

# Programming Techniques for Supercomputers: Modern Processors

Characterization of memory hierarchies

Data access optimization

Prof. Dr. G. Wellein<sup>(a,b)</sup> , Dr. G. Hager<sup>(a)</sup>

<sup>(a)</sup> Erlangen National High Performance Computing Center (NHR@FAU)

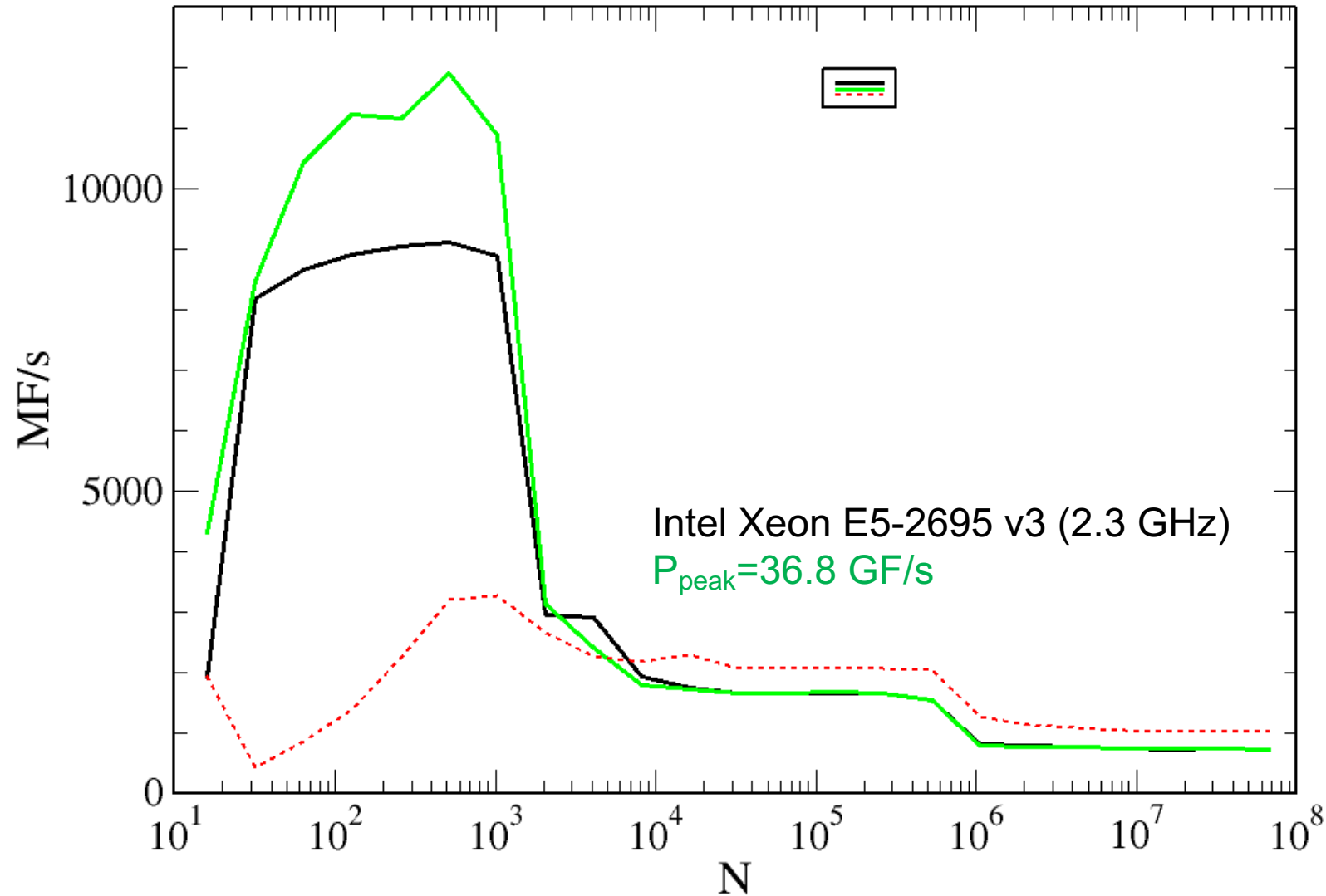
<sup>(b)</sup> Department für Informatik

Friedrich-Alexander-Universität Erlangen-Nürnberg, Sommersemester 2024



# Characterization of Memory Hierarchies – Motivation

- Vector Triad single core performance:  $\mathbf{A}[1:N] = \mathbf{B}[1:N] + \mathbf{C}[1:N] * \mathbf{D}[1:N]$



Can we explain performance based on hardware features?

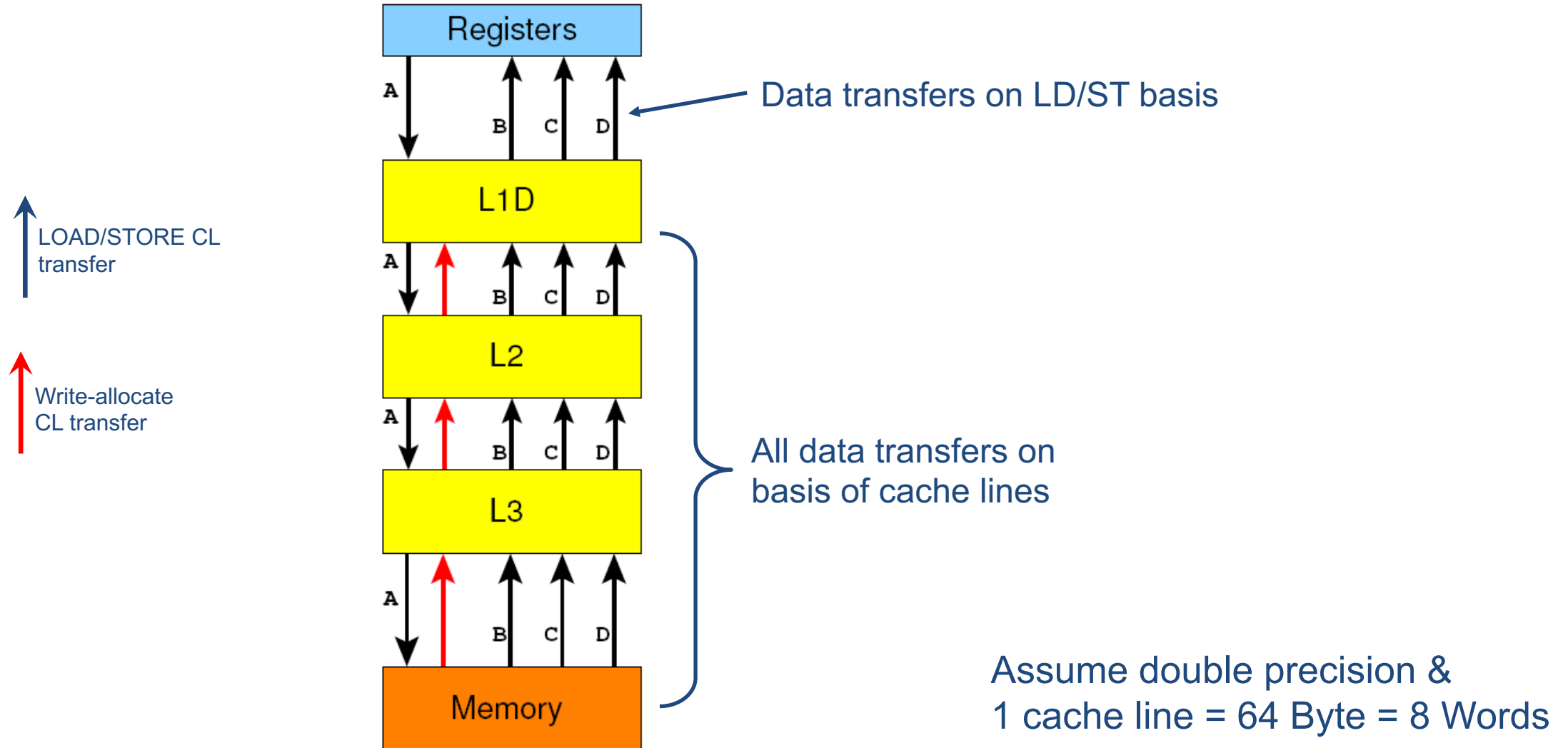
# Characterization of Memory Hierarchies

## Determine performance levels with low level benchmark: Vector Triad

```
DOUBLE PRECISION, dimension(SIZE):: A,B,C,D
DOUBLE PRECISION :: S,E,MFLOPS
! Input N .le. SIZE
DO i=1,N
    A(i) = 0.d0; B(i)=1.d0; C(i)=2.d0; D(i)=3.d0 ! initialize
ENDDO
call get_walltime(S)
DO ITER=1, NITER
    DO i=1, N
        A(i) = B(i) + C(i) * D(i)          ! 3 loads + 1 store; 2 FLOP
    ENDDO
    IF(A(2).lt.0) call dummy(A,B,C,D) ! Prevent loop interchange
ENDDO
call get_walltime(E)
MFLOPS = NITER * N * 2.d0 / ( (E-S) * 106 )
```

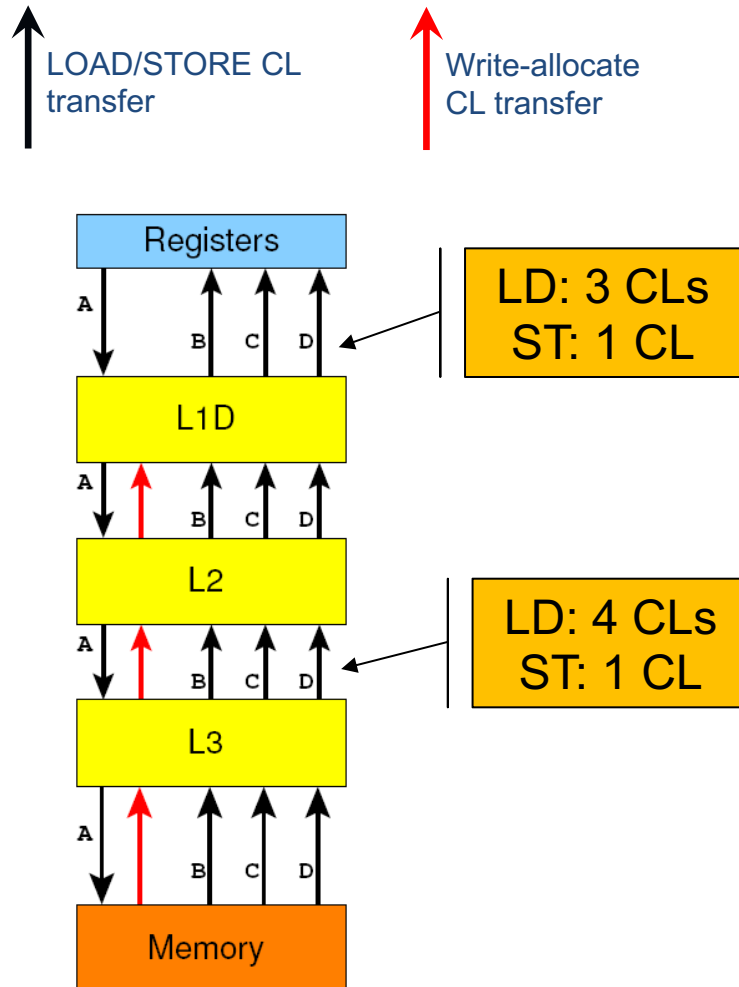
# Characterization of Memory Hierarchies: Vector Triads – Application model

Data transfer analysis: Vector Triad  $\mathbf{A}(\mathbf{i}) = \mathbf{B}(\mathbf{i}) + \mathbf{C}(\mathbf{i}) * \mathbf{D}(\mathbf{i})$



# Characterization of Memory Hierarchies: Vector Triads – Application model

## Data transfer analysis:



- **Unit of work:** 1 cache line update (1 CL update), i.e. 8 iterations:  
 $A(i:i+7) = B(i:i+7) + C(i:i+7) * D(i:i+7)$   
→ 16 F/CL-update

- Calculate data transfer time [#cy] for 1 CL update for every memory hierarchy (using machine model)  
→ Total data transfer time: #cy / CL update

→ Performance [F/s]:  
 $\{(16 \text{ F/CL-update}) / (\text{\#cy/CL-update})\} * \text{ClockSpeed}$

Consider pure data volume –  
no dependencies –  
no latencies

# Characterization of Memory Hierarchies: Processor Specs

## Intel Xeon E5-2695 v3 (“Haswell”) – Machine model

Microarchitecture	Haswell-EP
Shorthand	HSW
Xeon Model	E5-2695 v3
Year	09/2014
Clock speed (fixed)	2.3 GHz
Cores/Threads	14/28
<b>Load/Store throughput</b>	
AVX(2)	2 LD & 1 ST
SSE/scalar	2 LD & 1 ST
L1 port width	2×32+1×32 B
ADD throughput	1 / cy
MUL throughput	2 / cy
FMA throughput	2 / cy
<b>L2-L1 data bus</b>	
L2-L1 data bus	64 B
<b>L3-L2 data bus</b>	
L3-L2 data bus	32 B
LLC size	35 MiB
Main memory	4×DDR4-2133
Peak memory BW	34.2 GB/s
Load-only BW	32 GB/s
$T_{L3Mem}$ per CL	4.6 cy/CL

Assumptions: streaming  
(no latency penalty)

AXV LD/ST  
per cy

Calculate time per CL-  
transfer: #cy / CL

#cy/CL

Cluster-on-die  
Mode  
(BW for 7 cores)

Machine  
characteristics:

Arithmetic:  
2 FMA / cy

Registers

2 LD/cy + 1 ST/cy

L1

64 B/cy (→ 1 cy/CL)

L2

32 B/cy (→ 2 cy/CL)

L3

32 GB/s (→ 4.6 cy/CL)

Mem

“No overlap” assumption!?

# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3 (“Haswell”) – L1 cache performance

For 1 CL update from L1 data, i.e., for 8 iterations:

$$\mathbf{A}(i:i+7) = \mathbf{B}(i:i+7) + \mathbf{C}(i:i+7) * \mathbf{D}(i:i+7)$$

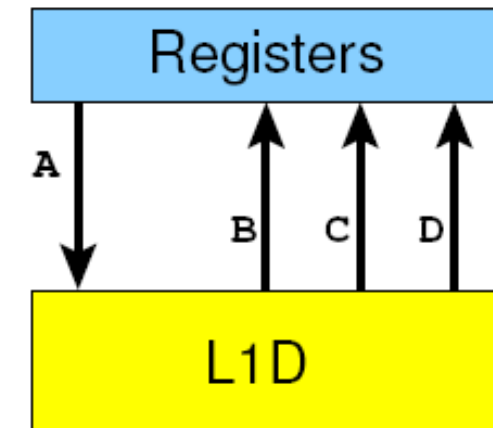
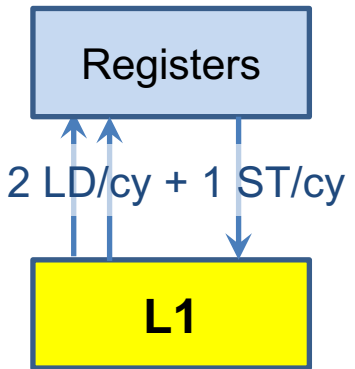
- 6 AVX LDs
  - $\mathbf{B}(i:i+3)$  ,  $\mathbf{B}(i+4:i+7)$
  - $\mathbf{C}(i:i+3)$  ,  $\mathbf{C}(i+4:i+7)$
  - $\mathbf{D}(i:i+3)$  ,  $\mathbf{D}(i+4:i+7)$
- 2 AVX STs
  - $\mathbf{A}(i:i+3)$  ,  $\mathbf{A}(i+4:i+7)$

→ Bottleneck: LD instructions → 6 LDs in 3 cy

→ 3 cy/CL-update for data in L1 cache

Machine characteristics:

Arithmetic:  
2 FMA / cy



# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3: L1 – L2 cache performance

For 1 CL update, i.e., for 8 iterations:

$$A(i:i+7) = B(i:i+7) + C(i:i+7) * D(i:i+7)$$

5 cache lines need to be transferred between L1 and L2 cache

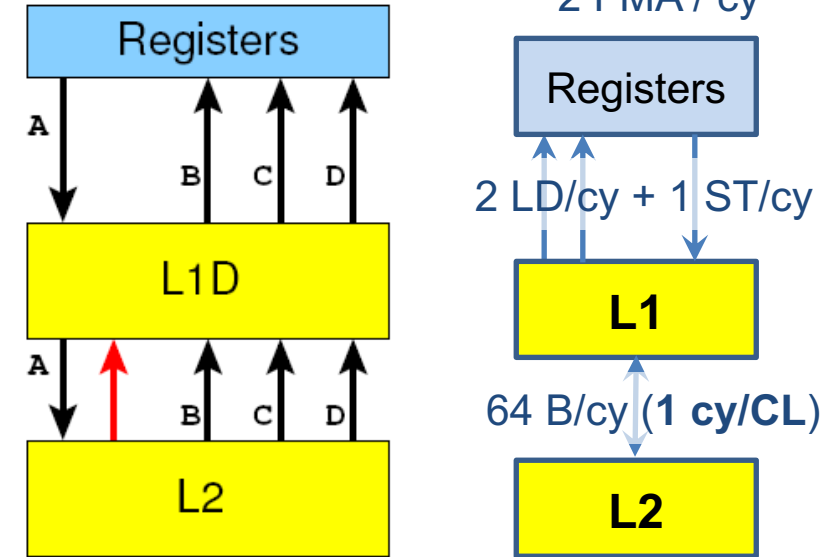
→ 5 cy / CL-update for L1 – L2 traffic

Total time for 1 CL update for L2 data

$$L2 \leftrightarrow L1 + L1 \leftrightarrow \text{Register} \rightarrow (5 \text{ cy} + 3 \text{ cy}) / \text{CL-update} = 8 \text{ cy} / \text{CL-update}$$

→ This assumes no overlap in data transfers (i.e., L1 cache is single ported)

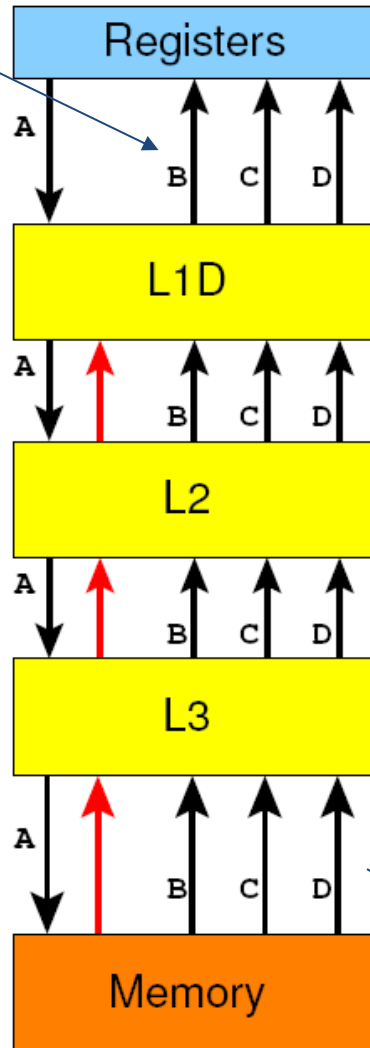
Machine characteristics:



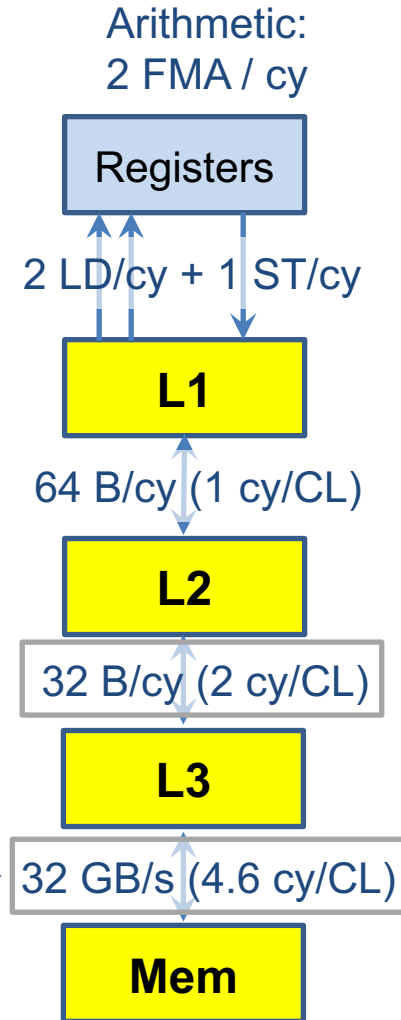


# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3 (“Haswell”)

Cache line (64 B)



Machine characteristics:



Where does data come from

Assuming no overlap throughout memory hierarchy

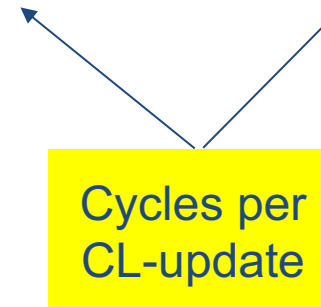
Hierarchy	Transfer time to next level	Total transfer time
L1	3 cy	3 cy
L2	5 cy	8 cy
L3	10 cy	18 cy
Memory	23 cy	41 cy

Cycles per CL-update

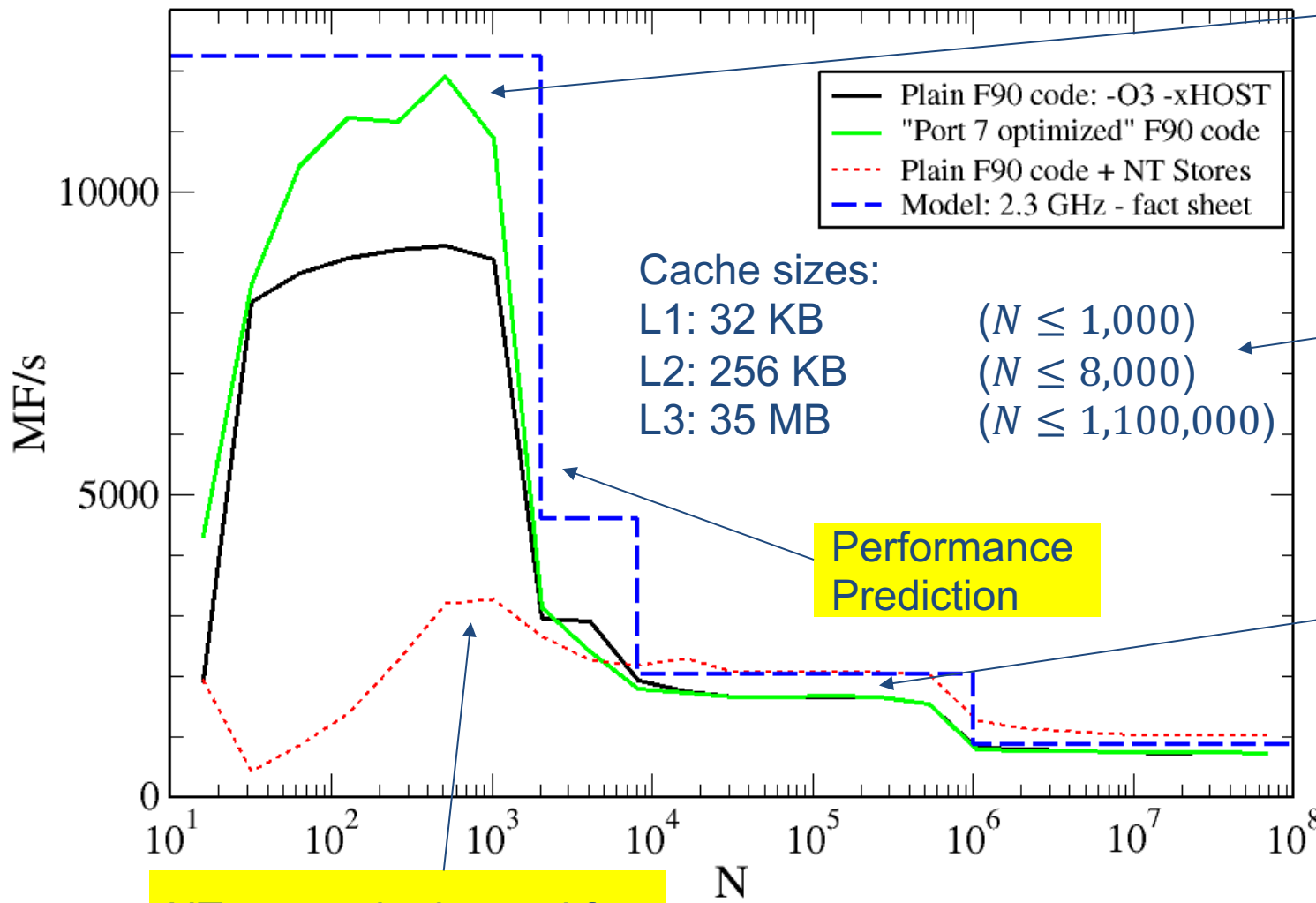
# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3 (“Haswell”)

- From cy/CL-update to MF/s
- Performance:  $\{(16 \text{ F/CL-update}) / (\# \text{cy/CL-update})\} * \text{ClockSpeed}$
- Clock speed of Xeon E5-2695 v3:  $2.3 \text{ GHz} = 2300 \text{ Mcy/s}$

Hierarchy	Transfer time to next level	Total transfer time	Performance prediction
L1	3 cy	3 cy	12266 MF/s
L2	5 cy	8 cy	4600 MF/s
L3	10 cy	18 cy	2044 MF/s
Memory	23 cy	41 cy	898 MF/s



# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3 (“Haswell”): Single core



Special addressing mode

Data set size  $N \cdot 4 \cdot 8$  B  
 $\leftrightarrow$  cache sizes

Performance Prediction

Good qualitative agreement

NT stores detrimental for inner cache performance

Underlying performance model: ECM model  
 H. Stengel, J. Treibig, G. Hager, and G. Wellein (2015) DOI:<https://doi.org/10.1145/2751205.2751240>

# Characterization of Memory Hierarchies: Vector Triads on Intel Xeon E5-2695 v3 (“Haswell”)

---

## Summary

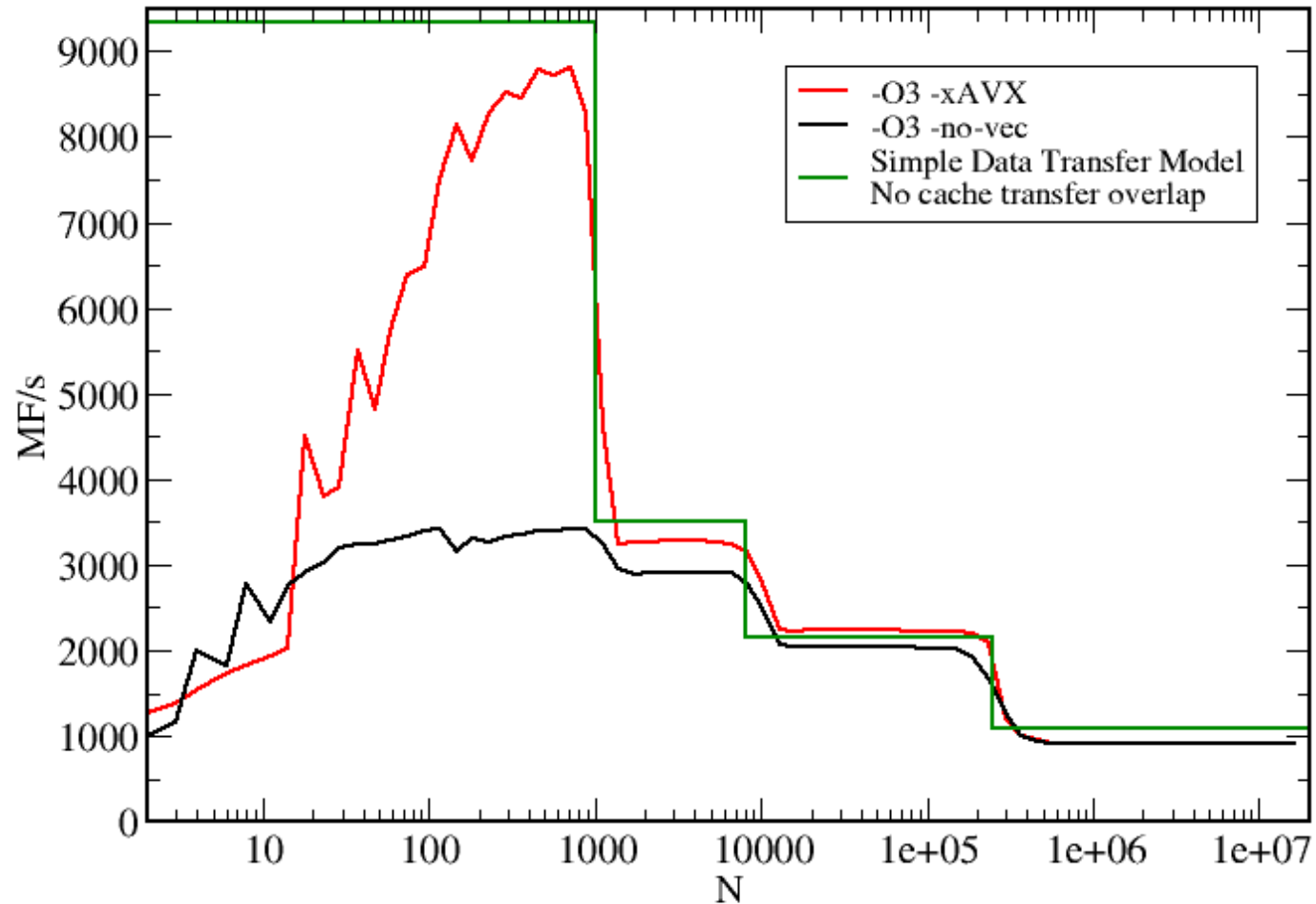
- Model/performance prediction purely based on fact sheet numbers and analysis of data transfers!
- Maximum attainable performance for triads in L1 ( $P_{max}$ ) is limited by LD port  
→ 2 FMA/3 cy → 1/3 peak performance (cf. lecture 3b)
- For lower cache levels:
  - Data transfer volume increases due to write allocate
  - No overlap assumption in hardware transfer fits well to Intel CPUs – individual transfer times within memory/cache hierarchy must be summed up
  - No overlap assumption does not hold on other architectures
  - L2 cache performance lower than expected: 64 B / cy too optimistic – low level benchmarks: ~ 32 B/cy – 48 B/cy

# Characterization of Memory hierarchies: Vector Triad

1 core Intel Sandy Bridge (AVX) desktop system

SNB 3.5 GHz (no Turbo, no SMT)

$A(:)=B(:)+C(:)*D(:)$  - ifort V12.1.0



Reg  $\leftrightarrow$  L1:  
256 Bit LD + 128 Bit ST

L1  $\leftrightarrow$  L2:  
256 Bit LD or ST

L2  $\leftrightarrow$  L3  
256 Bit LD or ST

L3  $\leftrightarrow$  MEM  
21.2 GB/s

# Data access optimization - case study: Dense Matrix Vector Multiplication (dMVM)



# Code balance metric: Quantify data traffic from various cache / memory levels

- Code balance ( $B_C$ ) quantifies how much data is transferred over a given data path per unit of work:

$$B_C = \frac{\text{data transfer [byte]}}{\text{amount of work [flops, it., CL updates,...]}}$$

- Code balance can be specified for each memory hierarchy level, e.g.,  $B_C^{mem}$ ,  $B_C^{L3}$ ,  $B_C^{L2}$
- Example: Vector triad  $A(:) = B(:) + C(:) * D(:)$  – double precision
- $B_C = (4+1) \text{ Words} / 2 \text{ Flops} = 2.5 \text{ W/F (including write allocate)} = 20 \text{ B/F}$   
(same for all memory hierarchies from L2 to main memory)
- “work” – often “flops,” but can be chosen problem specific

# Dense matrix-vector multiplication in DP

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

Left hand side  
(LHS) vector

Right hand side  
(RHS) vector

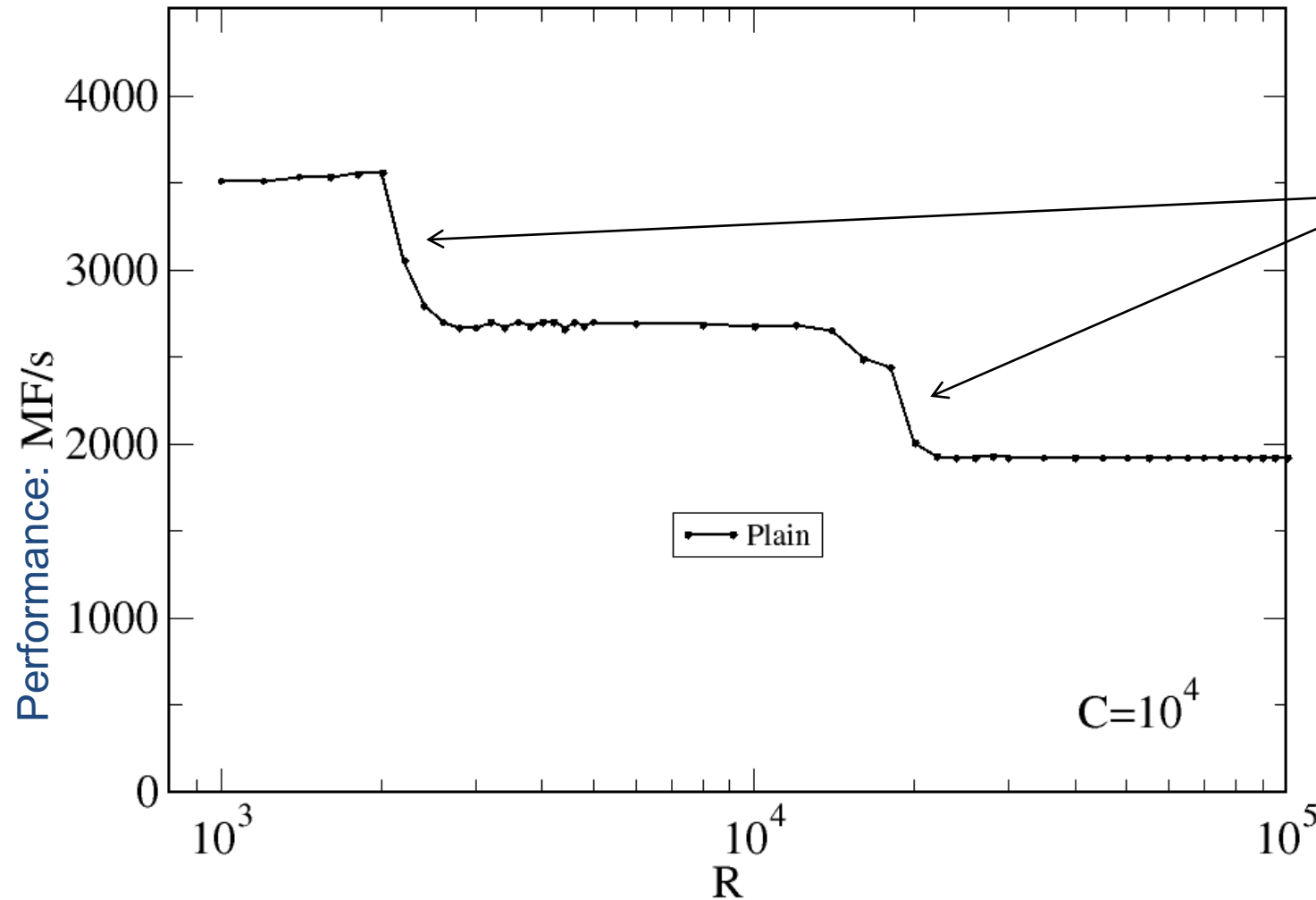
Work (inner loop):  
1 Iteration or 2 Flop

- Assume  $C = R \approx 10,000$  – double precision
- Size of data sets involved:
  - $\text{sizeof}(A(:, :)) = C * R * 8 \text{ Byte}$
  - $\text{sizeof}(y(:)) = R * 8 \text{ Byte}$
  - $\text{sizeof}(x(:)) = C * 8 \text{ Byte}$
- Total work (flops):  $2 * R * C \text{ Flop}$

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



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



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

Does code balance change?

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

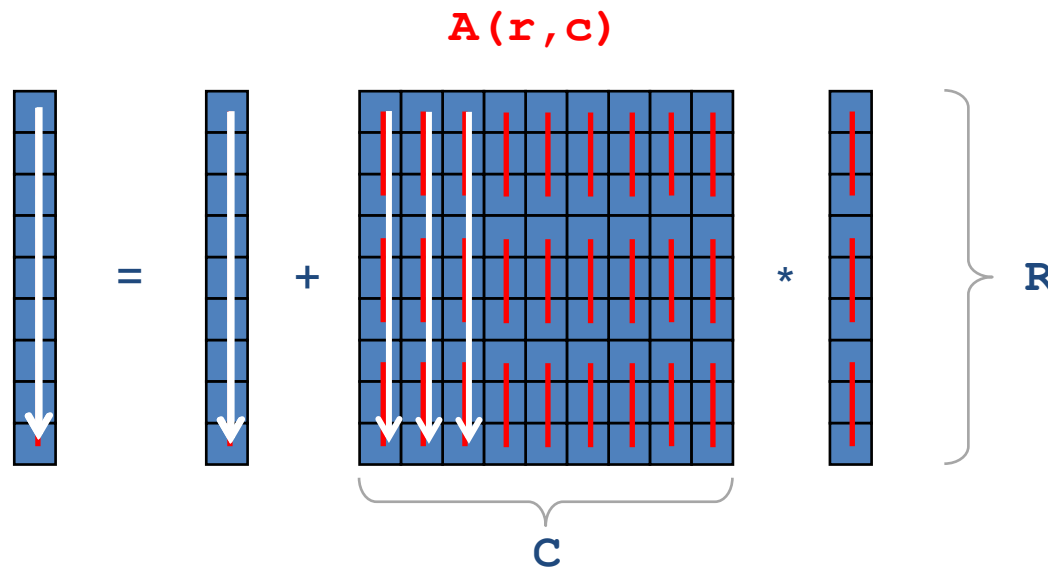
# DMVM data traffic analysis

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

`tmp` stays in a register during inner loop

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

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

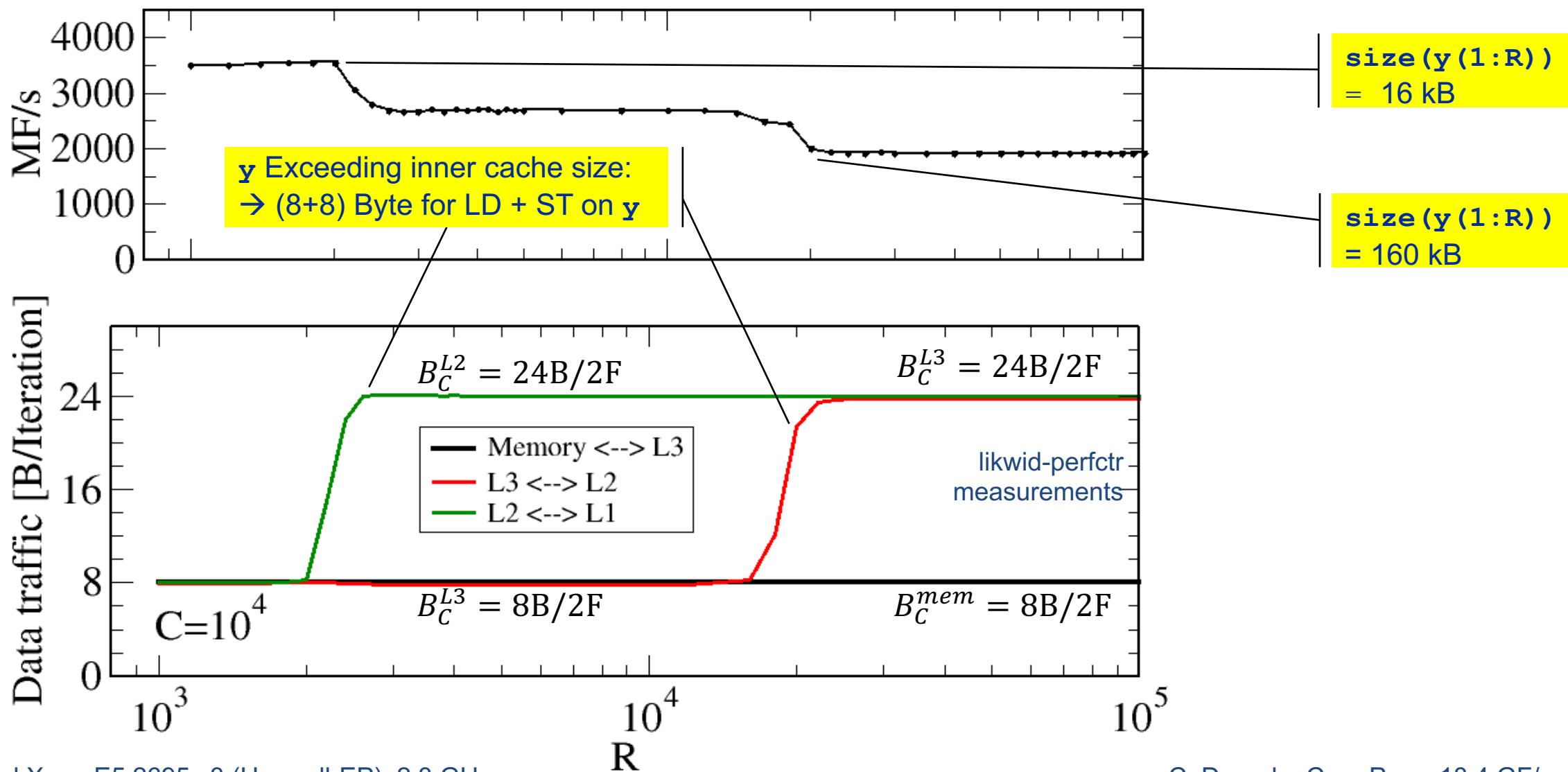


`y(:)` may not fit in innermost cache → more traffic from lower level caches for larger  $R$

Depending on  $R$ : Determine code balance in memory ( $B_C^{mem}$ ) and from relevant cache level(s) ( $B_C^{L3}, B_C^{L2}$ )!

See also discussion on [spatial/temporal](#) locality in lecture 4

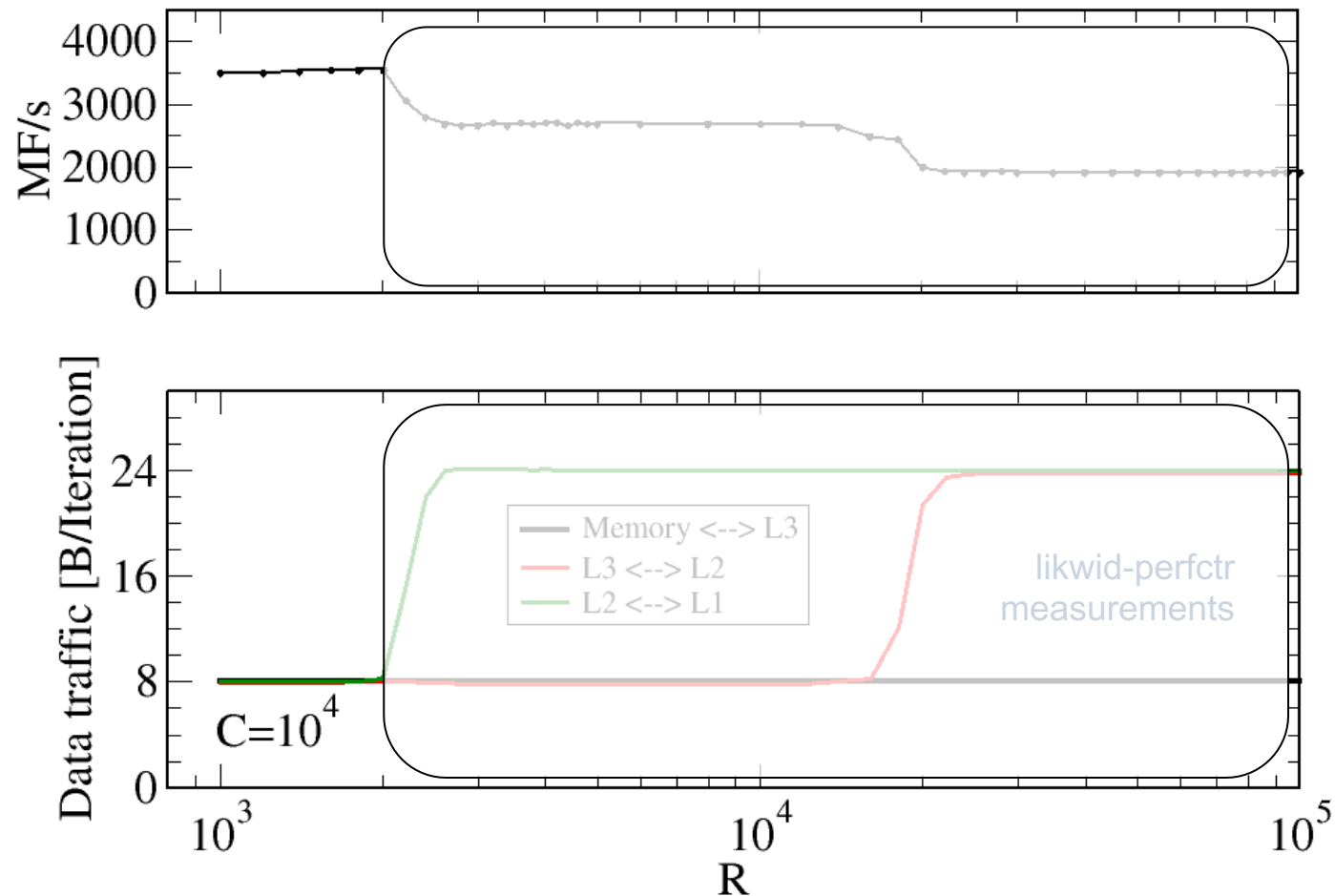
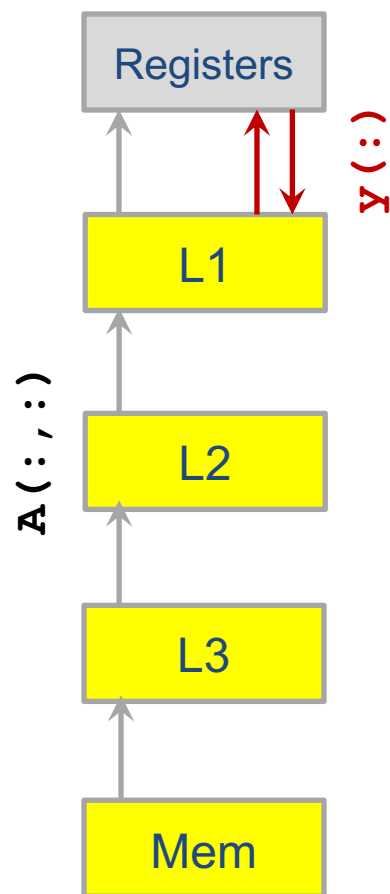
# DMVM (DP) – Single core data traffic analysis



Intel Xeon E5 2695 v3 (Haswell-EP), 2.3 GHz,  
 Caches: 32 KB / 256 KB / 35 MB, PageSize: 2 MB;

CoD mode, Core  $P_{peak} = 18.4$  GF/s,  
 ifort V15.0.1.133;  $b_S = 32$  Gbyte/s

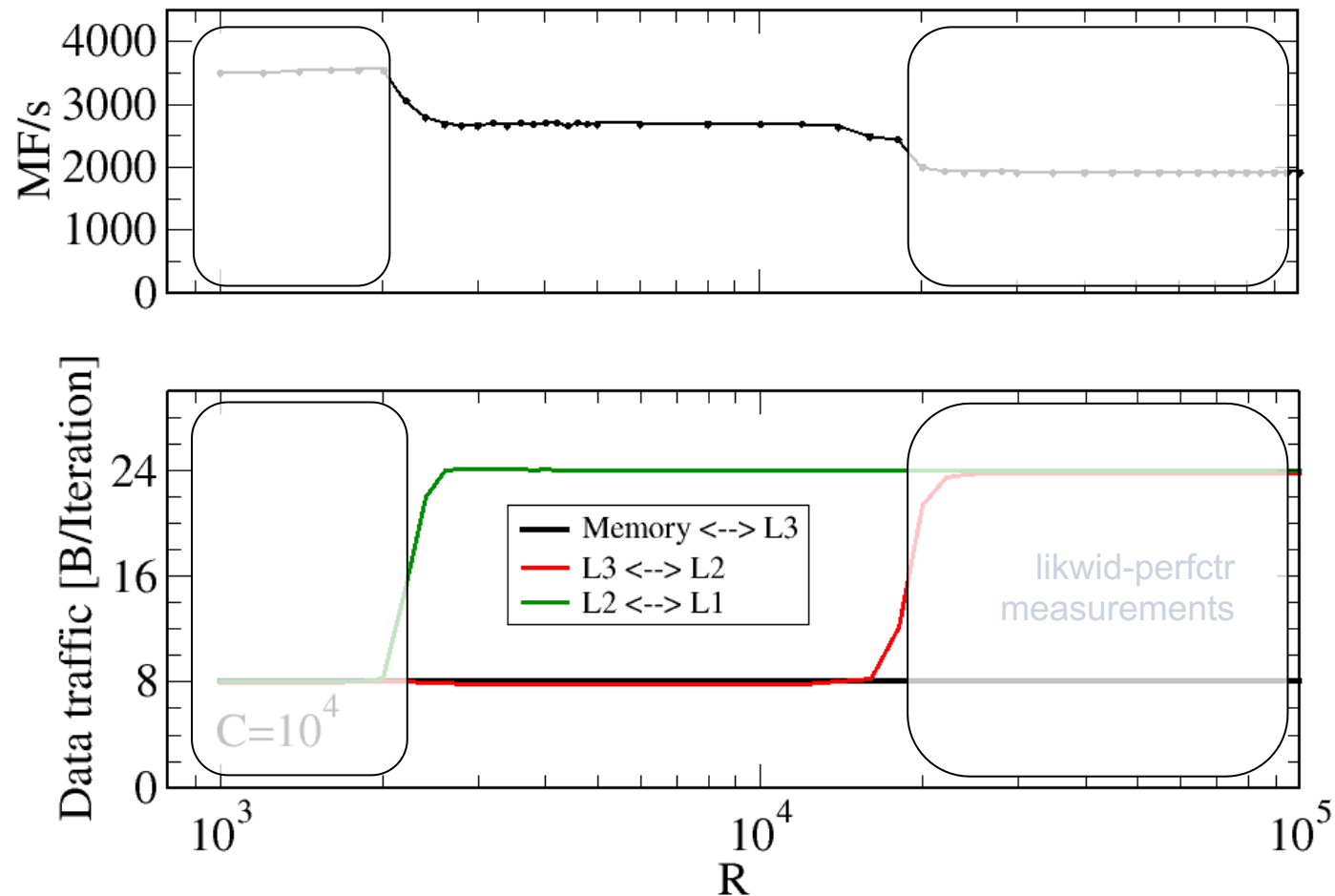
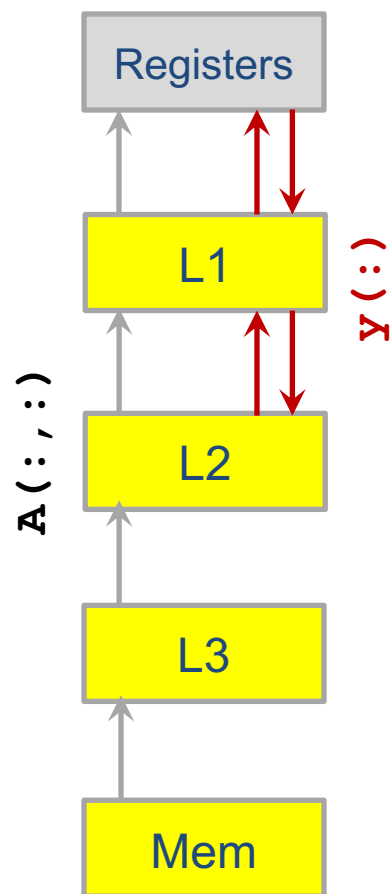
# DMVM (DP) – Single core data traffic analysis



Intel Xeon E5 2695 v3 (Haswell-EP), 2.3 GHz,  
Caches: 32 KB / 256 KB / 35 MB, PageSize: 2 MB;

CoD mode, Core  $P_{\text{peak}}=18.4$  GF/s,  
ifort V15.0.1.133;  $b_S = 32$  Gbyte/s

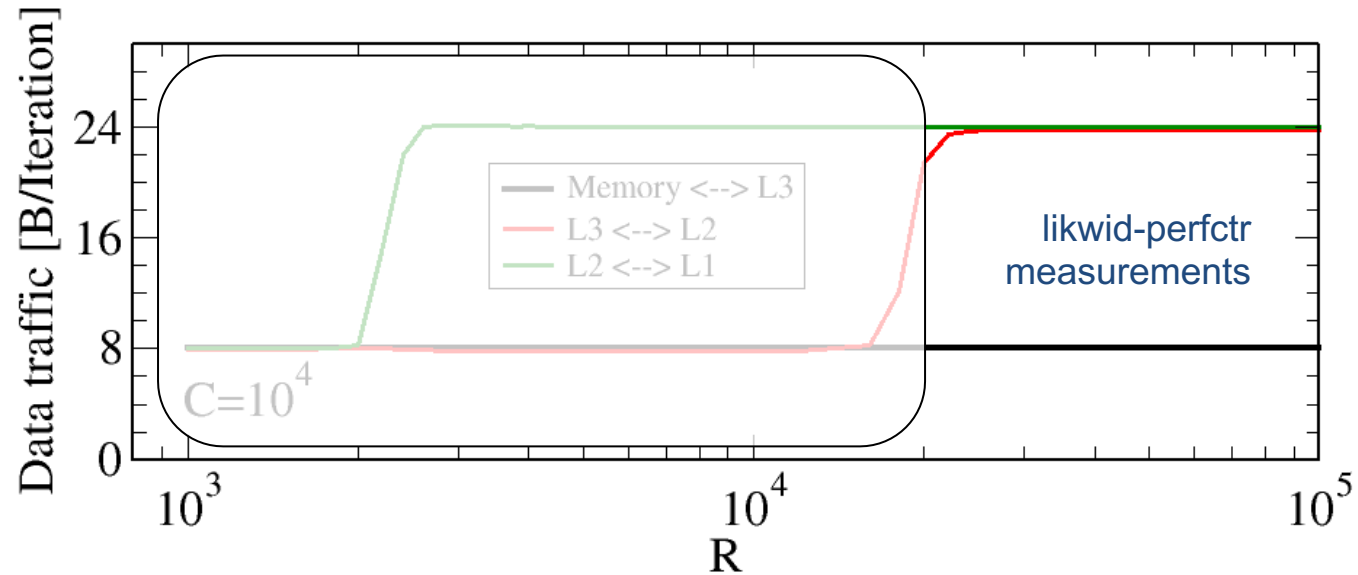
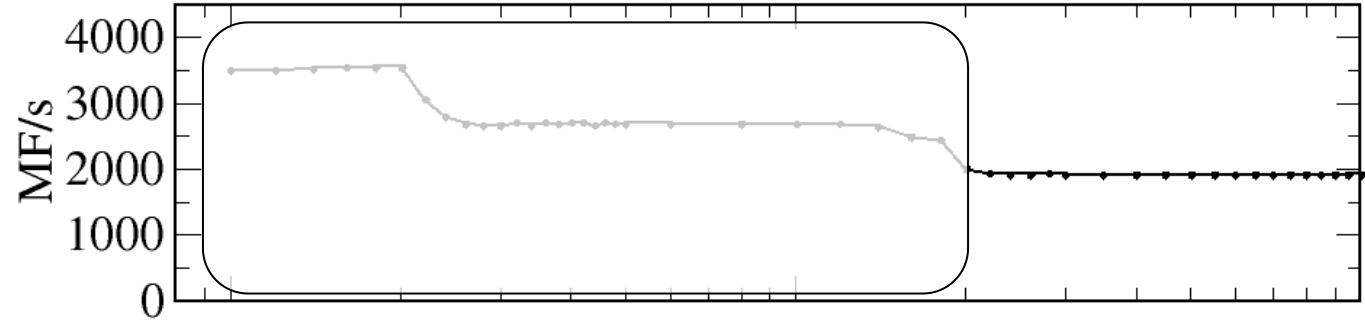
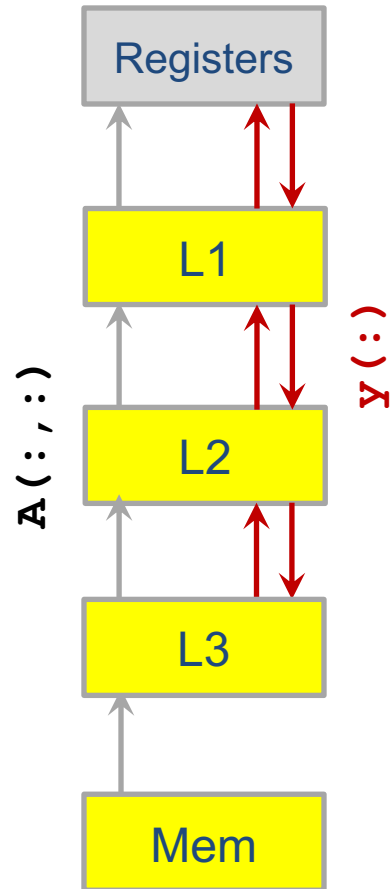
# DMVM (DP) – Single core data traffic analysis



Intel Xeon E5 2695 v3 (Haswell-EP), 2.3 GHz,  
Caches: 32 KB / 256 KB / 35 MB, PageSize: 2 MB;

CoD mode, Core  $P_{\text{peak}}=18.4$  GF/s,  
ifort V15.0.1.133;  $b_S = 32$  Gbyte/s

# DMVM (DP) – Single core data traffic analysis



Intel Xeon E5 2695 v3 (Haswell-EP), 2.3 GHz,  
Caches: 32 KB / 256 KB / 35 MB, PageSize: 2 MB;

CoD mode, Core  $P_{\text{peak}}=18.4$  GF/s,  
ifort V15.0.1.133;  $b_S = 32$  Gbyte/s

# DMVM (DP) – Single core data traffic analysis

Potential data transfer  
for y: 16 B / iteration

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

Data transfer for A:  
8 B / iteration

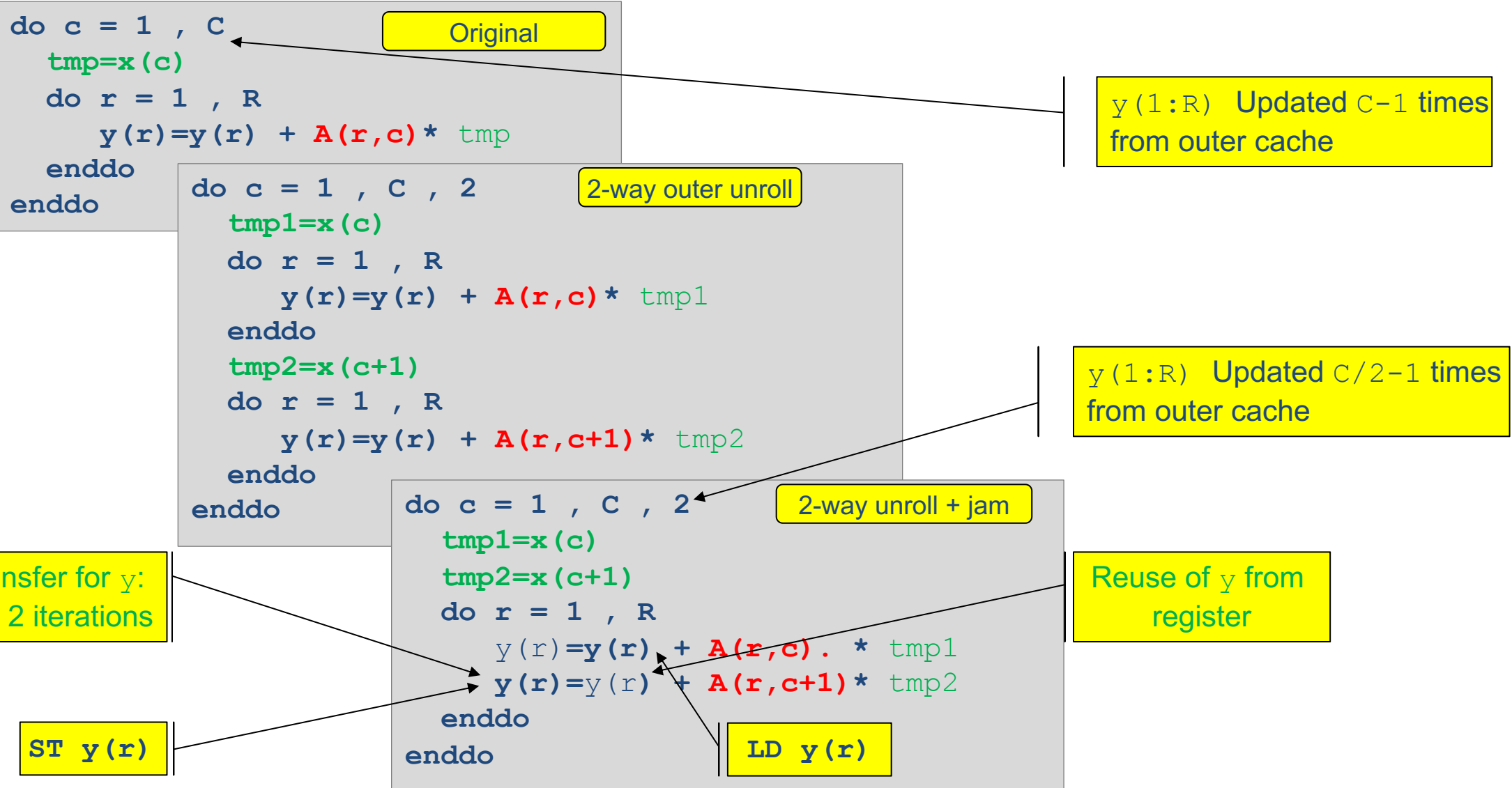
- Depending on  $R$  and cache size the code balance ( $B_C^i$ ) attains two values:
  - $B_C^i = 8 \frac{B}{it}$  if only the matrix data (8 B) is loaded from hierarchy  $i$  to inner caches (**best case**)
  - $B_C^i = (8 + 16) \frac{B}{it}$  if matrix data (8 B) is loaded and LHS data (16 B) is updated from hierarchy  $i$  (**worst case**)

# DMVM (DP) – reduce redundant LHS vector traffic

- Original version (summary)
  - Updating LHS vector ( $\underline{y} ( : )$ ) may dominate in-cache traffic
  - Worst case: Complete **vector  $\underline{y} (1 : R)$**  is **updated** in (travelling up & down to) some outer cache level **C-1 times**
- Strategies to **increase temporal locality** of LHS access in inner caches / register
  - **Outer Loop (c) Unroll and Jam** → Perform two “updates” of  $\underline{y} (r)$  in innermost loop  
→ Reuse of  $\underline{y} (r)$  in inner loop (register)
  - **Blocking/Tiling of inner (r) loop** such that “sufficiently” small parts of  $\underline{y} ( : )$  are updated  
→ Optimize block size for (L1) cache reuse.

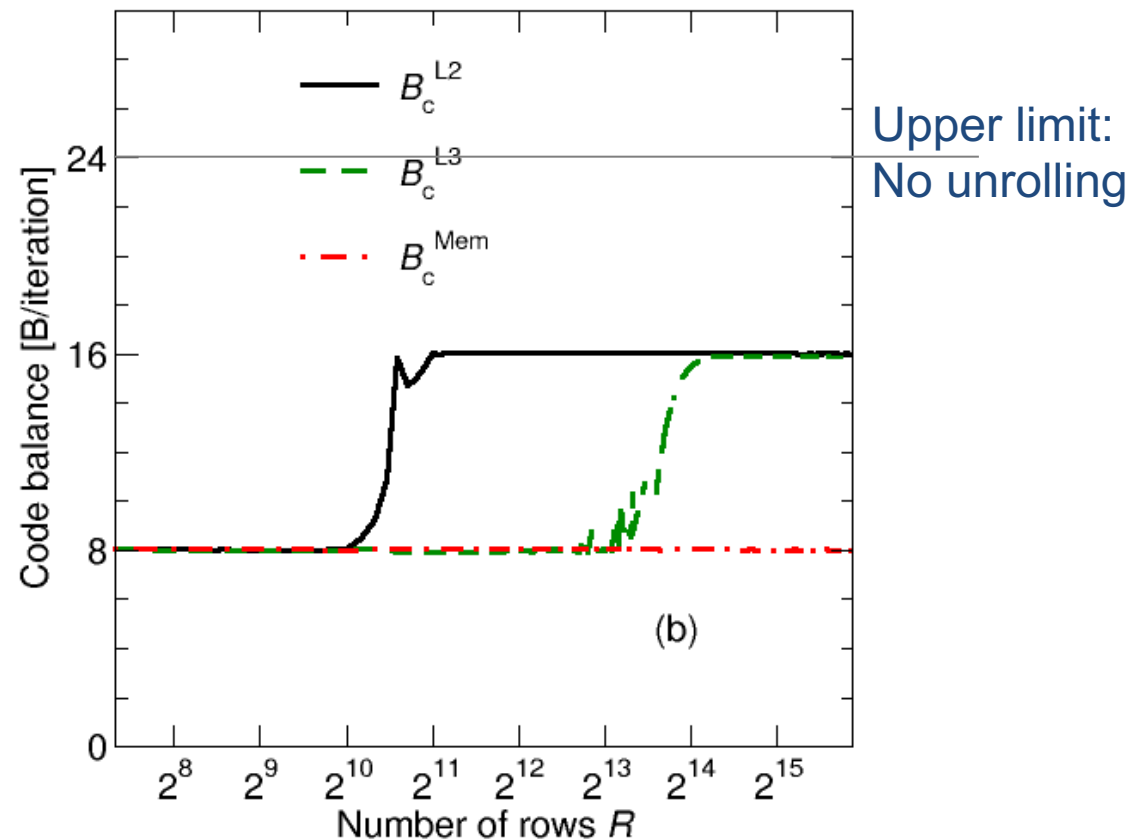
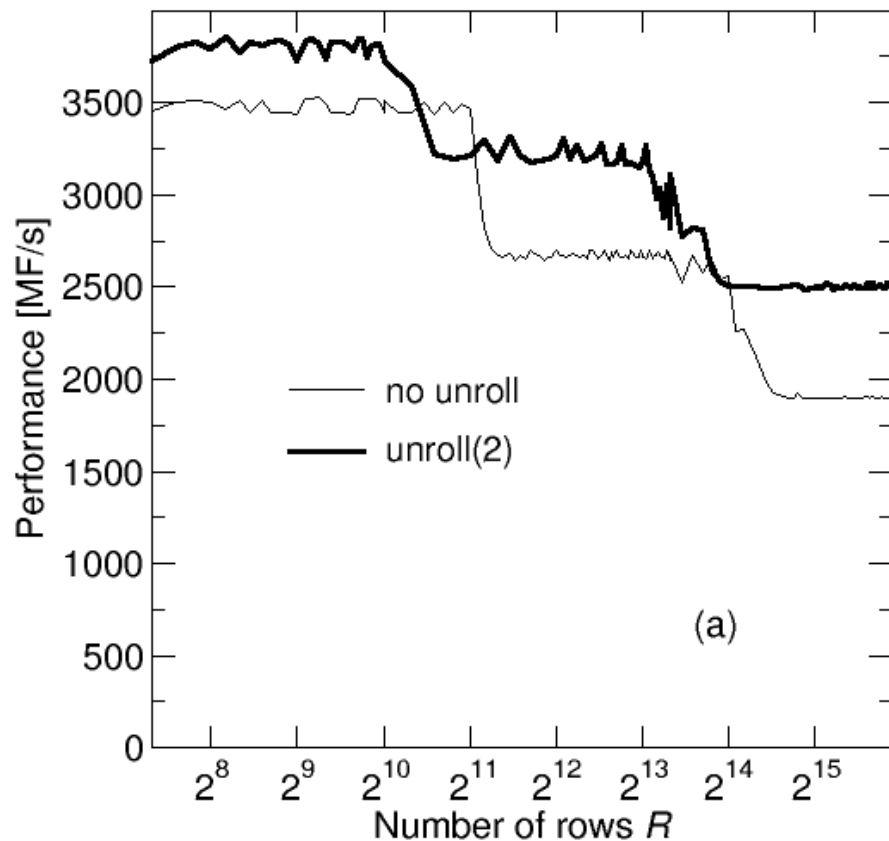


# Reducing traffic by “Outer Loop Unroll and Jam”



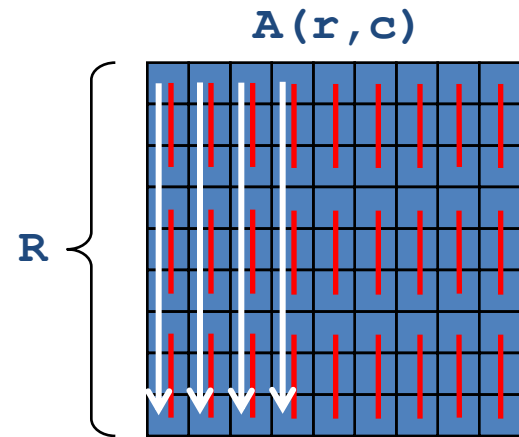
# Reducing traffic by “Unroll and Jam”

„2-way Unroll & Jam“ : Worst case balance is reduced:  $B_C^i = (8 + 16) B / \text{iteration} \rightarrow B_C^i = \frac{(16+16) B}{2 \text{ iterations}} = 16 B / \text{iteration}$



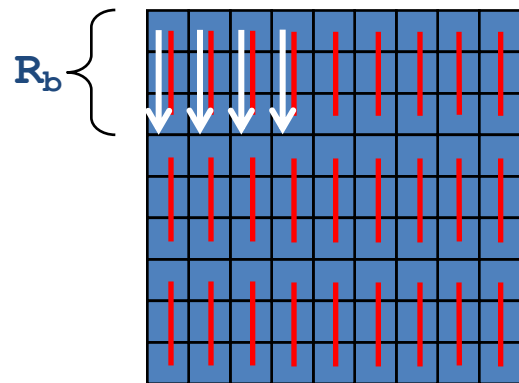
General case: For „m-way Unroll & Jam“ the worst case balance is  $B_C^i = (8 + \frac{16}{m}) B / \text{iteration}$

# Reducing traffic by “cache blocking/tiling”



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

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

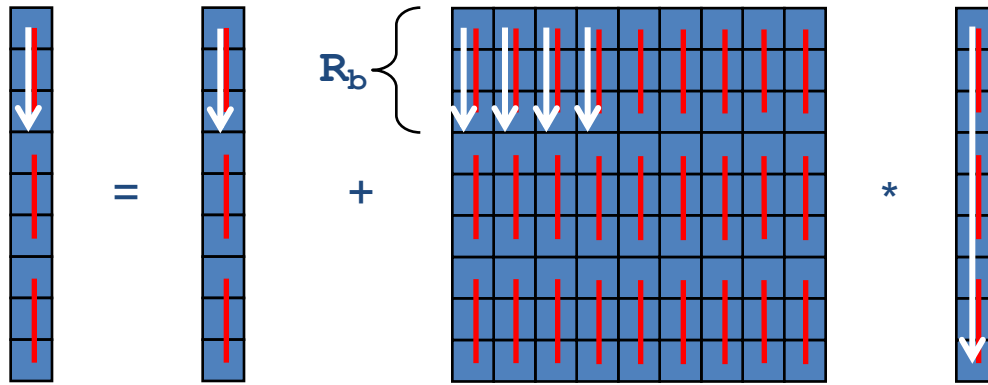


```
do rb = 1 , R ,  $R_b$ 
  rbS = rb
  rbE = min((rb+ $R_b$ -1) , R)
  do c = 1 , C
    do r = rbS , rbE
      y(r)=y(r) + A(r,c) * x(c)
    enddo
  enddo
enddo
```

$R_b$  free parameter – adapted to caches size

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

# Reducing traffic by “blocking/tiling”



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

- LHS only updated once in some cache level if blocking is applied
- Price: RHS is loaded  $R / R_b$  instead of once!

→ Contribution of  $y$  and  $x$  transfers to worst case code balance:

$$\frac{16B \times R \times C + 8B \times C}{R \times C \text{ iterations}} = \left(16 + \frac{8}{R}\right) \frac{B}{it.} \cong 16 \frac{B}{it.}$$

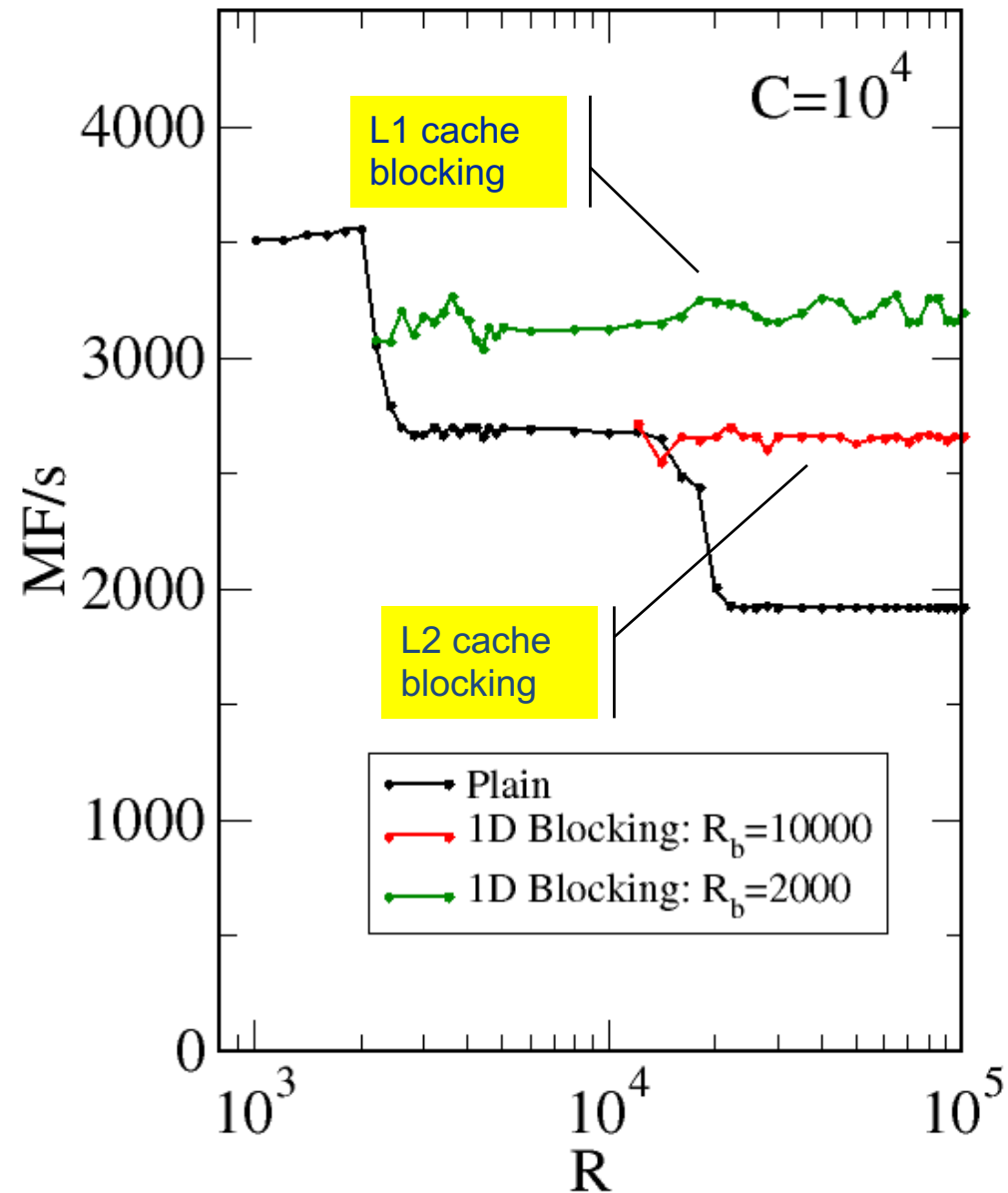
Original code

Blocking with factor  $R_b$

$$\frac{16B \times R + 8B \times C \times R / R_b}{R \times C \text{ iterations}} = \left(\frac{16}{C} + \frac{8}{R_b}\right) \frac{B}{it.} \cong \frac{8}{R_b} \frac{B}{it.}$$

→ Do not choose  $R_b$  too small

# DMVM (DP) – Reducing traffic by inner loop blocking

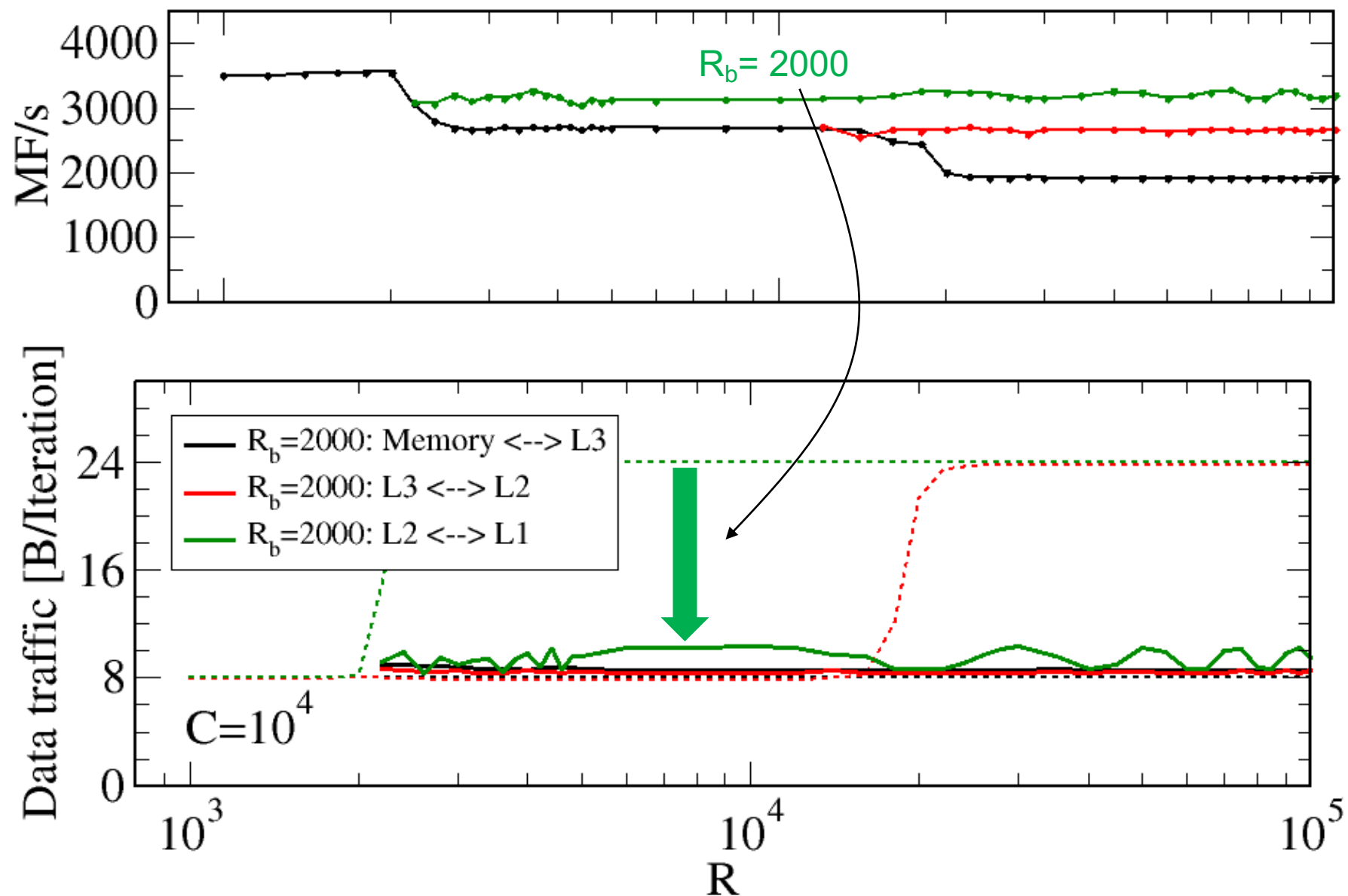


- “1D blocking” for inner loop
- Blocking factor  $R_b \leftrightarrow$  cache level

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

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

# DMVM (DP) – Validation of blocking optimization



# Conclusions from the dMVM example

- We have found the reasons for the **breakdown of single-core performance** with growing number of matrix rows
    - LHS vector fitting in different levels of the cache hierarchy
    - Validated theory by performance counter measurements
- Single core performance is sensitive to in-cache traffic volume
- **Inner loop blocking** was employed to improve code balance in L3 and/or L2
    - Validated by performance counter measurements
  - Outer Loop Unrolling also led to **better performance** – exploiting **temporal locality** in inner cache levels
  - Balance metric is useful to quantify data traffic per work ratio and estimate impact on performance

Data access optimizations:  
General considerations valid for any memory hierarchy levels

Classify basic operations classes with respect to their asymptotic balance characteristic and identify potential optimization strategies





# Basic idea

- Use “flop“-definition of balance for one hierarchy (memory):

$$B_C = \frac{\text{data transfer [B]}}{\text{amount of work [F]}}$$

- Consider characteristic balance scaling (as function of problem size) → lower balance is better
- For a given kernel determine as a function of problem size ( $N$ ):
  - **Minimum amount of data transfer** – a good lower bound is the size of the largest data structures involved
  - **Number of floating-point operations** to be executed – just count them
  - Consider leading order effects only ( $O(N^\alpha)$ )!

# Basic idea

- Example: Matrix-matrix multiplication (DGEMM)

```
do i=1,N
  do j=1,N
    do k=1,N
      c(j,i)=c(j,i)+a(k,i)*b(k,j)
    enddo
  enddo
enddo
```

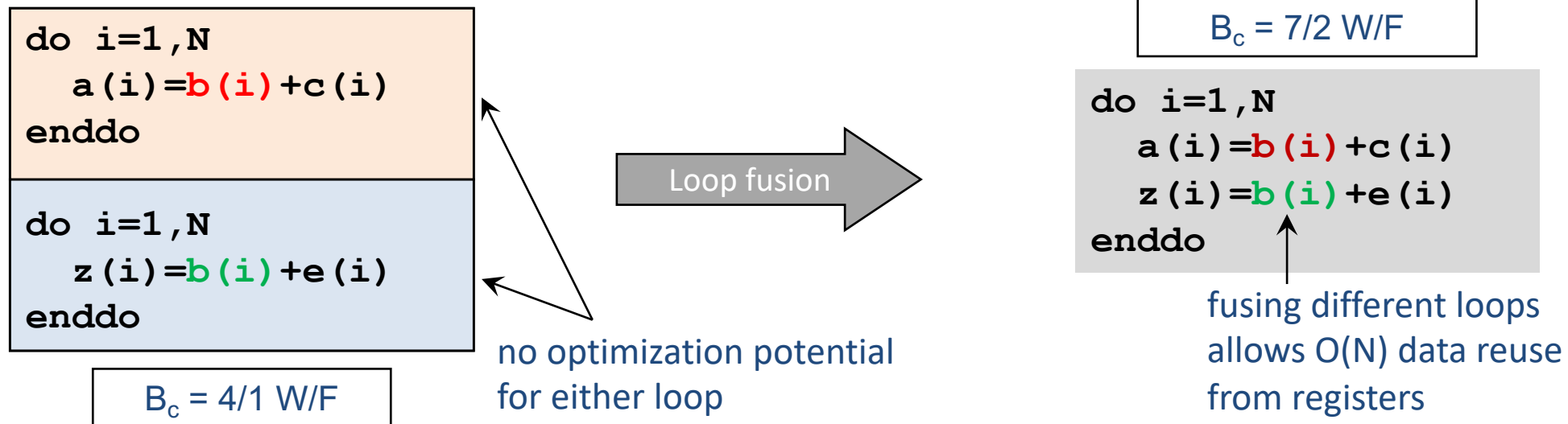
## Minimum Balance Analysis

- Amount of work  $\leftrightarrow$  3 nested loops  $\rightarrow 2 \times N^3 \times F$
- Minimum data transfer  $\leftrightarrow$  3+1 (NxN) matrices  $\rightarrow (3 + 1) \times N^2 \times 8 B$

$$\rightarrow B_C = \frac{32 * N^2}{2 * N^3} \frac{B}{F} = \frac{16}{N} \frac{B}{F} \rightarrow O(N^{-1}) \quad (\text{Minimum balance})$$

# Data access – general considerations $O(N)/O(N)$

- Case 1:  $O(N)/O(N)$  algorithms
  - $O(N)$  data access operations vs.  $O(N)$  arithmetic operations
  - Examples: Scalar product, vector addition, sparse MVM etc.
  - Performance **limited by memory BW** for large  $N$  (“memory bound”)
  - Limited optimization potential for single loops
    - ...**at most a constant factor** for multi-loop operations
- Example 1: successive vector additions (double precision: 1 W = 8 B)



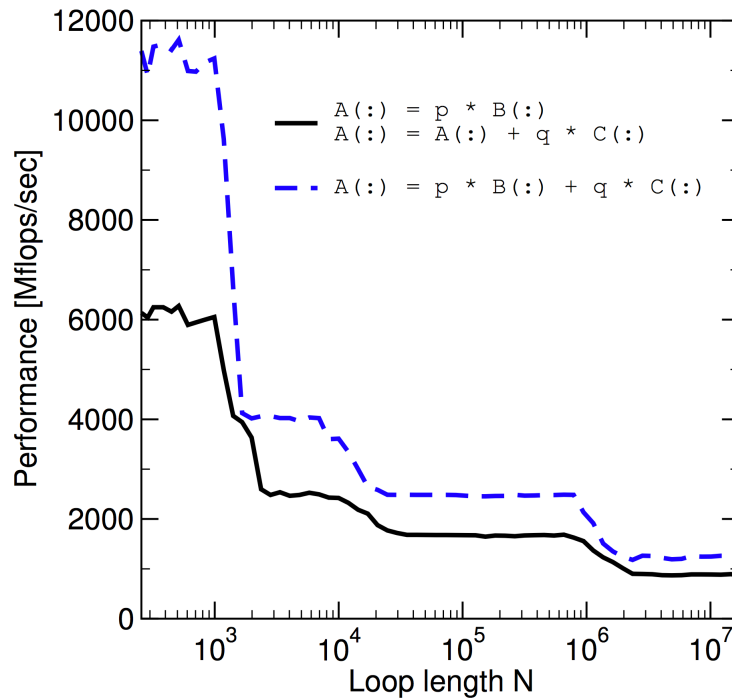
# Data access – general considerations $O(N)/O(N)$

## Example2

```
1 do i = 1,N ! 3 transfers, 1 flop
2   A(i) = p * B(i)
3 enddo
4 do i = 1,N ! 3 transfers, 2 flops
5   A(i) = A(i) + q * C(i)
6 enddo
```

loop fusion →

```
! optimized
do i = 1,N
! save two transfers for A(i)
! -> only 4 transfers
  A(i) = p * B(i) + q * C(i)
enddo
```



Intel Xeon E5-2660 v2 (“Ivy Bridge”):  
2.2 GHz; Caches: 32 KB / 256 KB / 25 MB

Below L1 cache reduction in balance directly correlates with increasing performance

In L1 cache: ST is bottleneck in both variants → Speed-up by 2x

# Data access – general guidelines

## ■ Case 2: $O(N^2)/O(N^2)$ algorithms

- Examples: dense matrix-vector multiply, matrix addition, dense matrix transposition etc.
  - Nested loops
- Memory bound for large N
- Some optimization potential (at most constant factor)
  - Can often enhance code balance by **outer loop unrolling** and/or **spatial blocking**
- Example: dense matrix-vector multiplication

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

- data transfer  $\leftrightarrow$  1 (N×N) matrix  
→  $N^2 \times 8$  B
- amount of work  $\leftrightarrow$  2 nested loops  
→  $2 \times N^2$  F

$$\rightarrow B_C = \frac{8 \times N^2}{2 \times N^2} \frac{B}{F} = 4 \frac{B}{F} \left( \frac{O(N^2)}{O(N^2)} \right)$$

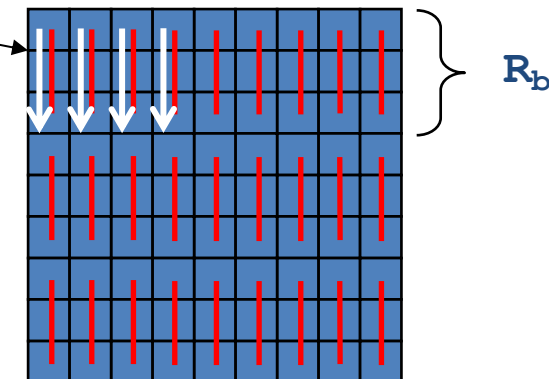

(Minimum balance)

# Data access – general guidelines

- $O(N^2)/O(N^2)$  algorithms – Optimization strategies
  - (Inner) Loop blocking/tiling (see slides 27 – 30)
  - (Outer) Loop unroll & Jam (see slides 25/26)
  - And combination of both
- Overheads to consider:
  - Significant code bloat
  - Short inner loops may cause overhead (e.g. fooling prefetcher: stop consecutive access and jump by large offset)
  - Loop Unrolling increases register pressure

```
do c = 1 , C , 2
  tmp1=x(c)
  tmp2=x(c+1)
  do r = 1 , R
    y(r)=y(r) + A(r,c) * tmp1
    y(r)=y(r) + A(r,c+1) * tmp2
  enddo
Enddo
```

5 registers



# Data access – general guidelines

- Case 3:  $O(N^{k-m}) / O(N^k)$  algorithms
  - Most favorable case – computation outweighs data traffic by factor of  $N^m$
  - Minimum balance  $\propto N^{-m}$  (see slide 31 for  $m=1$  / DGEMM)
  - Huge optimization potential: proper optimization can render the problem cache-bound if  $N$  is large enough
  - Examples Dense matrix-matrix multiplication ( $k=3; m=1$ ; DGEMM; see slide 31)
  - Naïve implementation may still have much worse balance:

```
do i=1,N
  do j=1,N
    do k=1,N
      c(j,i)=c(j,i)+a(k,i)*b(k,j)
    enddo
  enddo
enddo
```

Core task: dense MVM  
( $B_C = 4 \frac{B}{F}$ )  $\rightarrow O(N^2)/O(N^2)$   
 $\rightarrow$  memory bound

3  $N^2$  data elements involved BUT main memory traffic  $\sim N^3$  for large  $N$   
Reason:  $b(:,i)$  needs to be reloaded  $N$  times!

$\rightarrow$  Implement (spatial) blocking + unrolling!

# Data access – general guidelines

- $O(N^1)/O(N^2)$  Example:

---

```
1 do i = 1,N
2   do j = 1,N
3     sum = sum + A(i) * B(j)
4   enddo
5 enddo
```

---

Outer Loop Unroll  
& Jam

---

```
1 do jbs = 1,N,Rb
2   jstart = jbs; jend = min(jbs+Rb-1,N)
3   do i = 1,N,2
4     do j = jstart,jend
5       sum1 = sum1 + A(i) * B(j)
6       sum2 = sum2 + A(i+1) * B(j)
7     enddo
8     sum = sum + sum1 + sum2
9   enddo
10 enddo
```

---

Blocking Inner Loop



# Data access – general guidelines

## ■ DGEMM Example:

```
subroutine mmm(a,b,c,n)
integer :: n
double precision :: a(n,n),b(n,n),c(n,n)
integer :: i,j,k

do k=1,n
  do j=1,n
    do i=1,n
      c(i,k) = c(i,k) +
              a(j,k) * b(i,j)
    enddo
  enddo
enddo

end subroutine mmm
```

Compiler blocks all loops (125/125/128)  
& unrolls the two outer loops by 4x  
→ 9.8 GF/s out of 17.6 GF/s for n=5,000

```
vectorized
LOOP BEGIN at scan_f.f90(47,3)
remark #25442: blocked by 125 (pre-vector)
remark #25440: unrolled and jammed by 4 (pre-vector)
remark #15542: loop was not vectorized: inner loop was already
vectorized
remark #25015: Estimate of max trip count of loop=125

LOOP BEGIN at scan_f.f90(48,6)
remark #25442: blocked by 125 (pre-vector)
remark #25440: unrolled and jammed by 4 (pre-vector)
remark #15542: loop was not vectorized: inner loop was already
vectorized
remark #25015: Estimate of max trip count of loop=125

LOOP BEGIN at scan_f.f90(49,9)
<Peeled loop for vectorization>
remark #25456: Number of Array Refs Scalar Replaced In Loop: 36
remark #25015: Estimate of max trip count of loop=3
LOOP END

LOOP BEGIN at scan_f.f90(49,9)
remark #25442: blocked by 128 (pre-vector)
remark #15300: LOOP WAS VECTORIZED
remark #15442: entire loop may be executed in remainder
remark #15448: unmasked aligned unit stride loads: 1
remark #15449: unmasked aligned unit stride stores: 4
remark #15450: unmasked unaligned unit stride loads: 7
remark #15451: unmasked unaligned unit stride stores: 12
remark #15475: --- begin vector cost summary ---
remark #15476: scalar cost: 142
remark #15477: vector cost: 62.500
remark #15478: estimated potential speedup: 2.150
remark #15488: --- end vector cost summary ---
remark #25456: Number of Array Refs Scalar Replaced In Loop: 36
remark #25015: Estimate of max trip count of loop=32
LOOP END
LOOP END
LOOP END
```

# Summary

---

- The **cost of data transfers** increases rapidly as they come from outer level caches / main memory
- **Increase spatial and temporal locality** by
  - outer loop unrolling,
  - spatial blocking
  - or a combination of both.
- Things to consider with these transformations:
  - Prefetchers – “sufficiently long” contiguous memory accesses (i.e., inner loops)
  - Limited number of registers limits unrolling factor
  - Overhead at “block boundaries”
  - Size of cache to block for