



Programming Techniques for Supercomputers: Modern processors

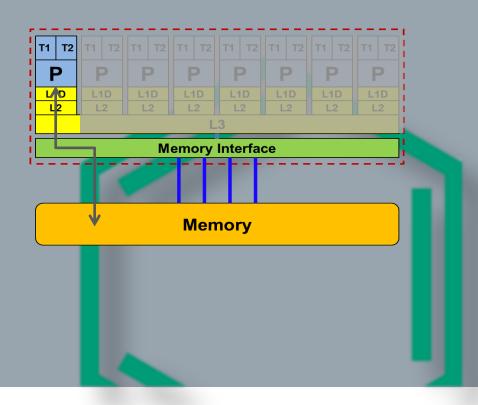
Architecture of the memory hierarchy

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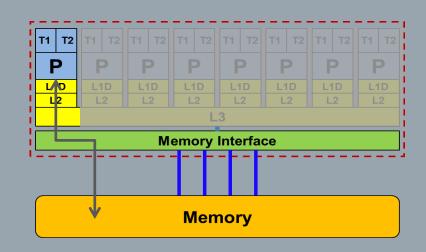
(b) Department für Informatik

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Architecture - Memory hierarchies:

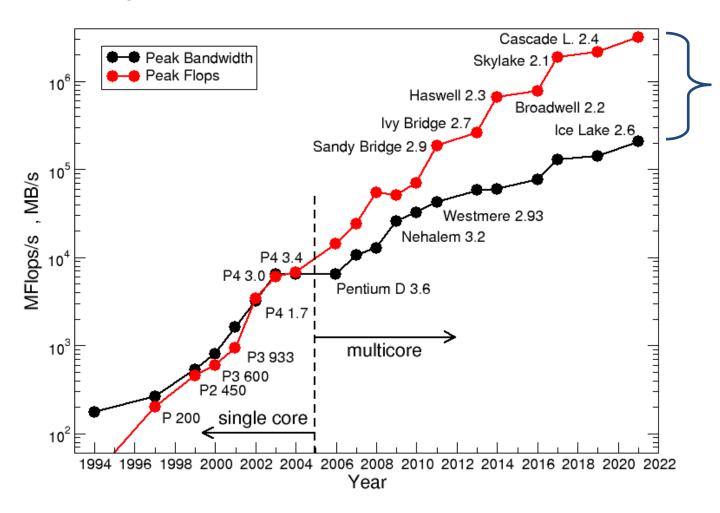
Caches - basics

Data access ←→ locality

Cache management

DRAM gap

DP peak performance and peak main memory bandwidth for a single Intel processor (chip)



Approx. 20 F/B

Main memory access speed not sufficient to keep CPU busy...

→ Fast on-chip caches, holding copies of recently used data items

Caches run at CPU clock → 5x-10x faster than memory

https://github.com/RRZE-HPC/TheBandwidthBenchmark/wiki/Memory-Wall

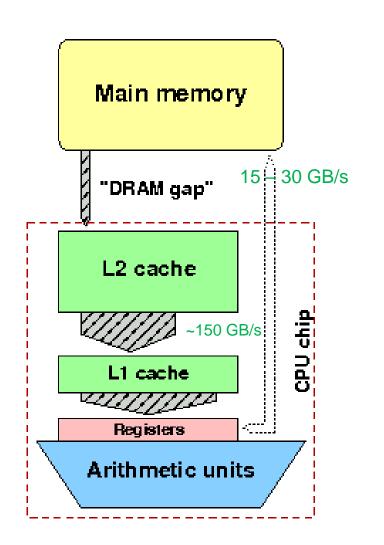
Schematic view of modern memory hierarchy & cache logic

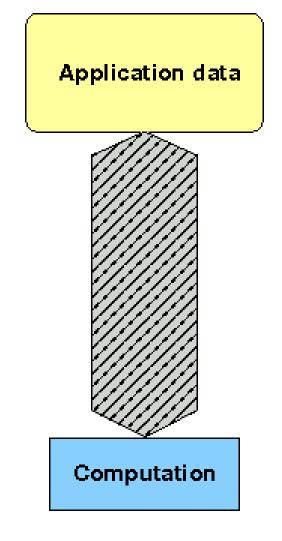
CPU issues a LOAD instruction Requests innermost cache to transfer a data item to a register

Cache logic automatically checks all cache levels whether data item is already in cache.

If data item is in cache ("cache hit") it is loaded to the register.

If data item is in no cache level ("cache miss") data item is loaded from main memory and a copy is held in cache.





Memory hierarchies: A model for effective bandwidth

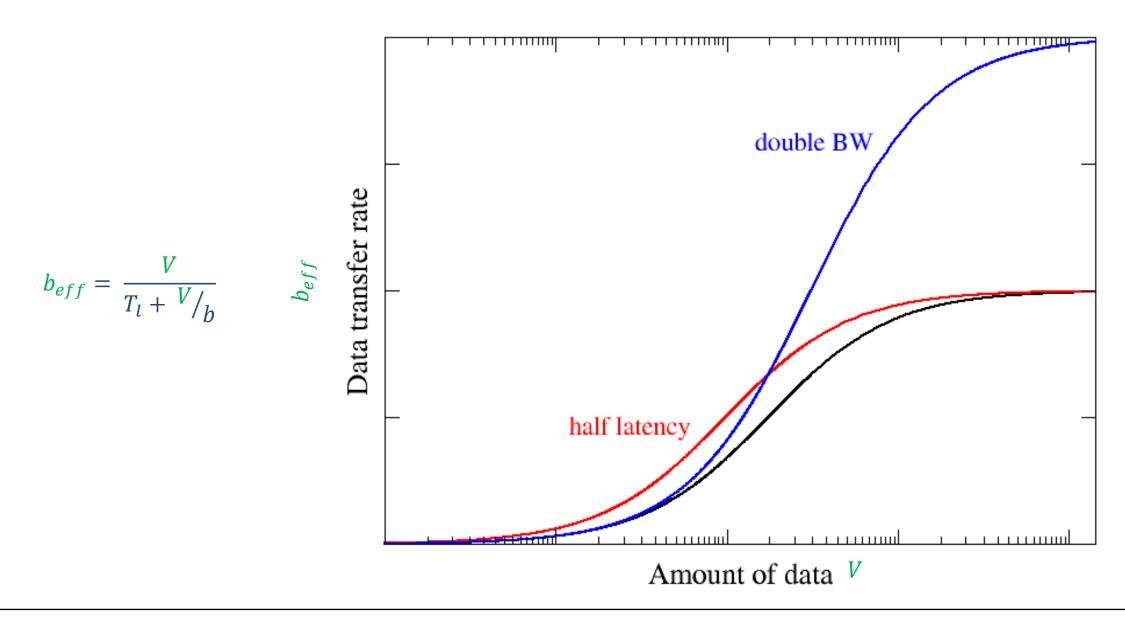
Hardware: Quantities to characterize the quality of a memory hierarchy:

- Latency (T_l) [s]: Set up time for data transfer from source (e.g., main memory or caches) to destination (e.g., registers)
- Bandwidth (b) [B/s]: Maximum amount of data per second which can be transferred between source (e.g., main memory or caches) and destination (e.g., registers)

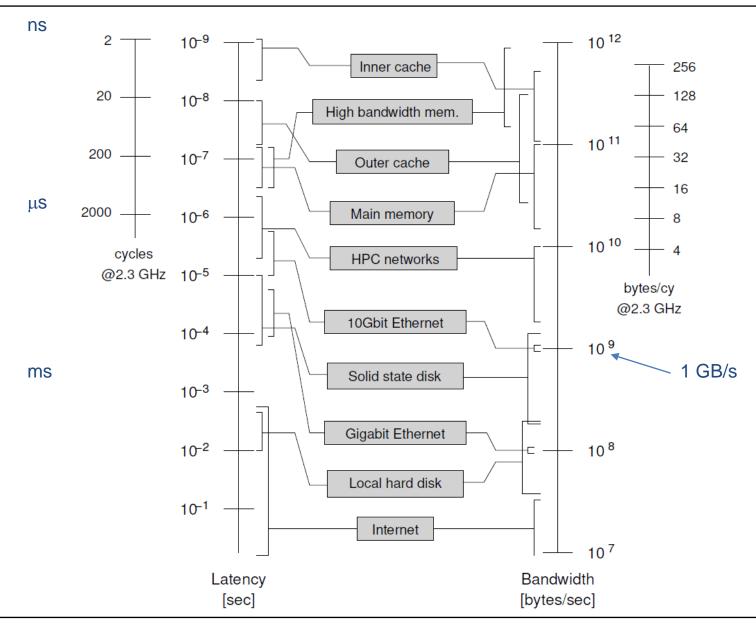
Application: Transfer time (T) and effective bandwidth (b_{eff}) depend on data volume (V) to be transferred:

- Transfer time: $T = T_l + \frac{V}{h}$ "Hockney's Model"
- Effective bandwidth: $b_{eff} = \frac{V}{T} = \frac{V}{T_l + V/b}$
 - "Low" data volume $(V \rightarrow 0)$: $b_{eff} \approx 0$
 - "Large" data volume $\left(\frac{V}{b} \gg T_l\right)$: $b_{eff} \approx b$

Memory hierarchies: A model for effective bandwidth



Latency and bandwidth in modern computer environments



Memory hierarchies: The latency problem

Main memory latency and bandwidth for modern multicore CPUs:

$$T_l = 64 \text{ ns } \& b = 64 \text{ GB/s}$$

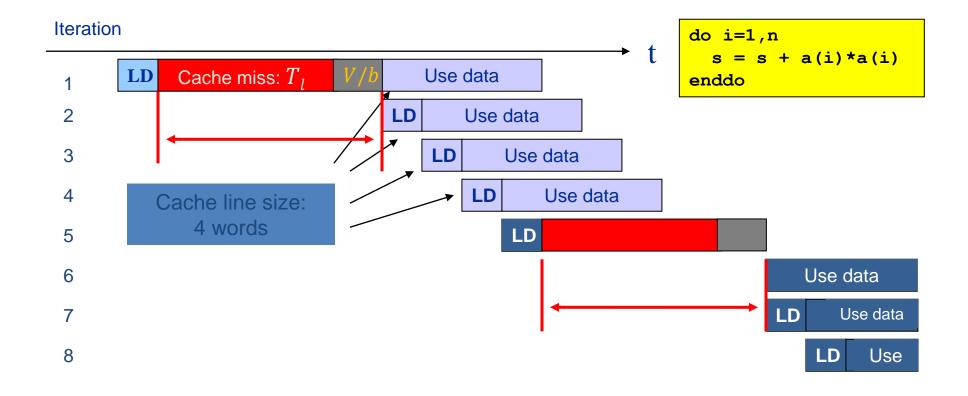
$$b_{eff} = \frac{V}{T} = \frac{V}{T_l + V/b}$$

V	T_l	V/b	T	b _{eff}
8 B	64 ns	0.125 ns	64.125 ns	0.13 GB/s
128 B	64 ns	2 ns	66 ns	1.9 GB/s
4096 B	64 ns	64 ns	128 ns	32 GB/s

- \rightarrow Data access is organized in cache lines (CL) always full cache line is transferred ($V = 64 \, \text{B}$ or $V = 128 \, \text{B}$ on modern architectures)
- → Multiple CLs must be loaded concurrently
 - → Multiple data requests by application code "non-blocking loads"
 - → Automatic hardware prefetching

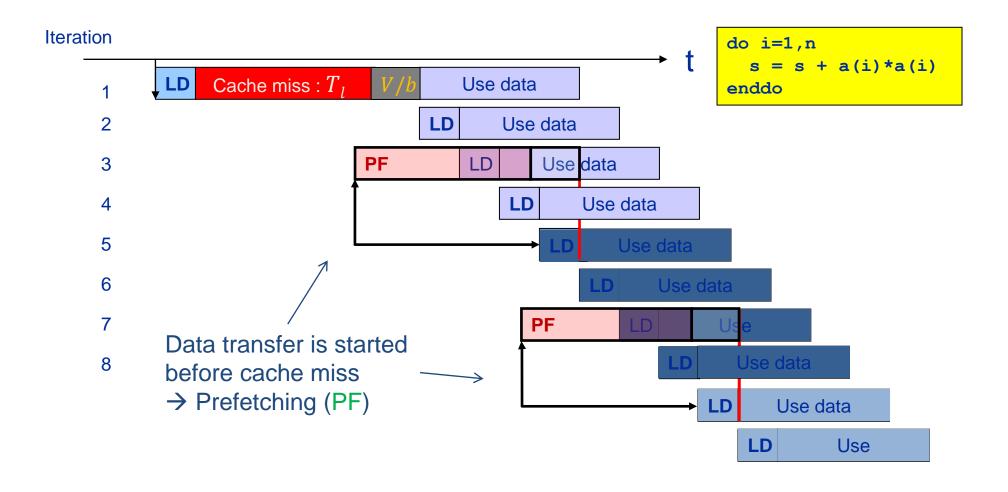
Memory hierarchies: Cache lines

- 1. If one data item is loaded from main memory ("cache miss"), whole cache line it belongs to is loaded
- 2. Cache lines are contiguous in main memory, i.e. "neighboring" items can then be used from cache



Memory hierarchies: (Automatic) Prefetching

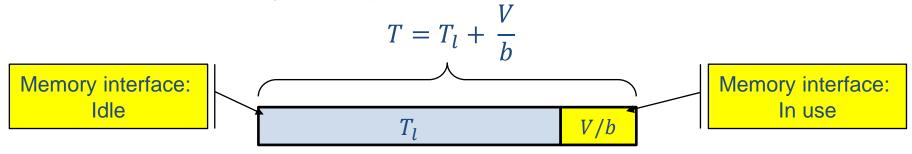
Prefetching data to hide memory latencies of CL transfers



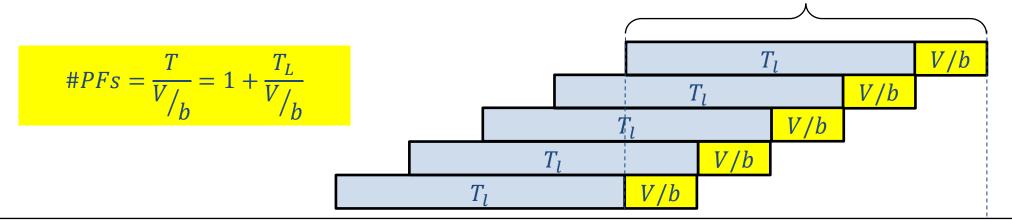
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Memory hierarchies: Hiding latency by concurrent PFs/LDs

- How many concurrent prefetches (or LDs) are required to
 - hide the latency (T_l) and eploit the full main memory bandwidth (b) ?
- Loading (LD) one cache line (V Bytes) requires total time



■ How many concurrent/outstanding PFs (or LDs) (P) are required to keep main memory interface busy for time?



Memory hierarchies: Hiding latency by concurrent PFs/LDs

- Example: CPU@2 GHz
 - Cache line size 64 B $\rightarrow V = 64B$
 - Cache: $T_l = 8 \text{ cy } \& b = 32 \text{ B/cy} \rightarrow P = 1 + \frac{8 \text{ cy}}{64 \text{ B/}_{32 \text{ B/cy}}} = 5$
 - → To hide latency, 5 PF/load operations must be active concurrently
 - Main memory: $T_l = 64 \text{ cy } \& b = 16 \text{ B/cy} \rightarrow P = 1 + \frac{64 \text{ cy}}{64 \text{ B/cy}} = 17$
 - → To hide latency, 17 PF/load operations must be active concurrently
 - \rightarrow This is 17*64 B = 1088 B (approx. 1 kB) of data "in-flight"

Memory Hierarchies: Prefetching – Hide memory latency

- Prefetch (PFT) instructions (limited use on modern architectures):
 - Transfer one cache line from memory to cache and then issue LD to registers
- Most architectures (Intel/AMD x86, IBM Power) use hardware-based automatic prefetch mechanisms
 - HW detects regular, consecutive memory access patterns (streams) and prefetches at will
 - Intel x86: Adjacent cache line prefetch loads 2 (64-byte) cache lines on L3 miss → Effectively doubles line length on loads (typical. enabled in BIOS)
 - Intel x86: Hardware prefetcher:
 Prefetches complete page (4 KB) if 2 successive CLs in this page are accessed
- Regular data access with long loops: Main memory latency is not an issue!
- Excessive data transfers for irregular access pattern or short consecutive loops

Memory Hierarchies: How to determine max. bandwidth from specifications

Intel® Xeon® Gold 6148 Processor

(see https://ark.intel.com/content/www/us/en/ark/products/120489/intel-xeon-gold-6148-processor-27-5m-cache-2-40-ghz.html)

Memory Specifications



Theoretical bandwidth of DDRx configuration:

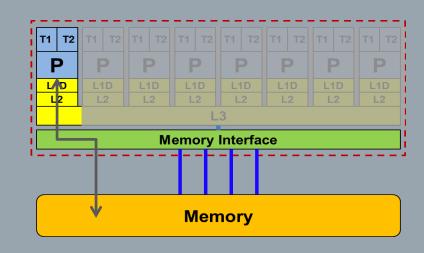
$$b_{peak} = \#Channels \times f_{MEM} \times 8 \frac{B}{cycle}$$

For above configuration we get:

$$b_{peak} = 6 \times 2,666 \frac{Mcycle}{s} \times 8 \frac{B}{cycle} = 127,968 \frac{MB}{s} = 128 \frac{GB}{s}$$







Architecture - Memory hierarchies:

Caches – basics

Data access ←→ locality

Cache management

Memory Hierarchies: Cache line ←→ Spatial access locality

- Cache line features
 - Cache line use is optimal for contiguous access ("stride 1") → STREAMING
 - Non-consecutive access reduces performance
 - Access with wrong stride (e.g. cache line size) can lead to disastrous performance breakdown
 - Typical CL sizes: 64 Byte (AMD/Intel) or 128 Byte (IBM)
- "Spatial locality": Ensure accesses to "neighboring" data items

```
GOOD ("Streaming")

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

```
BAD ("Strided")

do i=1,n,2
    s = s + a(i)*a(i)
enddo
```

If a (1:n) is loaded from main memory: ≈same runtime!

→ Performance of strided loop is half of the continuous one

- How to traverse multidimensional arrays?!
- Example: Initialize matrix A with A(i,j) = i*j
- What is the storage order of multidimensional-data structure?
- It depends, e.g. 2-dimensional 3x3 array A of doubles
- FORTRAN: column by column ("column major order")

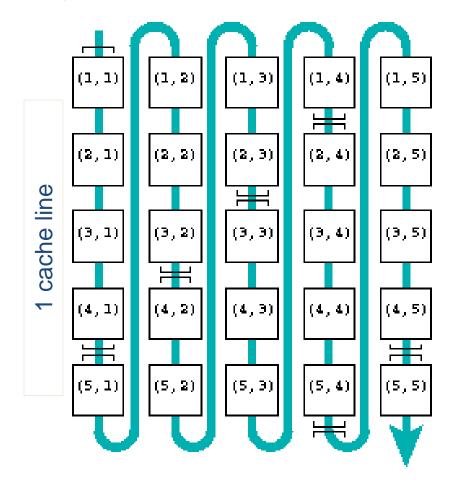
0 B Memory layout								71 B
A(1,1)	A(2,1)	A(3,1)	A(1,2)	A(2,2)	A(3,2)	A(1,3)	A(2,3)	A(3,3)

C/C++: row by row ("row major order")

0 B Memory layout								71 B
A[0][0]	A[0][1]	A[0][2]	A[1][0]	A[1][1]	A[1][2]	A[2][0]	A[2][1]	A[2][2]

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Default layout for FORTRAN: column by column (column major order)

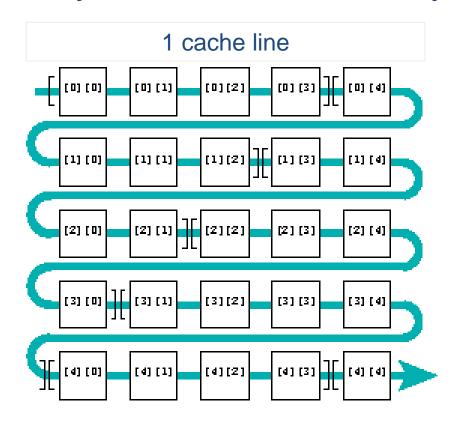


```
do i=1,n
do j=1,n
a(j,i)=i*j
enddo
enddo Continuous access!
```

```
do j=1,n
  do i=1,n
    a(j,i)=i*j
  enddo
enddo Stride n access!
```

FORTRAN: Inner loop must access innermost/left array index

Default layout for C/C++: row by row (row major order)



```
for (i=0; i<N; ++i) {
  for (j=0; j<N; ++j) {
    a[i][j] = i*j;
  }
} Continuous access!</pre>
```

```
for (j=0; j<N; ++j) {
  for (i=0; i<N; ++i) {
    a[i][j] = i*j;
  }
} Stride N access!</pre>
```

In C: Inner loop must access outermost/rightmost array index

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3-dimensional arrays in C/C++

```
for(i=0; i<N; ++i) {
  for(j=0; j<N; ++j) {
    for(k=0; k<N; ++k) {
      a[i][j][k] = i*j*k;
    }
  }
  Continuous access!</pre>
```

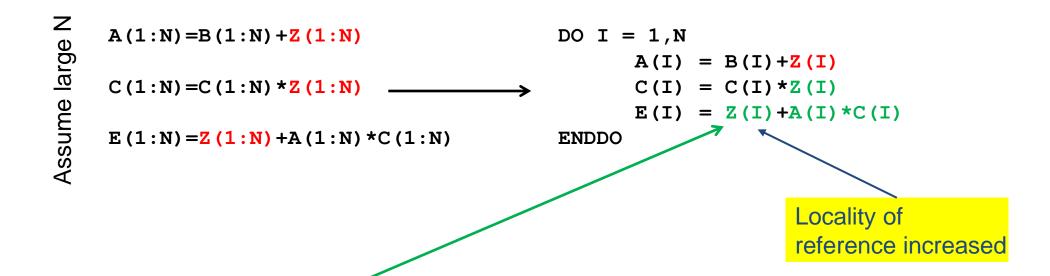
```
for (k=0; k<N; ++k) {
  for (j=0; j<N; ++j) {
    for (i=0; i<N; ++i) {
      a[i][j][k] = i*j*k;
    }
  }
  Stride N*N access!</pre>
```

- C/C++: Always start with rightmost index as inner loop index – if possible!
- Sometimes there are problems....
 (spatial blocking may improve the situation here)

```
for(i=0; i<N; ++i) {
  for(j=0; j<N; ++j) {
    a[i][j] = b[j][i];
  }
}</pre>
```

Memory Hierarchies: Data reuse - Temporal access locality

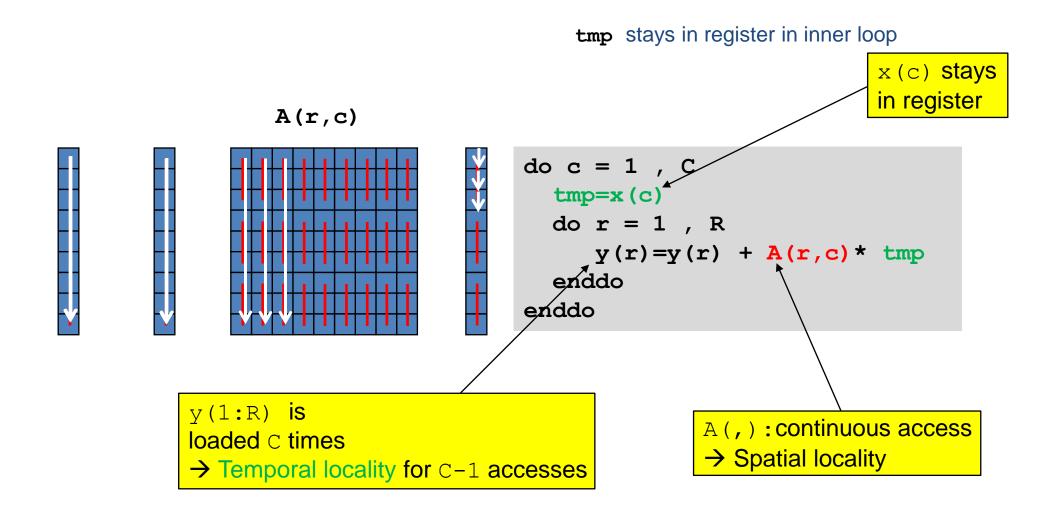
■ Efficient reuse of caches requires some "locality of reference", i.e. a data item loaded to register/cache needs to be reused several times "soon" before it gets old → "temporal locality"



Instead of reloading data from main memory (left), several accesses are served (right) by inner most cache or by register

Memory hierarchies: Temporal access locality

- Temporal locality: If data is already in cache reuse it from there!
- Example: Dense matrix vector multiplication (assume that cache is large enough to hold y (1:R))



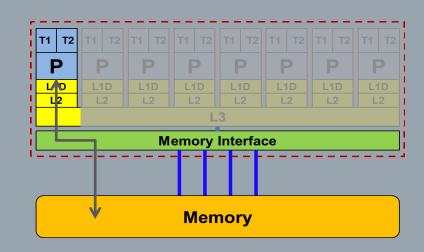
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Architecture - Memory hierarchies:

Caches – basics

Data access ←→ locality

Cache management

Memory Hierarchy: Cache management – Basics

- Size of caches (KB, MB) much smaller than main memory size (GB)
- If cache is full "data items" need to be replaced when new data comes in
- Transfer granularity
- Replacement based on "age" of cache line ←→ Last access time
- Cache lines get "old" if they are not accessed for some time
- Which "old" cache line to replace? ("Replacement policy")
 - Least recently used (LRU) Not recently used (NRU) (Random)

Important question: How is the pairing/mapping of memory addresses to cache locations?

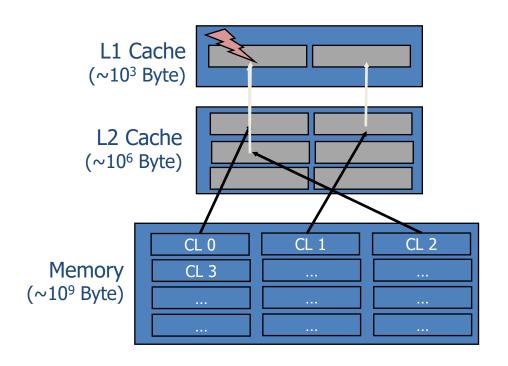
Memory Hierarchies: Cache Mapping

- Cache Mapping
 - Pairing of memory addresses with cache locations
 - Where is the CL to given memory addressed placed in the cache?

Memory address (32 Bit): 011100100000 1111010011111 001111

- Why (simple) strategies?
 - Hardware needs to search for data in cache, e.g.
 - is requested data in cache (hit or miss)?
 - If it is in cache where is it?
 - If new data comes in where is the old data to override

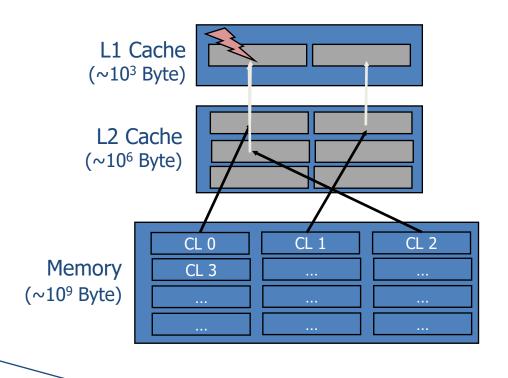




Memory Hierarchies: Cache Mapping – direct mapping

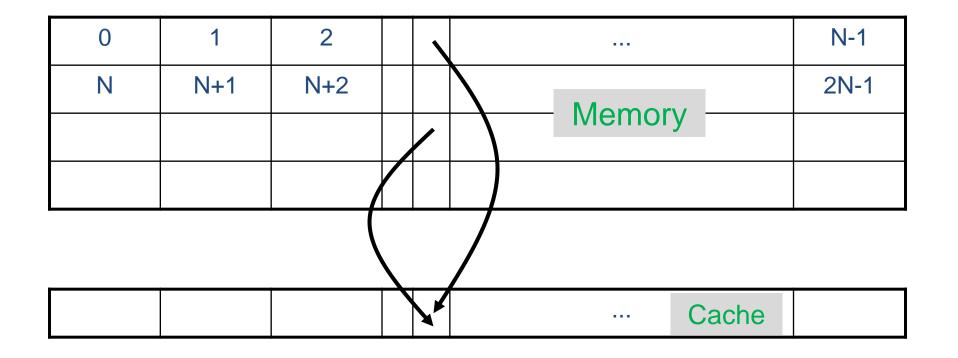
- Directly Mapped caches →
 each CL can only be mapped to
 one location in each cache
- If cache size is 1 MB choose "lowest" 20 bits of memory address as cache address

Memory address 32 Bit: 011100100000 1111010011111 0001111



- Remember: Each data transfer is on CL basis, e.g. 64 B → lowest 6 Bits address bytes within CL, which is mapped to a specific set in cache
- Bit 6-19: This identifies the location ("cache set") to which the CL is mapped in our 1 MB direct mapped cache
- Bit 20-31: This is information is stored in "Cache Tag"

Memory Hierarchies: Cache Mapping - Directly Mapped



Example: Directly mapped cache. Each memory location/cache line can be mapped to one cache location/cache set only.

E.g. Size of main memory= 64 GByte; Cache Size= 64 KB; CL=64 B

→ 10⁶ are Cache Lines mapped to the same cache location/set

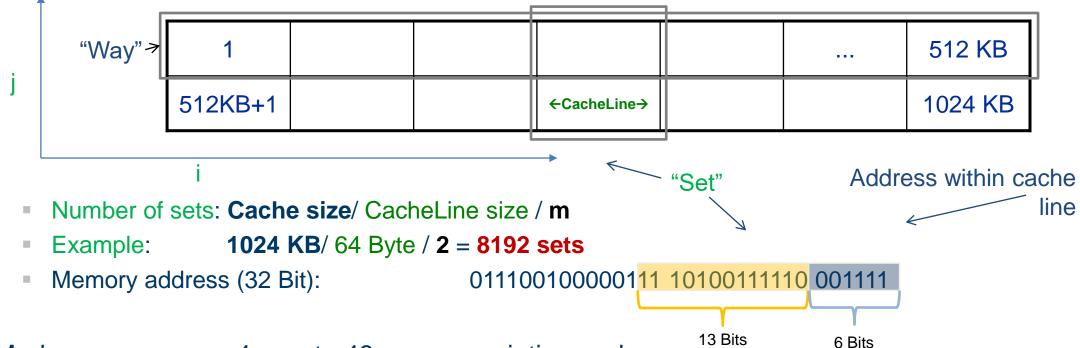
Memory Hierarchies: Cache Mapping – direct mapping

Advantages:

- Easy to implement
- Fast / low latency
- No penalty for stride 1 accesses (streaming)
- Disadvantages:
 - No flexibility → High chances of early evicts
 - Large stride accesses can substantially reduce the available cache size
- Rarely seen in real world processors
- Provide more flexibility: m-way set associative caches

Memory Hierarchies: Cache Mapping – Associative Caches

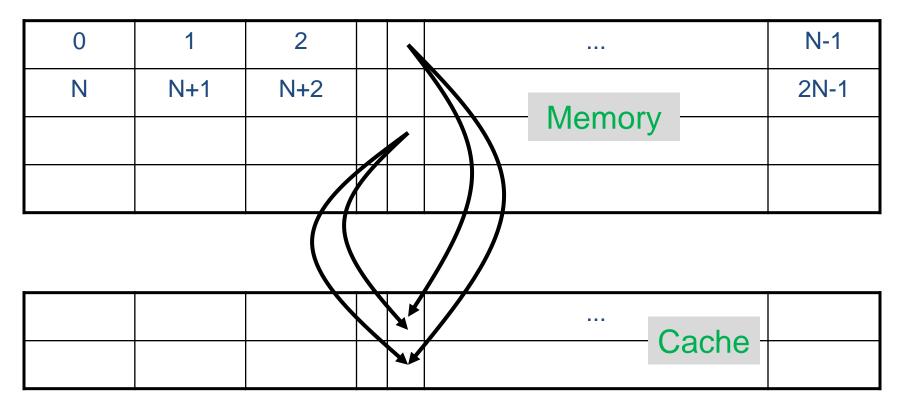
- Set-associative cache:
 - m-way associative cache of size m x n: each memory location i can be mapped to the m cache locations ("ways") i = j*n + mod(i,n); j=0..m-1
 - E.g.: 2-way set associative cache of size 1 Mbytes = **1024 KB** (Addresses: $0,...,20^{20}$ -1 \rightarrow 20 Bit):



- Modern processors: 4-way to 48-way associative caches
- Which way (j) is used within set: Age of data in the ways

0.....26-1

Memory hierarchies: Cache Mapping – Associative Caches



Example: 2-way associative cache. Each memory location can be mapped to two cache locations ("ways") within the same set:

Size of main memory= 64 GByte; Cache Size= 64 KB; CL = 64 B

→ 2*10⁶ Cache Lines are mapped to two cache locations / ways within a set

Memory hierarchies: Pitfalls & Problems

 If many memory locations are used that are mapped to same set, cache reuse can be very limited even with m-way associative caches

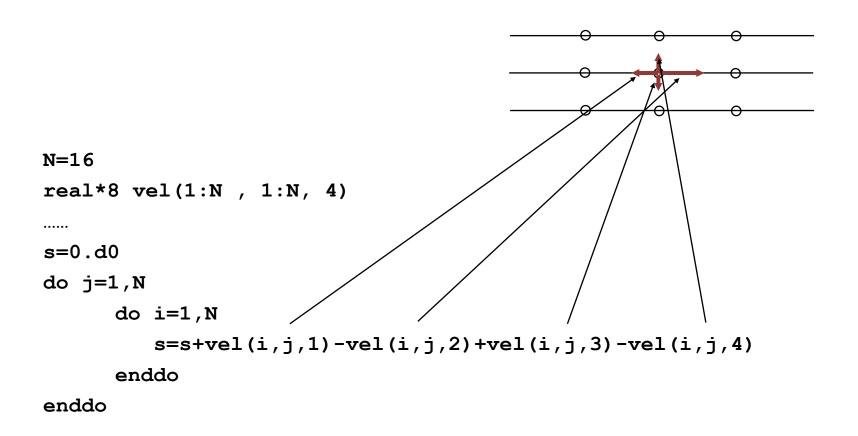
Warning: Using powers of 2 in the leading array dimensions of multi-dimensional arrays should be avoided! (Cache Thrashing)
double precision A(16384,16384)

If cache / m-ways are full and new data comes in from main memory, data in cache (full cache line)
 must be invalidated or written back

Ensure spatial and temporal data locality for data access!

Memory hierarchies: Cache thrashing - Example

Example: 2D – square lattice at each lattice point the 4 velocities for each of the 4 directions are stored

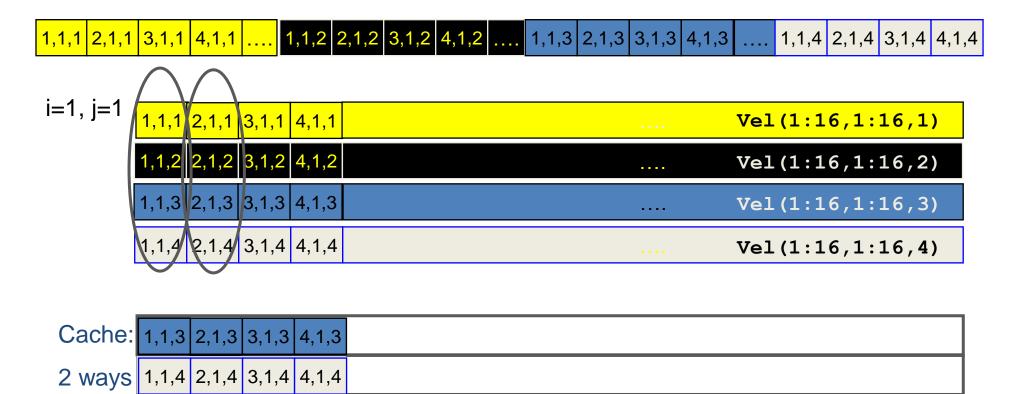


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Memory hierarchies: Cache thrashing - Example

Memory to cache mapping for vel (1:16, 1:16, 4)

Cache: 256 byte (=32 double) / 2-way associative / Cache line size=32 byte

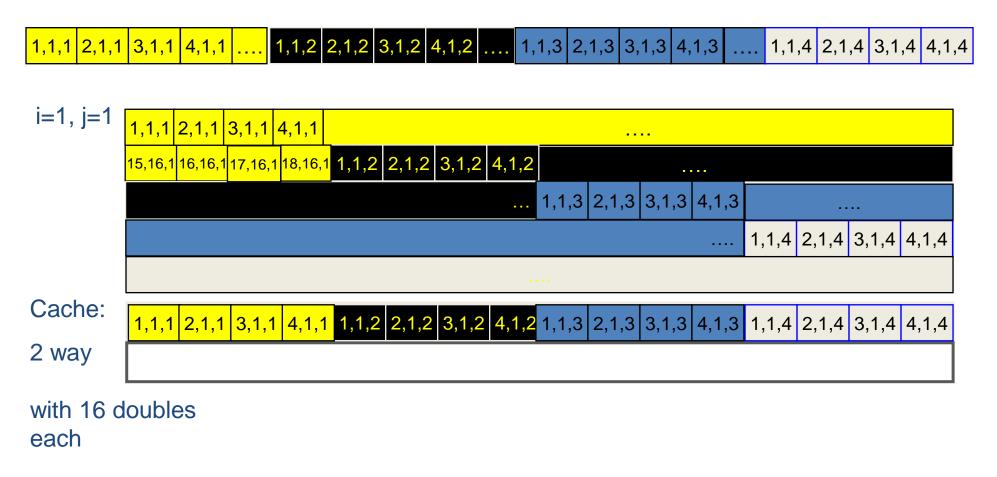


with 16 double each

Each cache line must be loaded 4 times from main memory to cache!

Memory hierarchies: Cache thrashing - Example

Memory to cache mapping for **vel(1:18, 1:18, 4)**Cache: 256 byte (=32 doubles) / 2-way associative / Cache line size=32 byte



Each cache line needs only be loaded **once** from memory to cache!

Memory hierarchies: Cache management details – states

- Handling of cached data to be replaced depends on the "cache line state"
- Basic "states" of cache line in cache:
 - NOT MODIFIED: Valid copy in lower cache levels/main memory → Cache line may be overwritten with new data or copied back to lower cache levels (see later: inclusive vs exclusive)
 - MODIFIED: Cache line has been modified and other copies in caches/main memory are invalid → Cache line needs to be evicted to lower cache levels/main memory before it can be overwritten
- Actual states are more diverse on modern multicore processors
- State of the cache line is stored cache line tag

Memory hierarchies: Cache management details – ST miss

Assume only one cache level:

- LOAD miss: If data item to be loaded to a register is not available in cache, the corresponding cache line is loaded from main memory
- STORE miss: Data item to be modified (e.g. a[2]=0.0) is not in cache?
 - Cache line is the minimum data transfer unit between main memory and cache (e.g. a[0:7]).
 - Load cache line from main memory to cache ("WRITE ALLOCATE")
 - Modify data item in cache
 - Later evict/write back modified cache line to main memory

```
do i=1,n
do j=1,n
a(j,i)= 0.0

enddo

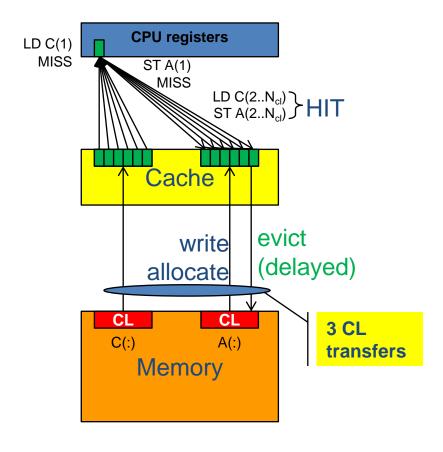
n² words are loaded from main memory to cache (WRITE ALLOCATE) and n² words are evicted/written back to main memory!
```

→ Overall data transfer volume may increases up to 2x! (NT stores: no increase)

Memory hierarchies: Cache management details

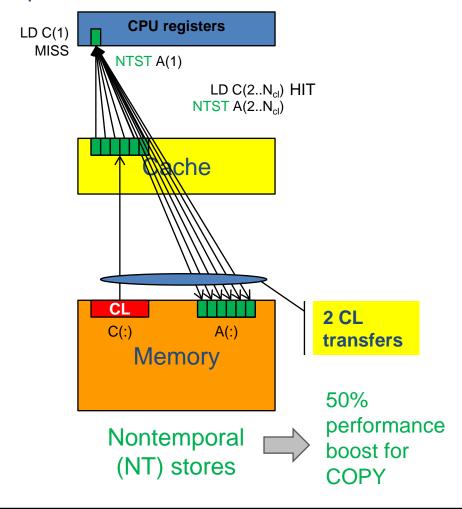
How does data travel from memory to the CPU and back?

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



Standard stores (WRITE ALLOCATE)

Special store instruction to avoid WA!



Memory management: Caches management details

Inclusive:

- 1. Cache line copy in all levels
- 2. Reduced effective size in outer cache levels
- 3. Cheap eviction for unmodified cache lines
- 4. Higher latency: cache lines have to load through hierarchy
- → All caches in Intel processors up to Broadwell

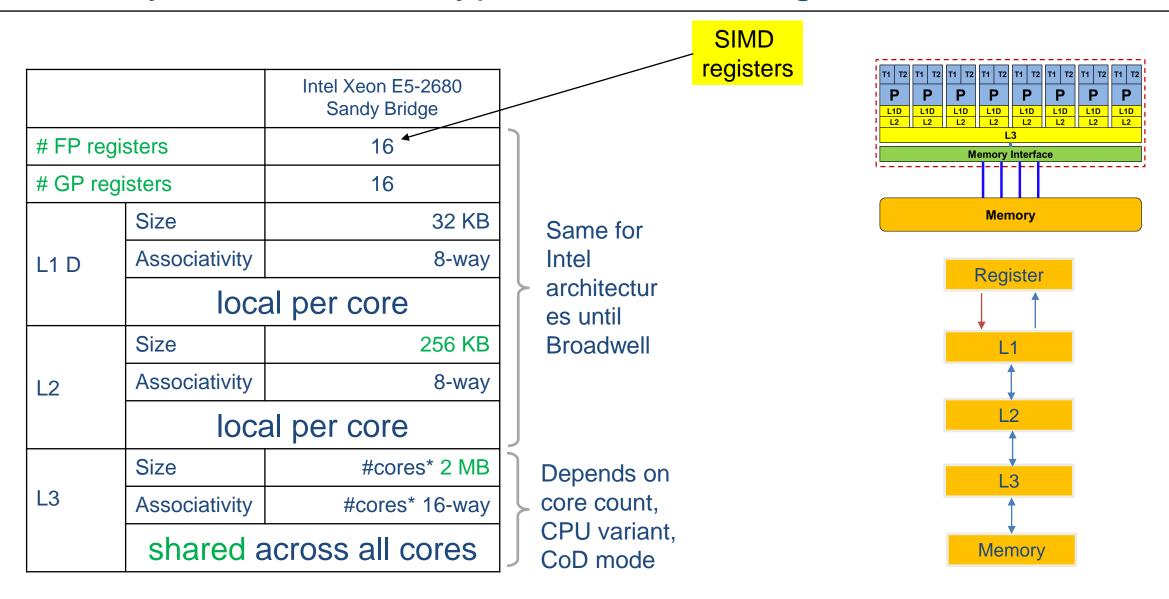
Exclusive / Non-inclusive:

- Only one cache line copy in cache hierarchy
- Full aggregate effective cache size
- 3. Eviction is expensive (copy back)
- 4. Lower latency: Data can be directly loaded in L1/L2 cache
- → AMD processors: L3 cache Intel Skylake (and later procs) L3 cache

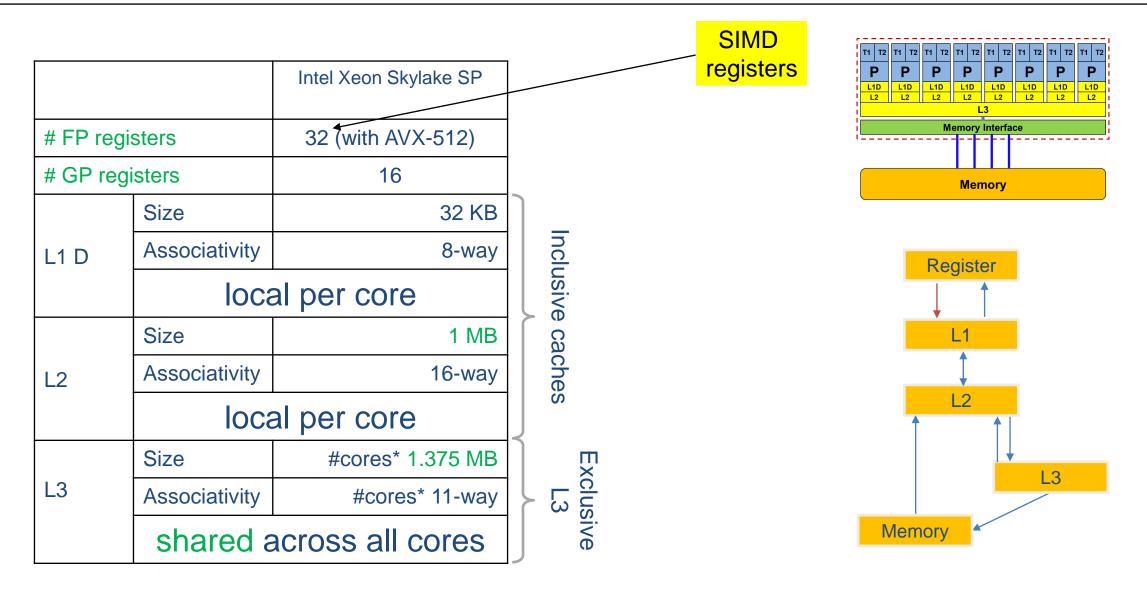
"Write back": A modified cache line is evicted to the next (lower) cache/memory level before it is overwritten by new data

"Write through": When a cache line is modified then the cache line copy in the next (lower) cache/memory level is updated as well

Memory Hierarchies: Typical cache configuration



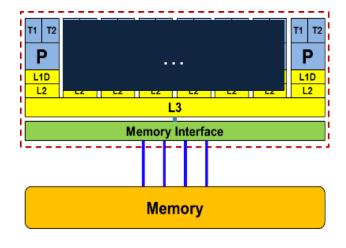
Memory Hierarchies: Typical cache configuration



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Intel Xeon E5 multicore processors

Microarchitecture	SandyBridge-EP	IvyBridge-EP	Haswell-EP
Shorthand	SNB	IVB	HSW
Xeon Model	E5-2680	E5-2690 v2	E5-2695 v3
Year	03/2012	09/2013	09/2014
Clock speed (fixed)	2.7 GHz	2.2 GHz	2.3 GHz
Cores/Threads	8/16	10/20	14/28
Load/Store through	out per cycle		
AVX(2)	1 LD & 1/2 ST	1 LD & 1/2 ST	2 LD & 1 ST
SSE/scalar	$2LD \parallel 1LD \& 1ST$	$2LD\ 1LD\&1ST$	2 LD & 1 ST
L1 port width	$2\times16+1\times16$ B	$2\times16+1\times16$ B	$2\times32+1\times32$ B
ADD throughput	1 / cy	1 / cy	1 / cy
MUL throughput	1 / cy	1 / cy	2 / cy
FMA throughput	n/a	n/a	2 / cy
L2-L1 data bus	32 B	32 B	64 B
L3-L2 data bus	32 B	32 B	32 B
LLC size	$20\mathrm{MiB}$	25 MiB	35 MiB
Main memory	4×DDR3-1600	4×DDR3-1866	4×DDR4-2133
Peak memory BW	51.2 GB/s	51.2 GB/s	68.3 GB/s
Load-only BW	43.6 GB/s (85%)	46.1 GB/s (90%)	60.6 GB/s (89%)
$T_{\rm L3Mem}$ per CL	3.96 cy	3.05 cy	2.43 cy



FP instructions throughput per core

Max. data transfer per cycle between caches

Peak main memory bandwidth

Max. attainable bandwidth

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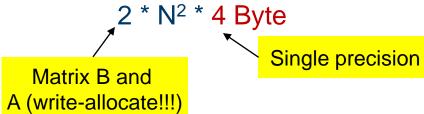
Matrix transpose & cache thrashing: A real-world example

Memory hierarchies: Cache traffic/thrashing – Example

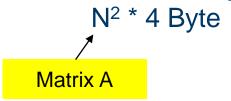
LIKWID

- Matrix transpose
- Minimum data traffic:

Min. Load from main memory



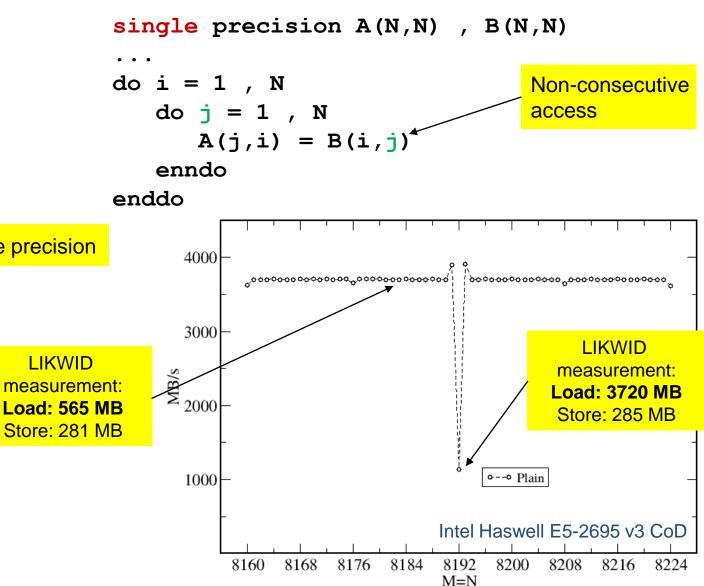
Min. Store to main memory:



For N= 8192 we expect

536 MB Load:

Store: 268 MB

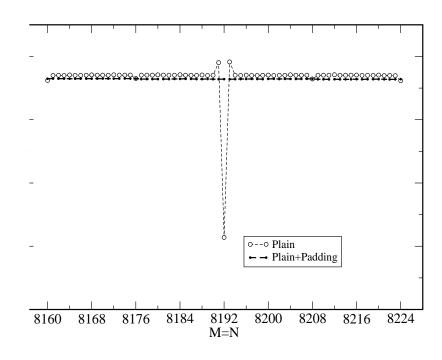


Memory hierarchies: Cache traffic/thrashing

Problem:

- L3 cache can hold 8192 cache lines (0.5 MB) of B to allow for spatial locality in next outer (i-) iteration
- But at N=8192 these cache lines are mapped to the same set in L3 cache (which has associativity of 7*32=224, i.e. only 224 CL can be stored)
- Thus in every j-iteration a full cache line is loaded from main memory (and only one entry is used)
- Solution: Padding
 - Chose leading dimension such that it is not power of 2, e.g.
 - Np is next number of N which is odd multiple of 16

```
single precision A(Np,N) , B(Np,N)
...
do i = 1 , N
    do j = 1 , N
        A(j,i) = B(i,j)
    enndo
enddo
```



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Architecture of memory hierarchy - Summary

- Deep cache hierarchies (typically 3 levels) between main memory and registers
- Granularity of data transfer below L1 cache:
 Cache lines (64 B or 128 B)
- Prefetchers to hide latencies
- STORE misses may trigger cache write allocate traffic
- m-way associative mapping in caches may reduce "usable" cache size
- Cache thrashing
- Can we quantify / understand the single core data access performance?

