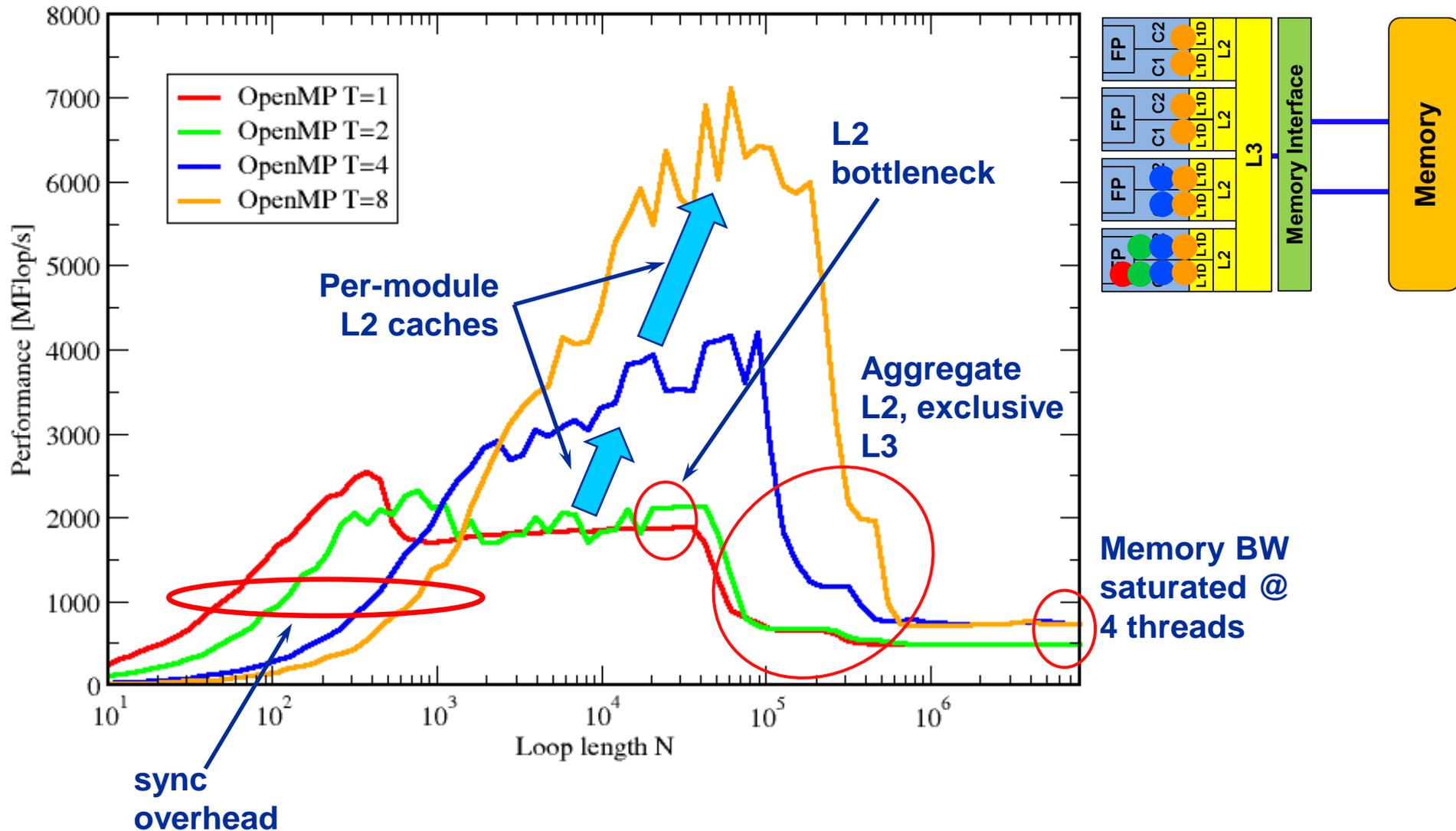
# The parallel vector triad benchmark

Single thread on Cray XE6 Interlagos node



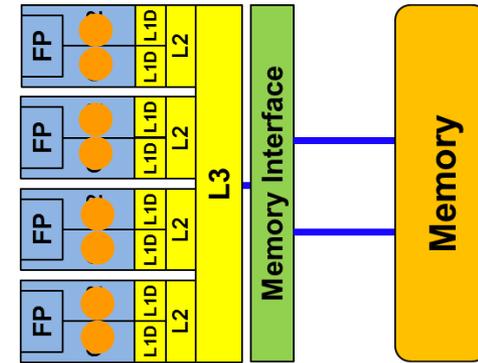
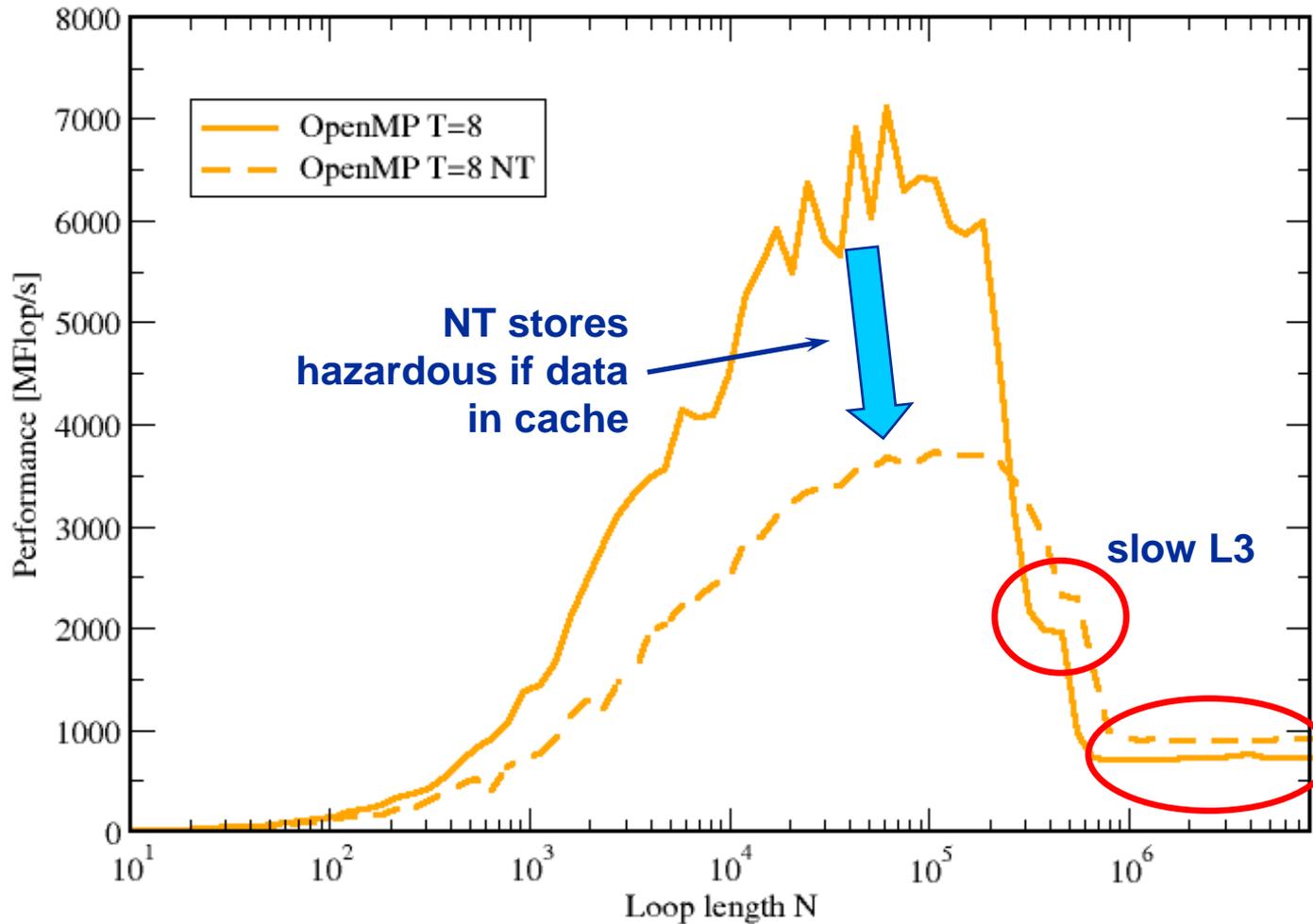
# The parallel vector triad benchmark

## Intra-chip scaling on Cray XE6 Interlagos node



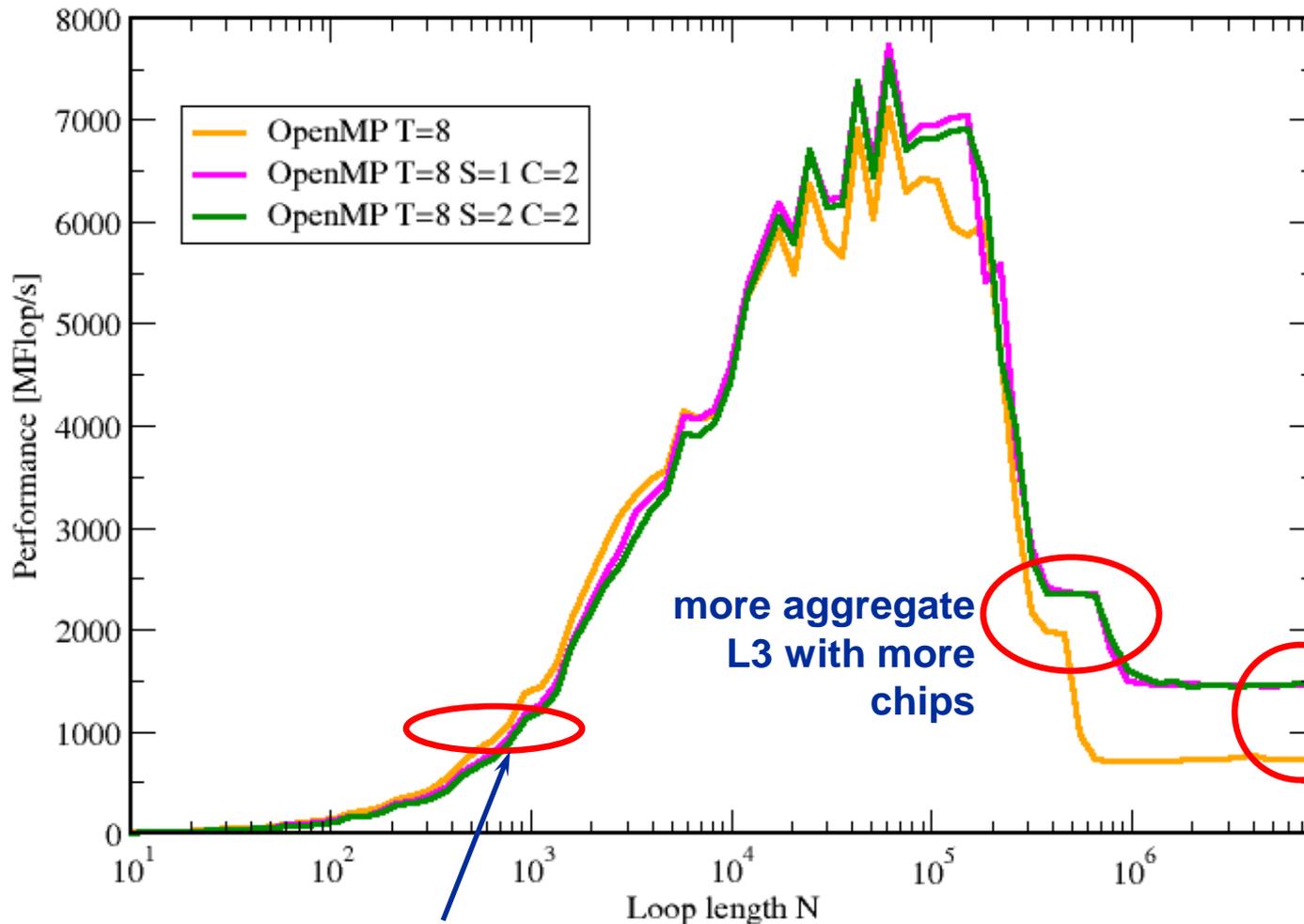
# The parallel vector triad benchmark

*Nontemporal stores on Cray XE6 Interlagos node*

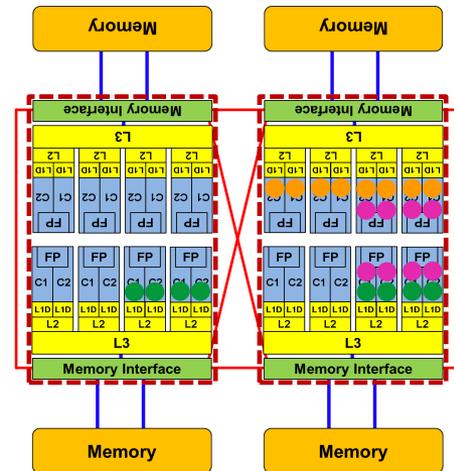


# The parallel vector triad benchmark

Topology dependence on Cray XE6 Interlagos node



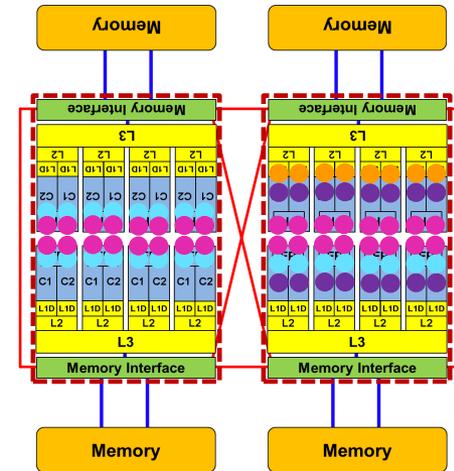
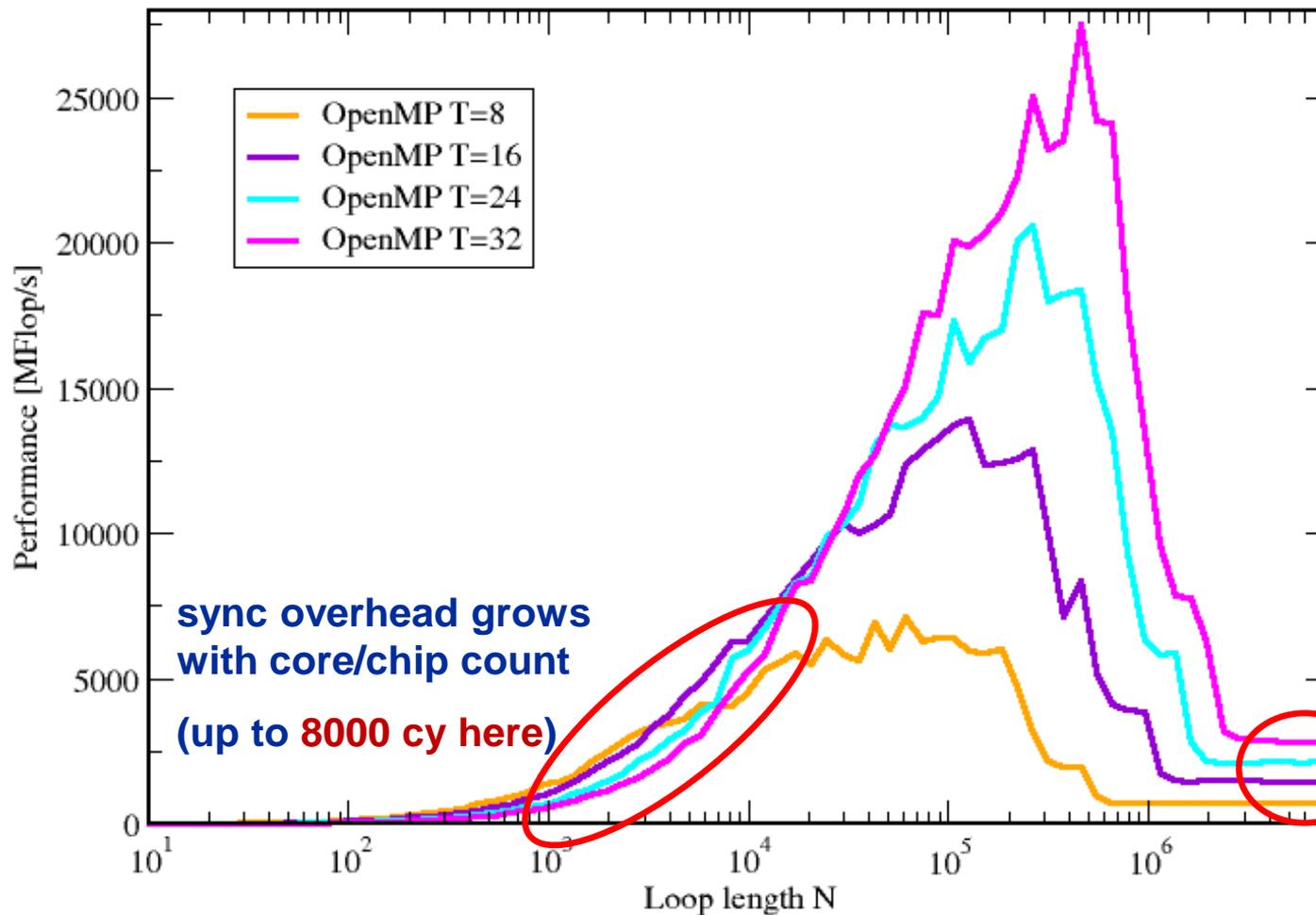
sync overhead nearly topology-independent @ constant thread count



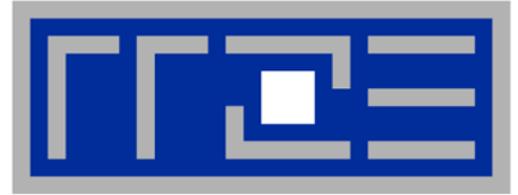
bandwidth scalability across memory interfaces

# The parallel vector triad benchmark

Inter-chip scaling on Cray XE6 Interlagos node





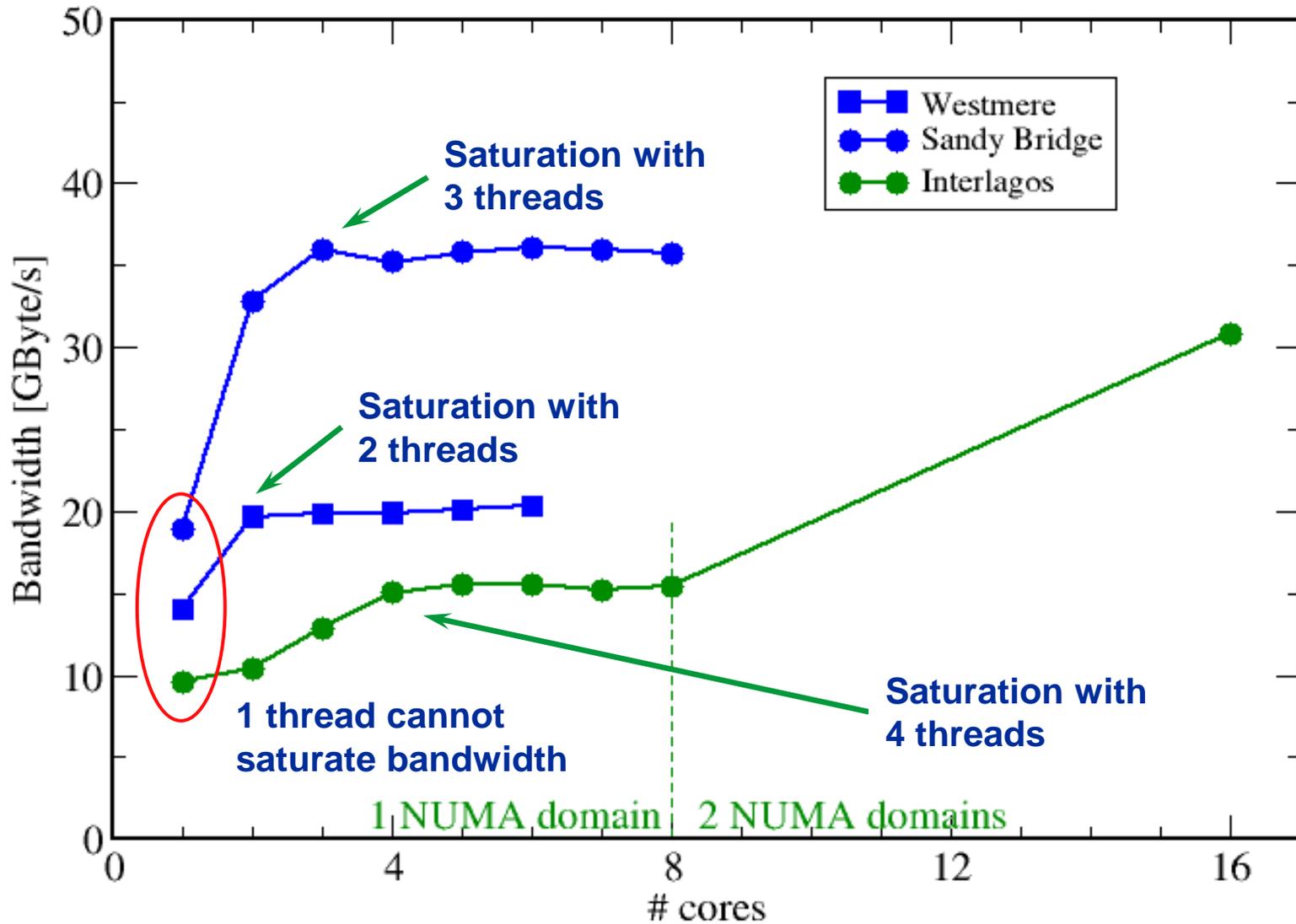


# **Bandwidth saturation effects in cache and memory**

**A look at different processors**

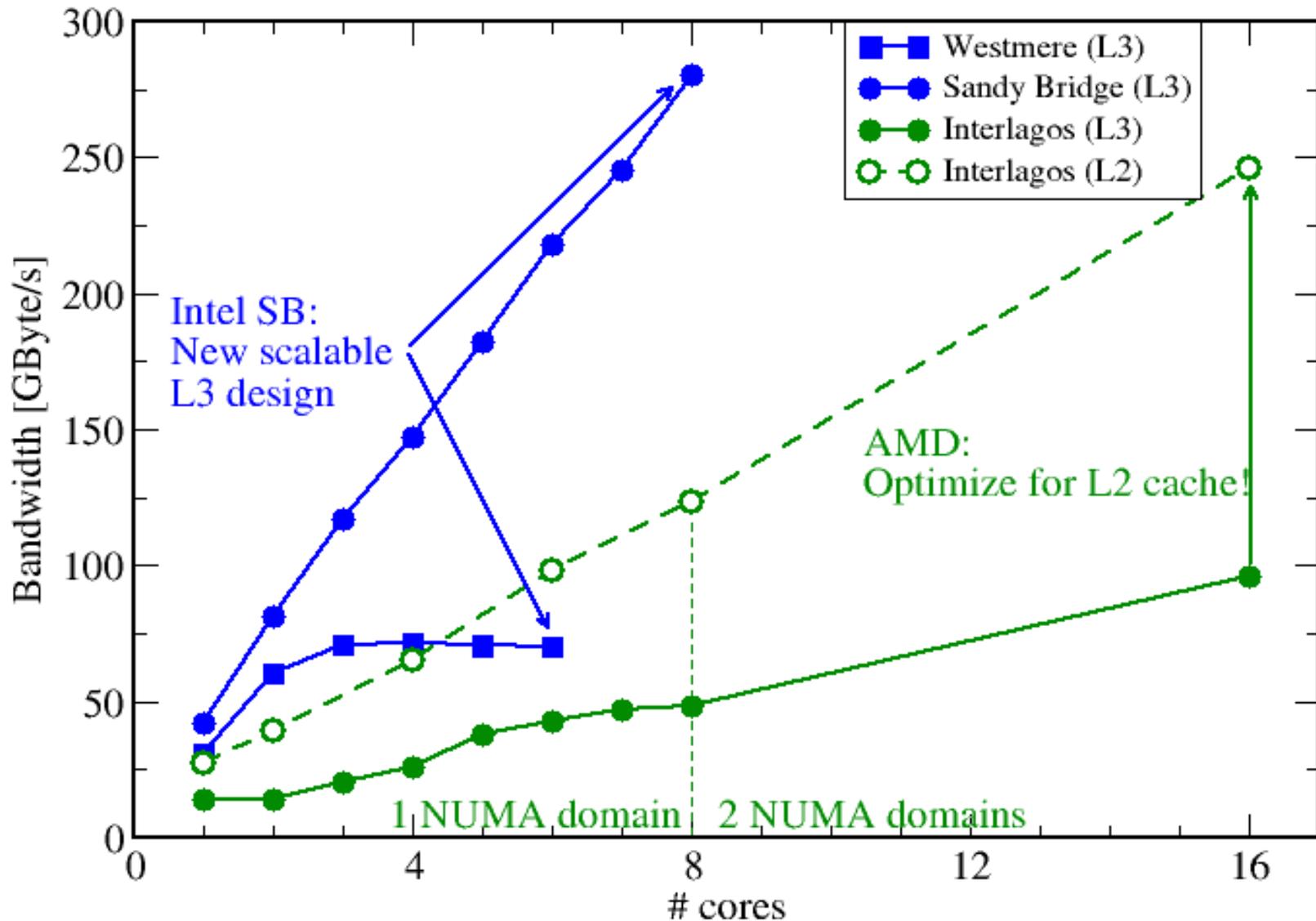
# Bandwidth limitations: Main Memory

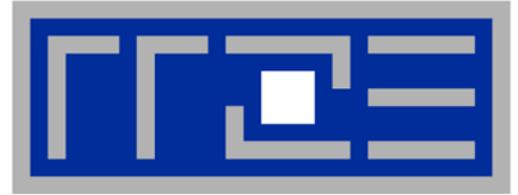
Scalability of shared data paths *inside a NUMA domain* (V-Triad)



# Bandwidth limitations: Outer-level cache

## Scalability of shared data paths in L3 cache





**Some data on  
OpenMP synchronization overhead**

# 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 programs.

Determine costs via modified OpenMP  
Microbenchmarks testcase (epcc)

## On x86 systems there is no hardware support for synchronization!

- Next slide: 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 AMD Interlagos

OpenMP barrier overhead in CPU cycles

2 Threads	Cray 8.03	GCC 4.6.2	PGI 11.8	Intel 12.1.3
Shared L2	258	3995	1503	128623
Shared L3	698	2853	1076	128611
Same socket	879	2785	1297	128695
Other socket	940	2740 / 4222	1284 / 1325	128718



Intel compiler barrier very expensive on Interlagos

OpenMP & Cray compiler 

Full domain	Cray 8.03	GCC 4.6.2	PGI 11.8	Intel 12.1.3
Shared L3	2272	27916	5981	151939
Socket	3783	49947	7479	163561
Node	7663	167646	9526	178892





# Thread synchronization overhead on Intel CPUs

*pthread*s vs. *OpenMP* vs. Spin loop

2 Threads	Q9550 (shared L2)	i7 920 (shared L3)
<code>pthread_barrier_wait</code>	<b>23739</b>	6511
<code>omp barrier gcc 4.3.3</code>	22603	7333
<code>omp barrier icc 11.0</code>	<b>399</b>	<b>469</b>
Spin loop	<b>231</b>	<b>270</b>

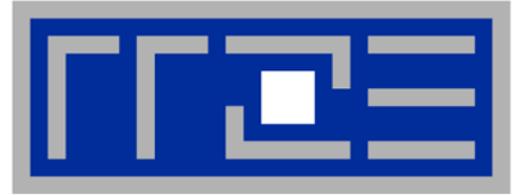
Nehalem 2 Threads	Shared SMT threads	shared L3	different socket
<code>pthread_barrier_wait</code>	<b>23352</b>	4796	49237
<code>omp barrier (icc 11.0)</code>	<b>2761</b>	<b>479</b>	<b>1206</b>
Spin loop	17388	<b>267</b>	787

**pthread**s → OS kernel call ☹️

Syncing SMT threads is expensive ☹️

Spin loop does fine for shared cache sync

**OpenMP & Intel compiler** 😊



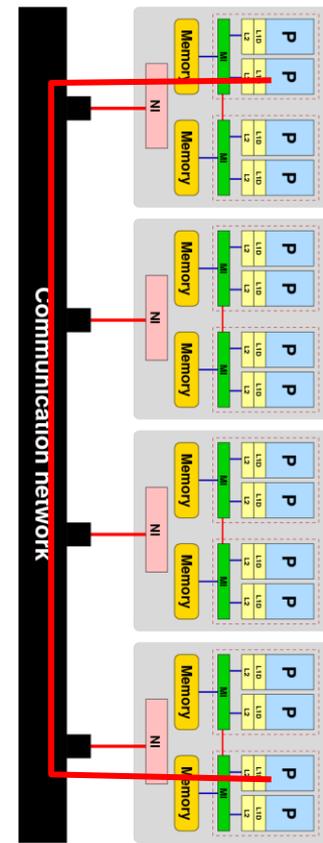
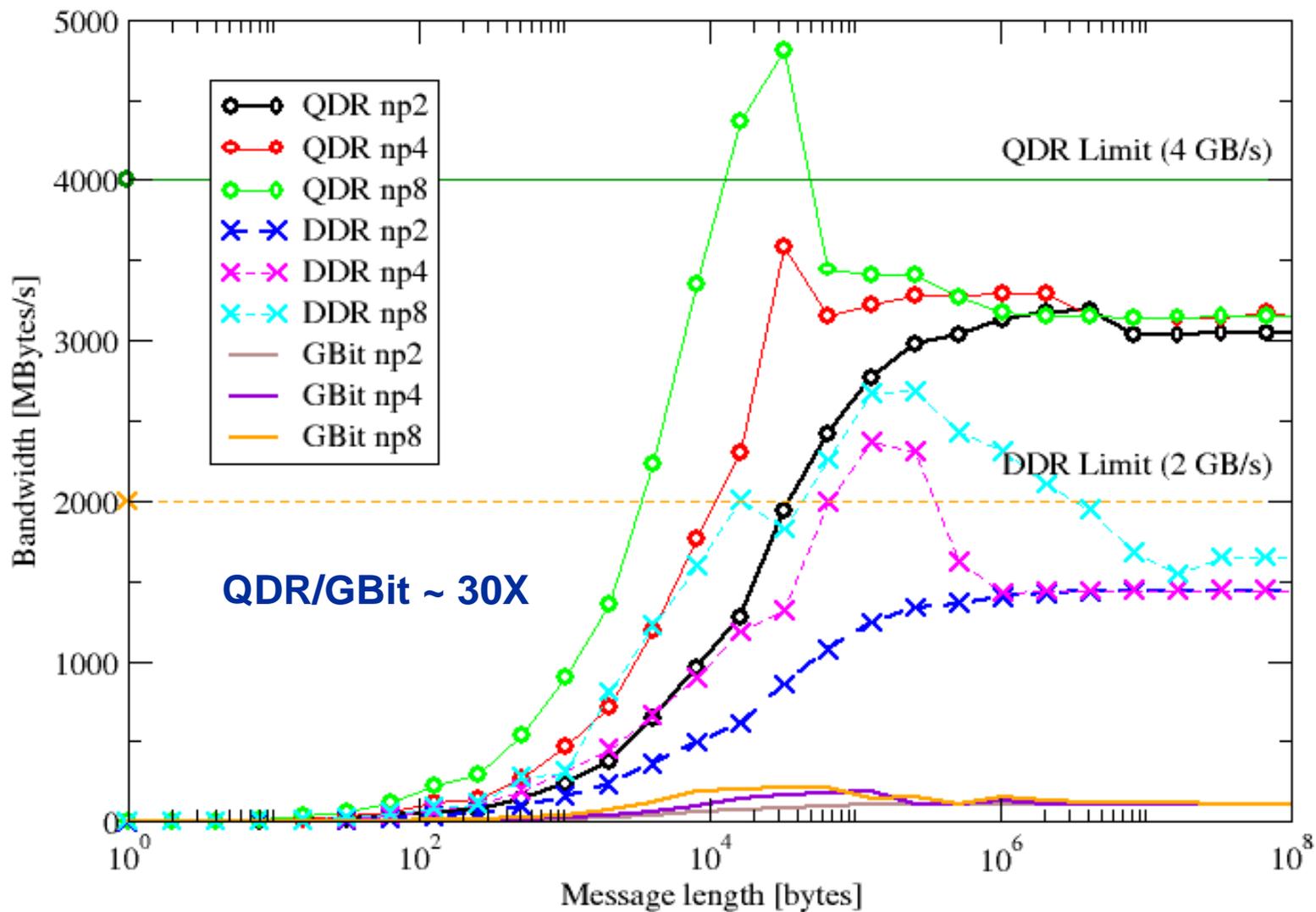
# Understanding MPI communication in multicore environments

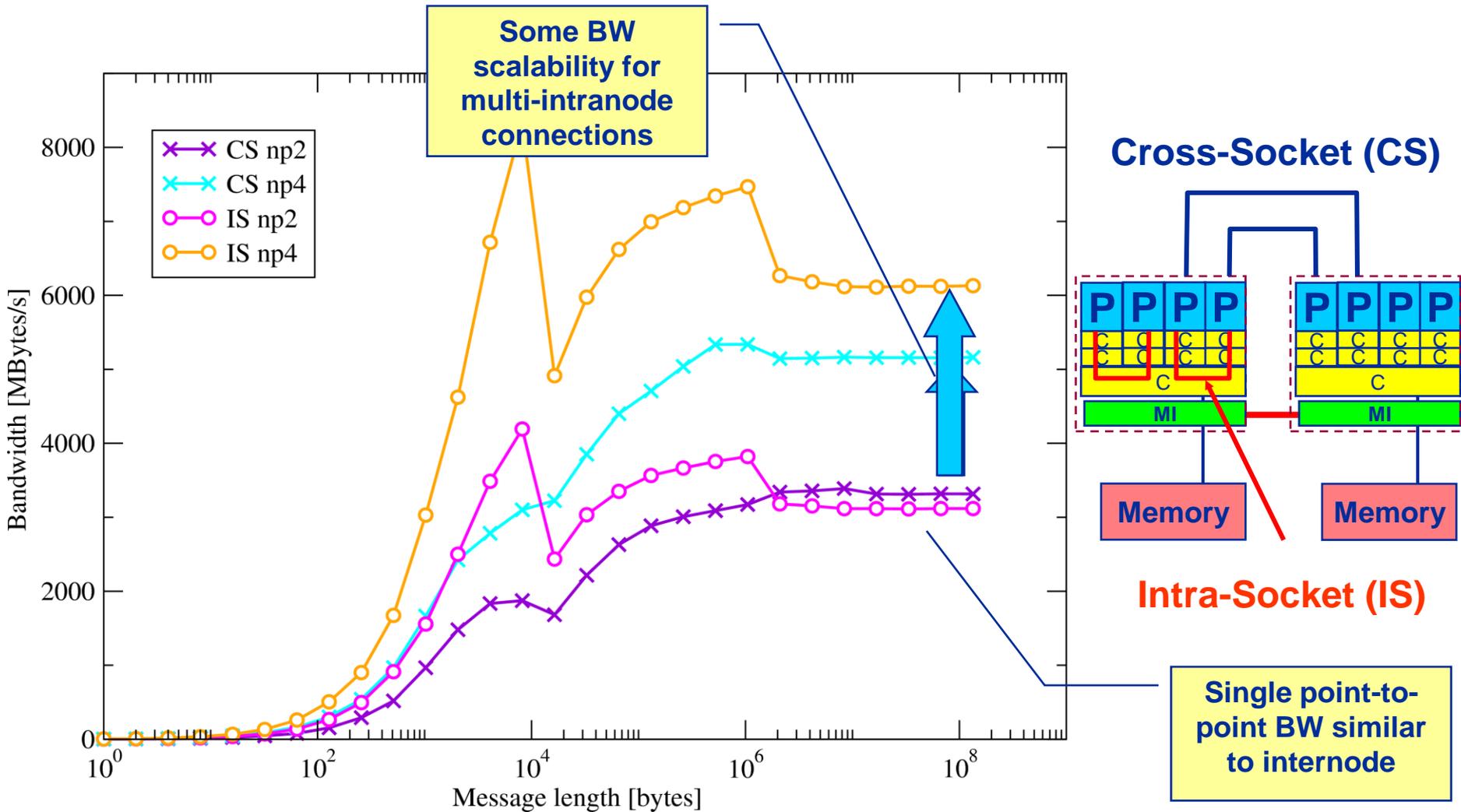
**Intra-node vs. inter-node MPI**

MPI Cartesian topologies and rank-subdomain mapping



- **Common misconception:** Intranode MPI is infinitely fast compared to internode
- **Reality**
  - Intranode **latency** is much smaller than internode
  - Intranode **asymptotic bandwidth** is surprisingly comparable to internode
  - Difference in saturation behavior
- **Other issues**
  - Mapping between ranks, subdomains and cores with Cartesian MPI topologies
  - Overlapping intranode with internode communication

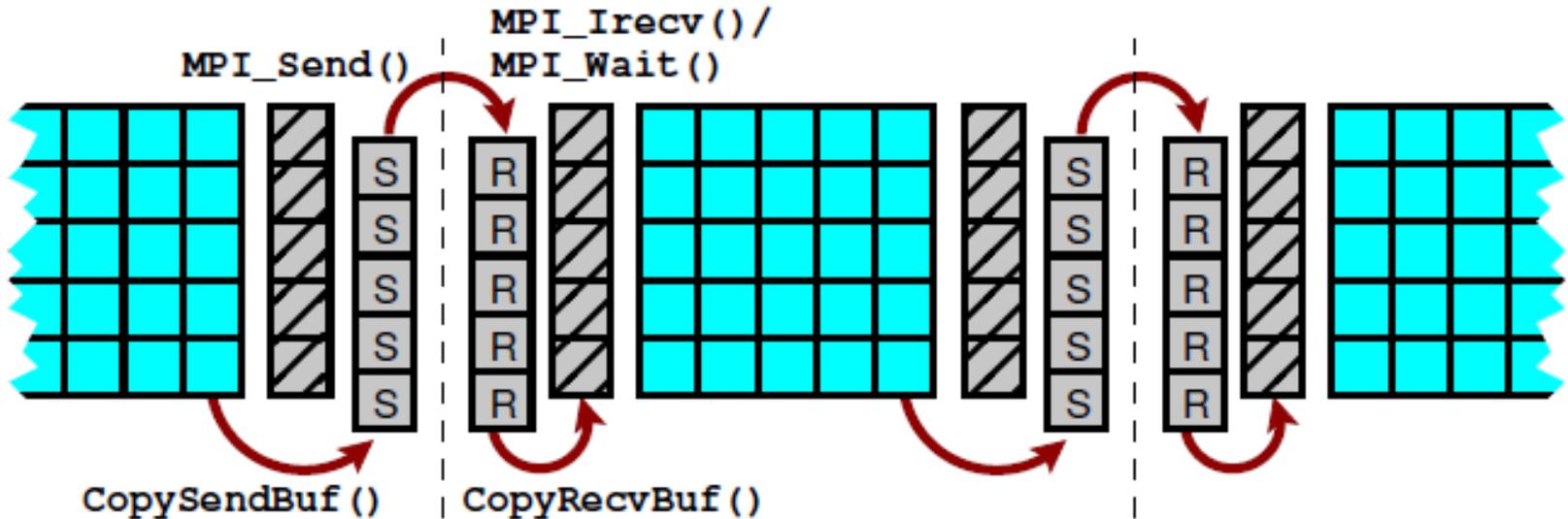




Mapping problem for most efficient communication paths!?



### ■ Example: Stencil solver with halo exchange



### ■ Goal: Reduce inter-node halo traffic

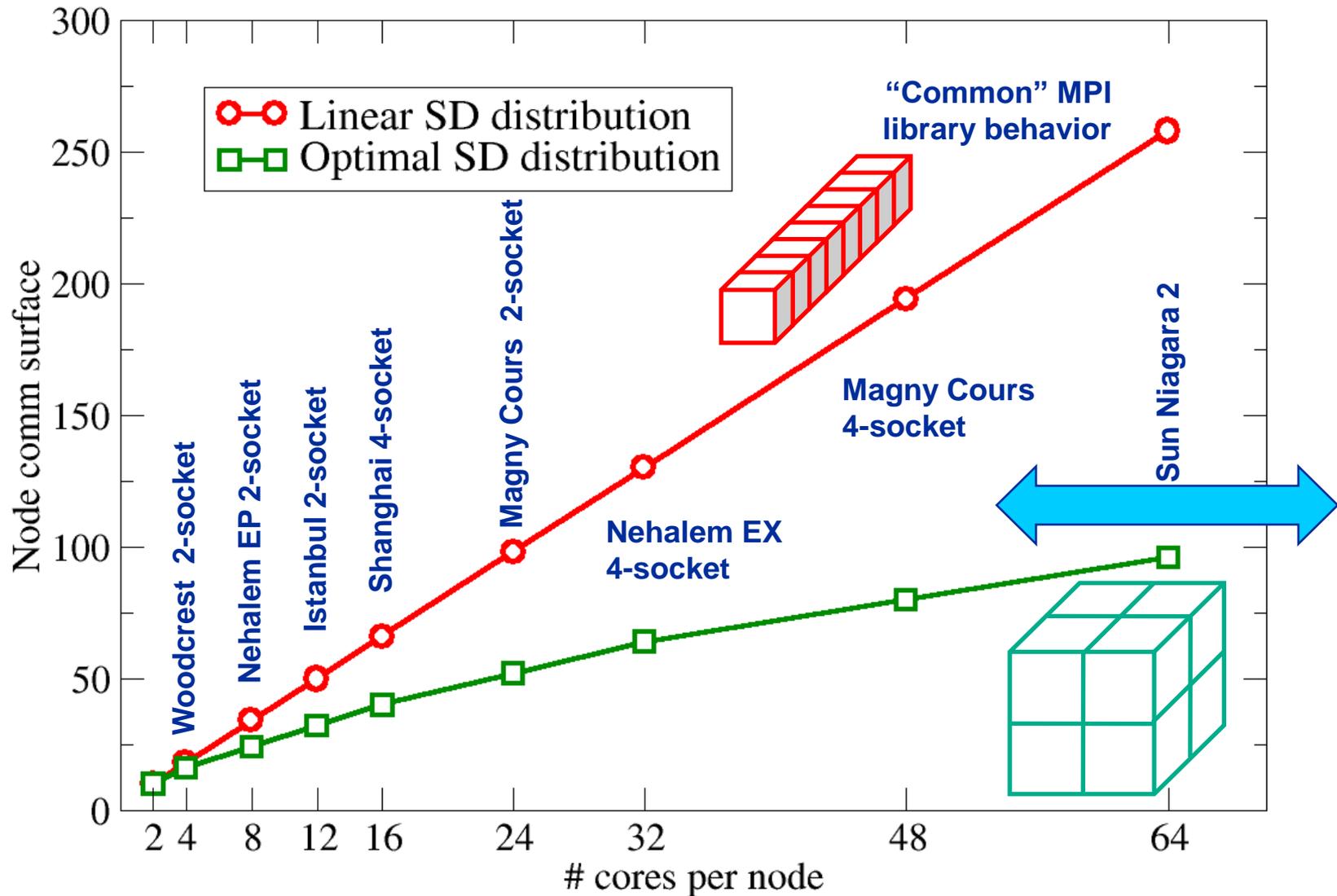
### ■ Subdomains exchange halo with neighbors

- Populate a node's ranks with “maximum neighboring” subdomains
- This minimizes a node's communication surface

### ■ Shouldn't MPI\_CART\_CREATE (w/ reorder) take care of this?

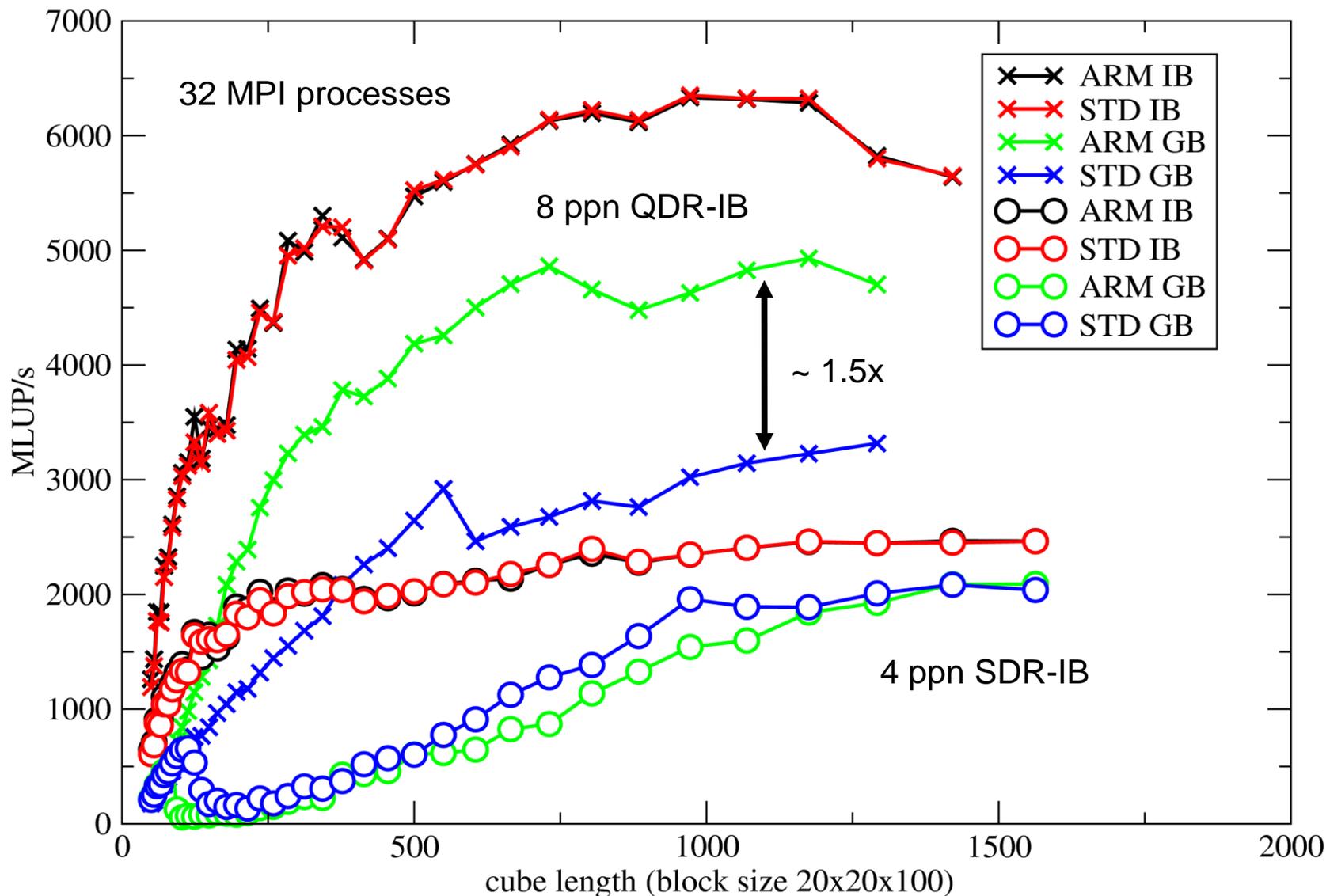
# MPI rank-subdomain mapping in Cartesian topologies:

*A 3D stencil solver and the growing number of cores per node*



# MPI rank-subdomain mapping:

3D stencil solver – measurements for 8ppn and 4ppn GBE vs. IB





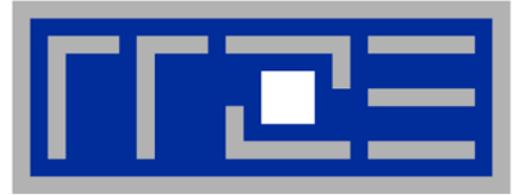
- **Intranode MPI**
  - May not be as fast as you think...
  - Becomes more important as core counts increase
  - May not be handled optimally by your MPI library
  
- **Rank-core mapping may be crucial for best performance**
  - Reduce inter-node traffic
  - Most MPIs do not recognize this
  - Some (e.g., Cray) can give you hints toward optimal placement



- **Affinity matters!**
  - Almost all performance properties depend on the position of
    - Data
    - Threads/processes
  - Consequences
    - **Know the topology of your machine**
    - **Know where your threads are running**
    - **Know where your data is**
  
- **Bandwidth bottlenecks are ubiquitous**
  - Bad scaling is not always a bad thing
  - Do you exhaust your bottlenecks?
  
- **Synchronization overhead may be an issue**
  - ... and also depends on affinity!



- **Motivation**
- **Performance Engineering**
  - Performance modeling
  - The Performance Engineering process
- **Modern architectures**
  - Multicore
  - Accelerators
  - Programming models
- **Data access**
- **Performance properties of multicore systems**
  - Saturation
  - Scalability
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- **Case study: OpenMP-parallel sparse MVM**
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- **Conclusions**



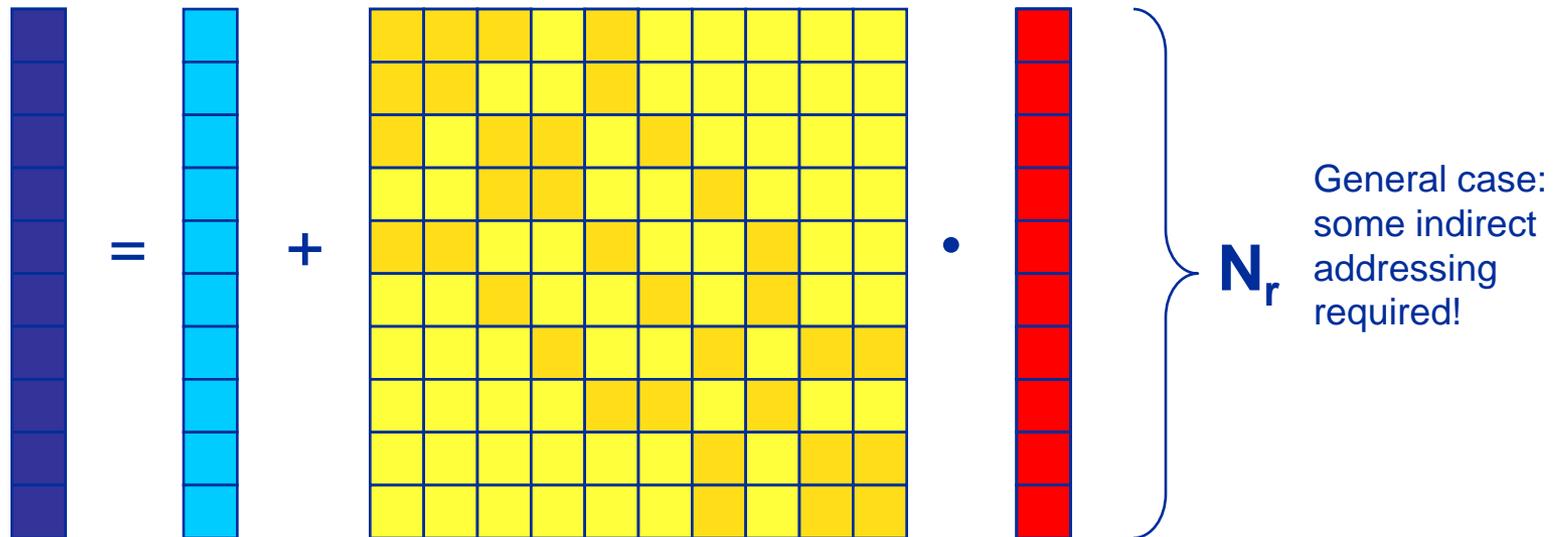
**Case study:  
OpenMP-parallel sparse matrix-vector  
multiplication**

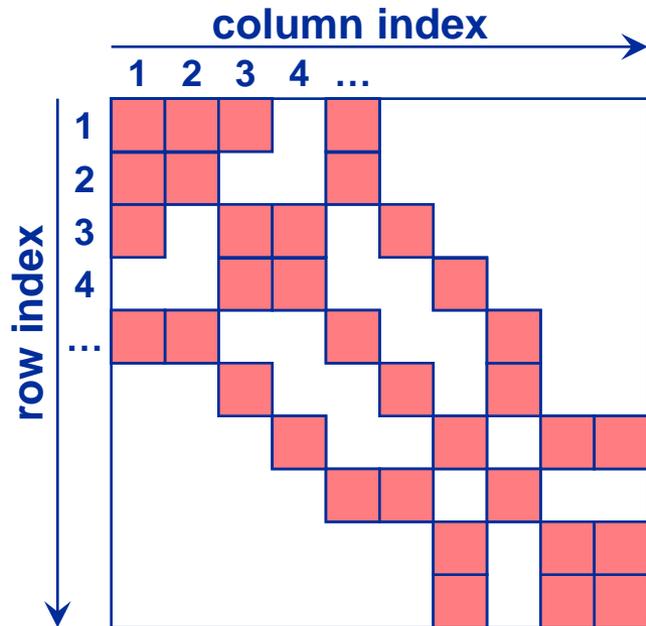
**A simple (but sometimes not-so-simple)  
example for bandwidth-bound code and  
saturation effects in memory**

# Sparse matrix-vector multiply (sMVM)

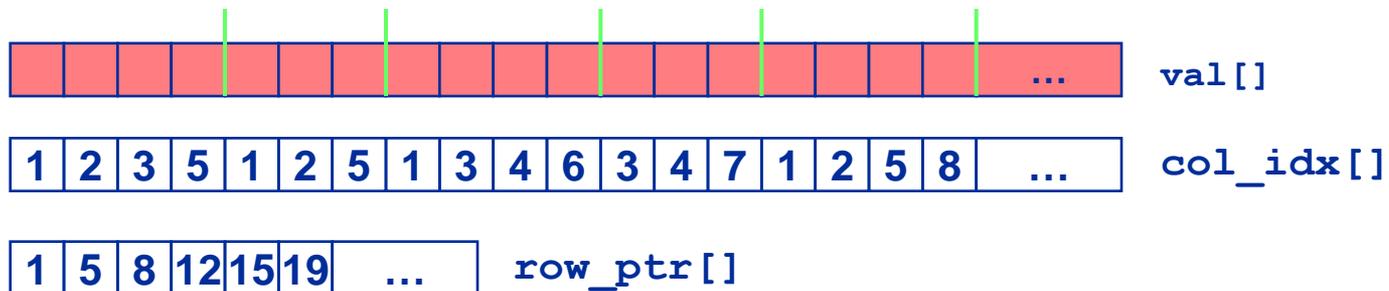


- Key ingredient in some matrix diagonalization algorithms
  - Lanczos, Davidson, Jacobi-Davidson
- Store only  $N_{nz}$  nonzero elements of matrix and RHS, LHS vectors with  $N_r$  (number of matrix rows) entries
- “Sparse”:  $N_{nz} \sim N_r$





- `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:  $N_r$ )





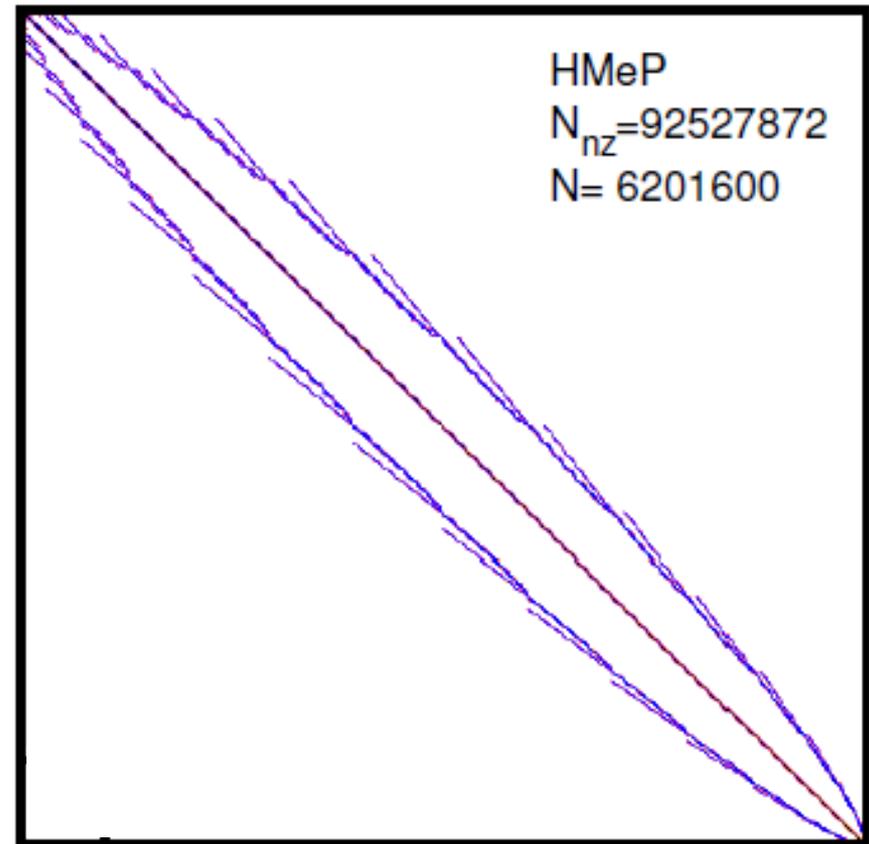
- **Strongly memory-bound for large data sets**
  - Streaming, with partially indirect access:

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

- Usually many spMVMs required to solve a problem
  - MPI parallelization possible and well-studied
- **Following slides: Performance data on one 24-core AMD Magny Cours node**



- **Data storage format is crucial for performance properties**
  - Most useful general format: Compressed Row Storage (**CRS**)
  - SpMVM is **easily parallelizable** in shared and distributed memory
  
- **For large problems, spMVM is inevitably memory-bound**
  - **Intra-LD saturation effect** on modern multicores
  
- **MPI-parallel spMVM is often communication-bound**
  - See later part for what we can do about this...

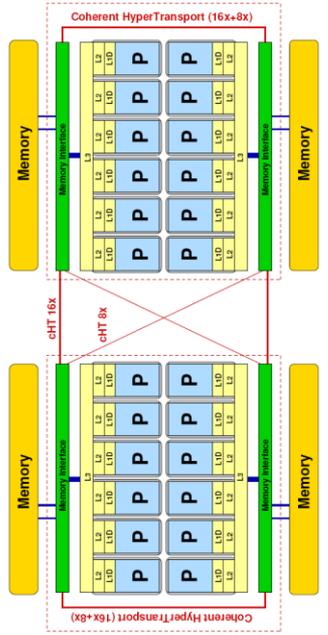


# Application: Sparse matrix-vector multiply

Strong scaling on one XE6 Magny-Cours node

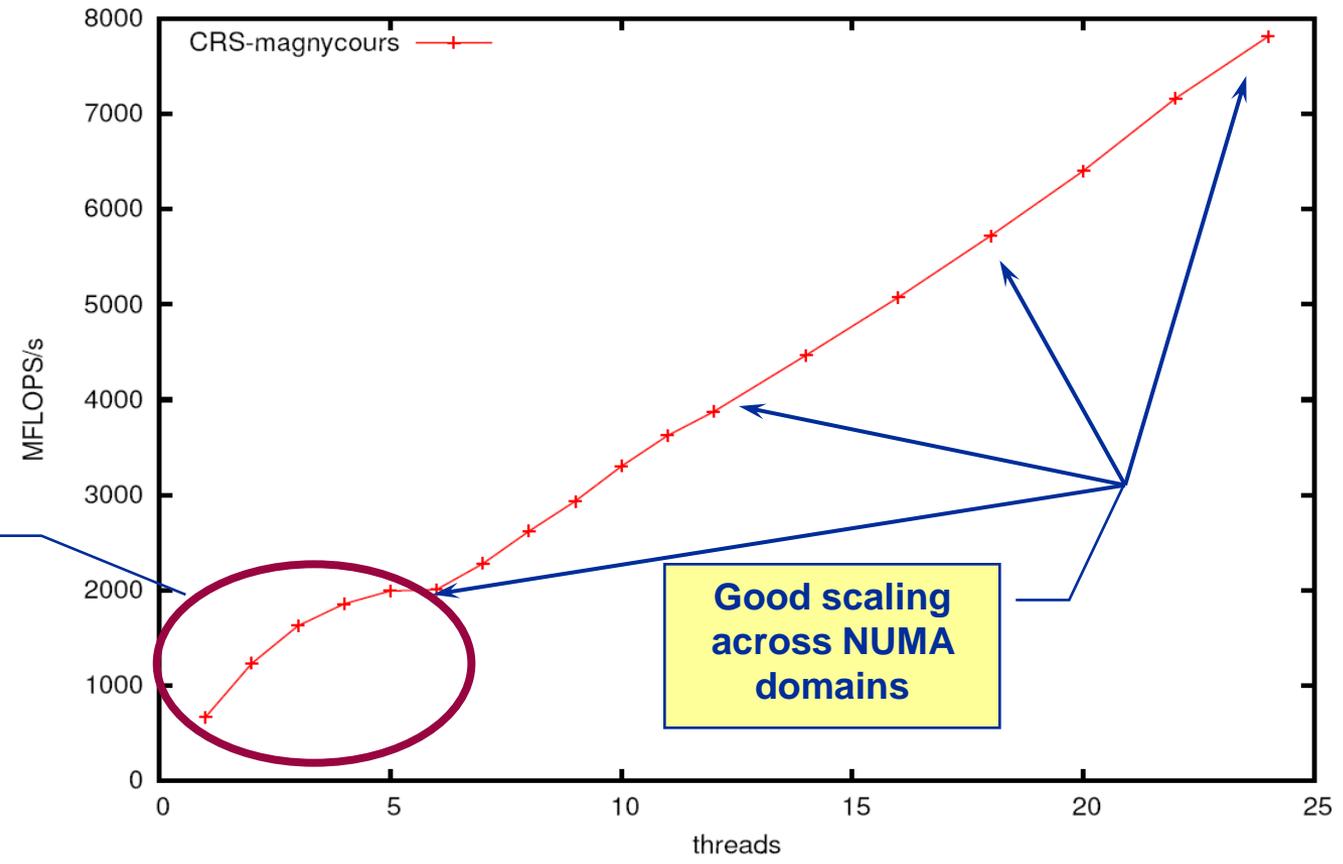


## Case 1: Large matrix



**Intrasocket bandwidth bottleneck**

cant, 62451x62451, non-zero: 4007383

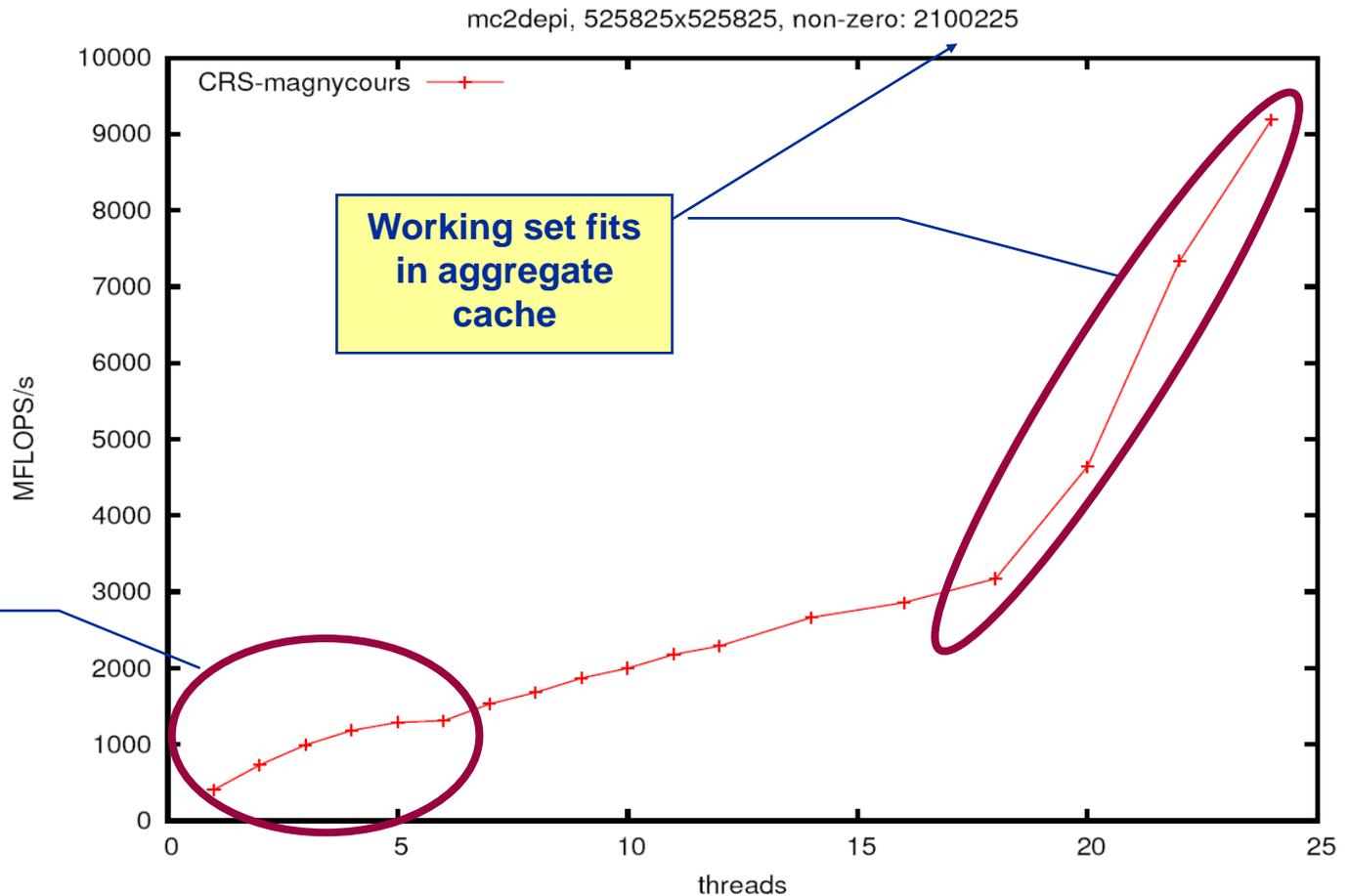




### Case 2: Medium size



Intrasocket bandwidth bottleneck

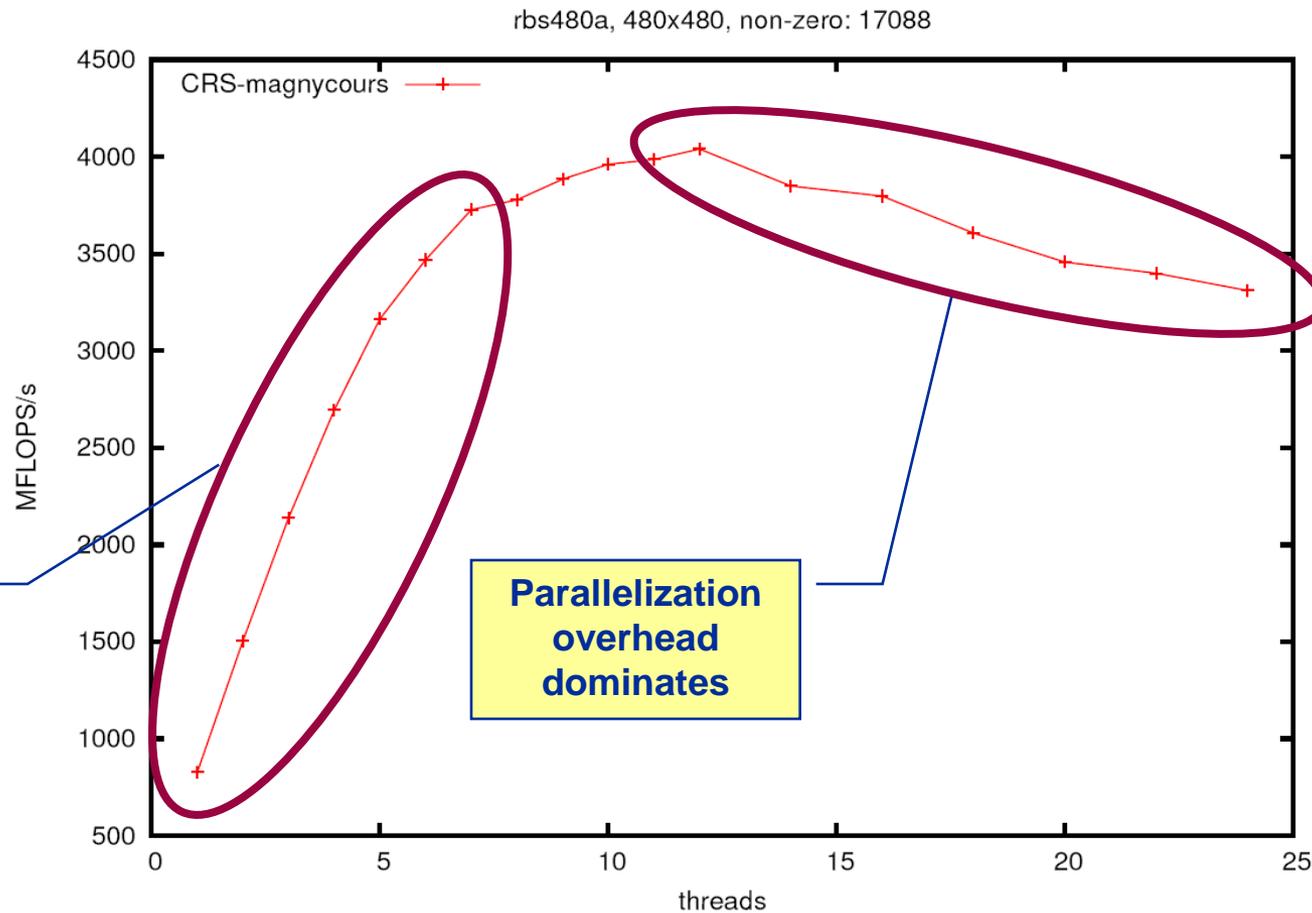




### Case 3: Small size



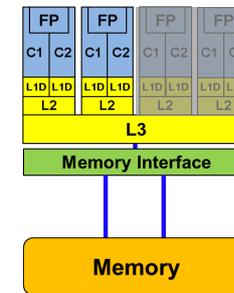
No bandwidth bottleneck



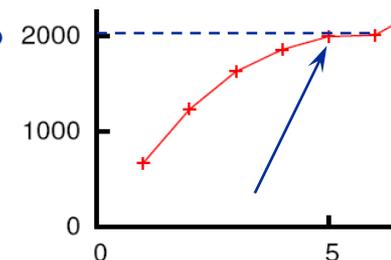
Parallelization overhead dominates



- If the problem is “large”, bandwidth saturation on the socket is a reality
  - → There are “**spare cores**”
  - Very **common performance pattern**
- **What to do with spare cores?**
  - Use them for other tasks, such as **MPI communication**
  - Let them **idle** → **saves energy** with minor loss in time to solution
- **Can we predict the saturated performance?**
  - Bandwidth-based performance **modeling!**
  - What is the significance of the **indirect access**? Can it be modeled?
- **Can we predict the saturation point?**
  - ... and why is this important?

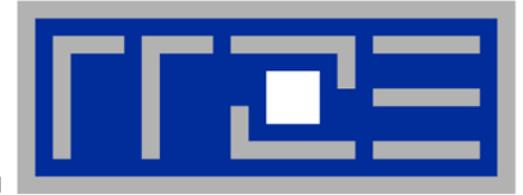


See later for answers!





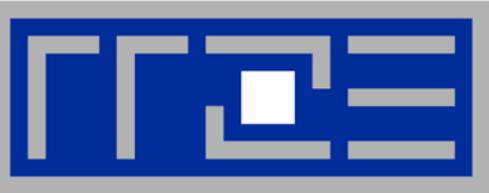
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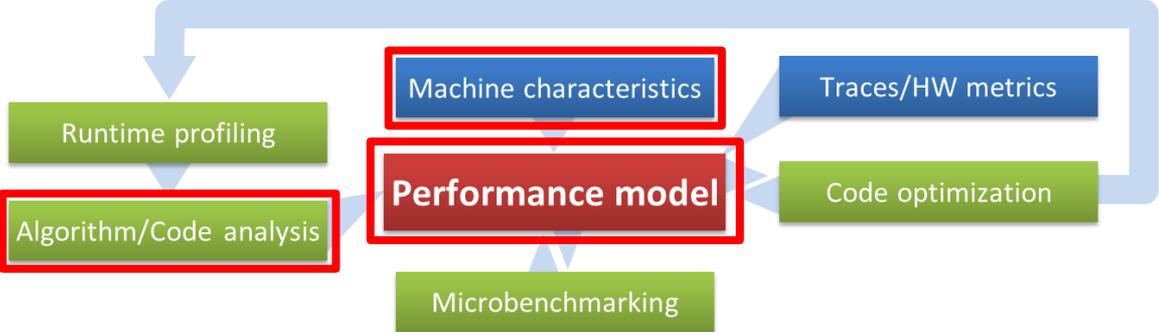
# **Basic performance modeling and “motivated optimizations”**

**The Roofline Model**

**Case study: The Jacobi smoother**

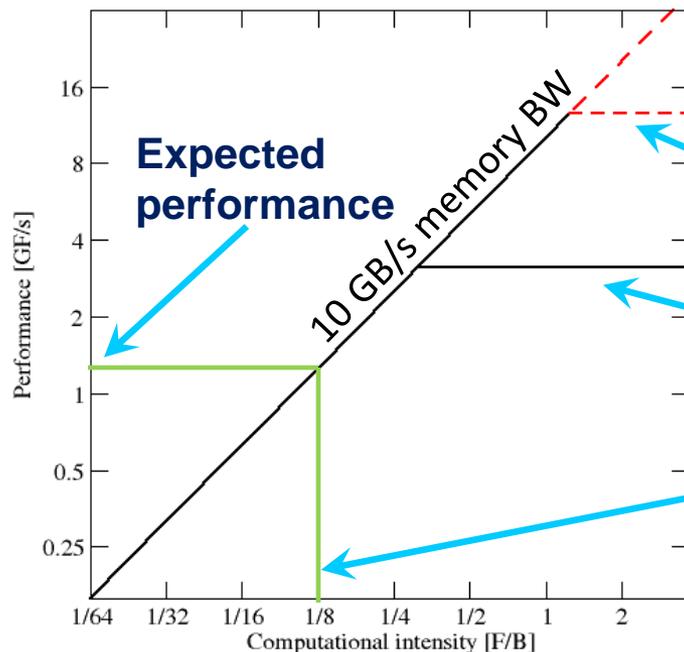


# The Roofline Model





1. Determine the **applicable peak performance** of a loop, assuming that data comes from L1 cache
2. Determine the **computational intensity (flops per byte transferred)** over the slowest data path utilized
3. Determine the **applicable peak bandwidth** of the slowest data path utilized



Example: `do i=1,N; s=s+a(i); enddo`  
in DP on hypothetical 3 GHz CPU, 4-way SIMD, N large

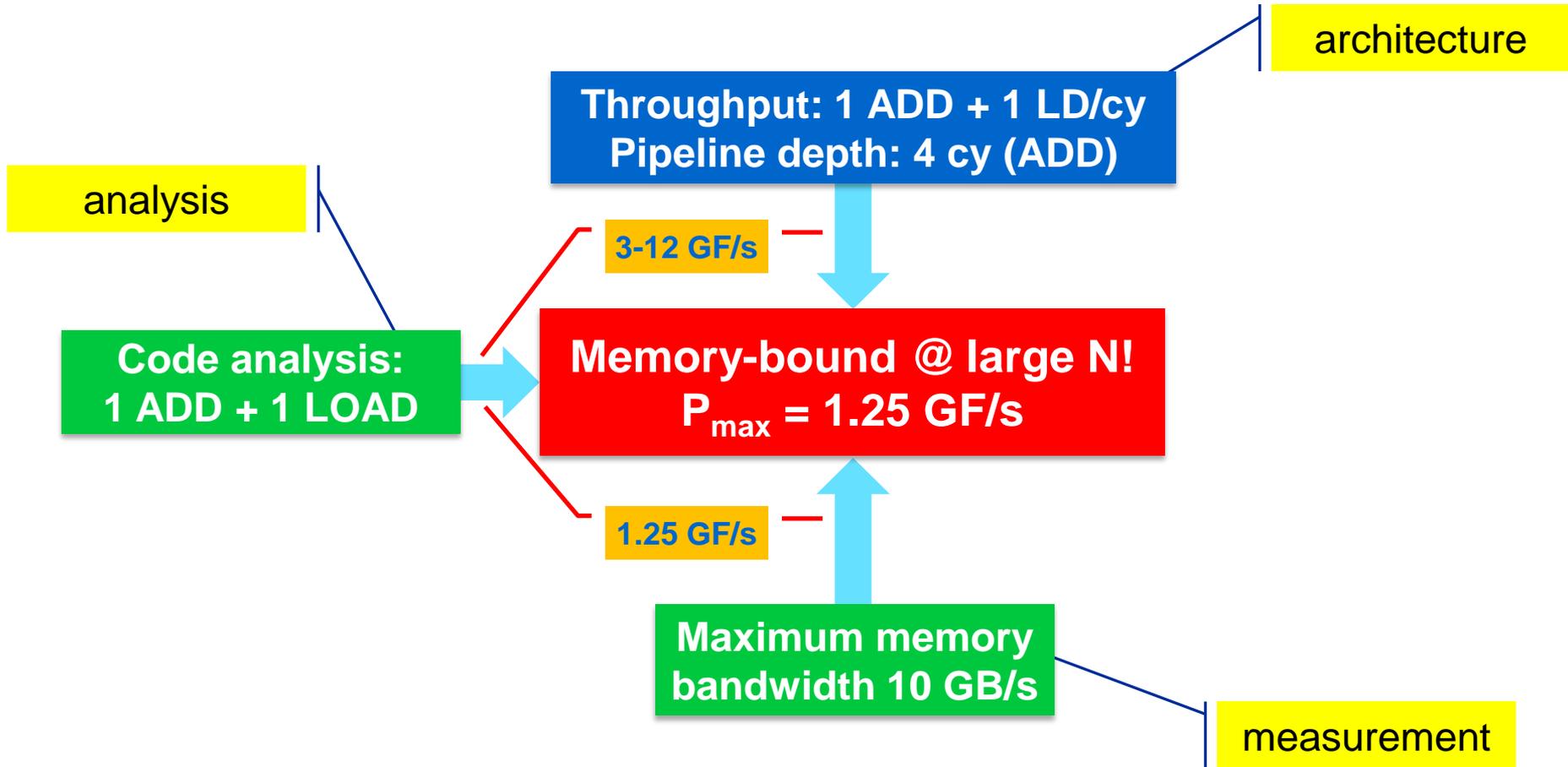
ADD peak (half of full peak)

4-cycle latency per ADD if not unrolled

Computational intensity [Flops/byte]



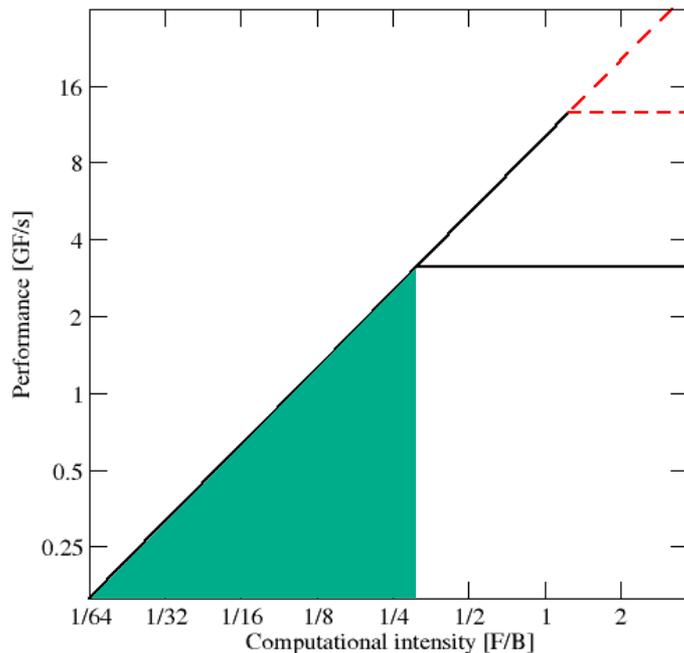
... on the example of `do i=1,N; s=s+a(i); enddo`





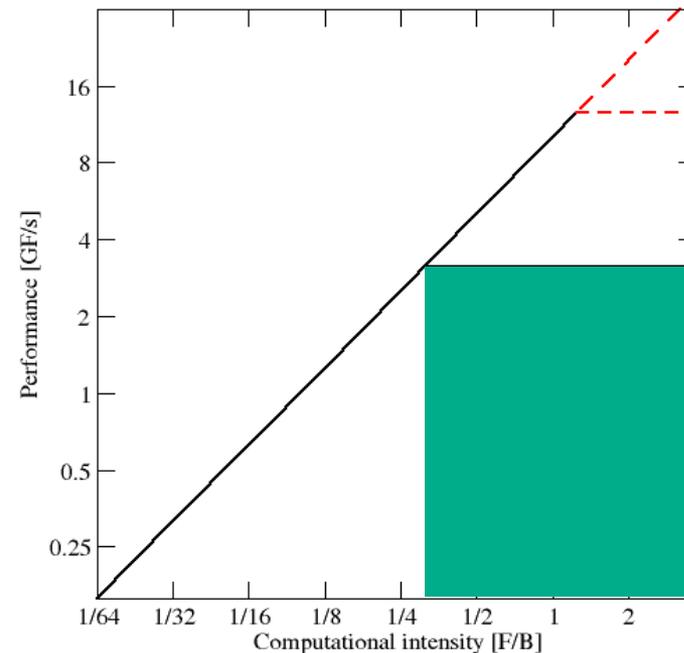
## Bandwidth-bound (simple case)

- Accurate traffic calculation (write-allocate, strided access, ...)
- Practical  $\neq$  theoretical BW limits
- **Erratic access patterns**



## Core-bound (may be complex)

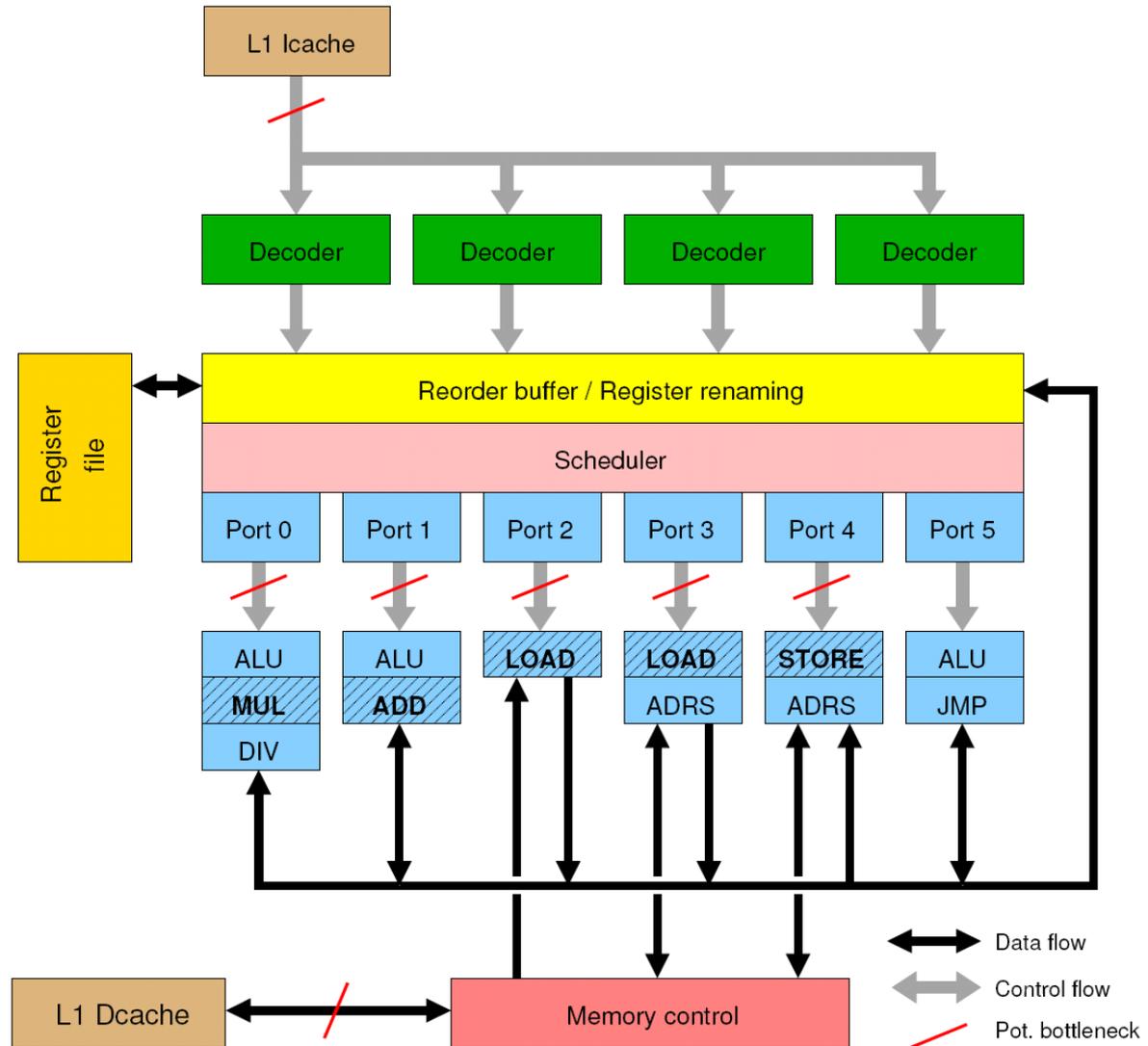
- **Multiple bottlenecks:** LD/ST, arithmetic, pipelines, SIMD, execution ports
- See next slide...





## Multiple bottlenecks:

- L1 Icache bandwidth
- Decode/retirement throughput
- Port contention (direct or indirect)
- Arithmetic pipeline stalls (dependencies)
- Overall pipeline stalls (branching)
- L1 Dcache bandwidth (LD/ST throughput)
- Scalar vs. SIMD execution
- ...
- Register pressure
- Alignment issues





- **Code balance ( $B_C$ )** quantifies the requirements of the code
  - Reciprocal of comp. intensity

$$B_C = \frac{\text{data transfer (LD/ST) [words]}}{\text{arithmetic operations [flops]}}$$

- **$b_S$  = achievable bandwidth over the slowest data path**
  - E.g., measured by suitable microbenchmark (STREAM, ...)

- **Lightspeed** for absolute performance: ( $P_{\max}$  : “applicable” peak performance)

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

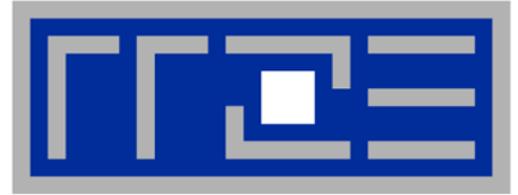
Newton's  
Second Law  
of  
performance  
modeling

- **Example: Vector triad  $A(:) = B(:) + C(:) * D(:)$  on 2.3 GHz Interlagos**
  - $B_C = (4+1) \text{ Words} / 2 \text{ Flops} = 2.5 \text{ W/F}$  (including write allocate)

$$b_S/B_C = 1.7 \text{ GF/s (1.2 \% of peak performance)}$$



- **The balance metric 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!**
  - **Slowest data path is modeled only;** all others are assumed to be infinitely fast
  - If data transfer is the limiting factor, the **bandwidth** of the slowest data path can be **utilized to 100%** (“saturation”)
  - Latency effects are ignored, i.e. **perfect streaming mode**



**Case study:**  
**A 3D Jacobi smoother**

**The basics in two dimensions**  
**Performance analysis and modeling**



- Laplace equation in 2D:  $\Delta\Phi = 0$
- **Solve** with Dirichlet boundary conditions using Jacobi iteration scheme:

```

double precision, dimension(0:imax+1,0:kmax+1,0:1) :: phi
integer :: t0,t1
t0 = 0 ; t1 = 1
do it = 1,itmax      ! choose suitable number of sweeps
  do k = 1,kmax
    do i = 1,imax
      ! four flops, one store, four loads
      phi(i,k,t1) = ( phi(i+1,k,t0) + phi(i-1,k,t0)
                    + phi(i,k+1,t0) + phi(i,k-1,t0) ) * 0.25
    enddo
  enddo
  ! swap arrays
  i = t0 ; t0=t1 ; t1=i
enddo

```

Reuse when computing  $\text{phi}(i+2,k,t1)$

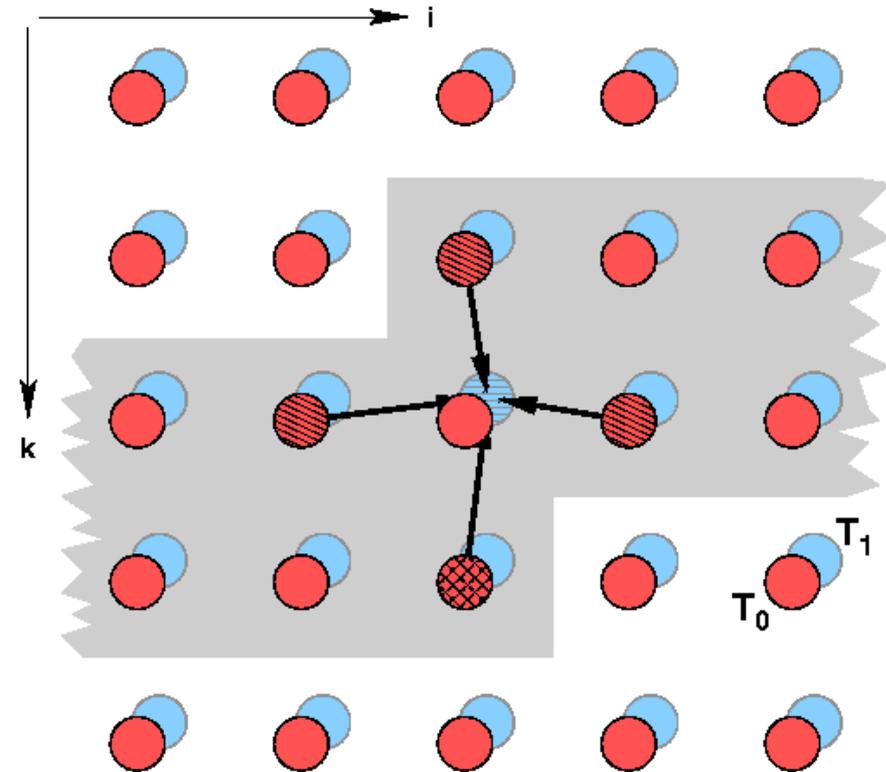
**Naive balance (incl. write allocate):**

**$\text{phi}(:, :, t0)$ : 3 LD +**  
 **$\text{phi}(:, :, t1)$ : 1 ST+ 1LD**

**$\rightarrow B_C = 5 W / 4 \text{ FLOPs} = 1.25 W / F$**

**WRITE ALLOCATE:**  
**LD + ST  $\text{phi}(i, k, t1)$**

- Modern cache subsystems may further reduce memory traffic



If cache is large enough to hold at least 2 rows (shaded region): Each  $\text{phi}(:, :, t_0)$  is loaded once from main memory and re-used 3 times from cache:

$$\text{phi}(:, :, t_0): 1 \text{ LD} + \text{phi}(:, :, t_1): 1 \text{ ST} + 1 \text{ LD} \\ \rightarrow B_C = 3W / 4F = 0.75W / F$$

If cache is too small to hold one row:  
 $\text{phi}(:, :, t_0): 2 \text{ LD} + \text{phi}(:, :, t_1): 1 \text{ ST} + 1 \text{ LD}$   
 $\rightarrow B_C = 5W / 4F = 1.25W / F$



- **Alternative implementation (“Macho FLOP version”)**

```
do k = 1, kmax
  do i = 1, imax
    phi(i, k, t1) = 0.25 * phi(i+1, k, t0) + 0.25 * phi(i-1, k, t0)
                  + 0.25 * phi(i, k+1, t0) + 0.25 * phi(i, k-1, t0)
  enddo
enddo
```

- **MFlops/sec increases by 7/4 but time to solution remains the same**
- **Better metric (for many iterative stencil schemes):**  
**Lattice Site Updates per Second (LUPs/sec)**

**2D Jacobi example: Compute LUPs/sec metric via**

$$P[LUPs / s] = \frac{it_{\max} \cdot i_{\max} \cdot k_{\max}}{T_{\text{wall}}}$$



- 3D sweep:

```
do k=1,kmax
  do j=1,jmax
    do i=1,imax
      phi(i,j,k,t1) = 1/6. * (phi(i-1,j,k,t0)+phi(i+1,j,k,t0) &
        + phi(i,j-1,k,t0)+phi(i,j+1,k,t0) &
        + phi(i,j,k-1,t0)+phi(i,j,k+1,t0))
    enddo
  enddo
enddo
```

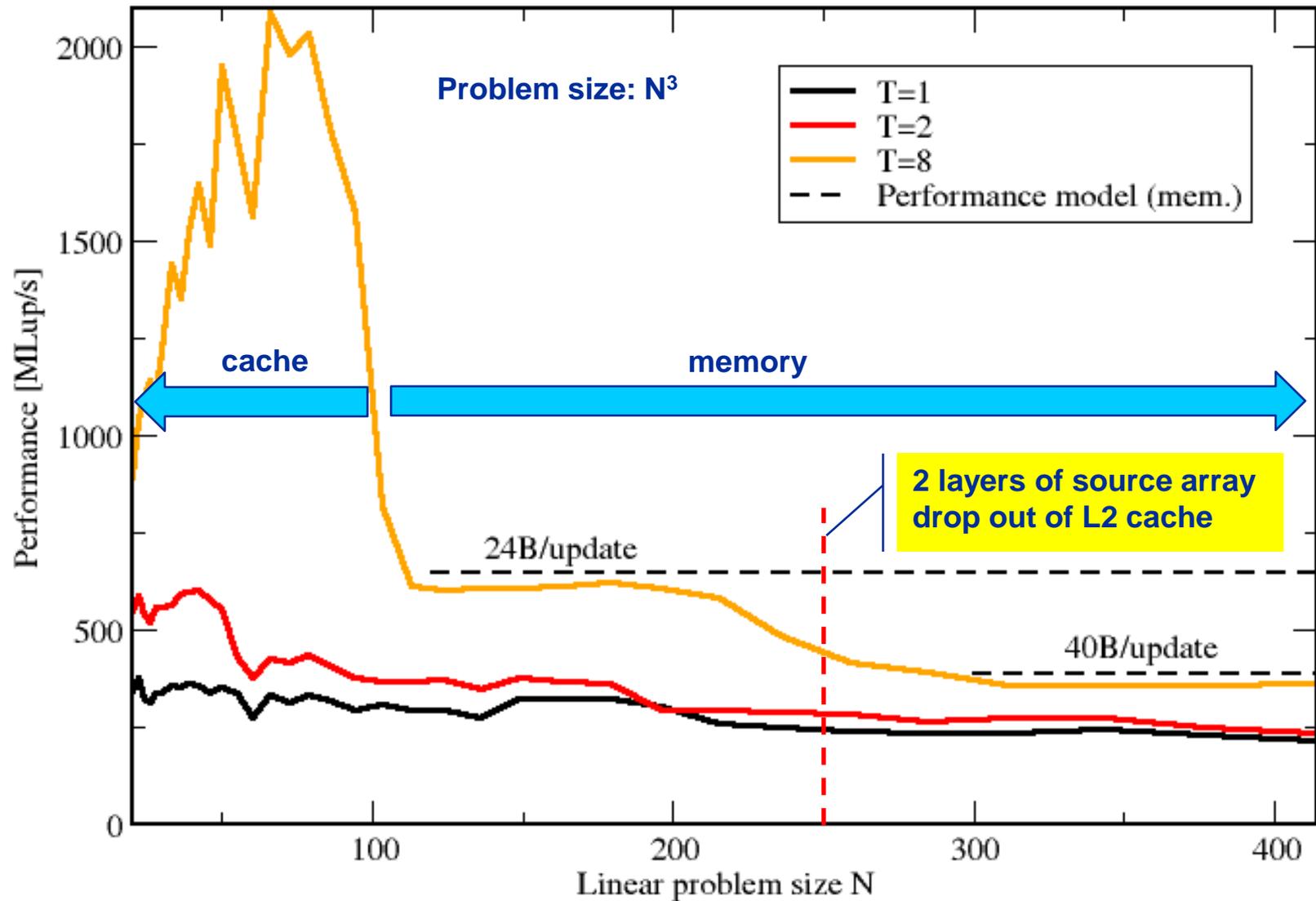
- Best case balance: 1 LD phi(i,j,k+1,t0)  
 1 ST + 1 write allocate phi(i,j,k,t1)  
 6 flops

→  $B_C = 0.5 \text{ W/F (24 bytes/update)}$

- No 2-layer condition but 2 rows fit:  $B_C = 5/6 \text{ W/F (40 bytes/update)}$
- Worst case (2 rows do not fit):  $B_C = 7/6 \text{ W/F (56 bytes/update)}$

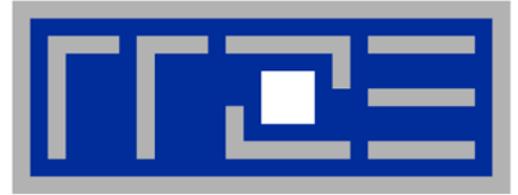
# 3D Jacobi solver

Performance of vanilla code on one Interlagos chip (8 cores)





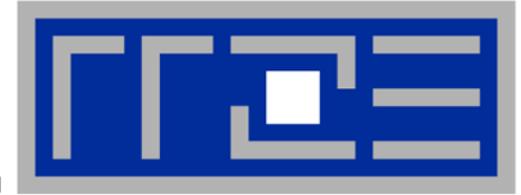
- We have **made sense** of the **memory-bound performance vs. problem size**
  - “Layer conditions” lead to **predictions of code balance**
  - Achievable memory bandwidth is input parameter
  
- **The model works only if the bandwidth is “saturated”**
  - In-cache modeling is more involved
  
- **Optimization == reducing the code balance by code transformations**
  - See below



# **Data access optimizations**

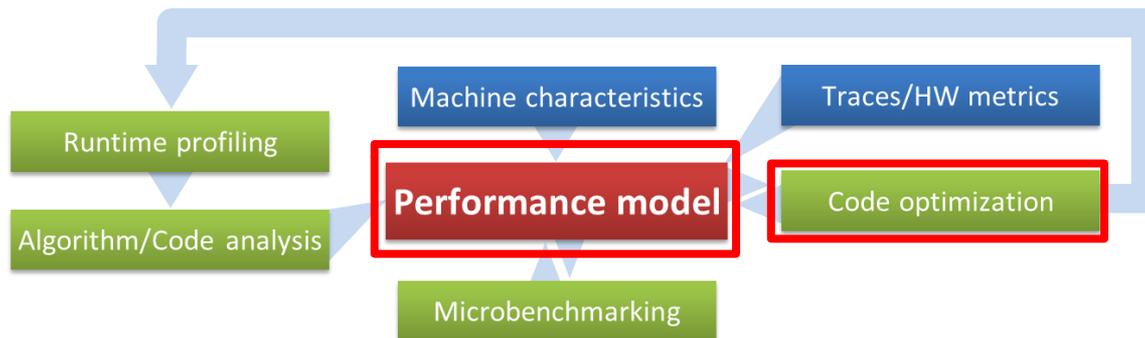
**Case study: Optimizing a Jacobi solver**

**Case study: Erratic RHS access for sparse MVM**

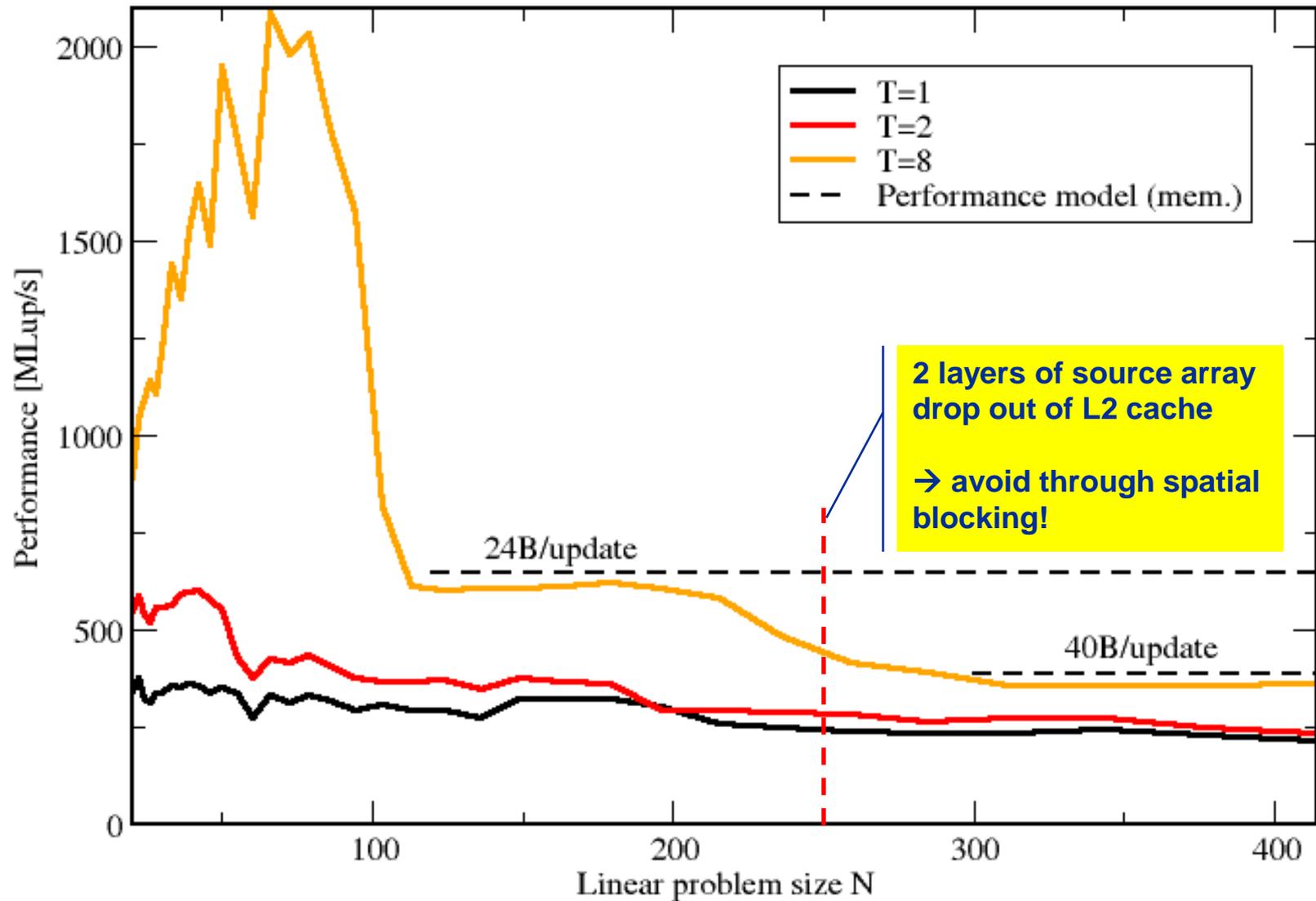


## Case study: 3D Jacobi solver

### Spatial blocking for improved cache re-use



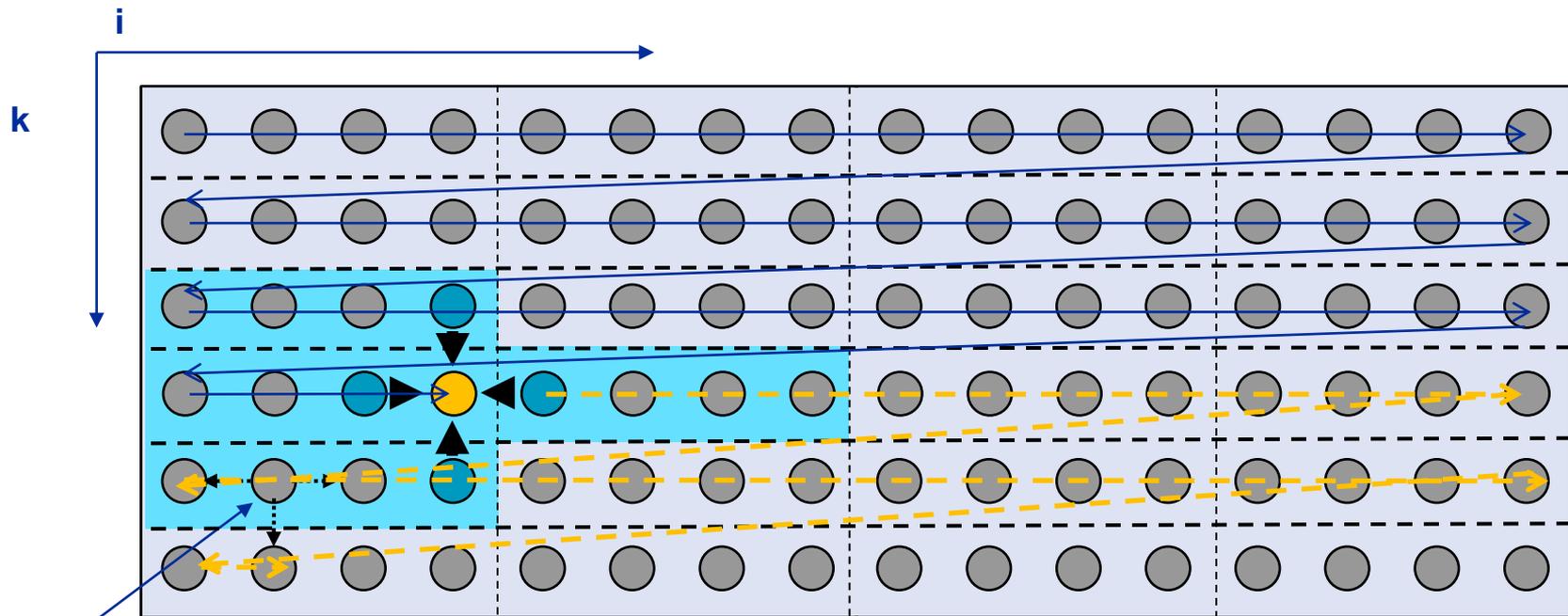
# Remember the 3D Jacobi solver on Interlagos?





## Assumptions:

- cache can hold 32 elements (16 for each array)
- Cache line size is 4 elements
- Perfect eviction strategy for source array

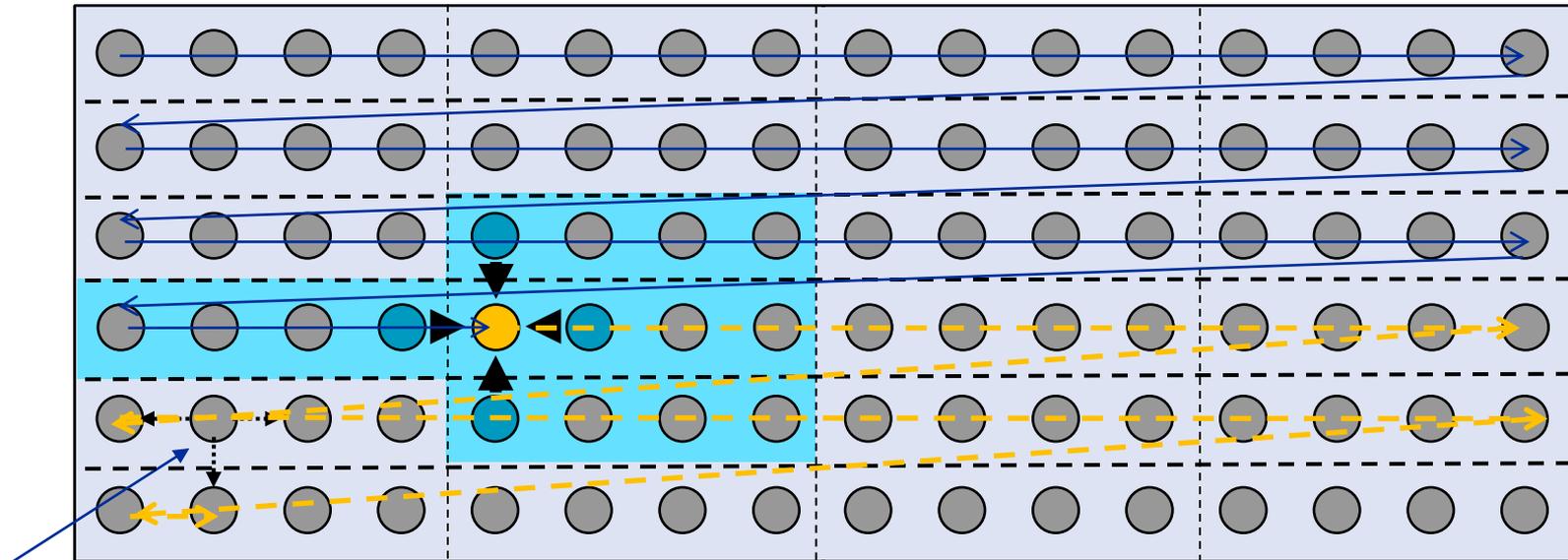


This element is needed for three more updates; but 29 updates happen before this element is used for the last time



## Assumptions:

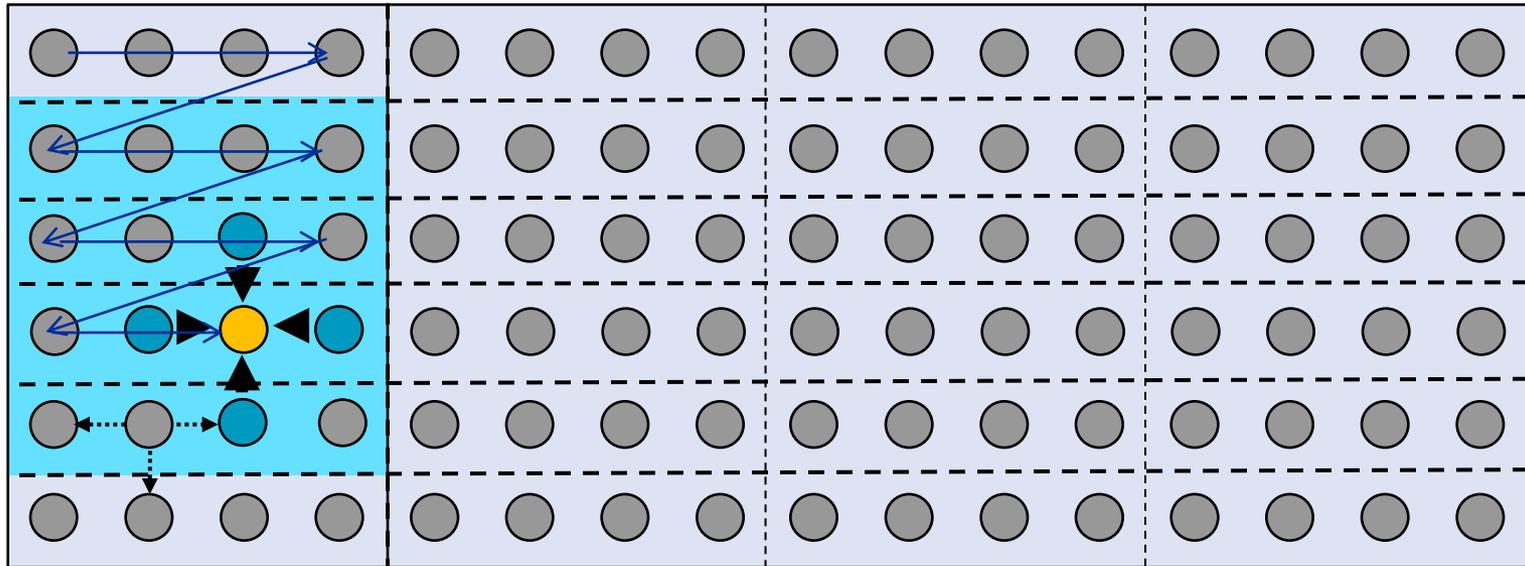
- cache can hold 32 elements (16 for each array)
- Cache line size is 4 elements
- Perfect eviction strategy for source array



**This element is needed for three more updates but has been evicted**

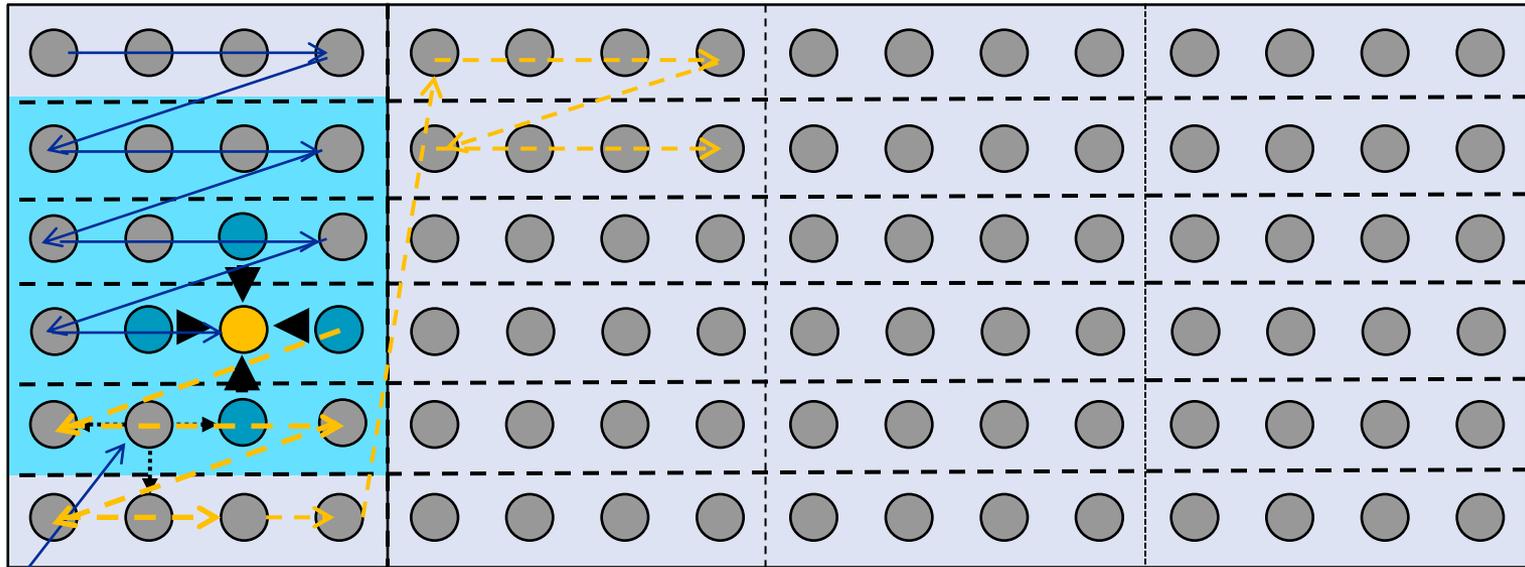


- divide system into blocks
- update block after block
- same performance as if three complete rows of the systems fit into cache





- **Spatial blocking reorders traversal of data to account for the data update rule of the code**
- **Elements stay sufficiently long in cache to be fully reused**
- **Spatial blocking improves temporal locality!**  
(Continuous access in inner loop ensures spatial locality)



**This element remains in cache until it is fully used (only 6 updates happen before last use of this element)**



## Implementation:

```
do ioffset=1,imax,iblock
  do joffset=1,jmax,jblock
    do k=1,kmax
      do j=joffset, min(jmax,joffset+jblock-1)
        do i=ioffset, min(imax,ioffset+iblock-1)
          phi(i,j,k,t1) = ( phi(i-1,j,k,t0)+phi(i+1,j,k,t0)
                        + ... + phi(i,j,k-1,t0)+phi(i,j,k+1,t0) )/6.d0
        enddo
      enddo
    enddo
  enddo
enddo
```

Diagram annotations:

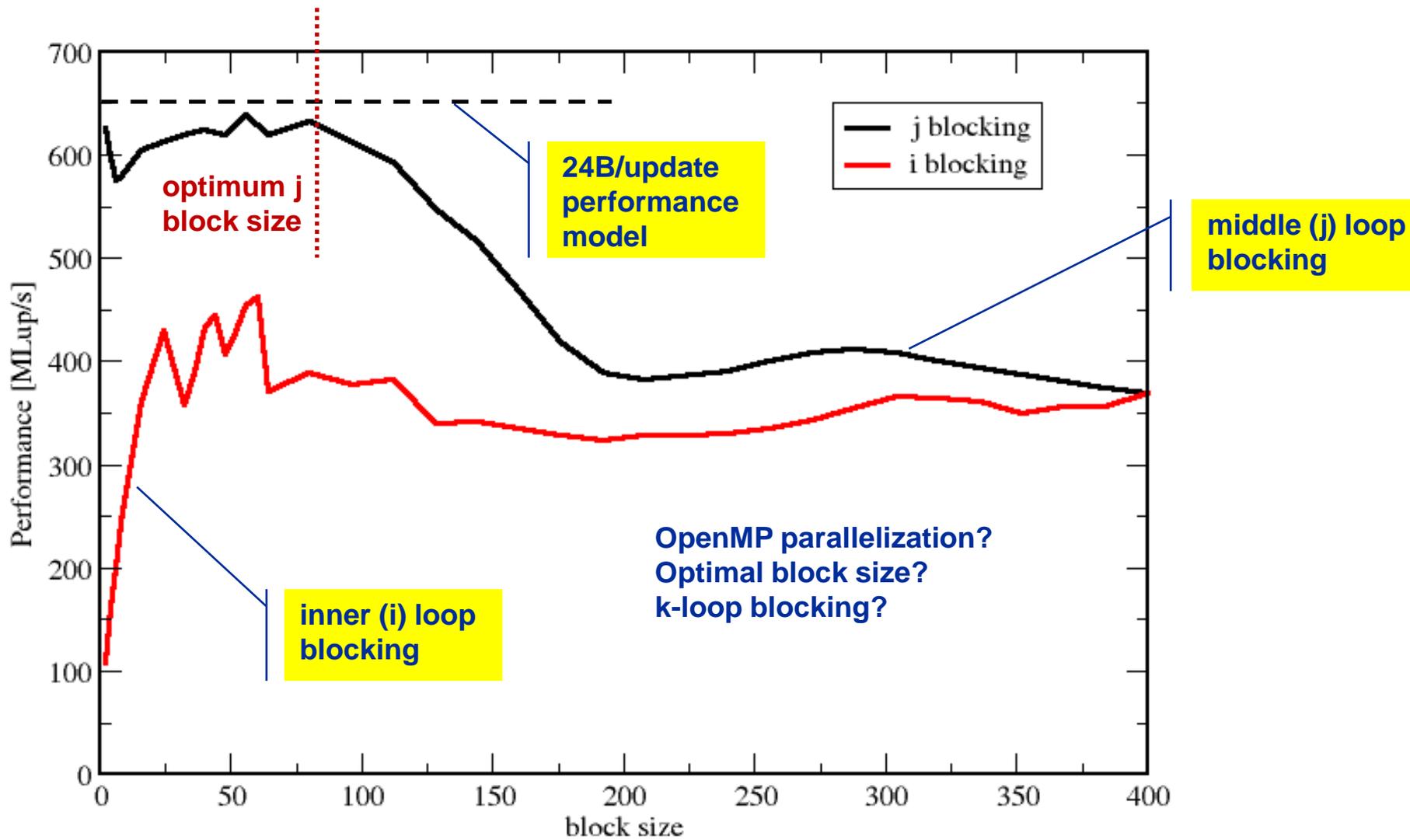
- A yellow box labeled "loop over i-blocks" has a line pointing to the innermost loop: `do i=ioffset, min(imax,ioffset+iblock-1)`.
- A yellow box labeled "loop over j-blocks" has a line pointing to the second loop: `do j=joffset, min(jmax,joffset+jblock-1)`.

## Guidelines:

- Blocking of inner loop levels (traversing continuously through main memory)
- **Blocking sizes** large enough to fulfill “**layer condition**”
- Cache size is a hard limit!
- Blocking loops may have some impact on ccNUMA page placement (see later)

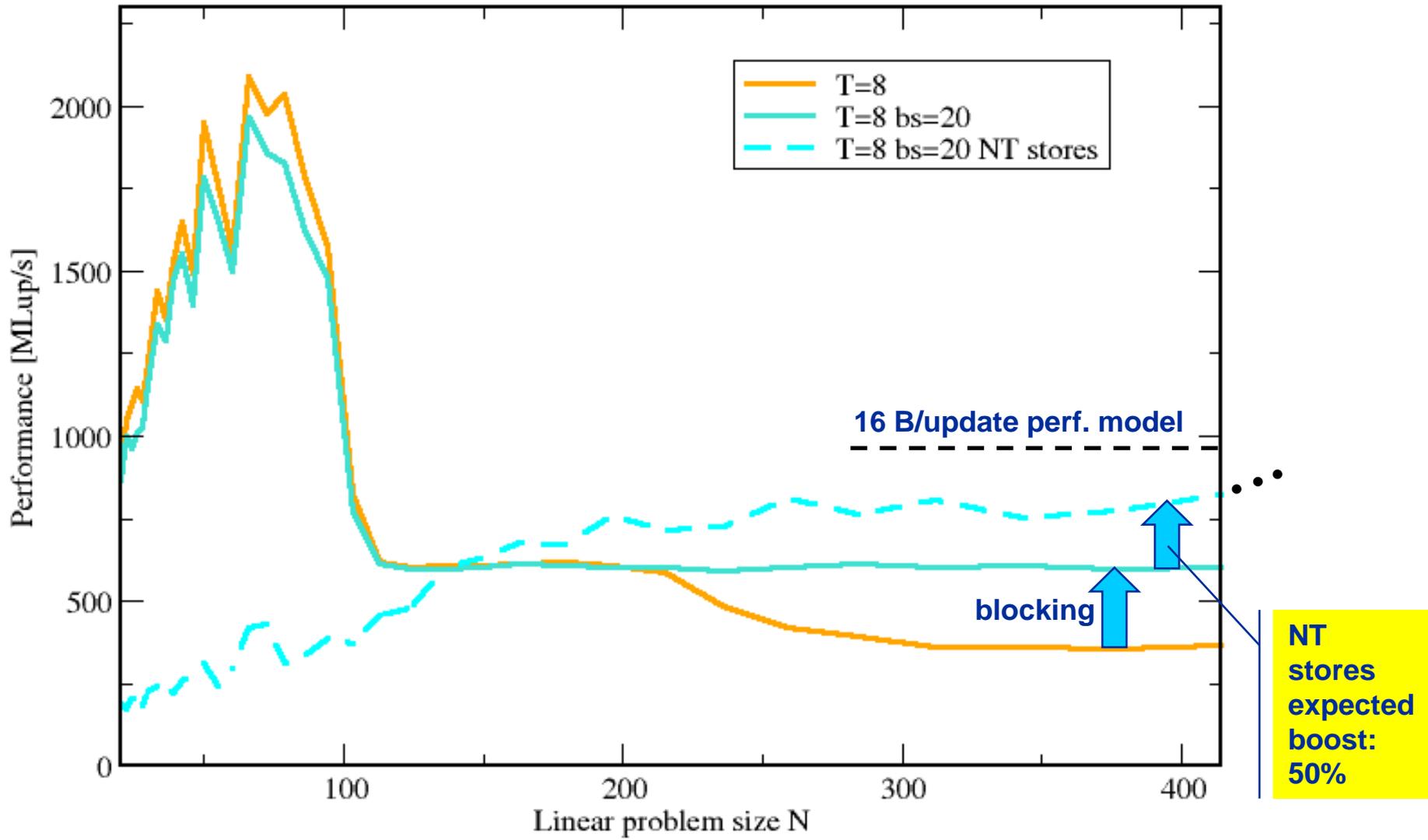
# 3D Jacobi solver (problem size $400^3$ )

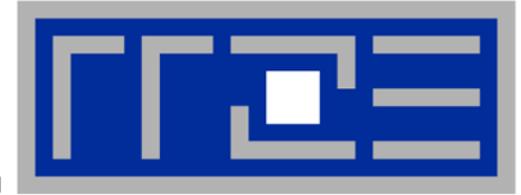
Blocking different loop levels (8 cores Interlagos)



# 3D Jacobi solver

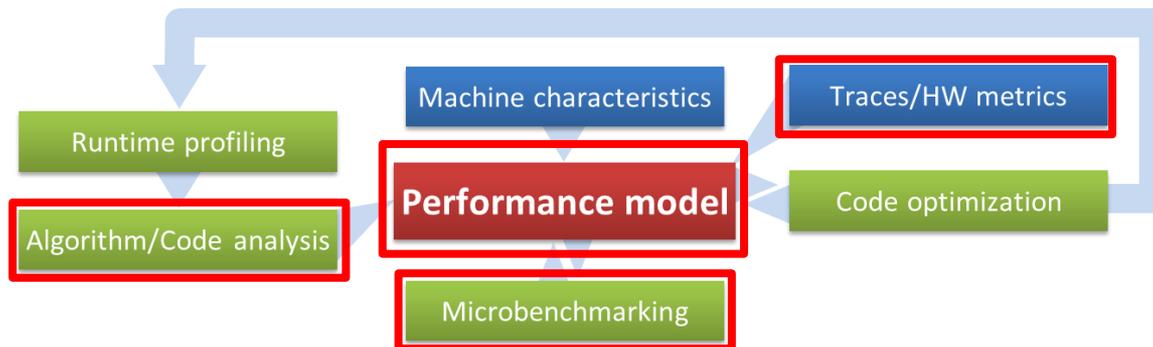
*Spatial blocking + nontemporal stores*





## Case study: Erratic RHS access in sparse MVM

“Modeling” indirect access





- **Sparse MVM in double precision w/ CRS:**

```
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 code balance**
  - $\kappa$  quantifies extra traffic for loading RHS more than once

$$B_{\text{CRS}} = \left( \frac{12 + 24/N_{\text{nzr}} + \kappa}{2} \right) \frac{\text{bytes}}{\text{flop}}$$

$$= \left( 6 + \frac{12}{N_{\text{nzr}}} + \frac{\kappa}{2} \right) \frac{\text{bytes}}{\text{flop}} .$$

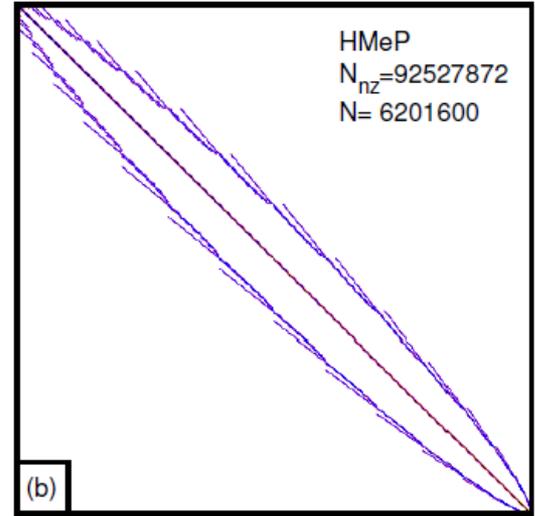
- Naive performance =  $b_s/B_{\text{CRS}}$
- Determine  $\kappa$  by measuring performance and **actual memory bandwidth**

G. Schubert, G. Hager, H. Fehske and G. Wellein: *Parallel sparse matrix-vector multiplication as a test case for hybrid MPI+OpenMP programming*. Workshop on Large-Scale Parallel Processing (LSPP 2011), May 20th, 2011, Anchorage, AK. [DOI:10.1109/IPDPS.2011.332](https://doi.org/10.1109/IPDPS.2011.332), Preprint: [arXiv:1101.0091](https://arxiv.org/abs/1101.0091)



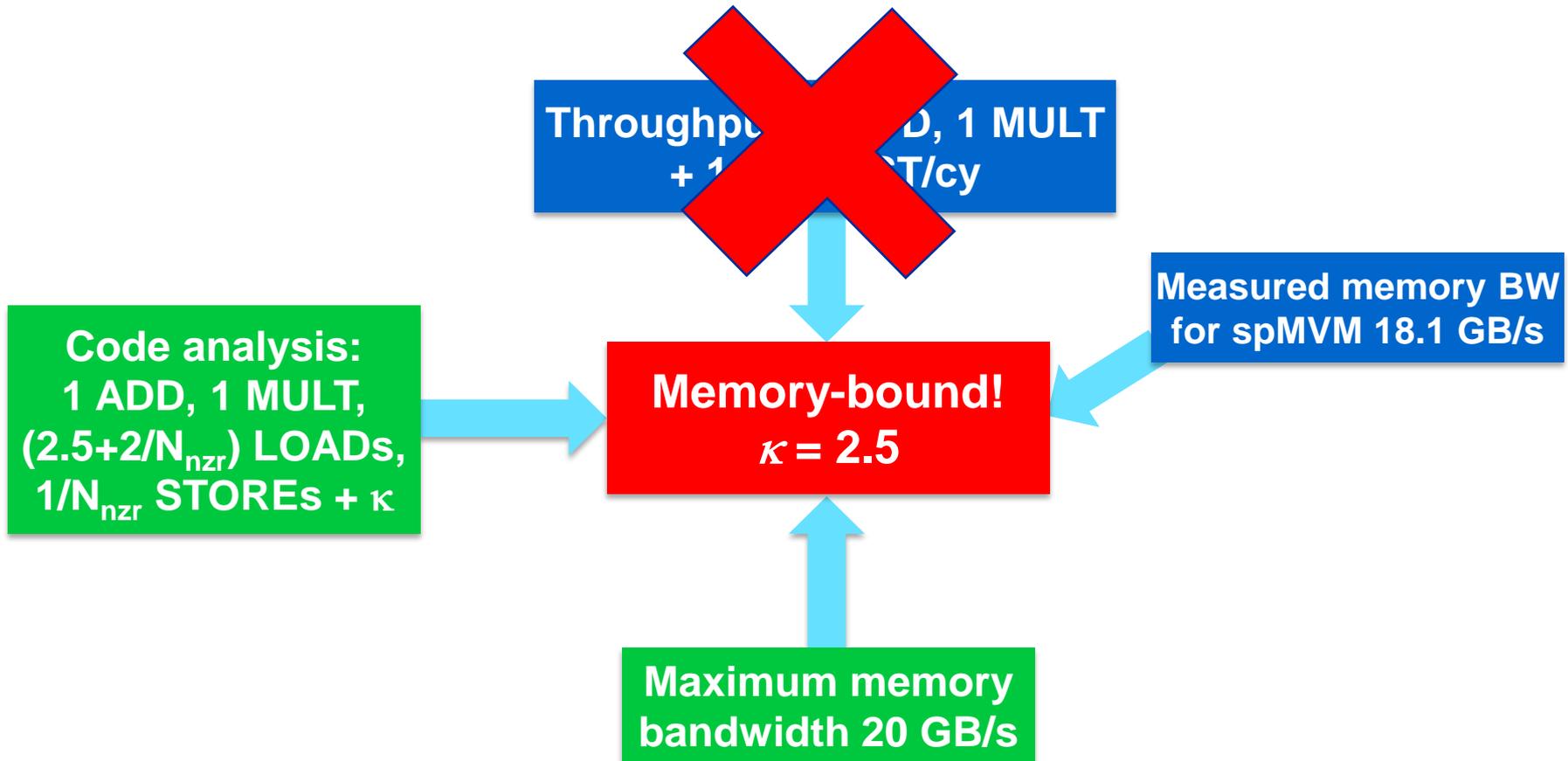
- **Analysis for HMeP matrix on Nehalem EP socket**

- BW used by spMVM kernel = 18.1 GB/s → should get  $\approx 2.66$  Gflop/s  
spMVM performance if  $\kappa = 0$
- Measured spMVM performance = 2.25 Gflop/s
- Solve  $2.25 \text{ Gflop/s} = b_S/B_{\text{CRS}}$  for  $\kappa \approx 2.5$ 
  - 37.5 extra bytes per row
  - RHS is loaded 6 times from memory
  - about 33% of BW goes into RHS



- **Conclusion:** Even if the roofline/bandwidth model does not work 100%, we can still learn something from the deviations
  - Optimization? Perhaps you can reorganize the matrix

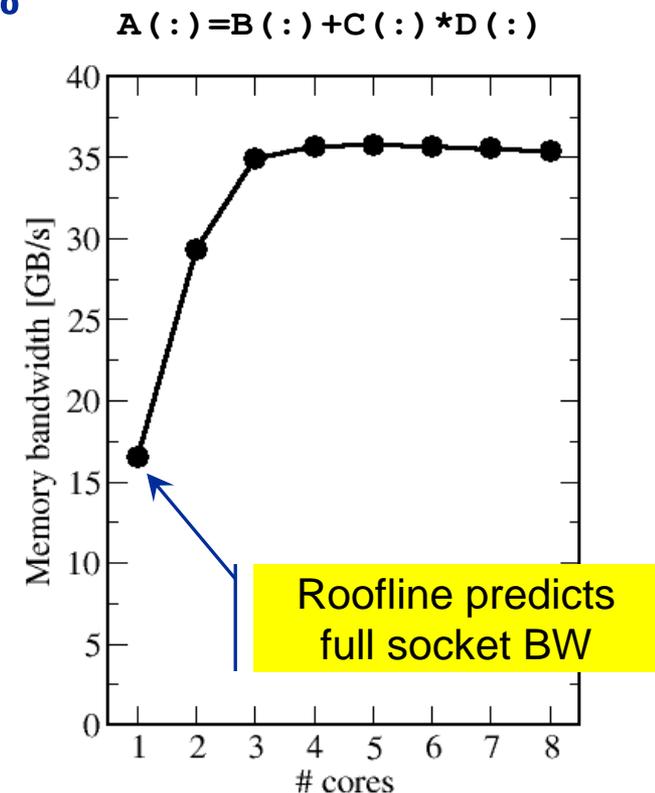
... on the example of spMVM with HMeP matrix





- Assumes one of two bottlenecks
  - In-core execution
  - Bandwidth of a single hierarchy level
- Latency effects are not modeled → pure data streaming assumed
- Data transfer and in-core time overlap 100%
- In-core execution is sometimes hard to model
- Saturation effects in multicore chips are not explained**
  - ECM model gives more insight

G. Hager, J. Treibig, J. Habich and G. Wellein: Exploring performance and power properties of modern multicore chips via simple machine models. Submitted. Preprint: [arXiv:1208.2908](https://arxiv.org/abs/1208.2908)

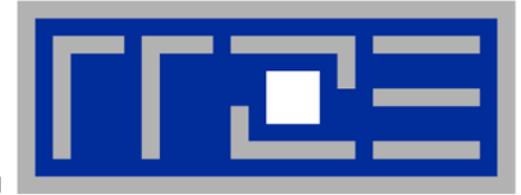




- There is no substitute for knowing what's going on between your code and the hardware
- **Make sense of performance behavior** through sensible application of performance models
  - However, there is no “golden formula” to do it all for you automagically
  - If the model does not work properly, you learn something new
- **Model inputs:**
  - Code analysis/inspection
  - Hardware counter data
  - Microbenchmark analysis
  - Architectural features
- **Simple models work best; do not try to make it more complex than necessary**



- **Motivation**
- **Performance Engineering**
  - Performance modeling
  - The Performance Engineering process
- **Modern architectures**
  - Multicore
  - Accelerators
  - Programming models
- **Data access**
- **Performance properties of multicore systems**
  - Saturation
  - Scalability
  - Synchronization
- **Case study: OpenMP-parallel sparse MVM**
- **Basic performance modeling: Roofline**
  - Theory
  - Case study: 3D Jacobi solver and guided optimizations
  - Modeling erratic access
- **Some more architecture**
  - **Simultaneous multithreading (SMT)**
  - **ccNUMA**
- **Putting cores to good use**
  - Asynchronous communication in spMVM
- **A simple power model for multicore**
  - Power-efficient code execution
- **Conclusions**



# **Boosting core efficiency: Simultaneous multithreading (SMT)**

**Principles and performance impact**

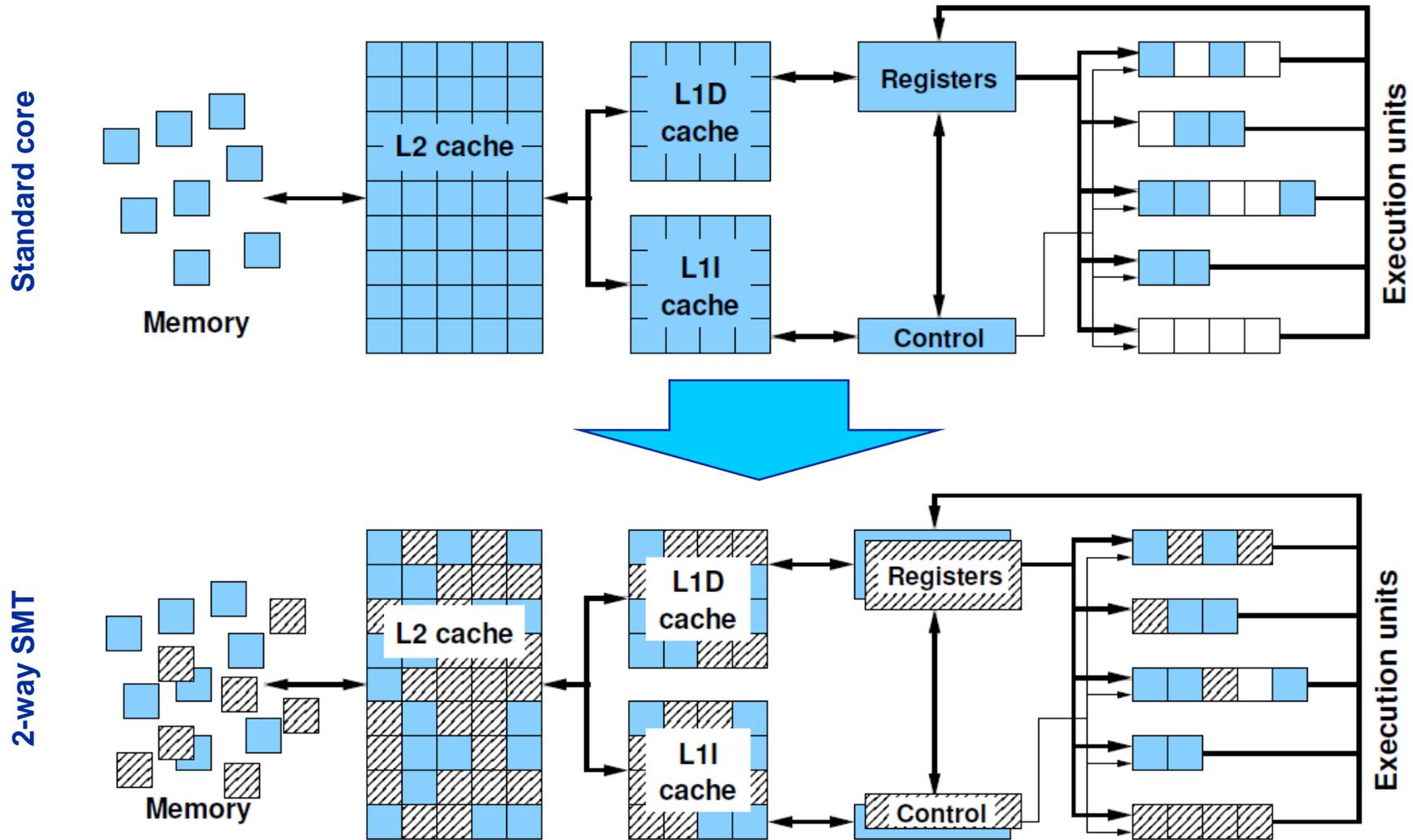
**SMT vs. independent instruction streams**

**Facts and fiction**

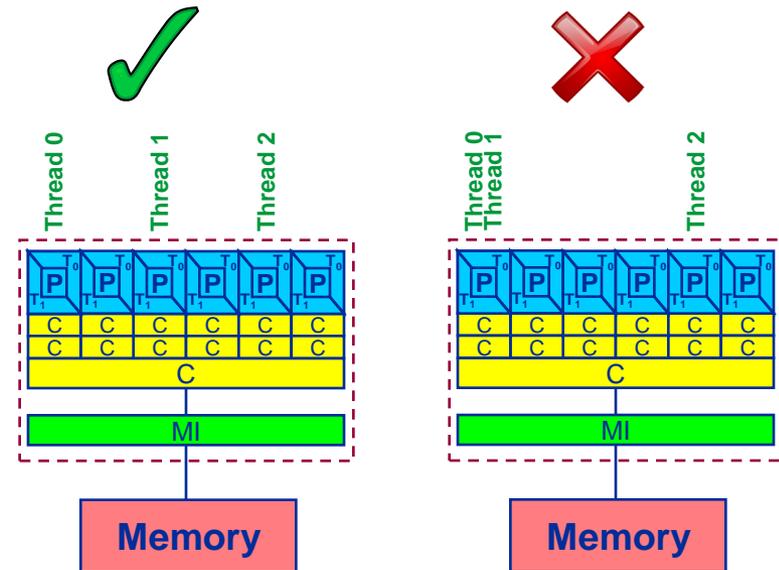
# SMT Makes a single physical core appear as two or more “logical” cores → multiple threads/processes run concurrently



- SMT principle (2-way example):



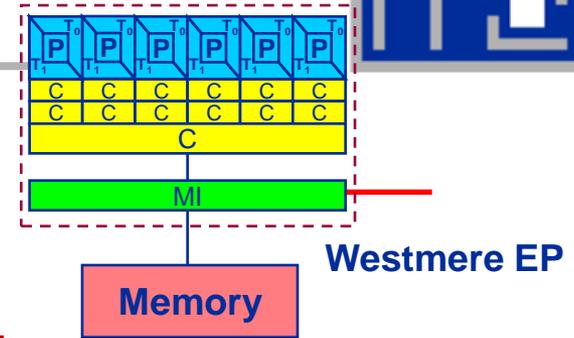
- **SMT is primarily suited for increasing processor throughput**
  - With multiple threads/processes running concurrently
- **Scientific codes tend to utilize chip resources quite well**
  - Standard optimizations (loop fusion, blocking, ...)
  - High data and instruction-level parallelism
  - Exceptions do exist
- **SMT is an important topology issue**
  - SMT threads share almost all core resources
    - Pipelines, caches, data paths
  - **Affinity matters!**
  - If SMT is not needed
    - pin threads to physical cores
    - or switch it off via BIOS etc.



# 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
```

Dependency → pipeline stalls until previous MULT is over

## Thread 1:

```
do i=1,N
  b(i) = func(i)*d
enddo
```

Unrelated work in other thread can fill the pipeline bubbles

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

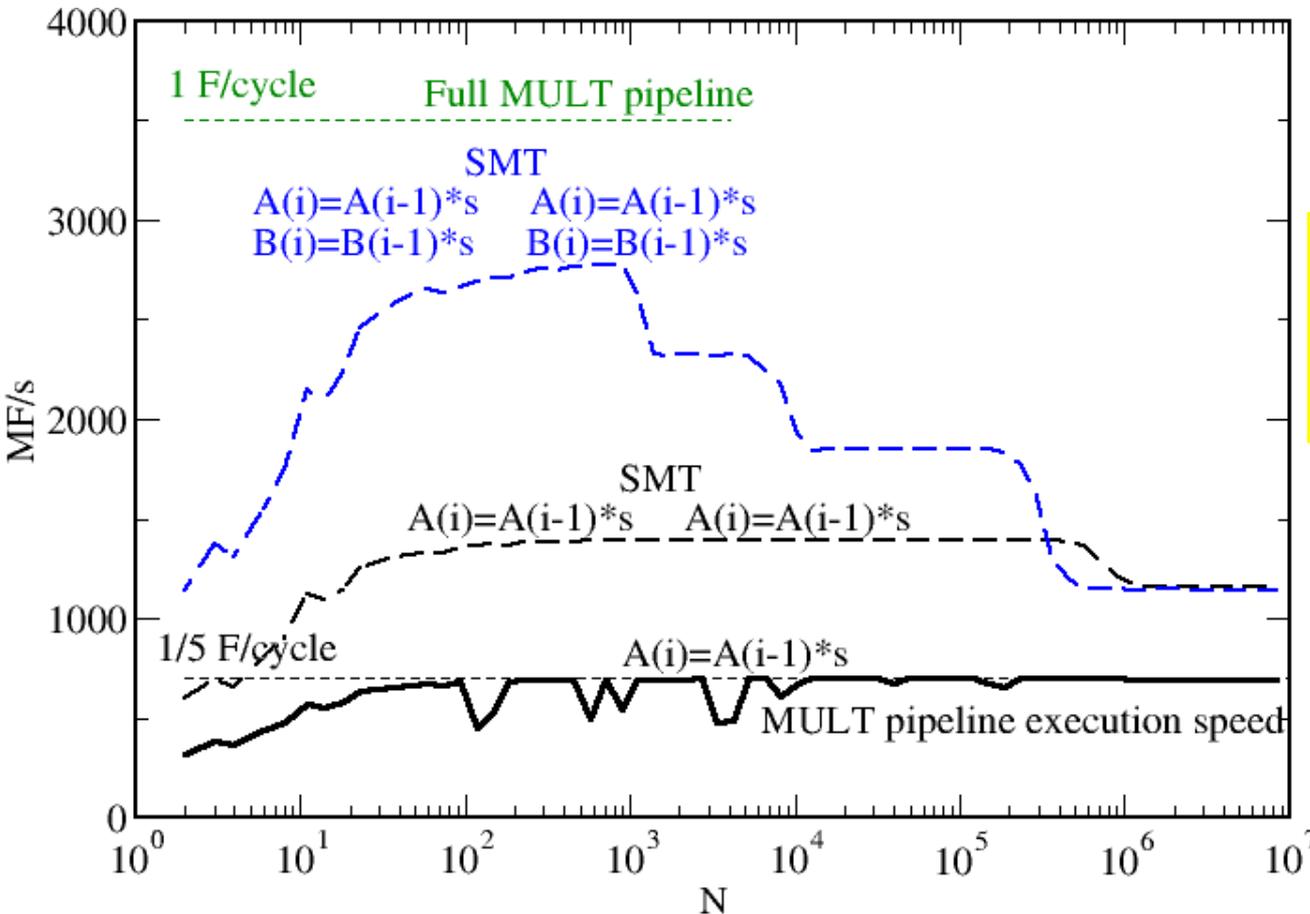
```
do i=1,N
  a(i) = a(i-1)*c
  b(i) = func(i)*d
enddo
```

# Simultaneous recursive updates with SMT



Intel Sandy Bridge (desktop) 4-core; 3.5 GHz; SMT

**MULT Pipeline depth: 5 stages** → 1 F / 5 cycles for recursive update



Fill bubbles via:

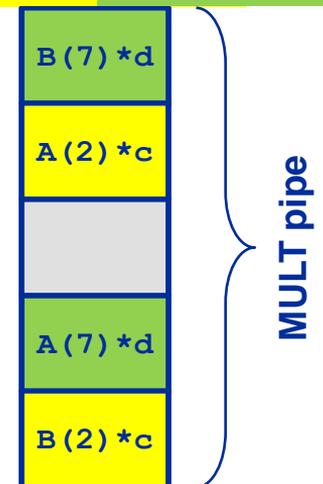
- SMT
- Multiple streams

Thread 0:

```
do i=1,N
A(i)=A(i-1)*c
B(i)=B(i-1)*d
enddo
```

Thread 1:

```
do i=1,N
A(i)=A(i-1)*c
B(i)=B(i-1)*d
enddo
```

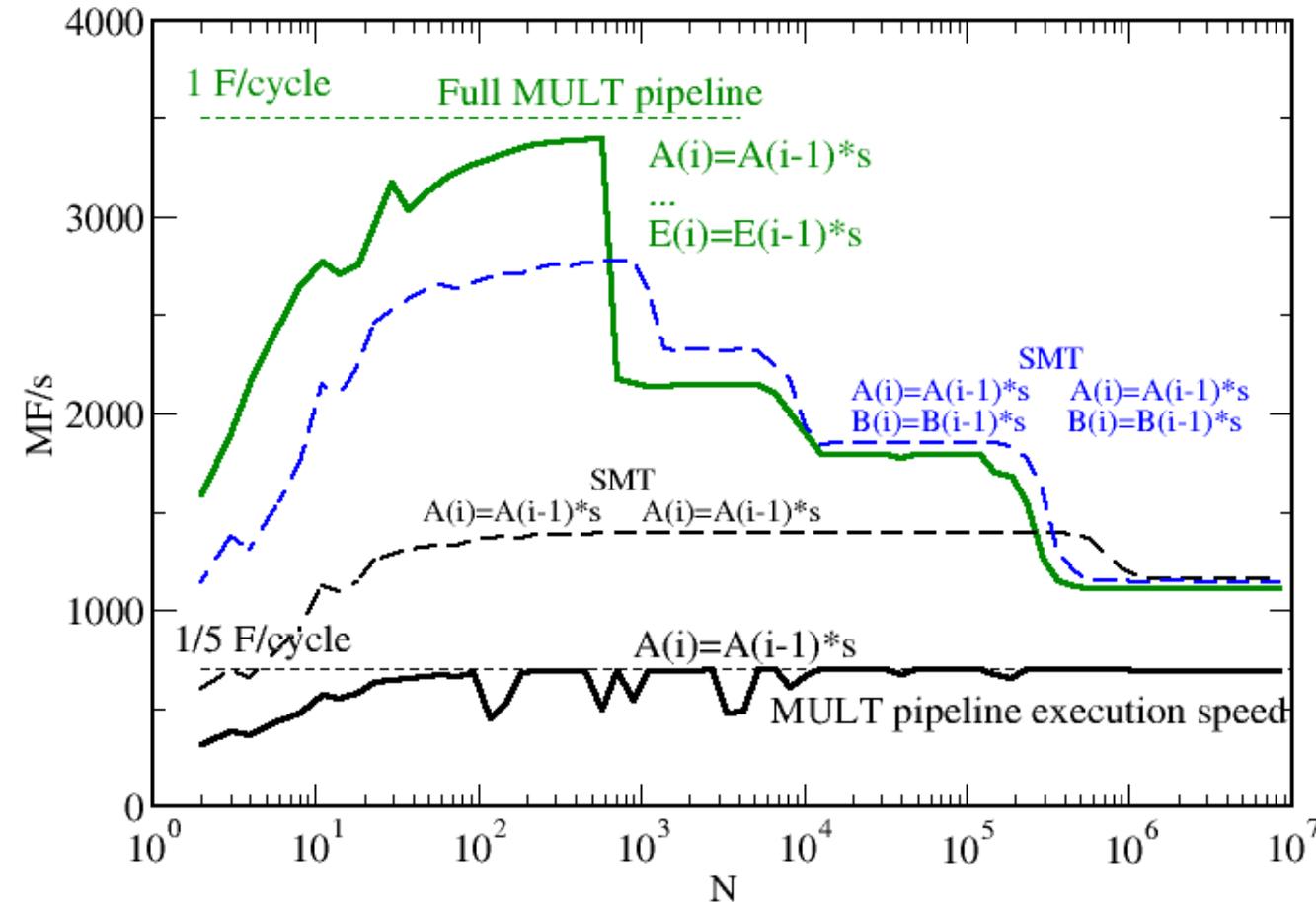


# Simultaneous recursive updates with SMT



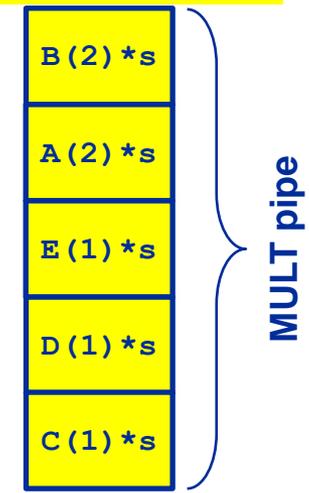
Intel Sandy Bridge (desktop) 4-core; 3.5 GHz; SMT

**MULT Pipeline depth: 5 stages** → 1 F / 5 cycles for recursive update



```

Thread 0:
do i=1,N
  A(i)=A(i-1)*s
  B(i)=B(i-1)*s
  C(i)=C(i-1)*s
  D(i)=D(i-1)*s
  E(i)=E(i-1)*s
enddo
    
```



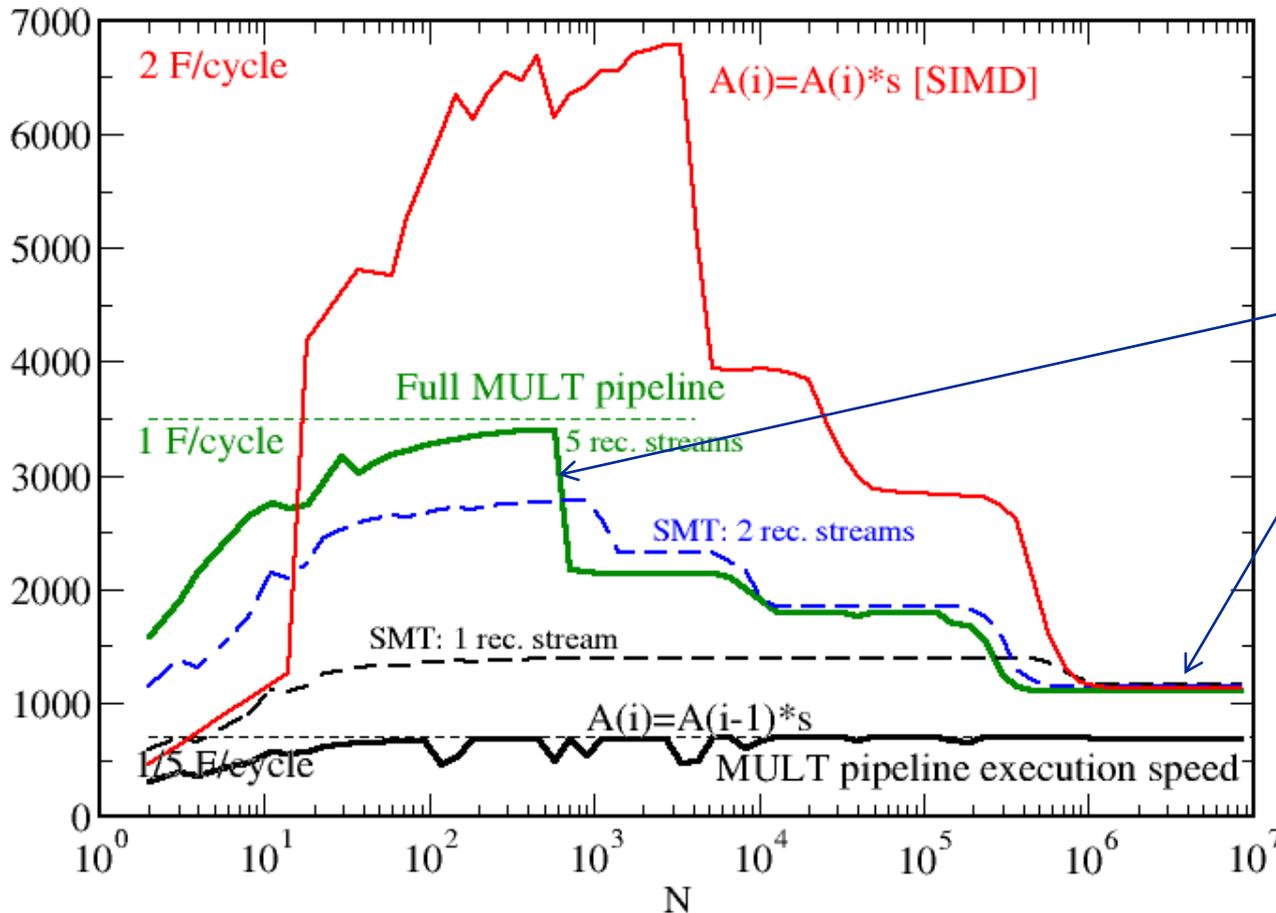
**5 independent updates on a single thread do the same job!**

# Simultaneous recursive updates with SMT



Intel Sandy Bridge (desktop) 4-core; 3.5 GHz; SMT

Pure update benchmark can be **vectorized** → **2 F / cycle (store limited)**



## Recursive update:

- SMT can fill pipeline bubbles
- A single thread can do so as well
- Bandwidth does not increase through SMT
- **SMT can not replace SIMD!**

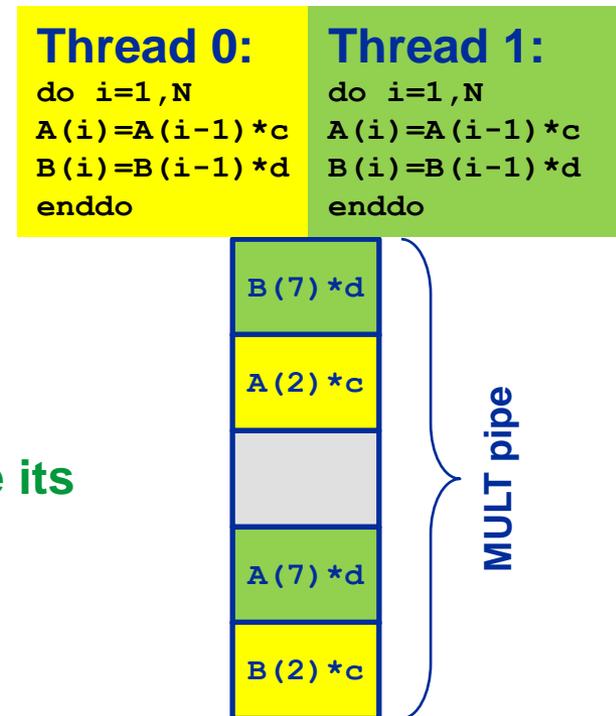
# SMT myths: Facts and fiction (1)



- **Myth: “If the code is compute-bound, then the functional units should be saturated and SMT should show no improvement.”**

- **Truth**

1. A compute-bound loop does not necessarily saturate the pipelines; dependencies can cause a lot of bubbles, which may be filled by SMT threads.
2. If a pipeline is already full, SMT will not improve its utilization



# SMT myths: Facts and fiction (2)



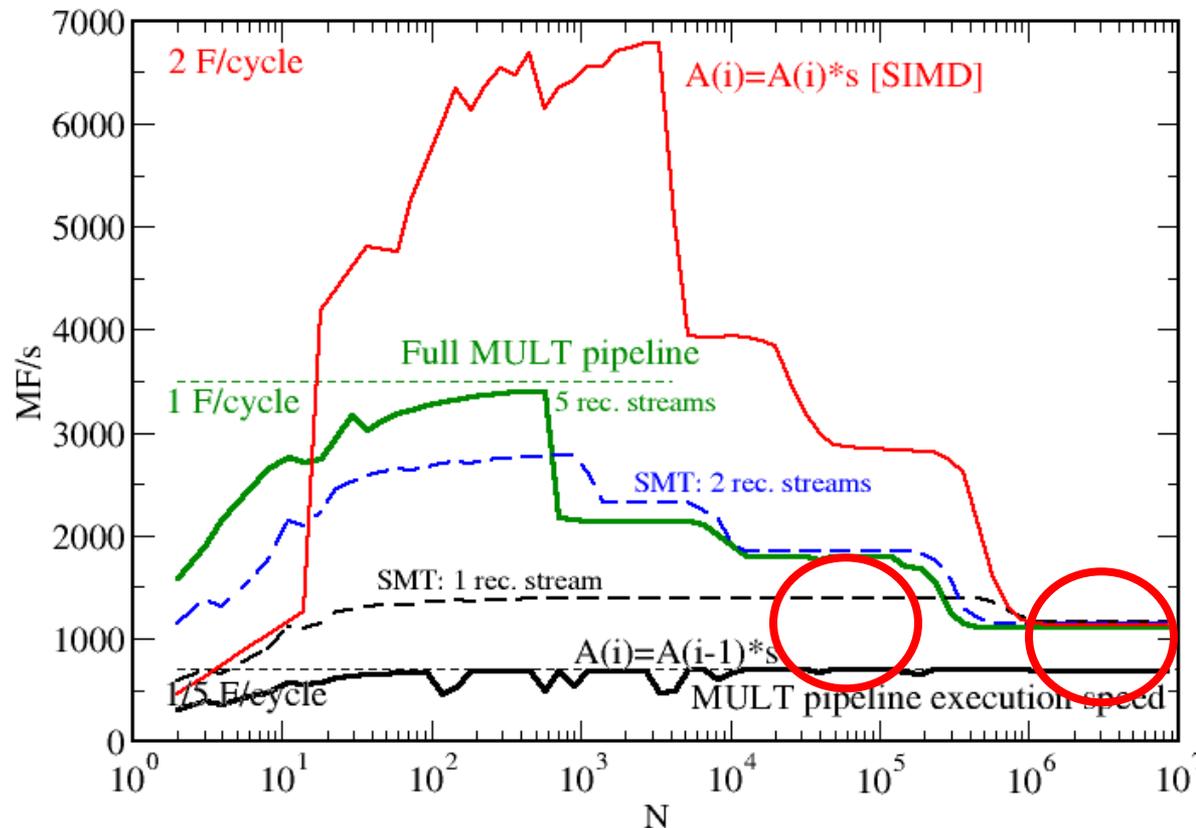
- Myth: “If the code is memory-bound, SMT should help because it can fill the bubbles left by waiting for data from memory.”

- Truth:

- If the maximum memory bandwidth is already reached, SMT will not help since the relevant resource (bandwidth) is exhausted.

- If the relevant bottleneck is not exhausted, SMT may help since it can fill bubbles in the LOAD pipeline.

This applies also to other “relevant bottlenecks!”

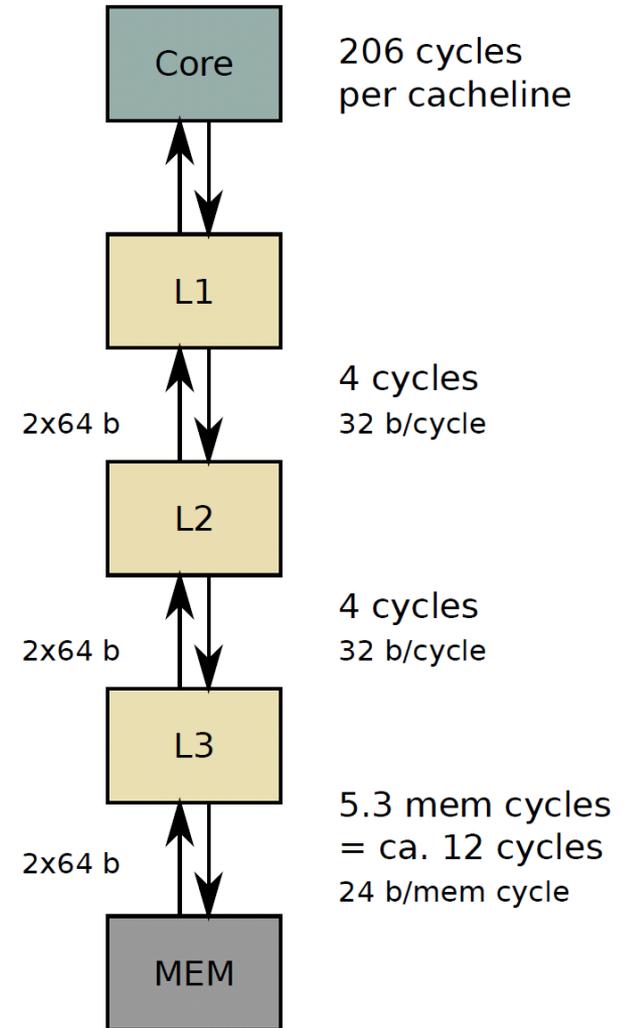


# SMT myths: Facts and fiction (3)



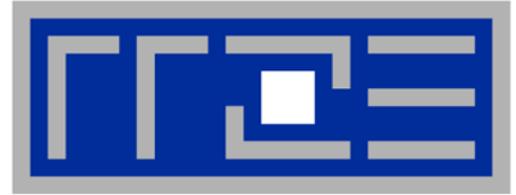
- **Myth:** “SMT can help bridge the latency to memory (more outstanding references).”
- **Truth:** Outstanding references may or may not be bound to SMT threads; they may be a resource of the memory interface and shared by all threads. The benefit of SMT with memory-bound code is usually due to better utilization of the pipelines so that less time gets “wasted” in the cache hierarchy.

See also the “**ECM Performance Model**” later on.





Functional parallelization	 
FP-only parallel loop code	 
Frequent thread synchronization	
Code sensitive to cache size	
Strongly memory-bound code	
Independent pipeline-unfriendly instruction streams	



## **Beyond the chip boundary: Efficient parallel programming on ccNUMA nodes**

**Performance characteristics of ccNUMA nodes**

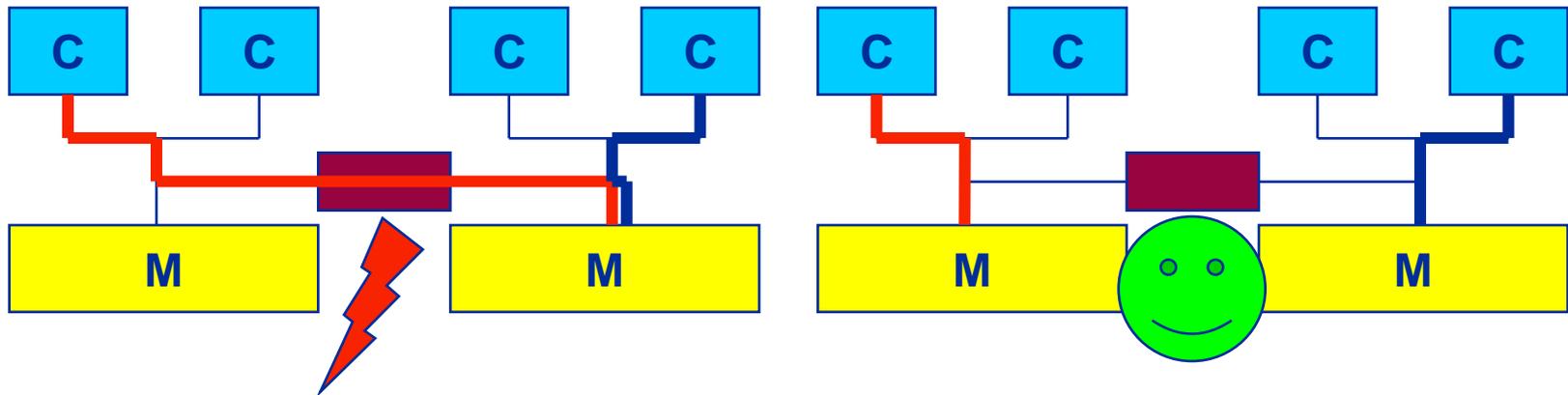
**First touch placement policy**

**ccNUMA locality and erratic access**



## ■ 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)

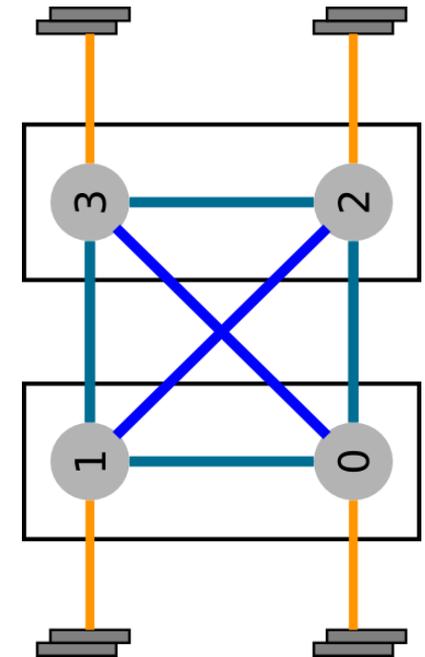
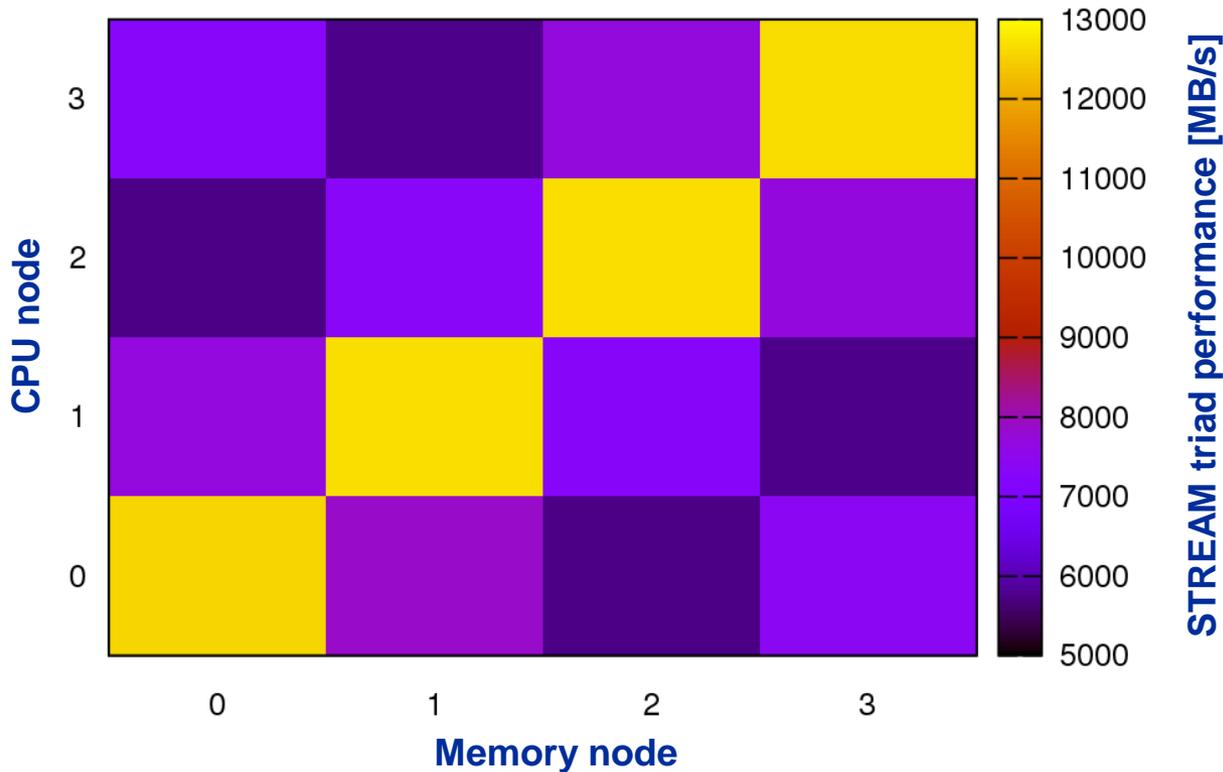
# Cray XE6 Interlagos node

4 chips, two sockets, 8 threads per ccNUMA domain



- **ccNUMA map: Bandwidth penalties for remote access**

- Run 8 threads per ccNUMA domain (1 chip)
- Place memory in different domain → 4x4 combinations
- STREAM triad benchmark using nontemporal stores





- **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:**

```
env OMP_NUM_THREADS=2 numactl --membind=0 --cpunodebind=1 ./stream
```

```
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?**



- "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

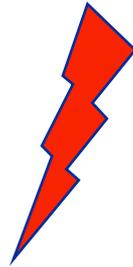
- **It is sufficient to touch a single item to map the entire page**



- 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
```

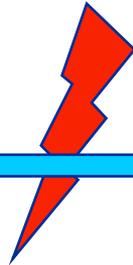




- Sometimes initialization is not so obvious: I/O cannot be easily parallelized, so “localize” arrays before I/O

```
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
```





- **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)
  - Presupposes that all **`worksharing loops`** with the **`same loop length`** have the **`same thread-chunk mapping`**
  - 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
- **`std::vector` in C++ is initialized serially by default**
  - **`STL allocators`** provide an elegant solution



- **Speaking of C++: 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)
```



- 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
  - But there may also be a general problem in your code...
- Try running with `numactl --interleave ...`
  - If performance goes up → ccNUMA problem!
- Consider using performance counters
  - **LIKWID-perfctr** can be used to measure nonlocal memory accesses
  - Example for Intel Nehalem (Core i7):

```
env OMP_NUM_THREADS=8 likwid-perfctr -g MEM -C N:0-7 ./a.out
```

# Using performance counters for diagnosing bad ccNUMA access locality



## Intel Nehalem EP node:

Uncore events only counted once per socket

Event	core 0	core 1	core 2	core 3	core 4	core 5
INSTR_RETIRED_ANY	5.20725e+08	5.24793e+08	5.21547e+08	5.23717e+08	5.28269e+08	5.29083e+08
CPU_CLK_UNHALTED_CORE	1.90447e+09	1.90599e+09	1.90619e+09	1.90673e+09	1.90583e+09	1.90746e+09
UNC_QMC_NORMAL_READS_ANY	8.17606e+07	0	0	0	8.07797e+07	0
UNC_QMC_WRITES_FULL_ANY	5.53837e+07	0	0	0	5.51052e+07	0
UNC_QHL_REQUESTS_REMOTE_READS	6.84504e+07	0	0	0	6.8107e+07	0
UNC_QHL_REQUESTS_LOCAL_READS	6.82751e+07	0	0	0	6.76274e+07	0

RDTSC timing: 0.827196 s

Metric	core 0	core 1	core 2	core 3	core 4	core 5	core 6	core 7
Runtime [s]	0.714167	0.714733	0.71481	0.715013	0.714673	0.715286	0.71486	0.71515
CPI	3.65735	3.63188	3.65488	3.64076	3.60768	3.60521	3.59613	3.60184
Memory bandwidth [MBytes/s]	10610.8	0	0	0	10513.4	0	0	0
Remote Read BW [MBytes/s]	5296	0	0	0	5269.43	0	0	0

Half of read BW comes from other socket!



- Even if all placement rules have been carefully observed, you may still see nonlocal memory traffic. Reasons?
  - Program has **erratic access patterns** → 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
```

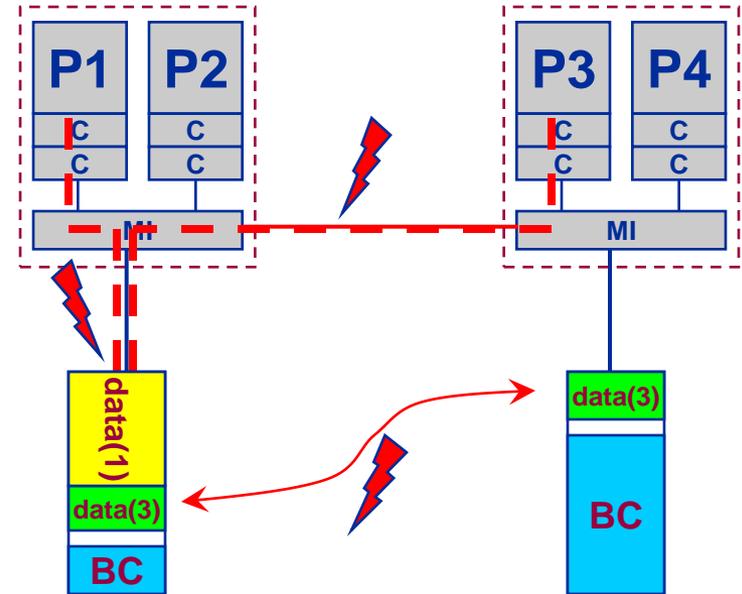
```
top - 14:18:25 up 92 days,  6:07,  2 users,  load average: 0.00, 0.02, 0.00  
Mem:   4065564k total, 1149400k used, 2716164k free,   43388k buffers  
Swap:  2104504k total,   2656k used, 2101848k free, 1038412k cached
```

A blue arrow originates from the text 'node 0 free: 906 MB' in the numactl output and points to the '1038412k cached' value in the top output, illustrating that the free memory on node 0 is being used as a buffer cache.



- **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



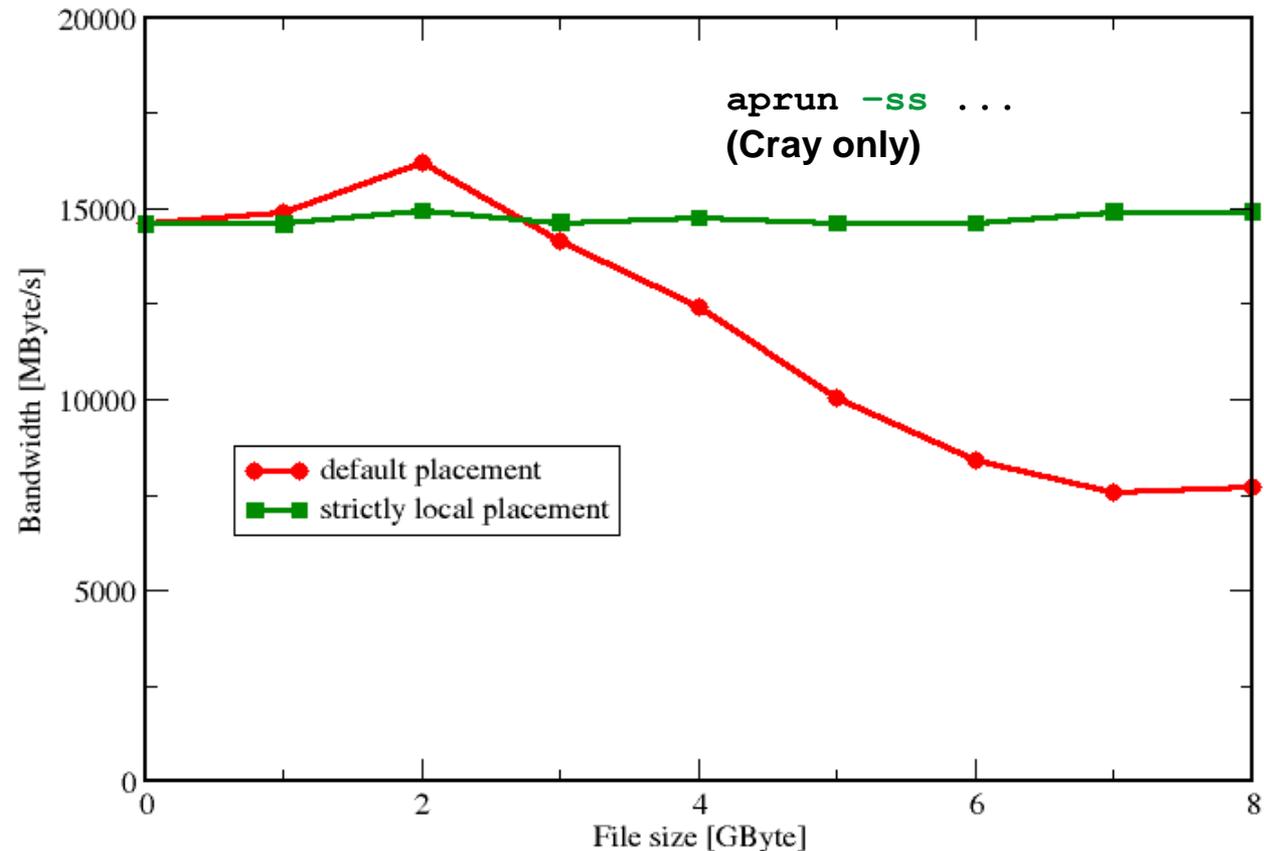
## Real-world example: ccNUMA and the Linux buffer cache

### 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!**





- Sometimes access patterns are just not nicely grouped into contiguous chunks:

```
double precision :: r, a(M)
!$OMP parallel do private(r)
do i=1,N
  call RANDOM_NUMBER(r)
  ind = int(r * M) + 1
  res(i) = res(i) + a(ind)
enddo
!OMP end parallel do
```

- Or you have to use tasking/dynamic scheduling:

```
!$OMP parallel
!$OMP single
do i=1,N
  call RANDOM_NUMBER(r)
  if(r.le.0.5d0) then
!$OMP task
    call do_work_with(p(i))
!$OMP end task
  endif
enddo
!$OMP end single
!$OMP end parallel
```

- In both cases page placement cannot easily be fixed for perfect parallel access



- **Worth a try: Interleave memory across ccNUMA domains to get at least some parallel access**

1. Explicit placement:

```
!$OMP parallel do schedule(static,512)  
do i=1,M  
  a(i) = ...  
enddo  
!$OMP end parallel do
```

Observe page alignment of array to get proper placement!

2. Using global control via `numactl`:

```
numactl --interleave=0-3 ./a.out
```

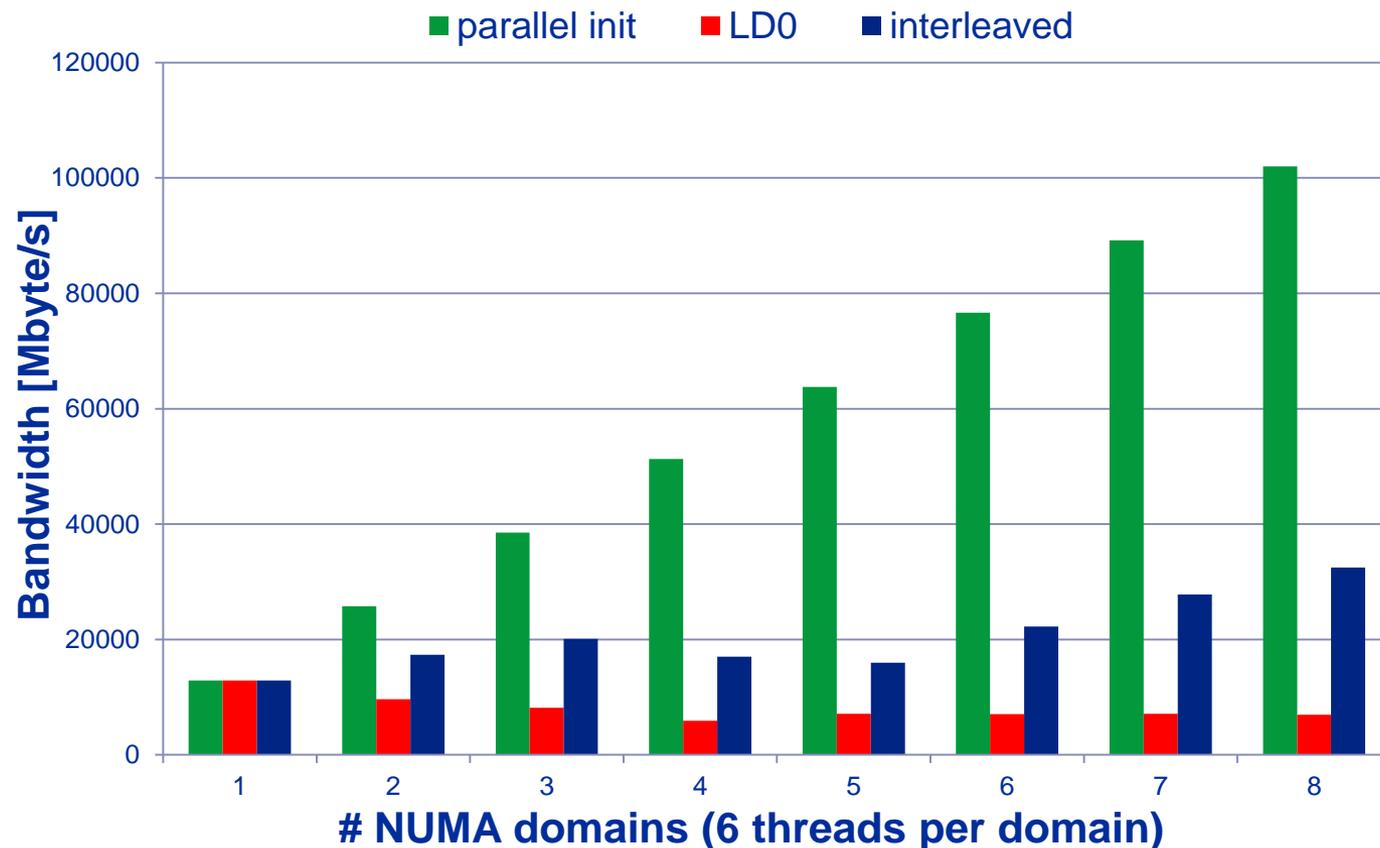
This is for **all** memory, not just the problematic arrays!

- **Fine-grained program-controlled placement via `libnuma` (Linux) using, e.g., `numa_alloc_interleaved_subset()`, `numa_alloc_interleaved()` and others**

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



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

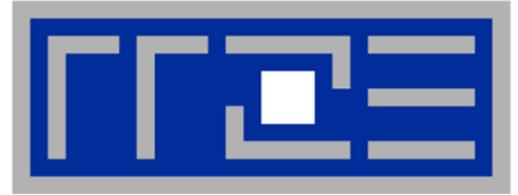




- ccNUMA is present on **all standard cluster architectures**
- With **pure MPI (and proper affinity control)** you **should be fine**
  - However, watch out for buffer cache
- With **threading**, you may be fine with **one process per ccNUMA domain**
- **Thread groups spanning more than one domain may cause problems**
  - Employ **first touch** placement (“**Golden Rule**”)
  - Experiment with round-robin placement
- **If access patterns are totally erratic, round-robin may be your only choice**
  - But there are advanced solutions (“locality queues”)

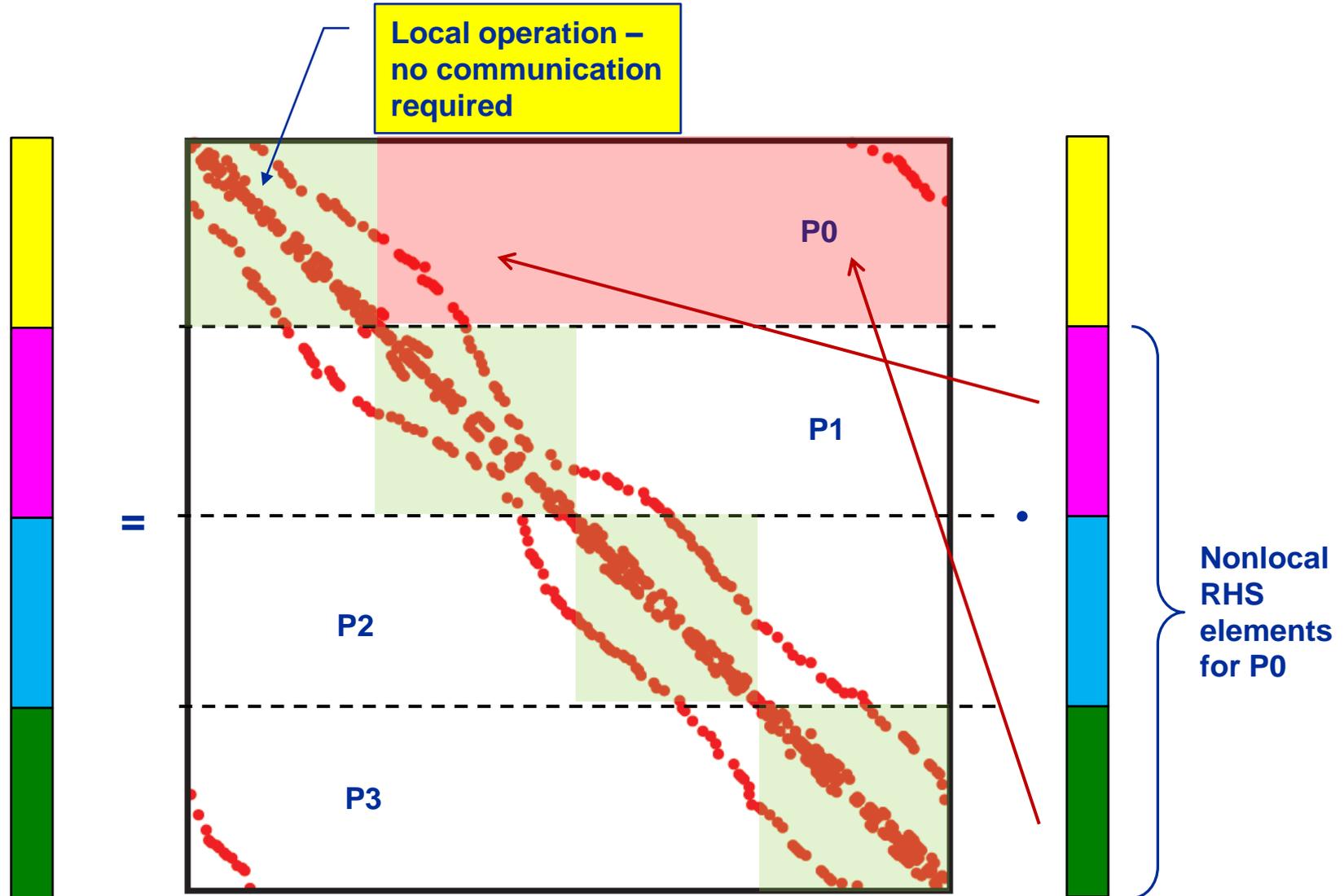


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  - Power-efficient code execution
- **Conclusions**



## **Case study: Asynchronous MPI communication in sparse MVM**

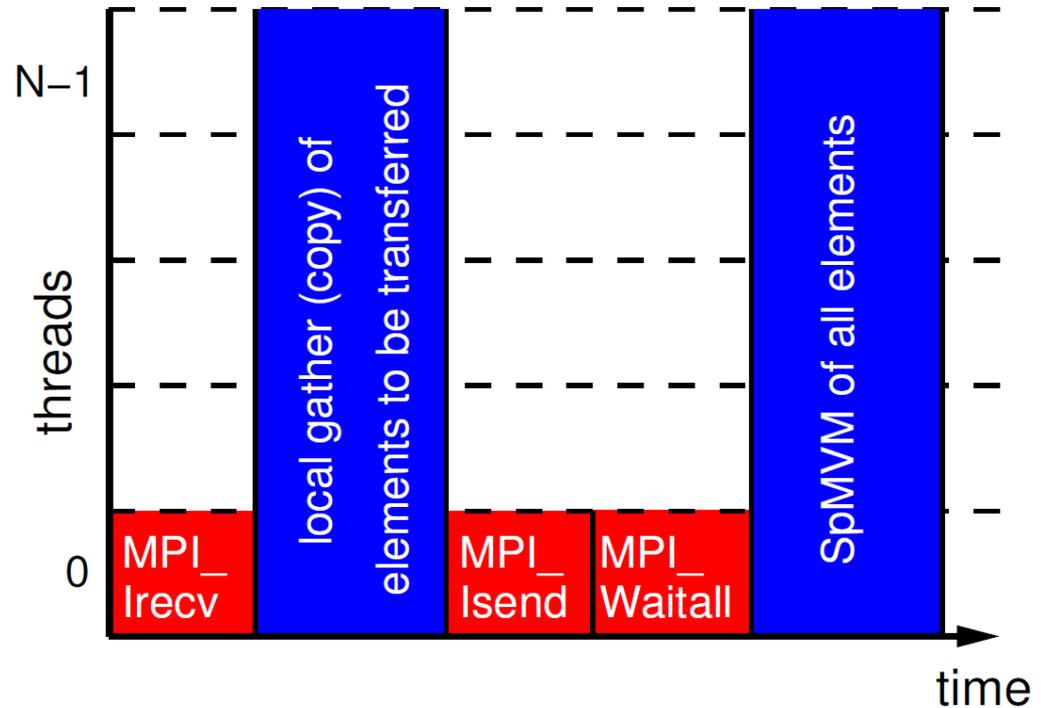
**What to do with spare cores**





- **Variant 1: “Vector mode” without overlap**

- **Standard concept for “hybrid MPI+OpenMP”**
- **Multithreaded computation (all threads)**
- **Communication only outside of computation**

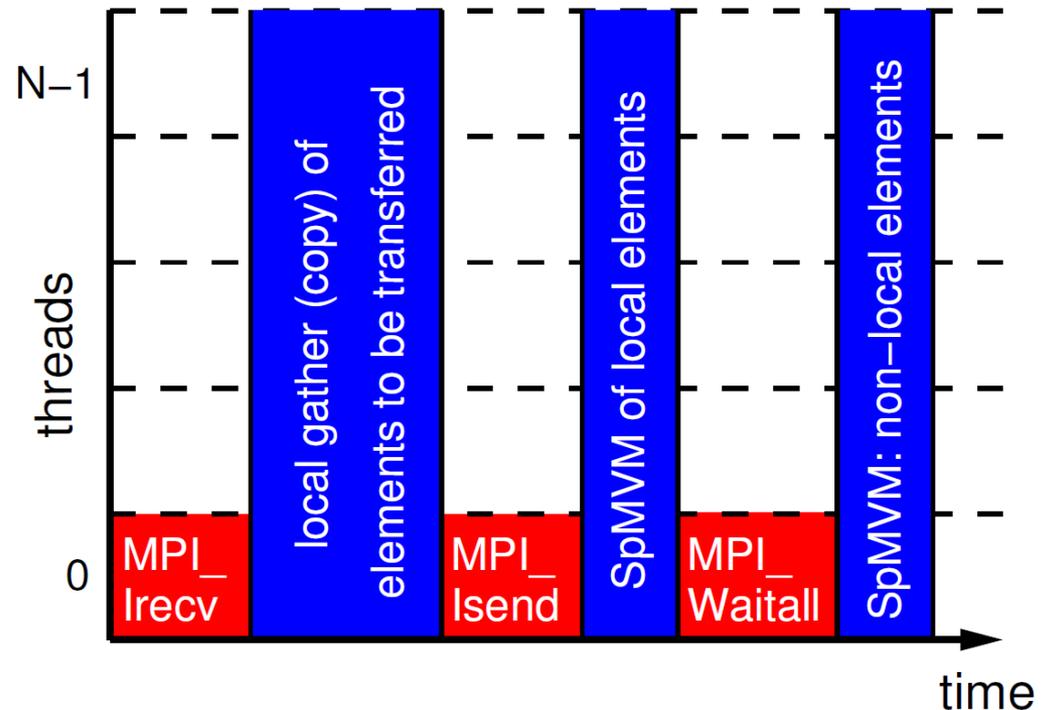


- **Benefit of threaded MPI process only due to message aggregation and (probably) better load balancing**

G. Hager, G. Jost, and R. Rabenseifner: *Communication Characteristics and Hybrid MPI/OpenMP Parallel Programming on Clusters of Multi-core SMP Nodes*. In: Proceedings of the Cray Users Group Conference 2009 (CUG 2009), Atlanta, GA, USA, May 4-7, 2009. [PDF](#)

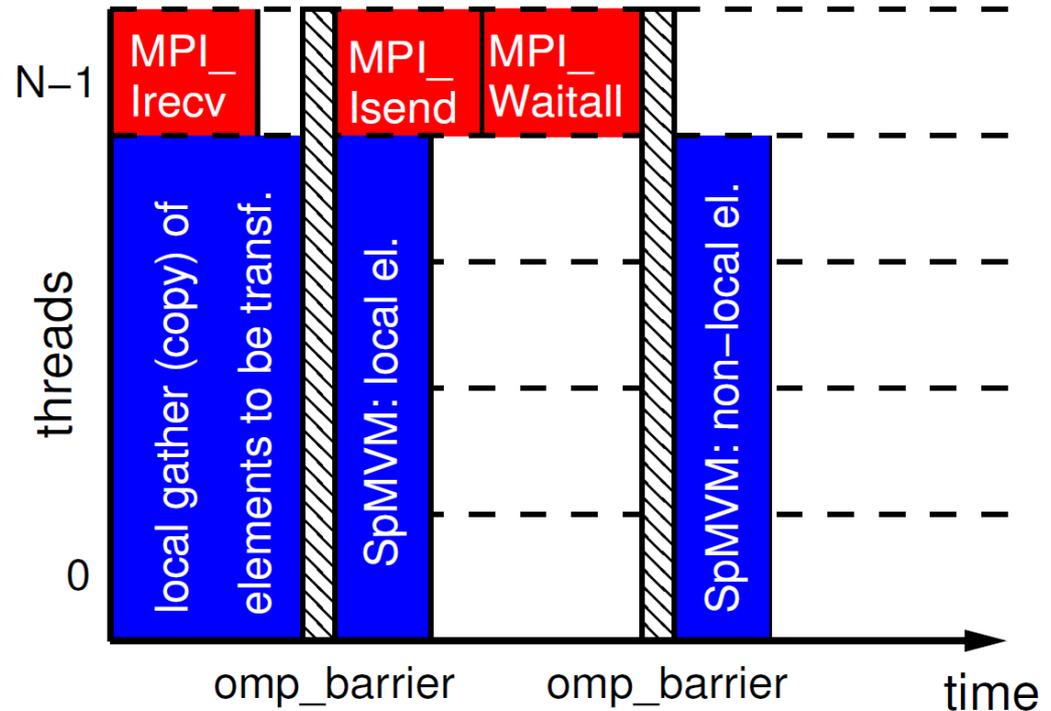


- **Variant 2: “Vector mode” with naïve overlap** (“good faith hybrid”)
- Relies on MPI to support async nonblocking PtP
- Multithreaded computation (all threads)
- Still simple programming
- **Drawback: Result vector is written twice to memory**
  - modified performance model



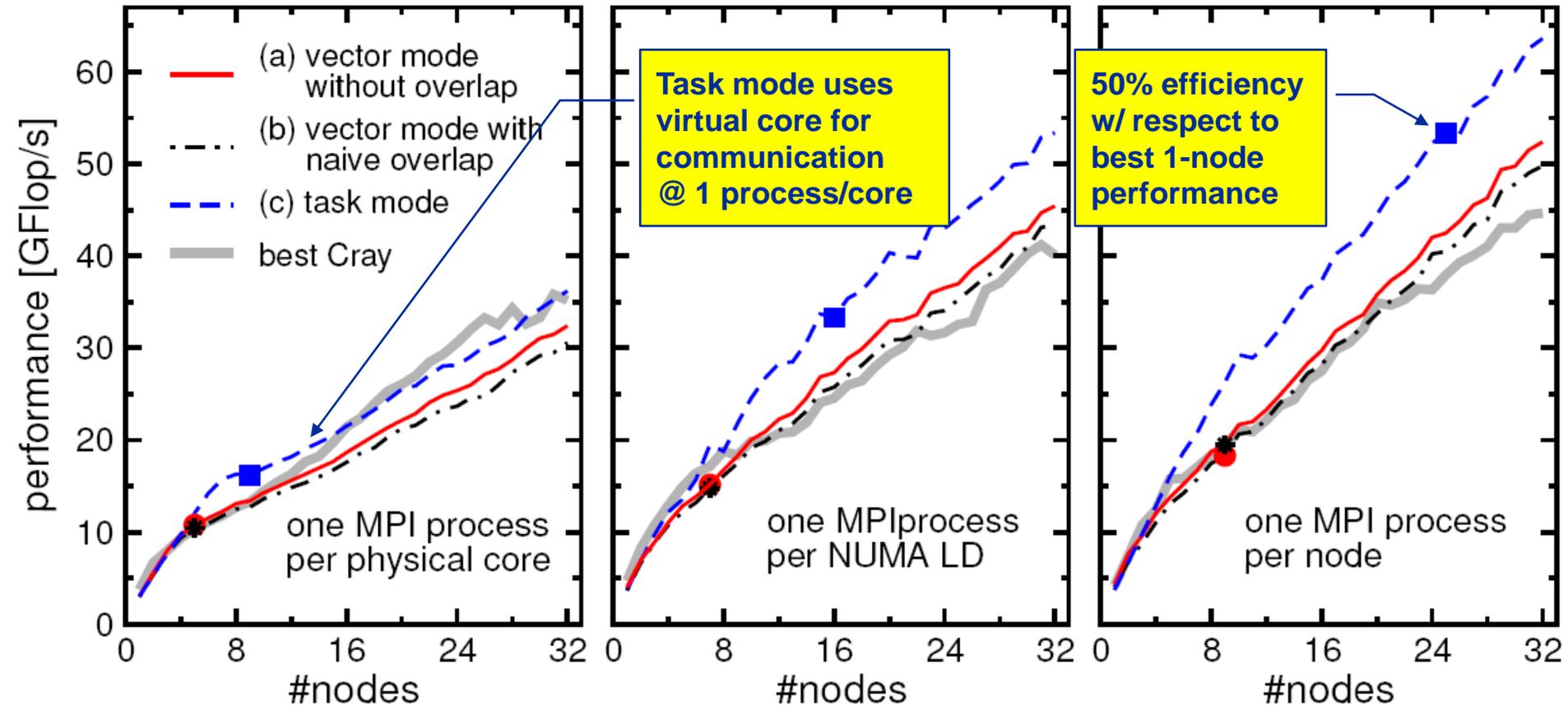


- **Variant 3: “Task mode” with dedicated communication thread**
- **Explicit overlap, more complex to implement**
- **One thread missing in team of compute threads**
  - But that doesn't hurt here...
  - Using tasking seems simpler but may require some work on NUMA locality
- **Drawbacks**
  - Result vector is written twice to memory
  - No simple OpenMP worksharing (manual, tasking)



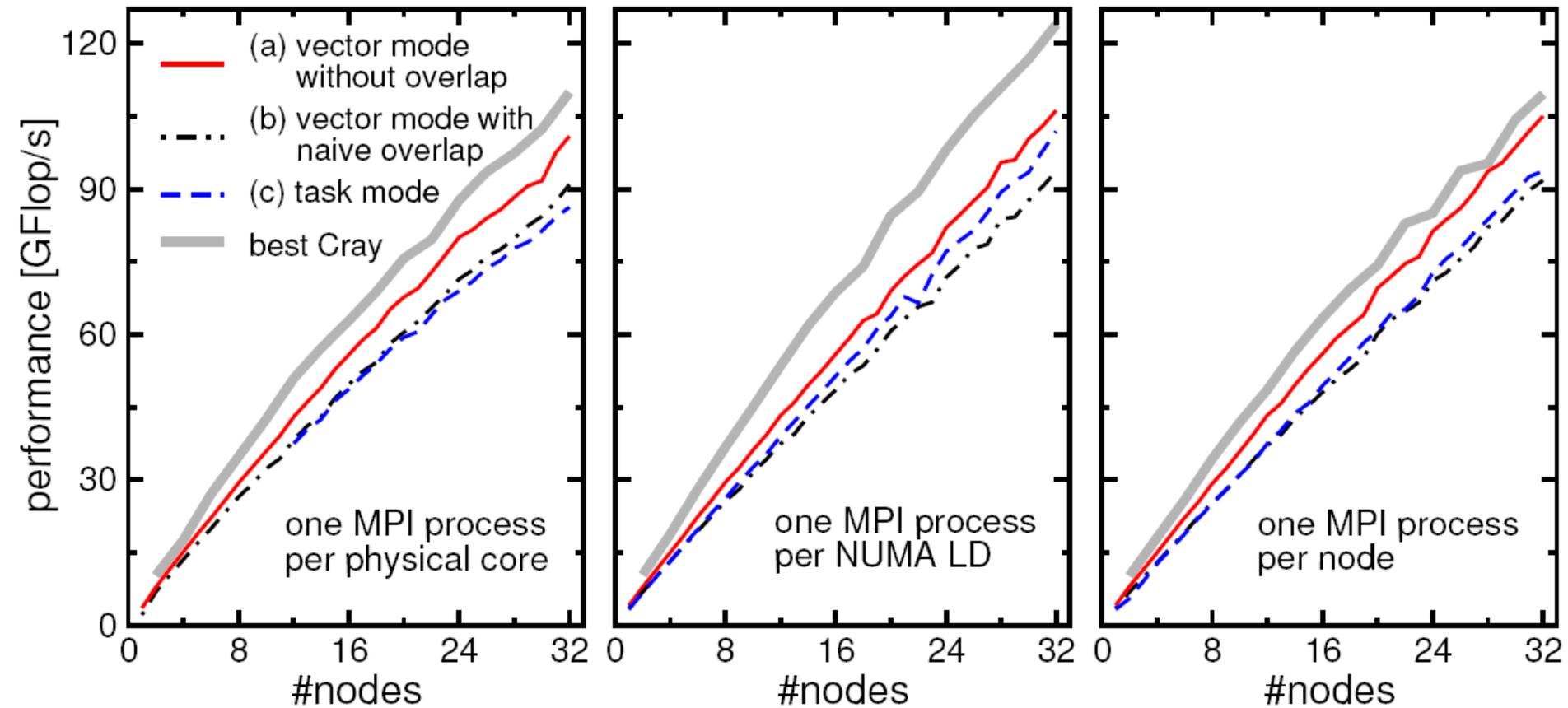
R. Rabenseifner and G. Wellein: *Communication and Optimization Aspects of Parallel Programming Models on Hybrid Architectures*. International Journal of High Performance Computing Applications 17, 49-62, February 2003.  
[DOI:10.1177/1094342003017001005](https://doi.org/10.1177/1094342003017001005)

# Performance results for the HMeP matrix



- **Dominated by communication (and some load imbalance for large #procs)**
- **Single-node Cray performance cannot be maintained beyond a few nodes**
- **Task mode pays off esp. with one process (12 threads) per node**
- **Task mode overlap (over-)compensates additional LHS traffic**

# Performance results for the sAMG matrix



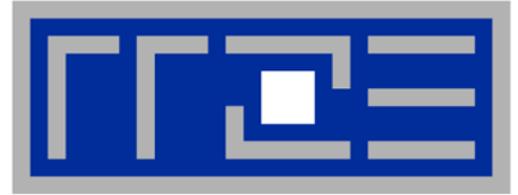
- **Much less communication-bound**
- **XE6 outperforms Westmere cluster, can maintain good node performance**
- **Hardly any discernible difference as to # of threads per process**
- **If pure MPI is good enough, don't bother going hybrid!**



- Do not rely on asynchronous MPI progress
- Sparse MVM leaves resources (cores) free for use by **communication threads**
- Simple **“vector mode” hybrid MPI+OpenMP parallelization is not good enough** if communication is a real problem
- **“Task mode” hybrid can truly hide communication and overcompensate penalty from additional memory traffic in spMVM**
- Comm thread can share a core with comp thread via **SMT** and still be asynchronous
- **If pure MPI scales ok and maintains its node performance according to the node-level performance model, don't bother going hybrid**
- **Extension to multi-GPGPU is possible**
  - See references



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# A simple power model for the Sandy Bridge processor

Assumptions

Validation using simple benchmarks

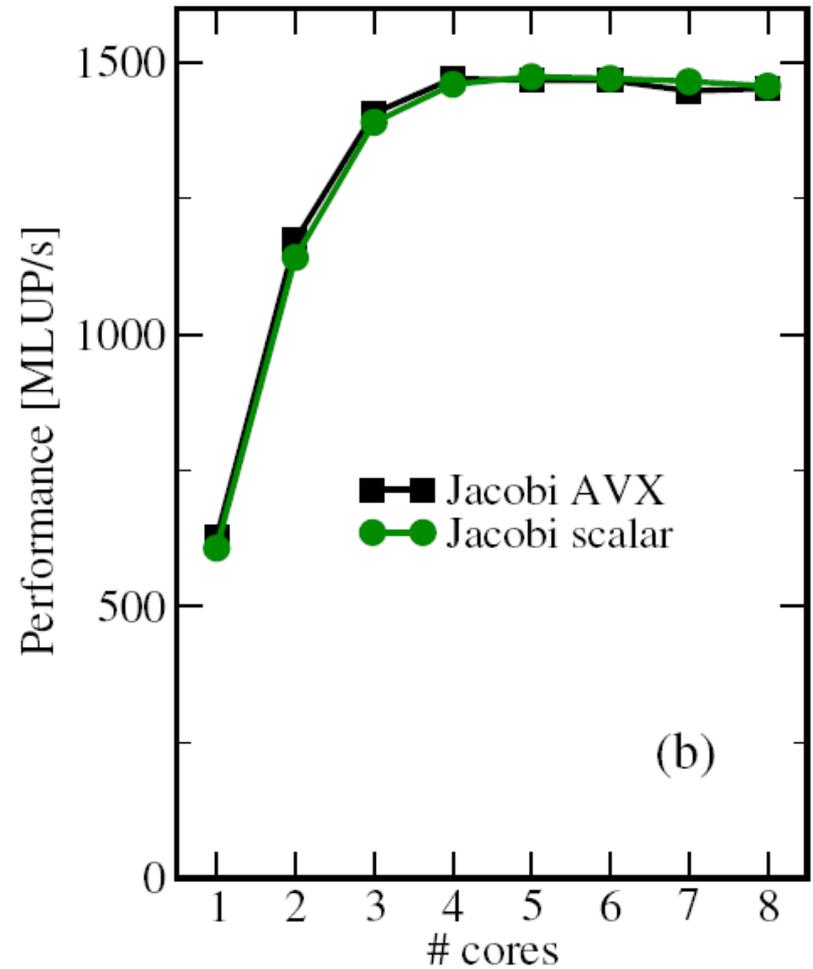
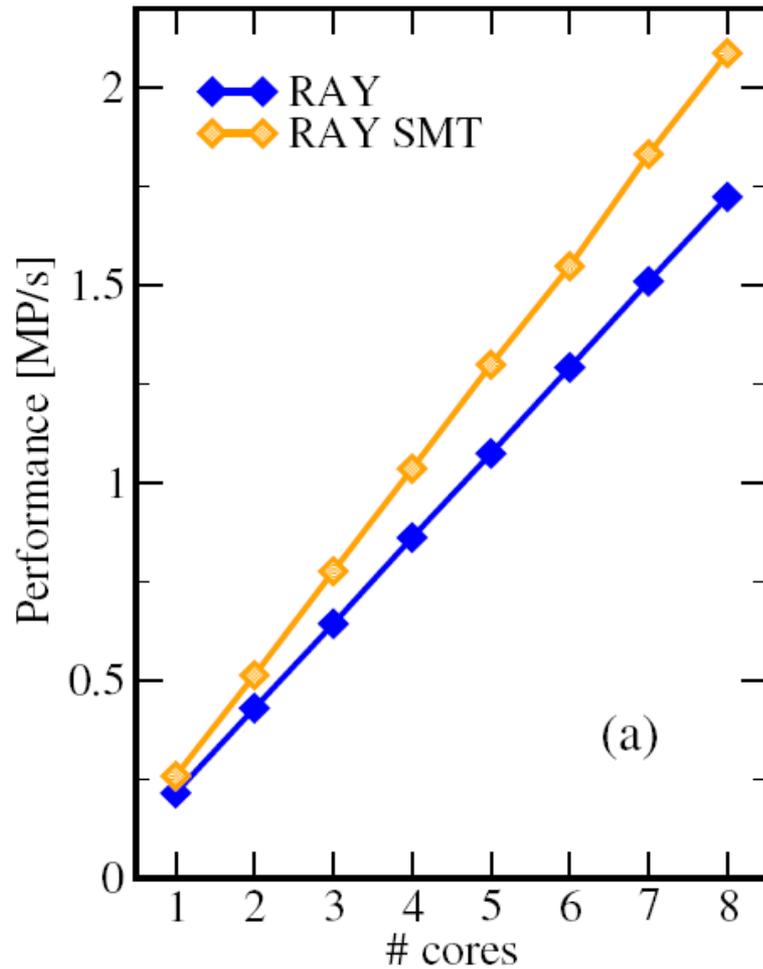
G. Hager, J. Treibig, J. Habich and G. Wellein: Exploring performance and power properties of modern multicore chips via simple machine models. Submitted.  
Preprint: [arXiv:1208.2908](https://arxiv.org/abs/1208.2908)



- **Goal: Establish model for chip power and program energy consumption with respect to**
  - Clock speed
  - Number of cores used
  - Single-thread program performance
- **Choose different characteristic benchmark applications to measure a chip's power behavior**
  - **Matrix-matrix-multiply** (“DGEMM”): “Hot” code, well scalable
  - **Ray tracer**: Sensitive to SMT execution (15% speedup), well scalable
  - **2D Jacobi solver**: 4000x4000 grid, strong saturation on the chip
    - AVX variant
    - Scalar variant
- **Measure characteristics of those apps and establish a power model**

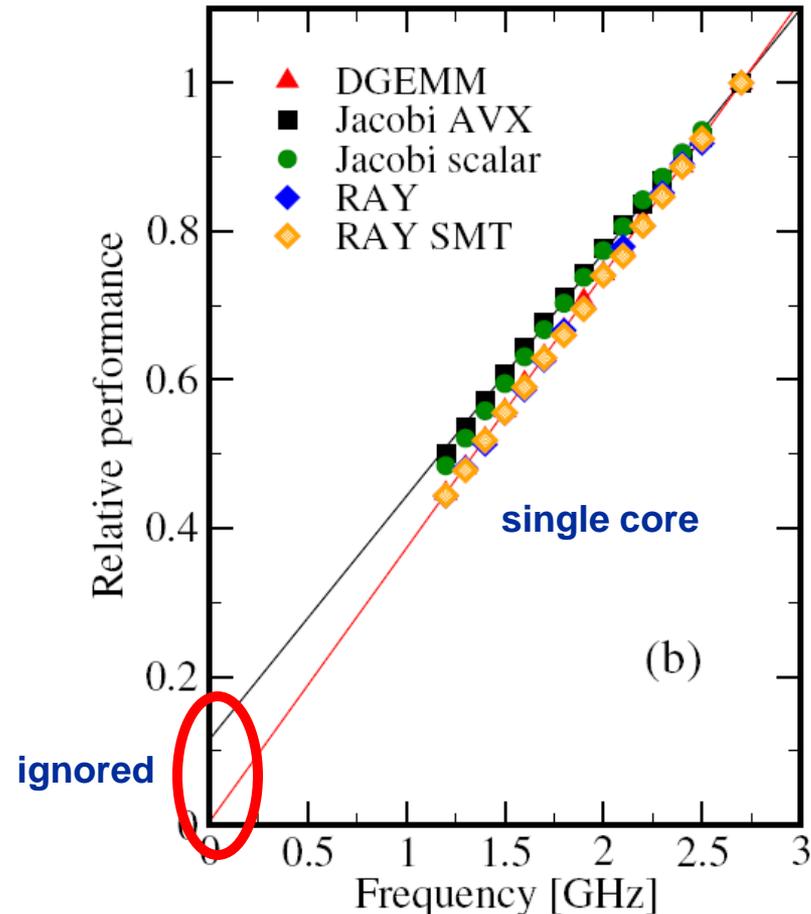
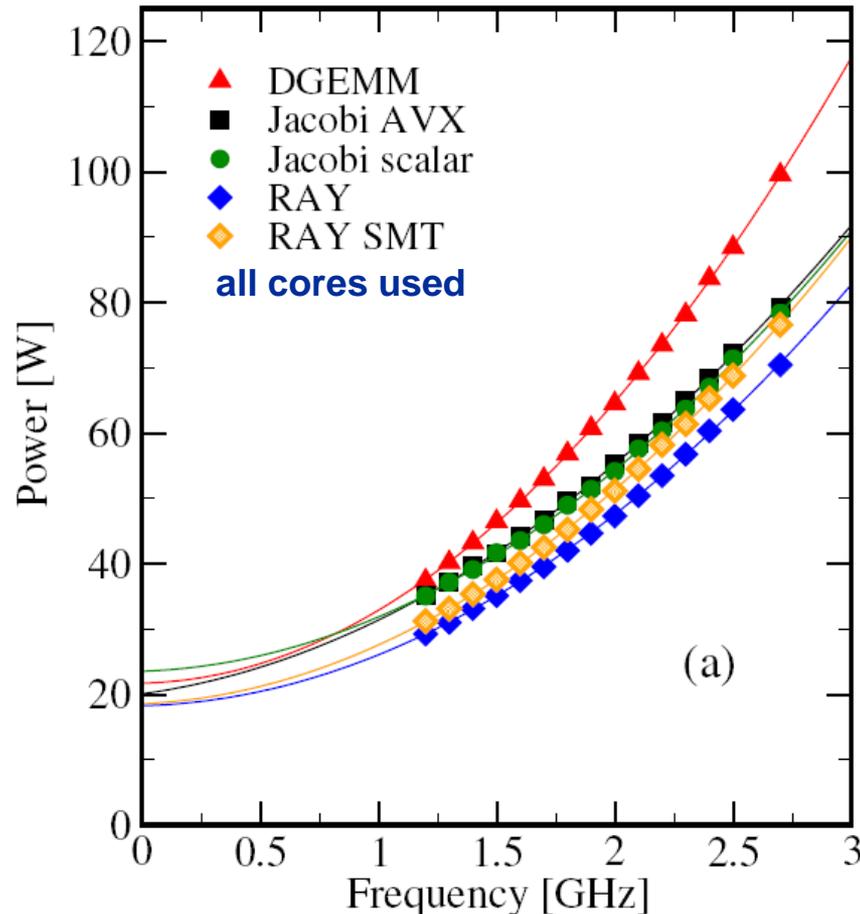


## Sandy Bridge EP (8-core) processor:



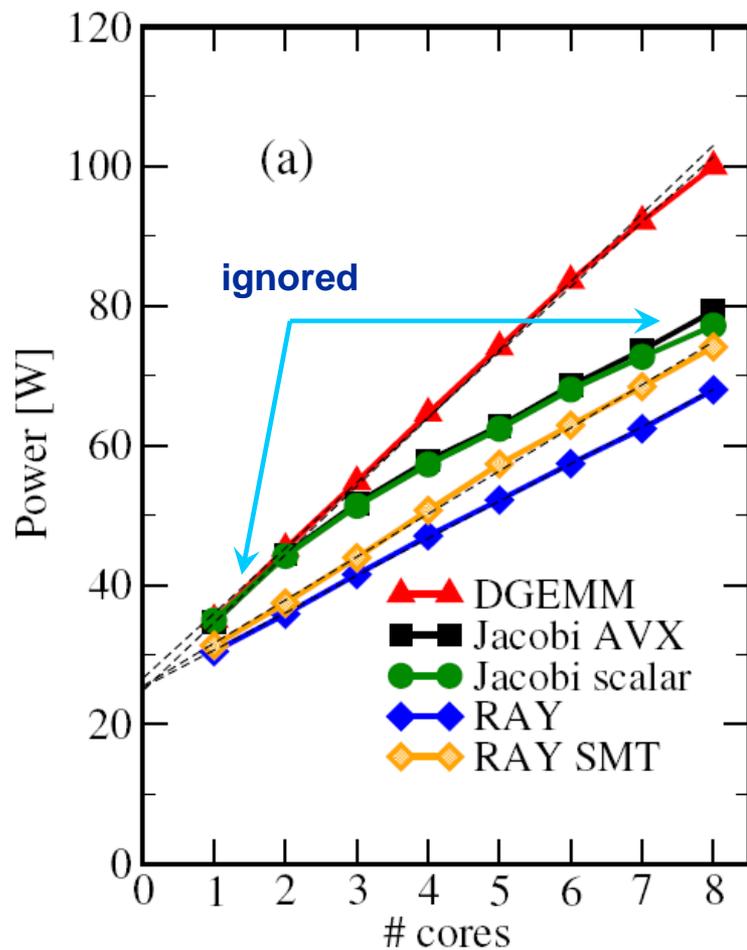


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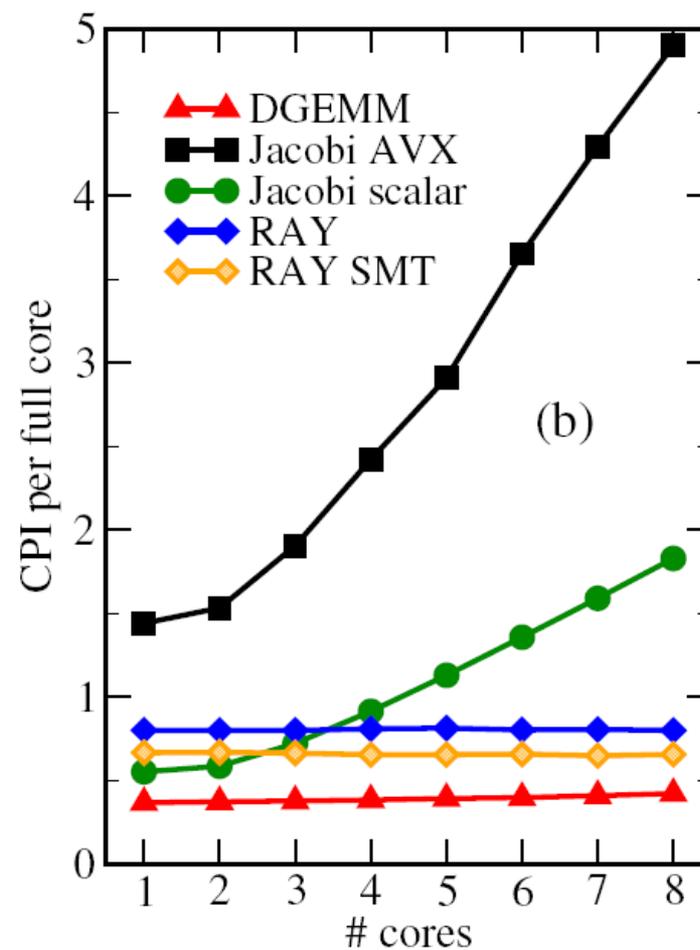




## Sandy Bridge EP (8-core) processor:



CPI and power correlated, but not proportional





## Assumptions:

1. Power is a quadratic polynomial in the clock frequency
2. Dynamic power is linear in the number of active cores  $t$
3. Performance is linear in the number of cores until it hits a bottleneck ( $\leftarrow$  ECM model)
4. Performance is linear in the clock frequency unless it hits a bottleneck
5. **Energy to solution** is power dissipation divided by performance

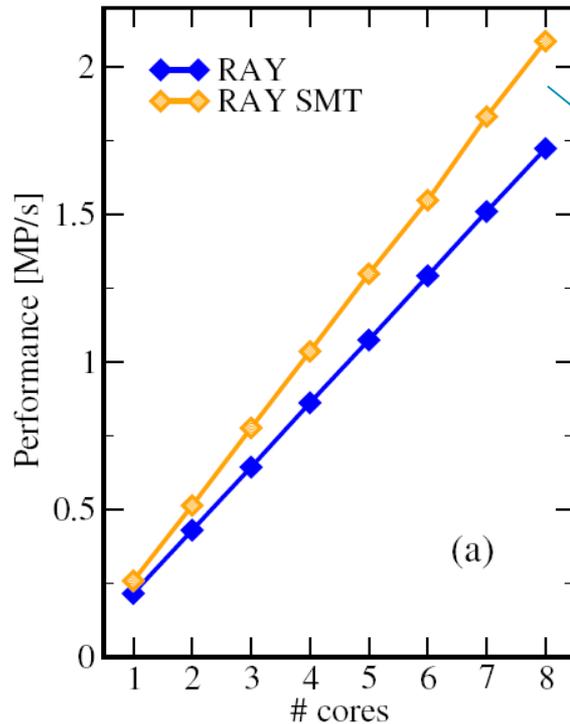
Model:

$$E = \frac{W_0 + (W_1 f + W_2 f^2)t}{\min((1 + \Delta v)t P_0, P_{\max})}$$

where  $f = (1 + \Delta v)f_0$

$$E = \frac{W_0 + (W_1 f + W_2 f^2)t}{\min((1 + \Delta v)tP_0, P_{\max})}$$

1. If there is **no saturation**, use **all available cores** to minimize  $E$



Minimum E here

$$\frac{\partial E}{\partial t} = -\frac{W_0}{(1 + \Delta v)t^2 P_0} < 0$$



$$E = \frac{W_0 + (W_1 f + W_2 f^2)t}{\min((1 + \Delta v)t P_0, P_{\max})}$$

2. There is an optimal frequency  $f_{\text{opt}}$  at which  $E$  is minimal in the **non-saturated** case, with

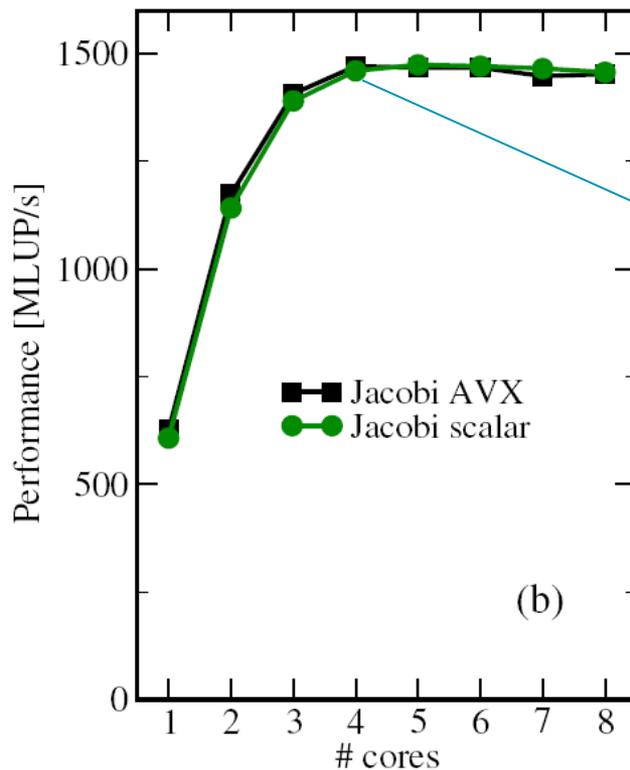
$$f_{\text{opt}} = \sqrt{\frac{W_0}{W_2 t}}, \text{ hence it depends on the baseline power}$$

- “**Clock race to idle**” if baseline accommodates whole system!
- May have to look at other metrics, e.g.,  $C = E/P$

$$\frac{\partial C}{\partial \Delta v} = -\frac{2W_0 + W_1 f t}{(f/f_0)^3 P_0^2} < 0$$

$$E = \frac{W_0 + (W_1 f + W_2 f^2)t}{\min((1 + \Delta v)tP_0, P_{\max})}$$

3. If there is saturation, ***E*** is minimal at the saturation point

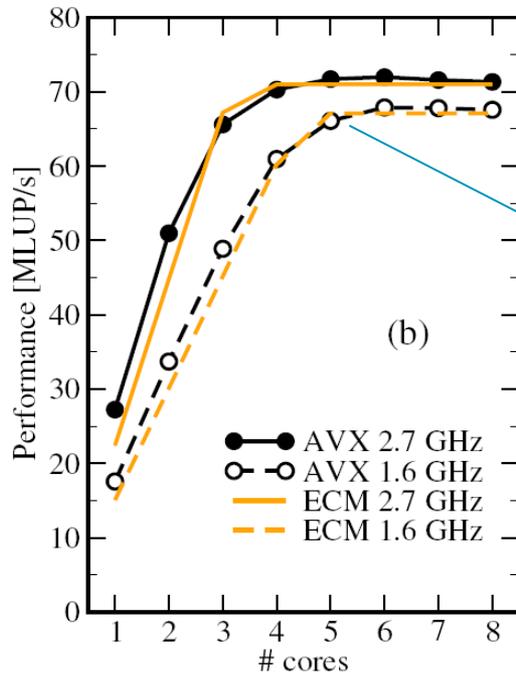


Minimum *E* here

$$t_s = \frac{P_{\max}}{(1 + \Delta v)P_0}$$

$$E = \frac{W_0 + (W_1 f + W_2 f^2)t}{\min((1 + \Delta v)t P_0, P_{\max})}$$

4. If there is saturation, **absolute minimum  $E$**  is reached if the **saturation point is at the number of available cores**

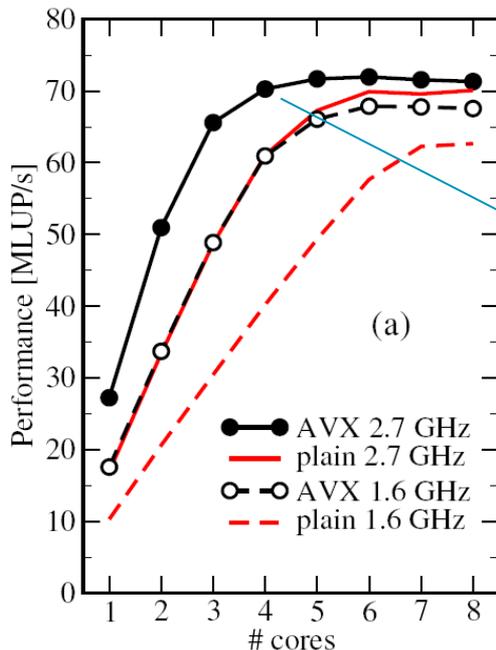


Slower clock  
 → more cores to saturation  
 → smaller  $E$

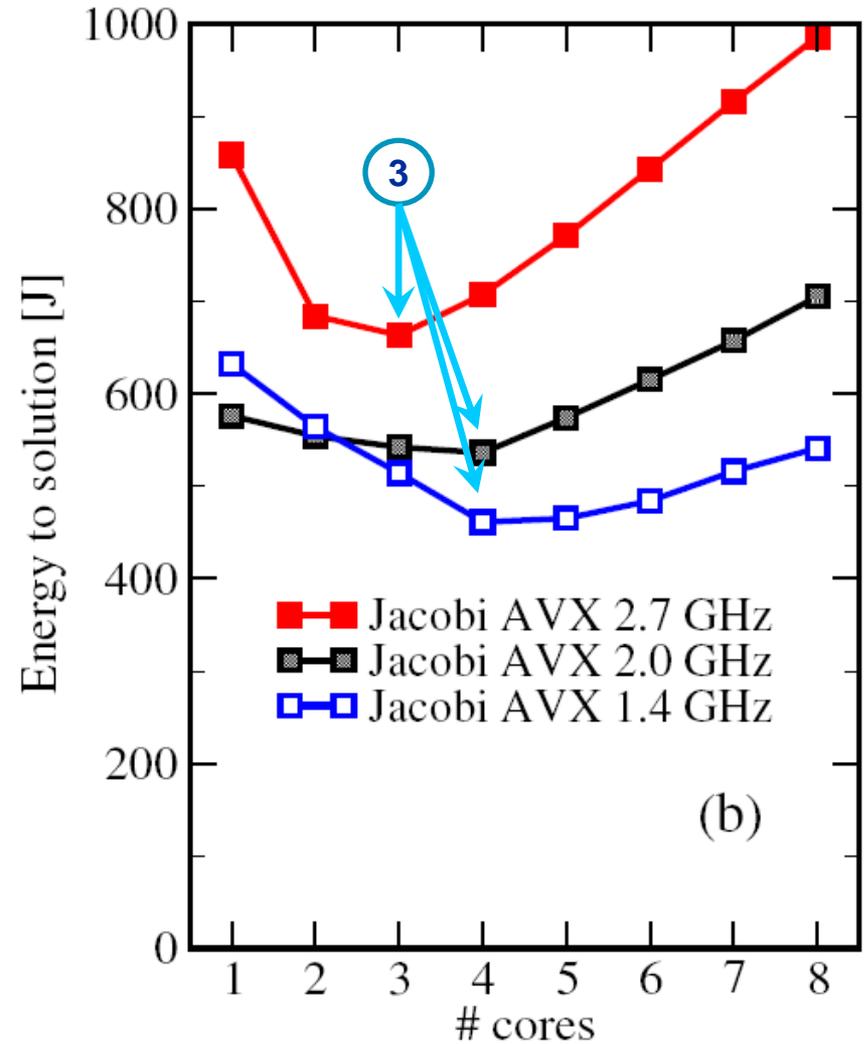
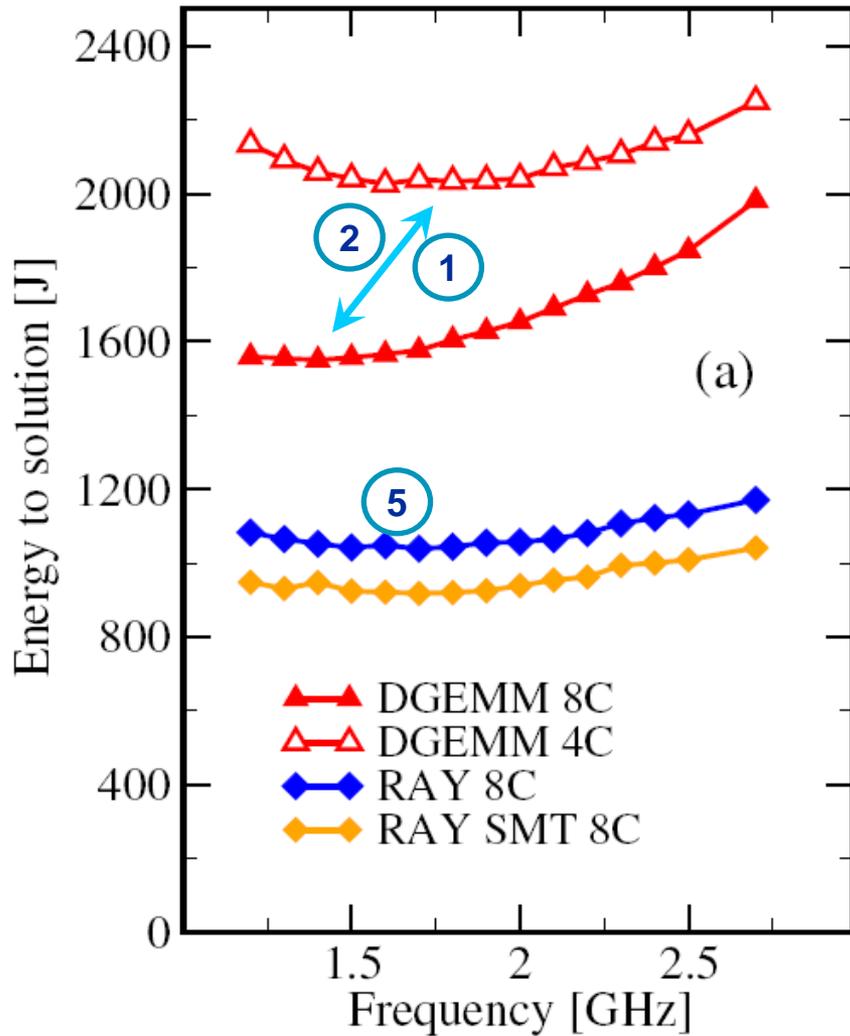
$$E = \frac{W_0 + (W_1 f + W_2 f^2) t}{\min((1 + \Delta v) t P_0, P_{\max})}$$

## 5. Making code execute faster on the core saves energy since

- The time to solution is smaller if the code scales (“Code race to idle”)
- We can use fewer cores to reach saturation if there is a bottleneck



**Better code**  
→ earlier saturation  
→ smaller E @ saturation





- Simple assumptions lead to surprising conclusions
- **Performance saturation** plays a key role
- **“Clock race to idle”** can be proven quantitatively
- **“Code race to idle”** (optimization saves energy) is a trivial result
  - Better: “Optimization makes better use of the energy budget”
- **Possible extensions to the power model**
  - Allow for per-core frequency setting (coming with Intel Haswell)
  - Accommodate load imbalance & sync overhead



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- **Basic performance modeling: Roofline**
  - Theory
  - Case study: 3D Jacobi solver and guided optimizations
  - Modeling erratic access
- **Some more architecture**
  - Simultaneous multithreading (SMT)
  - ccNUMA
- **Putting cores to good use**
  - Asynchronous communication in spMVM
- **A simple power model for multicore**
  - Power-efficient code execution
- **Conclusions**



- **LIKWID: Lightweight multicore performance tools**
  - <http://code.google.com/p/likwid>
- **Multicore-specific properties of MPI communication**
- **Sparse MVM on multiple GPGPUs: Performance modeling for viability analysis**
  - See references
- **Exploiting shared caches for temporal blocking of stencil codes**
- **Execution-Cache-Memory (ECM) model**
  - Predictive model for multicore scaling
  - Goes well with the power model
- **... and much more ☹**



- **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?
  - Leave surplus cores idle to save energy
- **Simple modeling techniques help us**
  - ... understand the limits of our code on the given hardware
  - ... identify optimization opportunities and hence save energy
  - ... learn more, especially when they do not work!



## Code:

```
double precision, dimension(100000000) :: a,b

do i=1,N
    s=s+a(i)*b(i)
enddo
```

**GPGPU:** 2880 cores,  $P_{\text{peak}} = 1.3 \text{ Tflop/s}$ ,  $b_S = 160 \text{ Gbyte/s}$

**Optimal  
performance?**

**Jan Treibig  
Johannes Habich  
Moritz Kreutzer  
Markus Wittmann  
Thomas Zeiser  
Michael Meier  
Faisal Shahzad  
Gerald Schubert**

**THANK YOU.**

**KONWIHR**  
**II**  
OMI4papps  
HQS@HPC II



**Bundesministerium  
für Bildung  
und Forschung**

**hpcADD  
SKALB**



- **Georg Hager** holds a PhD in computational physics from the University of Greifswald. He has been working with high performance systems since 1995, and is now 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. See his blog at <http://blogs.fau.de/hager> for current activities, publications, and talks.
- **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.





## Book:

- G. Hager and G. Wellein: [Introduction to High Performance Computing for Scientists and Engineers](#). CRC Computational Science Series, 2010. ISBN 978-1439811924

## Papers:

- G. Hager, J. Treibig, J. Habich and G. Wellein: [Exploring performance and power properties of modern multicore chips via simple machine models](#). Submitted. Preprint: [arXiv:1208.2908](#)
- J. Treibig, G. Hager and G. Wellein: [Performance patterns and hardware metrics on modern multicore processors: Best practices for performance engineering](#). Workshop on Productivity and Performance (PROPER 2012) at Euro-Par 2012, August 28, 2012, Rhodes Island, Greece. Preprint: [arXiv:1206.3738](#)
- M. Kreutzer, G. Hager, G. Wellein, H. Fehske, A. Basermann and A. R. Bishop: [Sparse Matrix-vector Multiplication on GPGPU Clusters: A New Storage Format and a Scalable Implementation](#). Workshop on Large-Scale Parallel Processing 2012 (LSPP12), DOI: [10.1109/IPDPSW.2012.211](#)
- J. Treibig, G. Hager, H. Hofmann, J. Hornegger and G. Wellein: [Pushing the limits for medical image reconstruction on recent standard multicore processors](#). International Journal of High Performance Computing Applications, (published online before print). DOI: [10.1177/1094342012442424](#)



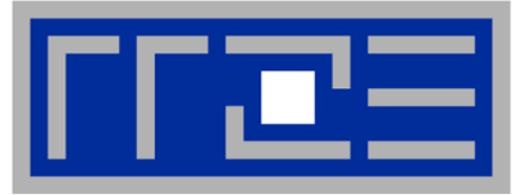
Papers continued:

- G. Wellein, G. Hager, T. Zeiser, M. Wittmann and H. Fehske: **Efficient temporal blocking for stencil computations by multicore-aware wavefront parallelization**. Proc. COMPSAC 2009.  
[DOI: 10.1109/COMPSAC.2009.82](https://doi.org/10.1109/COMPSAC.2009.82)
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[DOI: 10.1109/ICPPW.2010.38](https://doi.org/10.1109/ICPPW.2010.38). Preprint: [arXiv:1004.4431](https://arxiv.org/abs/1004.4431)
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[DOI: 10.1142/S0129626411000254](https://doi.org/10.1142/S0129626411000254)
- J. Treibig, G. Wellein and G. Hager: **Efficient multicore-aware parallelization strategies for iterative stencil computations**. Journal of Computational Science 2 (2), 130-137 (2011).  
[DOI 10.1016/j.jocs.2011.01.010](https://doi.org/10.1016/j.jocs.2011.01.010)

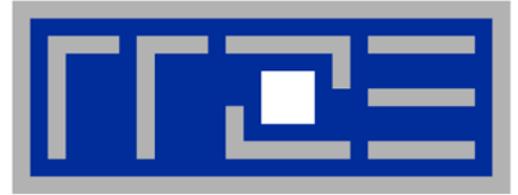


Papers continued:

- K. Iglberger, G. Hager, J. Treibig, and U. Rde: [Expression Templates Revisited: A Performance Analysis of Current ET Methodologies](#). *SIAM Journal on Scientific Computing* **34**(2), C42-C69 (2012). [DOI: 10.1137/110830125](#), Preprint: [arXiv:1104.1729](#)
- K. Iglberger, G. Hager, J. Treibig, and U. Rde: [High Performance Smart Expression Template Math Libraries](#). 2nd International Workshop on New Algorithms and Programming Models for the Manycore Era ([APMM 2012](#)) at [HPCS 2012](#), July 2-6, 2012, Madrid, Spain. [DOI: 10.1109/HPCSim.2012.6266939](#)
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- G. Hager, G. Jost, and R. Rabenseifner: [Communication Characteristics and Hybrid MPI/OpenMP Parallel Programming on Clusters of Multi-core SMP Nodes](#). In: *Proceedings of the Cray Users Group Conference 2009 (CUG 2009)*, Atlanta, GA, USA, May 4-7, 2009. [PDF](#)
- R. Rabenseifner and G. Wellein: [Communication and Optimization Aspects of Parallel Programming Models on Hybrid Architectures](#). *International Journal of High Performance Computing Applications* **17**, 49-62, February 2003. [DOI:10.1177/1094342003017001005](#)



**Backup material**



## Probing node topology

- Standard tools
- **likwid-topology**

# How do we figure out the node topology?



- **Topology =**

- Where in the machine does core #n reside? And do I have to remember this awkward numbering anyway?
- Which cores share which cache levels?
- Which hardware threads (“logical cores”) share a physical core?

- **Linux**

- `cat /proc/cpuinfo` is of limited use
- Core numbers may change across kernels and BIOSes even on identical hardware
- `numactl --hardware` prints ccNUMA node information
- Information on caches is harder to obtain



```
$ numactl --hardware
available: 4 nodes (0-3)
node 0 cpus: 0 1 2 3 4 5
node 0 size: 8189 MB
node 0 free: 3824 MB
node 1 cpus: 6 7 8 9 10 11
node 1 size: 8192 MB
node 1 free: 28 MB
node 2 cpus: 18 19 20 21 22 23
node 2 size: 8192 MB
node 2 free: 8036 MB
node 3 cpus: 12 13 14 15 16 17
node 3 size: 8192 MB
node 3 free: 7840 MB
```

- Lightweight command line tools for Linux
- Help to face the challenges without getting in the way
- Focus on X86 architecture

- **Philosophy:**

- Simple
- Efficient
- Portable
- Extensible



**Open source project (GPL v2):**

<http://code.google.com/p/likwid/>



- **Based on `cpuid` information**
- **Functionality:**
  - Measured clock frequency
  - Thread topology
  - Cache topology
  - Cache parameters (-c command line switch)
  - ASCII art output (-g command line switch)
- **Currently supported (more under development):**
  - Intel Core 2 (45nm + 65 nm)
  - Intel Nehalem + Westmere (Sandy Bridge in beta phase)
  - AMD K10 (Quadcore and Hexacore)
  - AMD K8
  - Linux OS

# Output of `likwid-topology -g`

on one node of Cray XE6 "Hermit"



```
-----
CPU type:      AMD Interlagos processor
*****
Hardware Thread Topology
*****
Sockets:      2
Cores per socket: 16
Threads per core: 1
-----

HWThread      Thread      Core      Socket
0              0           0         0
1              0           1         0
2              0           2         0
3              0           3         0
[...]
16             0           0         1
17             0           1         1
18             0           2         1
19             0           3         1
[...]
-----
Socket 0: ( 0 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 )
Socket 1: ( 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 )
-----

*****
Cache Topology
*****
Level:  1
Size:   16 kB
Cache groups: ( 0 ) ( 1 ) ( 2 ) ( 3 ) ( 4 ) ( 5 ) ( 6 ) ( 7 ) ( 8 ) ( 9 ) ( 10 ) ( 11 ) ( 12 ) ( 13 )
              ( 14 ) ( 15 ) ( 16 ) ( 17 ) ( 18 ) ( 19 ) ( 20 ) ( 21 ) ( 22 ) ( 23 ) ( 24 ) ( 25 ) ( 26 ) ( 27 ) (
              28 ) ( 29 ) ( 30 ) ( 31 )
```

# Output of likwid-topology continued



```
-----  
Level: 2  
Size: 2 MB  
Cache groups: ( 0 1 ) ( 2 3 ) ( 4 5 ) ( 6 7 ) ( 8 9 ) ( 10 11 ) ( 12 13 ) ( 14 15 ) ( 16 17 ) ( 18  
19 ) ( 20 21 ) ( 22 23 ) ( 24 25 ) ( 26 27 ) ( 28 29 ) ( 30 31 )  
-----
```

```
Level: 3  
Size: 6 MB  
Cache groups: ( 0 1 2 3 4 5 6 7 ) ( 8 9 10 11 12 13 14 15 ) ( 16 17 18 19 20 21 22 23 ) ( 24 25 26  
27 28 29 30 31 )  
-----
```

```
*****  
NUMA Topology  
*****  
NUMA domains: 4  
-----
```

```
Domain 0:  
Processors: 0 1 2 3 4 5 6 7  
Memory: 7837.25 MB free of total 8191.62 MB  
-----
```

```
Domain 1:  
Processors: 8 9 10 11 12 13 14 15  
Memory: 7860.02 MB free of total 8192 MB  
-----
```

```
Domain 2:  
Processors: 16 17 18 19 20 21 22 23  
Memory: 7847.39 MB free of total 8192 MB  
-----
```

```
Domain 3:  
Processors: 24 25 26 27 28 29 30 31  
Memory: 7785.02 MB free of total 8192 MB  
-----
```

# Output of likwid-topology continued



\*\*\*\*\*

Graphical:

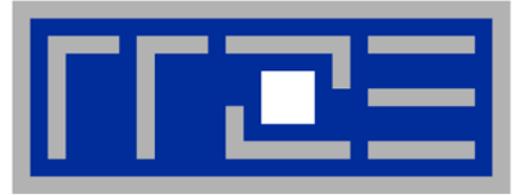
\*\*\*\*\*

Socket 0:

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
16kB															
2MB															
6MB								6MB							

Socket 1:

16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31
16kB															
2MB															
6MB								6MB							



# **Enforcing thread/process-core affinity under the Linux OS**

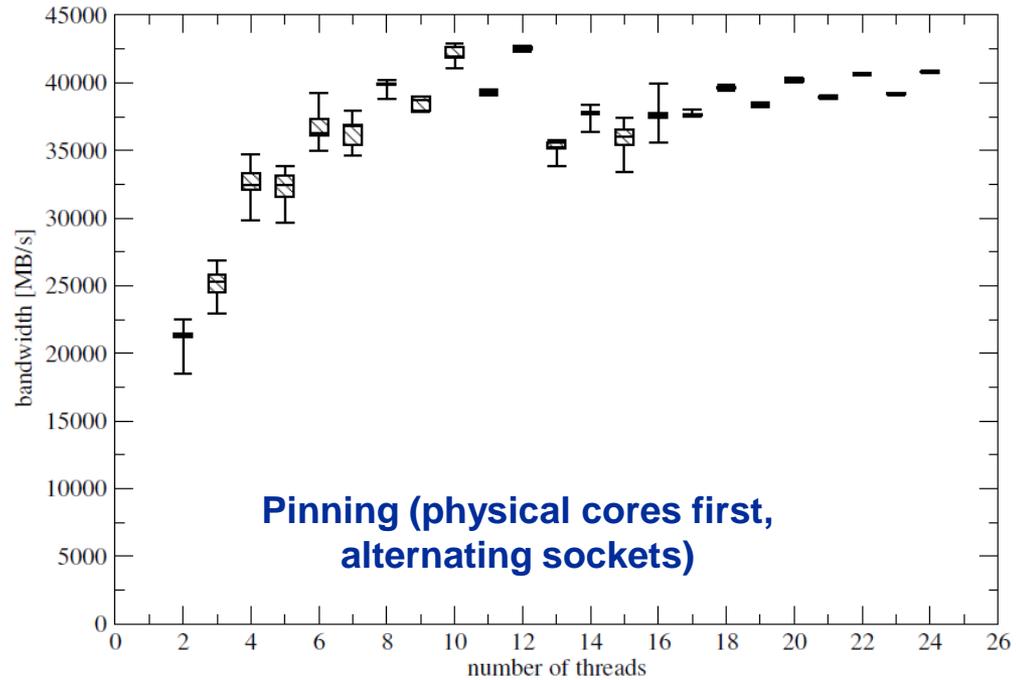
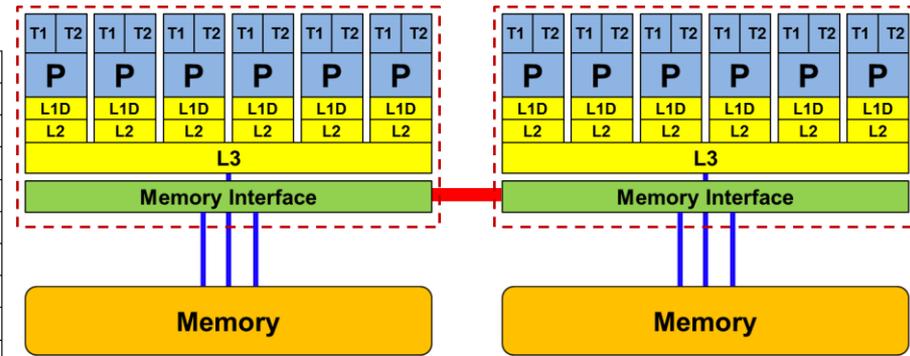
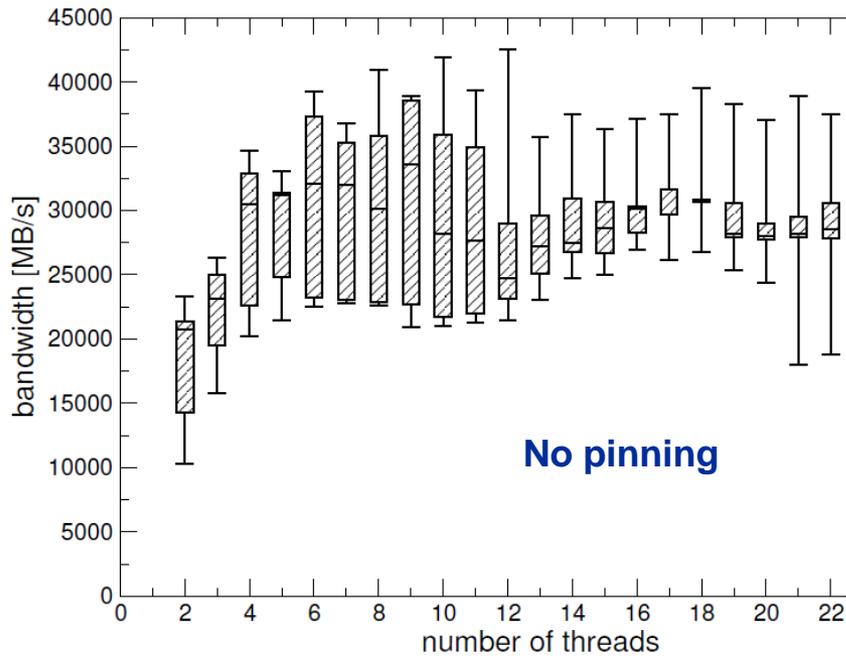
**Standard tools and OS affinity facilities under  
program control**

**likwid-pin**

# Motivation: STREAM benchmark on 12-core Intel Westmere



## Anarchy vs. thread pinning



There are several reasons for caring about affinity:

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



- `taskset [OPTIONS] [MASK | -c LIST ] \  
[PID | command [args]...]`
- **taskset binds processes/threads to a set of CPUs. Examples:**  
  

```
taskset 0x0006 ./a.out  
taskset -c 4 33187  
mpirun -np 2 taskset -c 0,2 ./a.out # doesn't always work
```
- **Processes/threads can still move within the set!**
- **Alternative: let process/thread bind itself by executing syscall**  

```
#include <sched.h>  
int sched_setaffinity(pid_t pid, unsigned int len,  
                     unsigned long *mask);
```
- **Disadvantage: which CPUs should you bind to on a non-exclusive machine?**
- **Still of value on multicore/multisocket cluster nodes, UMA or ccNUMA**



- **Complementary tool:** `numactl`

**Example:** `numactl --physcpubind=0,1,2,3 command [args]`

**Bind process to specified physical core numbers**

**Example:** `numactl --cpunodebind=1 command [args]`

**Bind process to specified ccNUMA node(s)**

- **Many more options (e.g., interleave memory across nodes)**
  - → see section on ccNUMA optimization
- **Diagnostic command (see earlier):**  
`numactl --hardware`
- **Again, this is not suitable for a shared machine**



- **Highly OS-dependent system calls**

- But available on all systems

Linux: `sched_setaffinity()`, PLPA (see below) → `hwloc`

Solaris: `processor_bind()`

Windows: `SetThreadAffinityMask()`

...

- **Support for “semi-automatic” pinning in some compilers/environments**

- Intel compilers > V9.1 (`KMP_AFFINITY` environment variable)
- PGI, Pathscale, GNU
- SGI Altix `dp1ace` (works with logical CPU numbers!)
- Generic Linux: `taskset`, `numactl`, `likwid-pin` (see below)

- **Affinity awareness in MPI libraries**

- SGI MPT
- OpenMPI
- Intel MPI
- ...



If combined with OpenMP,  
issues may arise



- Part of the LIKWID tool suite: <http://code.google.com/p/likwid>
- Pins processes and threads to specific cores **without touching code**
- Directly supports pthreads, gcc OpenMP, Intel OpenMP
  - Detects OpenMP implementation automatically
- Based on combination of wrapper tool together with overloaded pthread library → **binary must be dynamically linked!**
- Can also be used as a superior **replacement for taskset**
  
- Usage examples:
  - Physical numbering:  
`likwid-pin -c 0,2,4-6 ./myApp parameters`
  - Logical numbering (4 cores on socket 0) with “**skip mask**” specified:  
`likwid-pin -s 3 -c S0:0-3 ./myApp parameters`



- Running the STREAM benchmark with likwid-pin:

```
$ export OMP_NUM_THREADS=4
$ likwid-pin -s 0x1 -c 0,1,4,5 ./stream
[likwid-pin] Main PID -> core 0 - OK
-----
Double precision appears to have 16 digits of accuracy
Assuming 8 bytes per DOUBLE PRECISION word
-----
[... some STREAM output omitted ...]
The *best* time for each test is used
*EXCLUDING* the first and last iterations
[pthread wrapper] PIN_MASK: 0->1 1->4 2->5
[pthread wrapper] SKIP MASK: 0x1
[pthread wrapper 0] Notice: Using libpthread.so.0
    threadid 1073809728 -> SKIP
[pthread wrapper 1] Notice: Using libpthread.so.0
    threadid 1078008128 -> core 1 - OK
[pthread wrapper 2] Notice: Using libpthread.so.0
    threadid 1082206528 -> core 4 - OK
[pthread wrapper 3] Notice: Using libpthread.so.0
    threadid 1086404928 -> core 5 - OK
[... rest of STREAM output omitted ...]
```

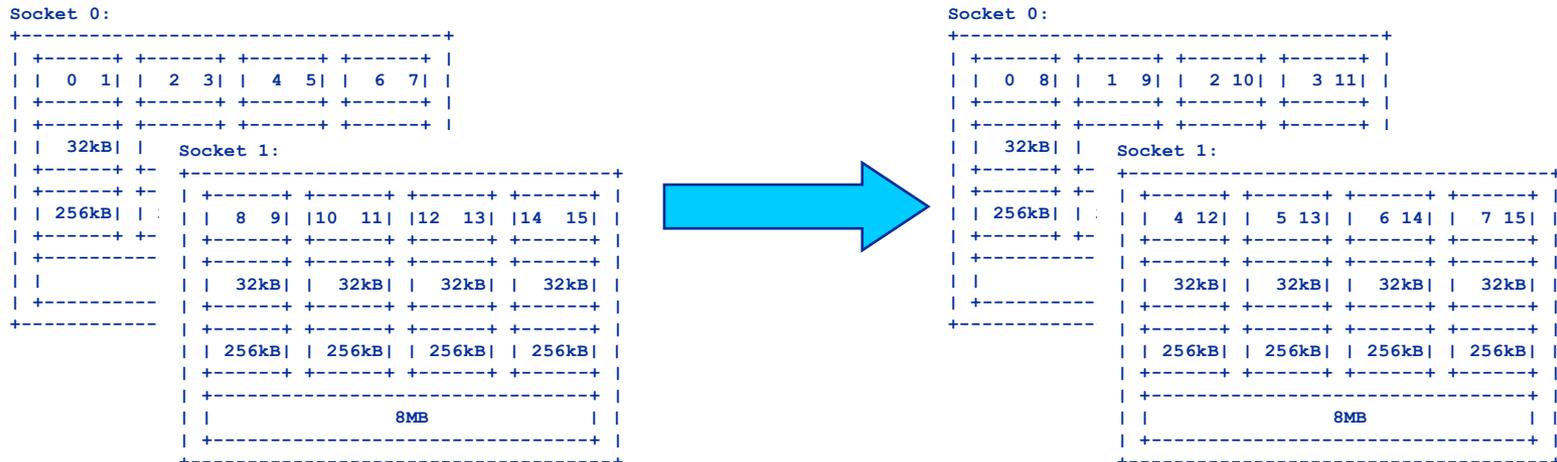
Main PID always pinned

Skip shepherd thread

Pin all spawned threads in turn



- Core numbering may vary from system to system even with identical hardware
  - Likwid-topology delivers this information, which can then be fed into likwid-pin
- Alternatively, likwid-pin can abstract this variation and provide a purely **logical** numbering (**physical cores first**)

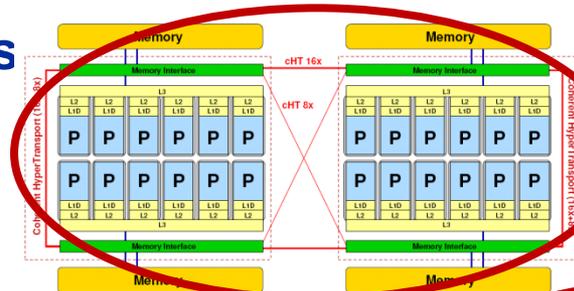


- Across all cores in the node:  
`OMP_NUM_THREADS=8 likwid-pin -c N:0-7 ./a.out`
- Across the cores in each socket and across sockets in each node:  
`OMP_NUM_THREADS=8 likwid-pin -c S0:0-3@S1:0-3 ./a.out`



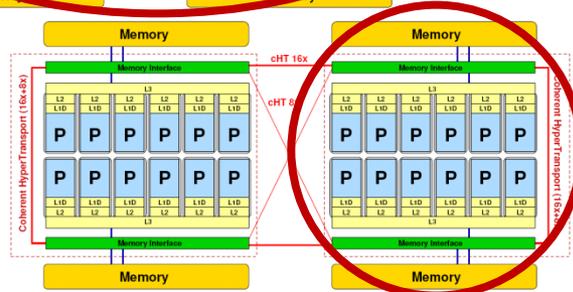
### Possible unit prefixes

**N** node

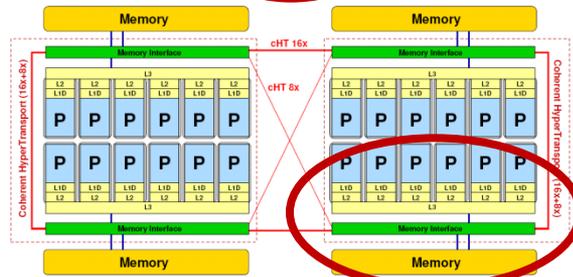


Default if -c is not specified!

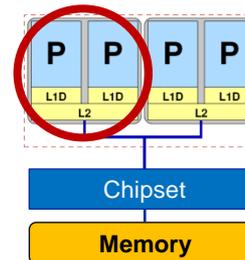
**S** socket



**M** NUMA domain



**C** outer level cache group





- How do you manage **affinity with MPI or hybrid MPI/threading?**
- In the long run a unified standard is needed
- Till then, **likwid-mpirun** provides a portable/flexible solution
- The examples here are for Intel MPI/OpenMP programs, but are also applicable to other threading models

### Pure MPI:

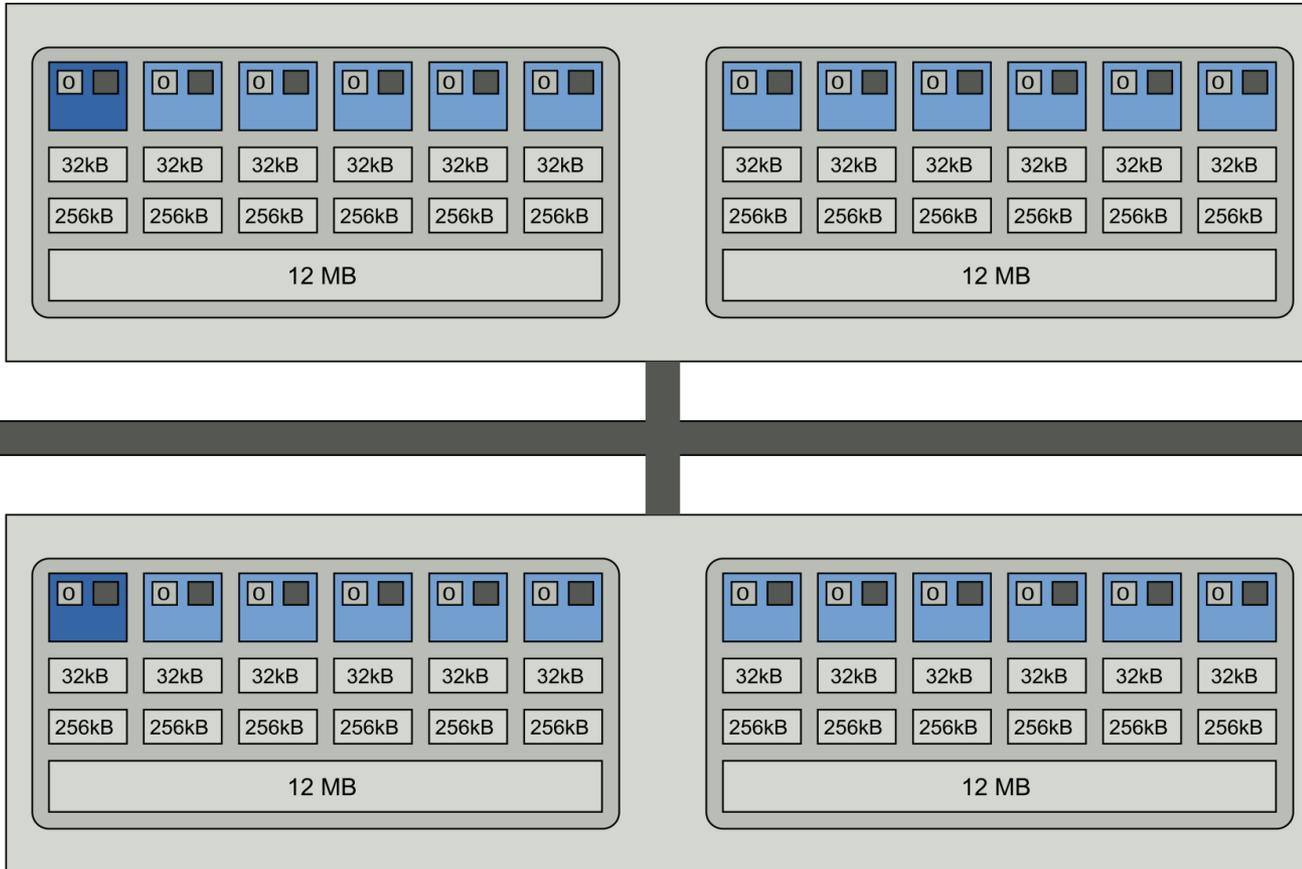
```
$ likwid-mpirun -np 16 -nperdomain S:2 ./a.out
```

### Hybrid:

```
$ likwid-mpirun -np 16 -pin S0:0,1_S1:0,1 ./a.out
```



```
likwid-mpirun -np 2 -pin N:0-11 ./a.out
```

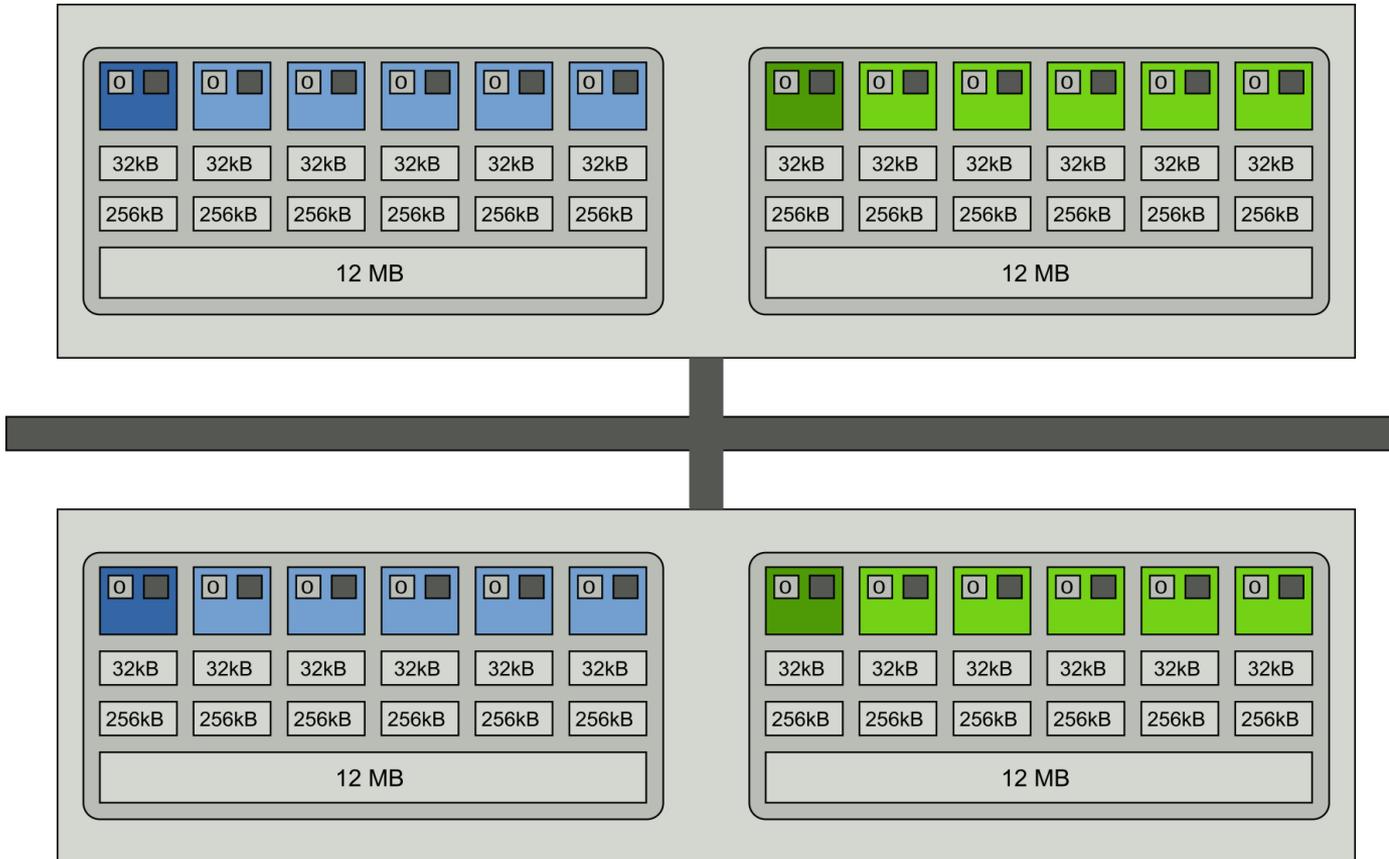


### Intel MPI+compiler:

```
OMP_NUM_THREADS=12 mpirun -ppn 1 -np 2 -env KMP_AFFINITY scatter ./a.out
```



```
likwid-mpirun -np 4 -pin s0:0-5_s1:0-5 ./a.out
```



### Intel MPI+compiler:

```
OMP_NUM_THREADS=6 mpirun -ppn 2 -np 4 \  
-env I_MPI_PIN_DOMAIN socket -env KMP_AFFINITY scatter ./a.out
```



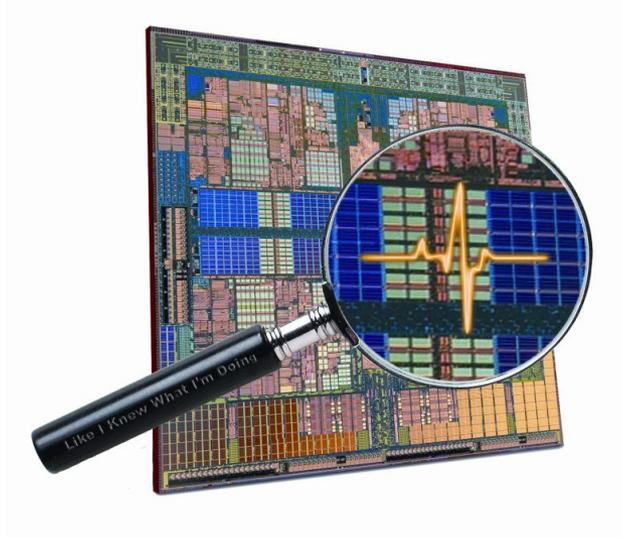
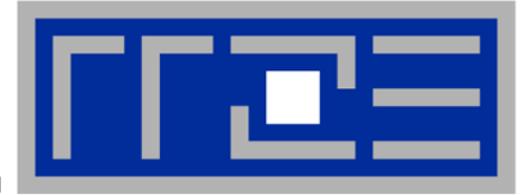
- **likwid-mpirun can optionally set up likwid-perfctr for you**

```
$ likwid-mpirun -np 16 -nperdomain S:2 -perf FLOPS_DP \  
-marker -mpi intelmpi ./a.out
```

- **likwid-mpirun generates an intermediate perl script which is called by the native MPI start mechanism**
- **According the MPI rank the script pins the process and threads**
- **If you use perfctr after the run for each process a file in the format Perf-<hostname>-<rank>.txt**

**Its output which contains the perfctr results.**

- **In the future analysis scripts will be added which generate reports of the raw data (e.g. as html pages)**



# Best practices for using hardware performance metrics

`likwid-perfctr`



- 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

- Operating modes:

- Wrapper
- Stethoscope
- Timeline
- Marker API

- 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



```
$ env OMP_NUM_THREADS=4 likwid-perfctr -C N:0-3 -t intel -g FLOPS_DP ./stream.exe
```

```
-----
CPU type:      Intel Core Lynnfield processor
CPU clock:    2.93 GHz
-----
```

```
Measuring group FLOPS_DP
```

```
YOUR PROGRAM OUTPUT
```

Event	core 0	core 1	core 2	core 3
INSTR_RETIRED_ANY	1.97463e+08	2.31001e+08	2.30963e+08	2.31885e+08
CPU_CLK_UNHALTED_CORE	9.56999e+08	9.58401e+08	9.58637e+08	9.57338e+08
FP_COMP_OPS_EXE_SSE_FP_PACKED	4.00294e+07	3.08927e+07	3.08866e+07	3.08904e+07
FP_COMP_OPS_EXE_SSE_FP_SCALAR	882	0	0	0
FP_COMP_OPS_EXE_SSE_SINGLE_PRECISION	0	0	0	0
FP_COMP_OPS_EXE_SSE_DOUBLE_PRECISION	4.00303e+07	3.08927e+07	3.08866e+07	3.08904e+07

Always measured

Configured metrics (this group)

Metric	core 0	core 1	core 2	core 3
Runtime [s]	0.326242	0.32672	0.326801	0.326358
CPI	4.84647	4.14891	4.15061	4.12849
DP MFlops/s (DP assumed)	245.399	189.108	189.024	189.304
Packed MUOPS/s	122.698	94.554	94.5121	94.6519
Scalar MUOPS/s	0.00270351	0	0	0
SP MUOPS/s	0	0	0	0
DP MUOPS/s	122.701	94.554	94.5121	94.6519

Derived metrics



### Things to look at (in roughly this order)

- **Load balance** (flops, instructions, BW)
- In-socket **memory BW saturation**
- Shared **cache 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 overrated**
  - If I really know my code, I can often *calculate* the misses
  - Runtime and resource utilization is much more important



- Instructions retired / CPI may not be a good indication of useful workload – at least for numerical / FP intensive codes....
- Floating Point Operations Executed** is often a better indicator
- Waiting / “Spinning” in barrier generates a high instruction count

Event	core 0	core 1	core 2	core 3	core 4	core 5
INSTR_RETIRED_ANY	2.10045e+10	1.90983e+10	1.729e+10	1.60898e+10	1.67958e+10	1.84689e+10
CPU_CLK_UNHALTED_CORE	1.82569e+10	1.81203e+10	1.81802e+10	1.82084e+10	1.82334e+10	1.82484e+10
CPU_CLK_UNHALTED_REF	1.66053e+10	1.6473e+10	1.65274e+10	1.65531e+10	1.65758e+10	1.65894e+10
FP_COMP_OPS_EXE_SSE_FP_PACKED	2.77016e+08	7.83476e+08	1.39355e+09	1.94365e+09	2.38059e+09	2.85981e+09
FP_COMP_OPS_EXE_SSE_FP_SCALAR	1.70802e+08	2.64065e+08	2.23153e+08	2.60835e+08	2.30434e+08	2.07293e+08
FP_COMP_OPS_EXE_SSE_SINGLE_PRECISION	19	0	0	0	0	0
FP_COMP_OPS_EXE_SSE_DOUBLE_PRECISION	4.47818e+08	1.04754e+09	1.61671e+09	2.20448e+09	2.61102e+09	3.0671e+09

```
!$OMP PARALLEL DO
```

```
DO I = 1, N
```

```
DO J = 1, I
```

```
    x(I) = x(I) + A(J,I) * y(J)
```

```
ENDDO
```

```
ENDDO
```

```
!$OMP END PARALLEL DO
```

Metric	core 0	core 1	core 2	core 3	core 4	core 5
Runtime [s]	6.84594	6.79471	6.81716	6.82773	6.83711	6.84274
Clock [MHz]	2932.07	2933.51	2933.51	2933.51	2933.51	2933.51
CPI	0.869191	0.948789	1.05148	1.13167	1.08559	0.988061
DP MFlops/s	109.192	275.833	453.48	624.893	751.96	892.857



```
env OMP_NUM_THREADS=6 likwid-perfctr -t intel -C S0:0-5 -g FLOPS_DP ./a.out
```

Event	core 0	core 1	core 2	core 3	core 4	core 5
INSTR_RETIRED_ANY	1.83124e+10	1.74784e+10	1.68453e+10	1.66794e+10	1.76685e+10	1.91736e+10
CPU_CLK_UNHALTED_CORE	2.24797e+10	2.23789e+10	2.23802e+10	2.23808e+10	2.23799e+10	2.23805e+10
CPU_CLK_UNHALTED_REF	2.04416e+10	2.03445e+10	2.03456e+10	2.03462e+10	2.03453e+10	2.03459e+10
FP_COMP_OPS_EXE_SSE_FP_PACKED	3.45348e+09	3.43035e+09	3.37573e+09	3.39272e+09	3.26132e+09	3.2377e+09
FP_COMP_OPS_EXE_SSE_FP_SCALAR	2.93108e+07	3.06063e+07	2.9704e+07	2.96507e+07	2.41141e+07	2.37397e+07
FP_COMP_OPS_EXE_SSE_SINGLE_PRECISION	19	0	0	0	0	0
FP_COMP_OPS_EXE_SSE_DOUBLE_PRECISION	3.48279e+09	3.46096e+09	3.40543e+09	3.42237e+09	3.28543e+09	3.26144e+09

Higher CPI but  
better performance

Metric	core 0	core 1	core 2	core 3	core 4	core 5
Runtime [s]	8.42938	8.39157	8.39206	8.3923	8.39193	8.39218
Clock [MHz]	2932.73	2933.5	2933.51	2933.51	2933.51	2933.51
CPI	1.22757	1.28037	1.32857	1.34182	1.26666	1.16726
DP MFlops/s	850.727	845.212	831.703	835.865	802.952	797.113
Packed MUOPS/s	423.566	420.729	414.03	416.114	399.997	397.101
Scalar MUOPS/s	3.59494	3.75383	3.64317	3.63663	2.95757	2.91165
SP MUOPS/s	2.33033e-06	0	0	0	0	0
DP MUOPS/s	427.161	424.483	417.673	419.751	402.955	400.013

```
!$OMP PARALLEL DO
```

```
DO I = 1, N
```

```
DO J = 1, N
```

```
  x(I) = x(I) + A(J,I) * y(J)
```

```
ENDDO
```

```
ENDDO
```

```
!$OMP END PARALLEL DO
```



- **likwid-perfctr counts events on cores; it has no notion of what kind of code is running (if any)**

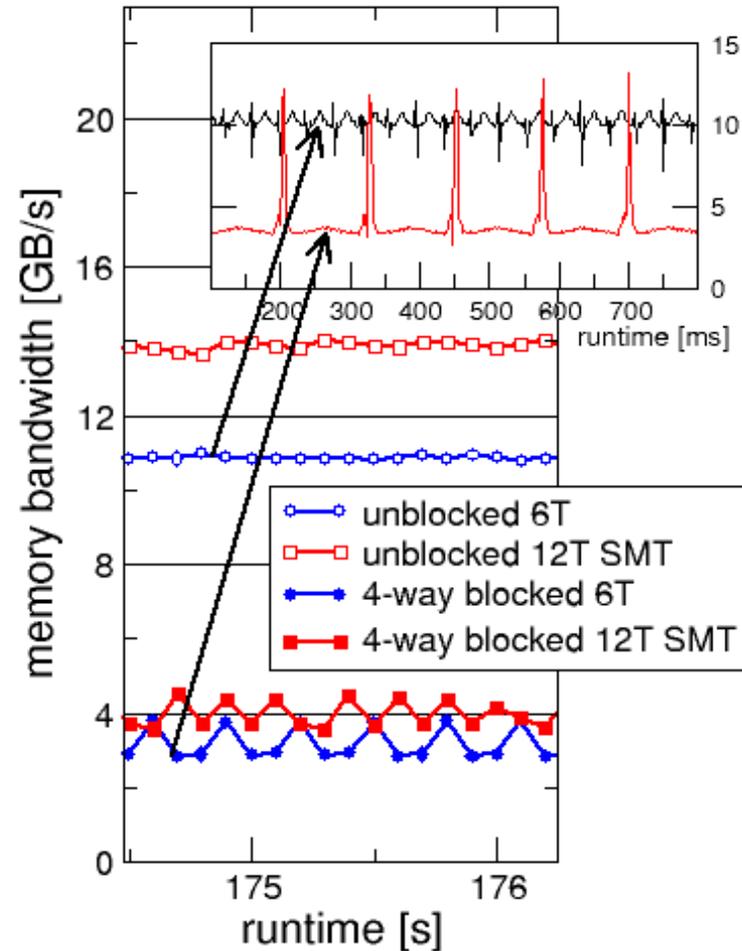
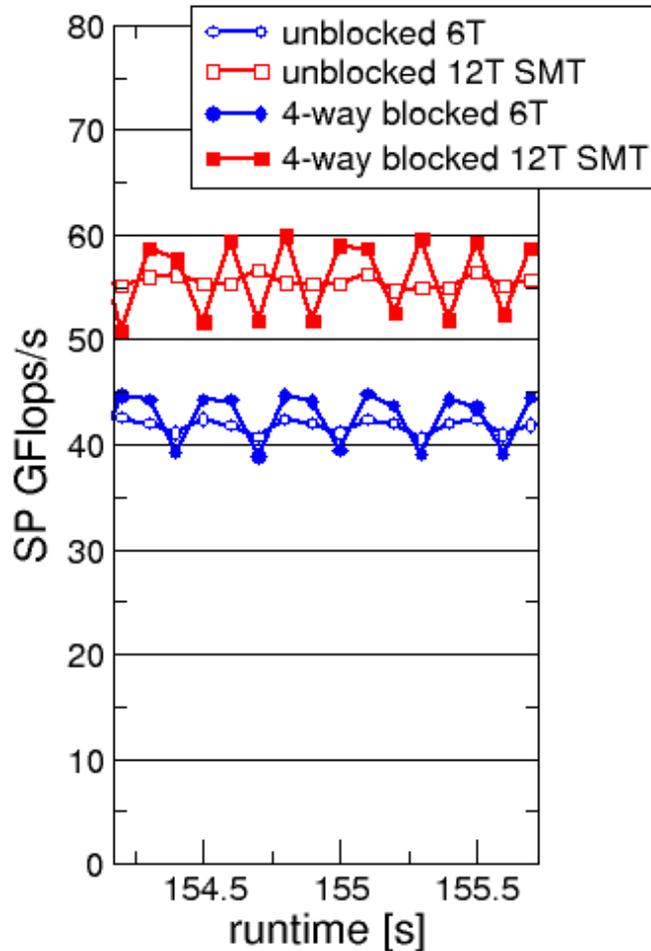
**This enables to listen on what currently happens without any overhead:**

```
likwid-perfctr -c N:0-11 -g FLOPS_DP -s 10
```

- **It can be used as cluster/server monitoring tool**
- **A frequent use is to measure a certain part of a long running parallel application from outside**

- likwid-perfctr supports time resolved measurements of full node:

```
likwid-perfctr -c N:0-11 -g MEM -d 50ms > out.txt
```





- **To measure only parts of an application a marker API is available.**
- **The API only turns counters on/off. The configuration of the counters is still done by likwid-perfctr application.**
- **Multiple named regions can be measured**
- **Results on multiple calls are accumulated**
- **Inclusive and overlapping Regions are allowed**

```
likwid_markerInit(); // must be called from serial region
```

```
likwid_markerStartRegion("Compute");
```

```
...
```

```
likwid_markerStopRegion("Compute");
```

```
likwid_markerStartRegion("postprocess");
```

```
...
```

```
likwid_markerStopRegion("postprocess");
```

```
likwid_markerClose(); // must be called from serial region
```



SHORT PSTI

### EVENTSET

```
FIXC0 INSTR_RETIRED_ANY
FIXC1 CPU_CLK_UNHALTED_CORE
FIXC2 CPU_CLK_UNHALTED_REF
PMC0 FP_COMP_OPS_EXE_SSE_FP_PACKED
PMC1 FP_COMP_OPS_EXE_SSE_FP_SCALAR
PMC2 FP_COMP_OPS_EXE_SSE_SINGLE_PRECISION
PMC3 FP_COMP_OPS_EXE_SSE_DOUBLE_PRECISION
UPMC0 UNC_QMC_NORMAL_READS_ANY
UPMC1 UNC_QMC_WRITES_FULL_ANY
UPMC2 UNC_QHL_REQUESTS_REMOTE_READS
UPMC3 UNC_QHL_REQUESTS_LOCAL_READS
```

### METRICS

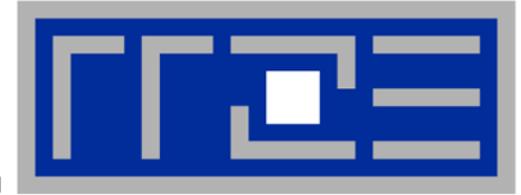
```
Runtime [s] FIXC1*inverseClock
CPI FIXC1/FIXC0
Clock [MHz] 1.E-06*(FIXC1/FIXC2)/inverseClock
DP MFlops/s (DP assumed) 1.0E-06*(PMC0*2.0+PMC1)/time
Packed MUOPS/s 1.0E-06*PMC0/time
Scalar MUOPS/s 1.0E-06*PMC1/time
SP MUOPS/s 1.0E-06*PMC2/time
DP MUOPS/s 1.0E-06*PMC3/time
Memory bandwidth [MBytes/s] 1.0E-06*(UPMC0+UPMC1)*64/time;
Remote Read BW [MBytes/s] 1.0E-06*(UPMC2)*64/time;
```

### LONG

Formula:

```
DP MFlops/s = (FP_COMP_OPS_EXE_SSE_FP_PACKED*2 + FP_COMP_OPS_EXE_SSE_FP_SCALAR)/ runtime.
```

- Groups are architecture-specific
- They are defined in simple text files
- Code is generated on recompile of likwid
- likwid-perfctr -a outputs list of groups
- For every group an extensive documentation is available



## **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

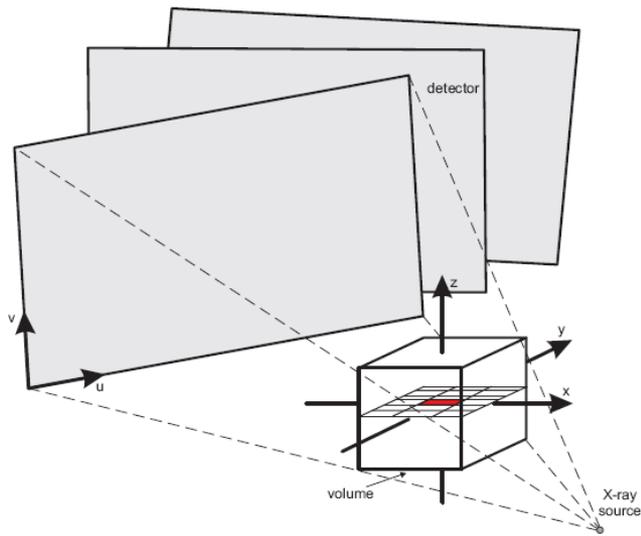
Minimum Power: 20 Watts

Maximum Power: 95 Watts

Maximum Time Window: 0.15625 micro sec  
-----

# Example:

A medical image reconstruction code on Sandy Bridge



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

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

