DTU Compute
Department of Applied Mathematics and Computer Science

High-Performance Computing

Getting good performance from your application

Tuning techniques for serial programs on cache-based computer systems

Application Tuning

Overview

- Introduction
- Memory Hierarchy
- General Optimization Techniques
-
- Compilers
- Analysis Tools
- Tuning Guide

Application Tuning

Introduction

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Introduction

Moore's Law

- Popular version:
  - *“CPU speed usually doubles every 18 months.”*
- More correct version:
  - *“The number of transistors per integrated circuit will double every 18 months.”*

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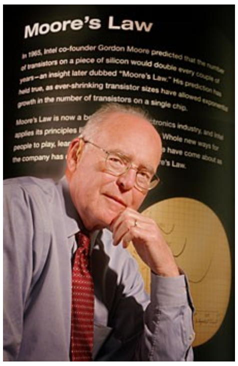
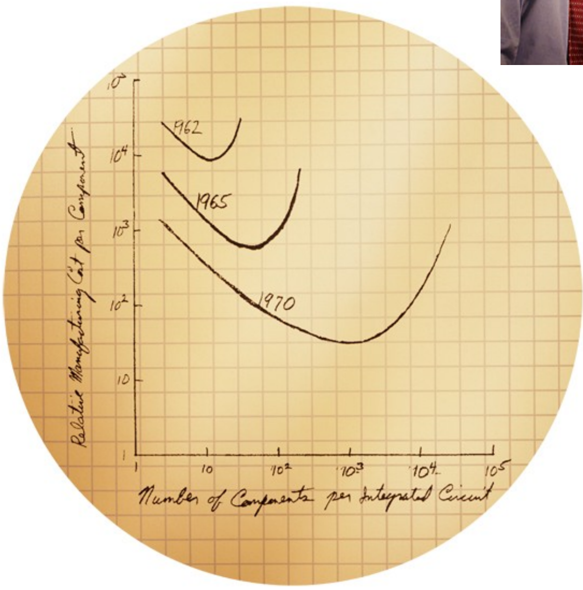
Introduction

Gordon Moore – co-founder of Intel



"I never said 18 months. I said one year, and then two years ... Moore's Law has been the name given to everything that changes exponentially. ... If Gore invented the Internet, I invented the exponential."

- Gordon Moore in an interview (2000)



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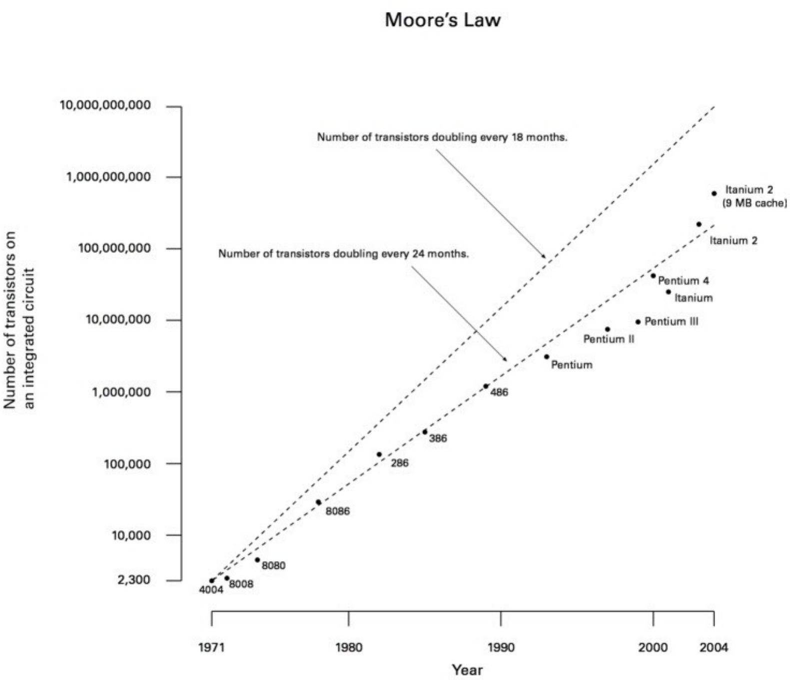

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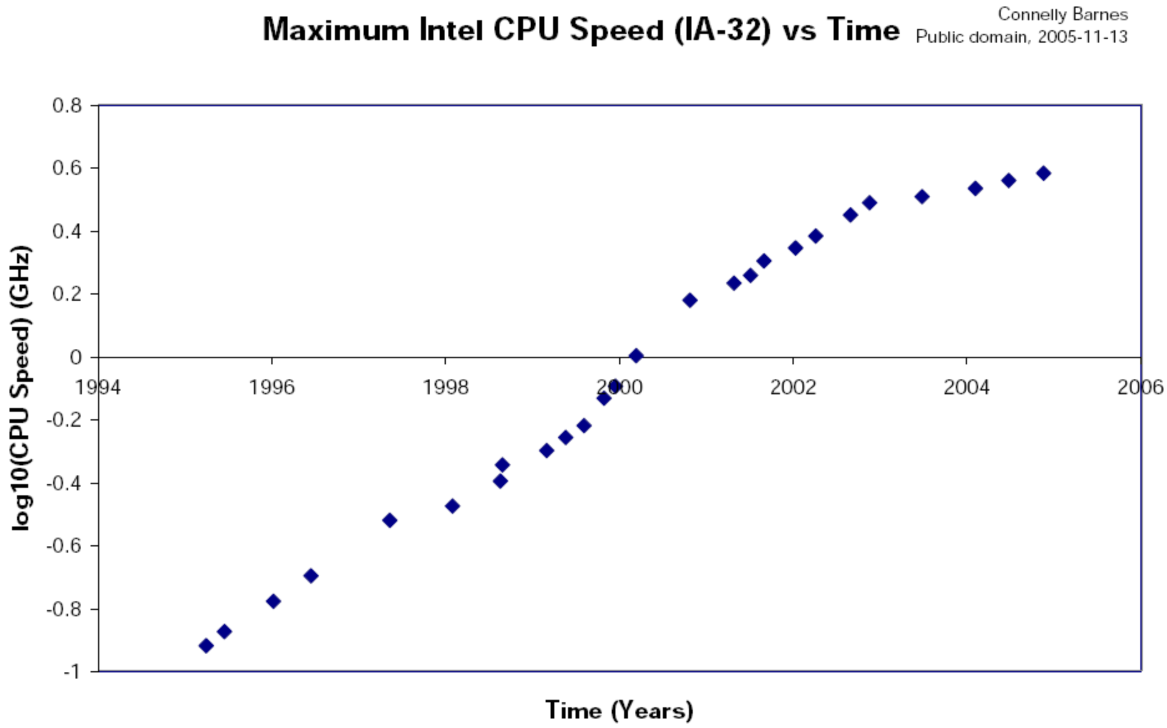

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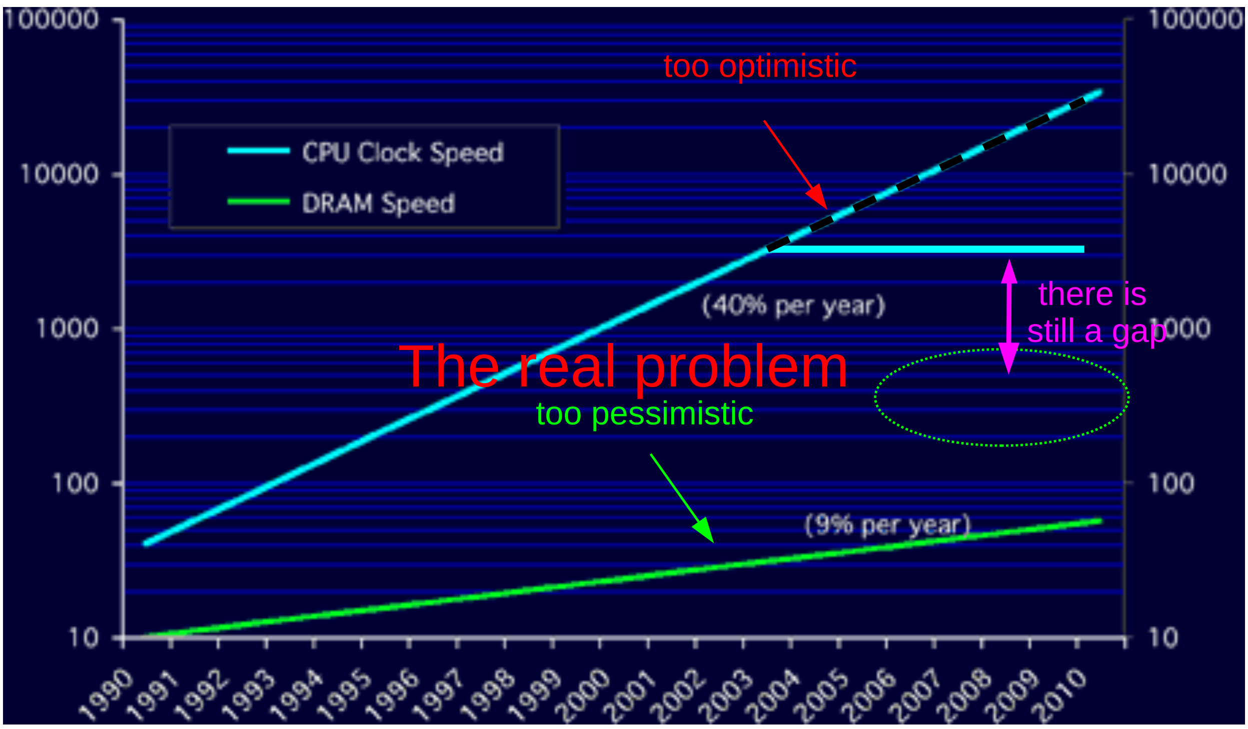
Introduction



Introduction

- CPU speed usually doubles every 18-24 months (not true any longer – we got other improvements, instead!).
- Development on the memory side is much slower (~ 6 years!).
- Memory speeds catch up – but also have to serve more cores!
- Something you should have in mind when designing your program!

Application Tuning

Motivation for Application Tuning

time flow in a computational task (simplified picture):

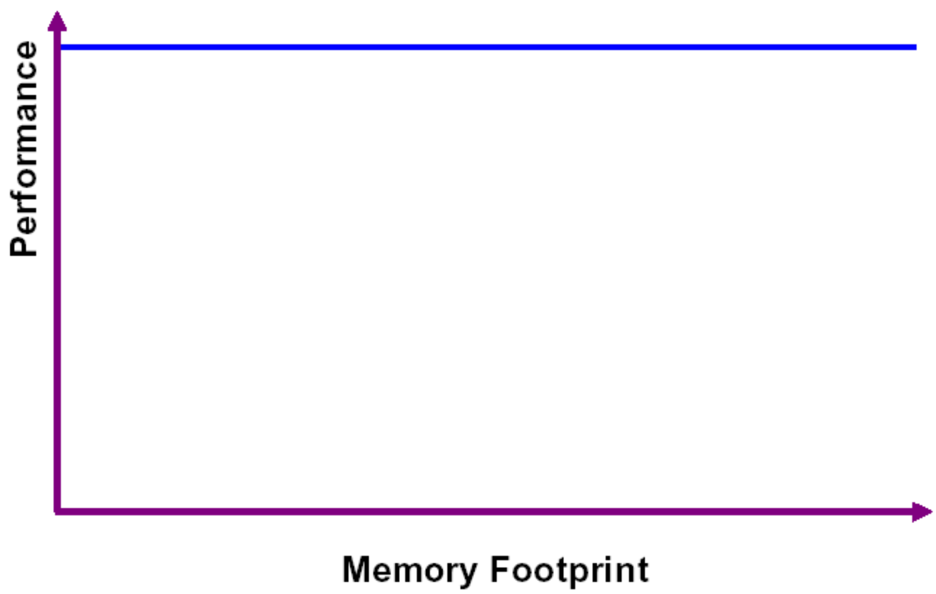
Application Tuning

The Memory Hierarchy

Application Tuning

The Memory Hierarchy

Intuitive Performance Graph:



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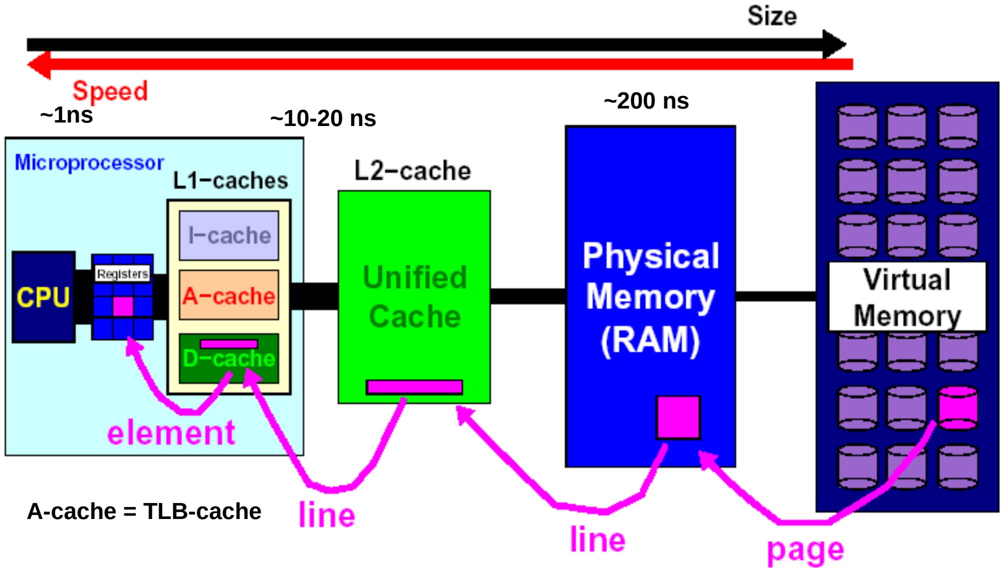
The Memory Hierarchy



Memory Optimization:
Keep frequently used data close to the processor

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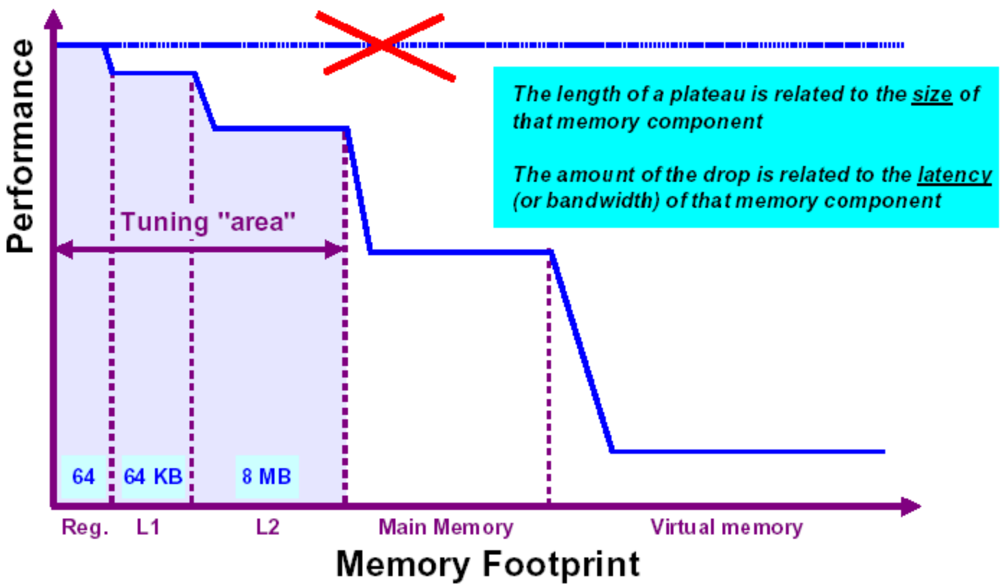
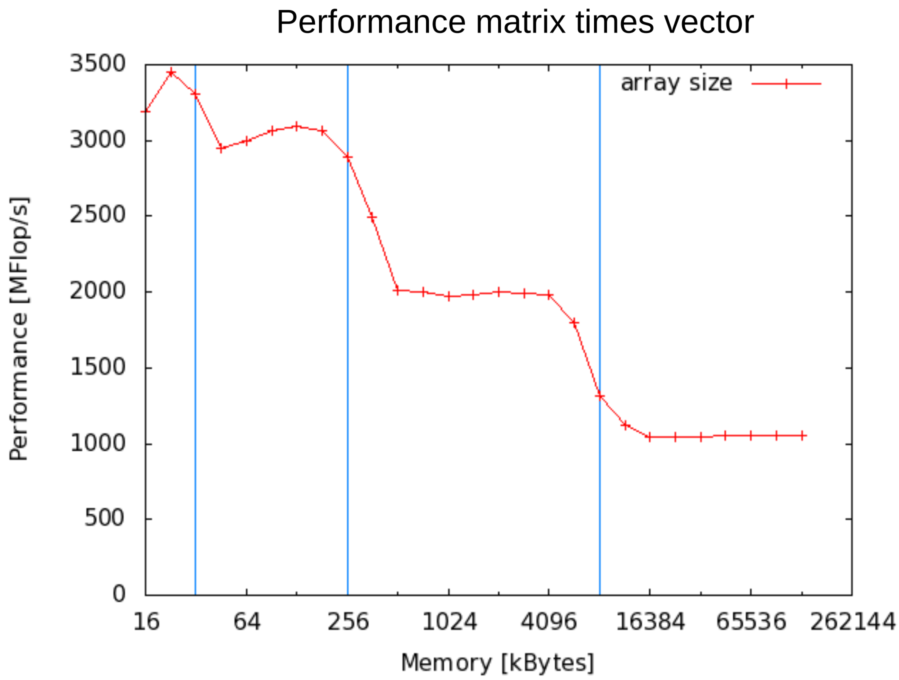
The Memory Hierarchy

Performance is not uniform:

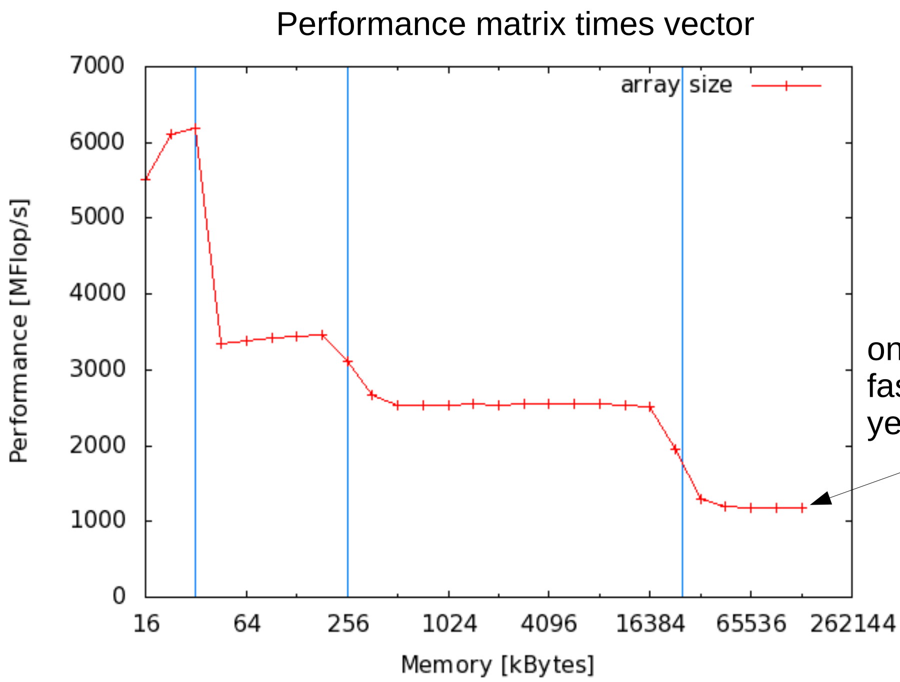


The Memory Hierarchy



Intel Xeon X5550, 2.67 GHz, 8 MB L3 cache (release: Q1/2009)

The Memory Hierarchy



only ~10% faster than 5 years ago!

Intel Xeon E5-2660v3, 2.66 GHz, 25 MB L3 (release: Q3/2014)

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The Memory Hierarchy

- Memory plays a crucial role in performance
- Not accessing memory in the right way will degrade performance on **all** computer systems
- The extent of degradation will depend on the system
- Knowledge about the relevant memory characteristics helps to write code that minimizes those problems

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Caches – and all that ...

How do those caches work?

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Caches

- Cache memory or cache for short (from French: cacher – to hide): fast buffers that help to hide the memory latency
- One distinguishes between
  - data cache
  - instruction cache
  - address cache (also called TLB – Translation Lookaside Buffer) – mapping between virtual and physical addresses

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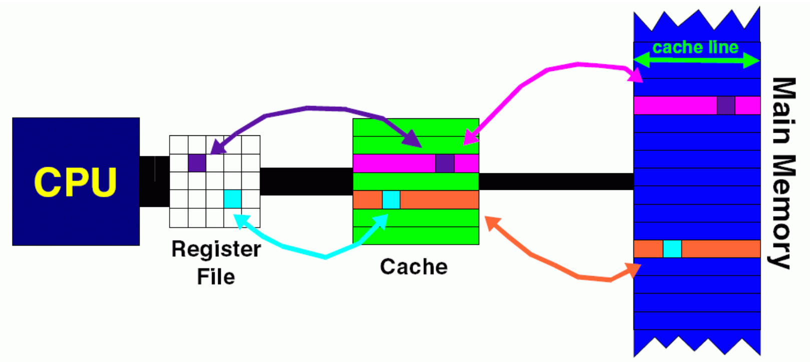
Cache Lines

- To get good performance, optimal use of the caches is crucial
- The unit of transfer is a "*cache line*":
  - linear structure of fixed length (bytes)
  - fixed starting address in memory



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Cache Organisation

Direct Mapped:

- Each memory address maps onto exactly one line in cache
- simple and efficient
- built-in replacement policy
- easy to scale to larger sizes
- downside: no control by usage – danger of replacing data that will be needed again soon

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Cache Organisation

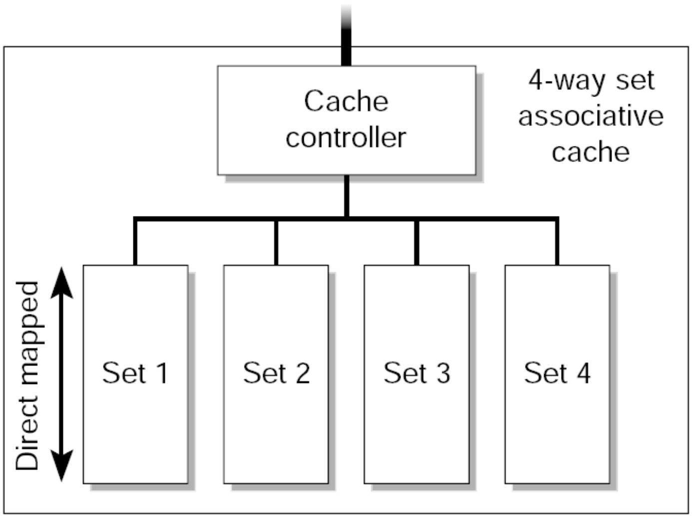
Fully Associative:

- Every memory address can be mapped anywhere in cache
- Need to track usage of cache lines
- Requires a replacement policy, e.g.
  - *least recent used* (LRU),
  - *least frequent used* (LFU),
  - random, etc
- Doesn't scale well to large sizes
- Costly design

Cache Organisation

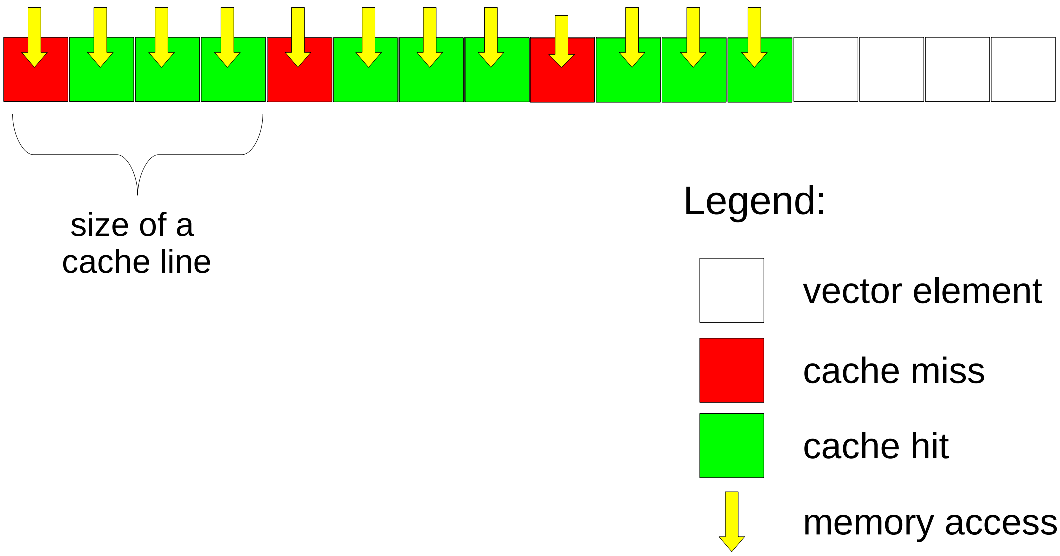
N-way Set Associative:

- Sets of direct mapped caches:



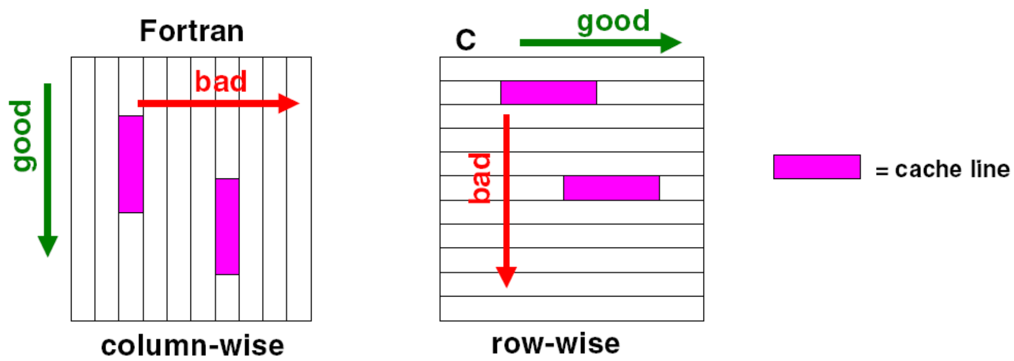
Memory access

- Memory has a 1-dimensional linear structure
- Accessing vector elements:



Memory access

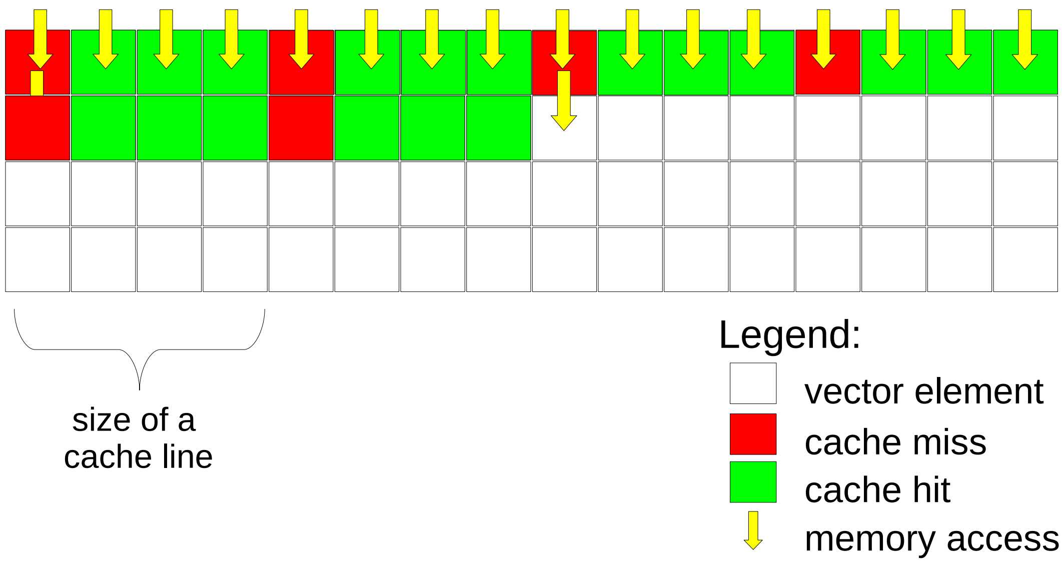
Access to multi-dimensional arrays depends on how data is stored:



Bad memory access has a huge impact on performance!!!

Memory access

Accessing 2d arrays in C – row wise:



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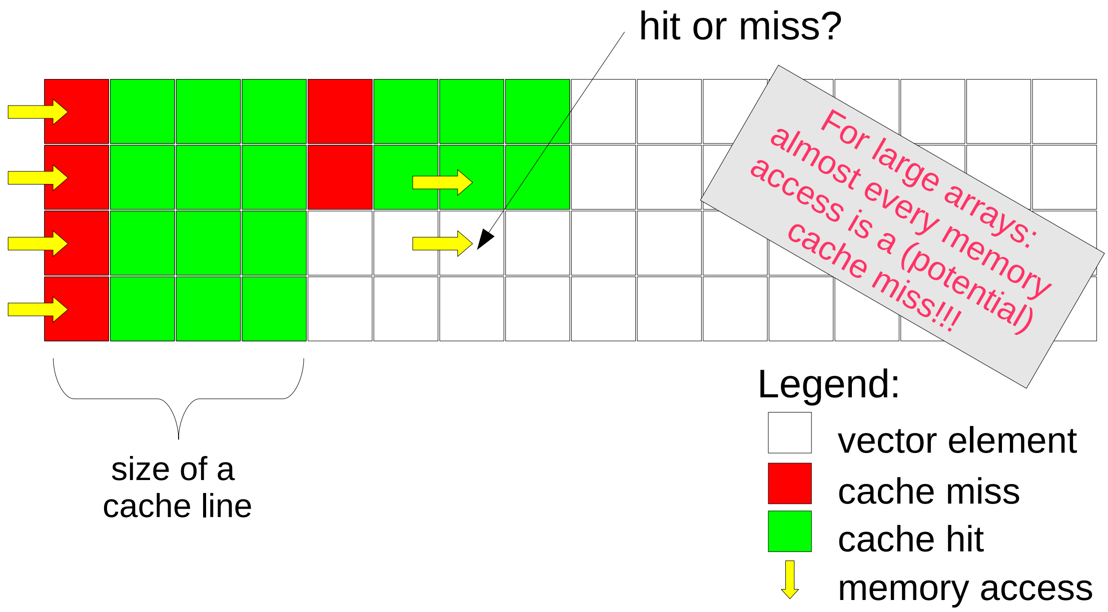
Memory access

Accessing 2d arrays in C – column wise:



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The TLB cache

- the Translation Lookaside Buffer (TLB) translates virtual memory addresses (in your application) to physical addresses
- also called 'address cache'
- unit: page – typical size 4kB
- creation of lookup table is an expensive operation
- cost: 10 – 100 clock cycles/miss
- modern CPUs are having advanced TLBs
  - support for variable page sizes

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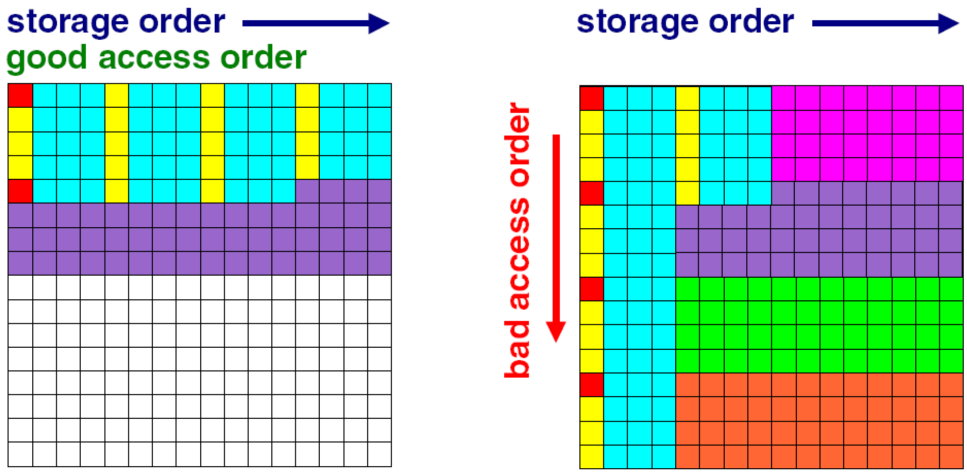
Memory access – TLB misses



- = TLB miss
- = D-cache miss
- = Cached elements
- = Virtual memory page

- If the entire matrix fits in the cache, the access pattern *hardly* matters.
- For large (out-of-cache) matrices, the access pattern **does** matter – both data cache and TLB misses

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About cache misses

Some simple rules:

- You cannot avoid cache misses – they are part of the nature of cache-based systems ...
- ... but you should try to minimize them to get good performance

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Cache Line Utilization

Two key rules: Maximize ...

- Spatial locality ⇒ Use all data in one cache line
  - depends on storage layout
  - depends on access patterns
    - stride = 1 is good
    - random access is really bad
- Temporal locality ⇒ Re-use data in a cache line
  - depends on algorithm used

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Some Terminology

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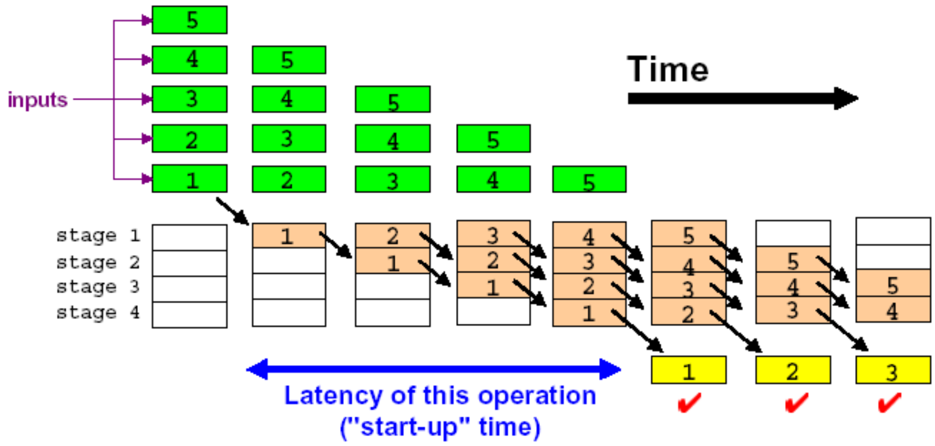
Terminology: Pipelining

stage 1
stage 2
stage 3
stage 4

Let's assume we have an operation that takes 4 stages per iteration



Rule of thumb: keep the pipeline filled for good performance!

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Terminology: Superscalar (or ILP)

- ***N-way superscalar:***
  - ***Execute N instructions at the same time***
- ***This is also called Instruction Level Parallelism (ILP)***

	slot 1	slot 2	slot 3	slot 4	
cycle 1					4-way superscalar
cycle 2	not used				3-way superscalar
cycle 3		not used	not used		2-way superscalar
cycle 4	not used			not used	2-way superscalar
cycle 5			not used		3-way superscalar

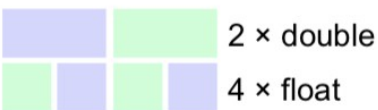
- ***The hardware has to support this, but it is up to the software to take advantage of it***
- ***Often there are restrictions which instructions can be "bundled"***
- ***These are documented in the Architecture Reference Manual for the microprocessor***

Terminology: Vectorization (SIMD)

- Vectorization is the process of transforming a scalar operation that acts on a single data element at a time (Single Instruction Single Data – SISD) to an operation that that acts on multiple data elements at a time (Single Instruction Multiple Data – SIMD).
- SIMD units are hardware arithmetic vector units that can perform the same operation on multiple data points simultaneously by using vector registers.

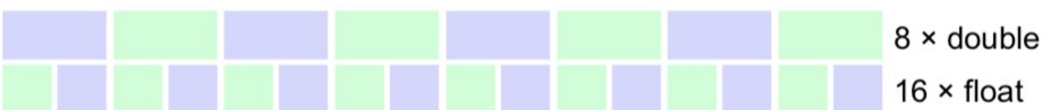
Terminology: Vectorization (SIMD)

- Vector types
  - 128 bit: SSE = Streaming SIMD Extension (1999)



  - 256 bit: AVX = Advanced Vector Extension (2011)

  - 512 bit: AVX-512 (2013)



Latency and Bandwidth

Latency:

- the time it takes from the initiation of an action till you have the first result
- unit: time

Bandwidth:

- how many
  - actions can be carried out,
  - results can be obtained,

  within a given time
- unit: #/time

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General Optimization Techniques

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Optimization Techniques - Overview

- Most optimization techniques are “loop based”
- Loop based optimizations:
  - Interchange
  - Fission and Fusion
  - Unrolling
  - Blocking

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Optimization Techniques - Overview

- Designing your data structures the “right way” can also be important
- Other techniques:
  - De-vectorization
  - Stripmining

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Loop based optimizations

Application Tuning

Coding style: array indexing

- To apply safe transformations, the compilers have to analyze data dependencies in a loop
- Explicit expressions will help the compilers to do a good job in loop optimization

Good	(*)Reasonable

`for(i=0; i<m; i++)`
`  for (j=0; j<n; j++)`
`    .. a[i][j] ..`
	`for(i=0; i<m; i++)`
	`  for (j=0; j<n; j++)`
	`    .. a[i*n+j] ..`

Bad	**Caution**

`k = 0;`
`for(i=0; i<m; i++)`
`  for (j=0; j<n; j++)`
`    .. a[k++] ..`
	`for(i=0; i<m; i++)`
	`  for (j=0; j<n; j++)`
	`    .. a[indx[i][j]] ..`

(*) harder to read for a human, but might be better for the compiler!

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Loop Interchange

```
DO I = 1, M
   DO J = 1, N
      A(I,J)=B(I,J)+C(I,J)
   END DO
END DO
```

Interchange loops

```
DO J = 1, N
   DO I = I, M
      A(I,J)=B(I,J)+C(I,J)
   END DO
END DO
```

- The matrices are accessed over the second dimension first
- This is the wrong order in Fortran
- A loop interchange solves the problem
- In C, the situation is reversed:
  - row access is okay
  - column access is bad

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Loop Fission

```
for (j=0; j<n; j++)
{
   c[j] = exp(j/n);
   for (i=0; i<m; i++)
      a[i][j]=b[i][j]+d[i]*e[j];
}
```

- *Access on arrays 'a' and 'b' is bad*
- *We can not simply interchange the loops*
- *Fission/splitting is the solution*

Fission

```
for (j=0; j<n; j++)
   c[j] = exp(j/n);
```

New loop created

This loop can now also be vectorized

```
for (j=0; j<n; j++)
   for (i=0; i<m; i++)
      a[i][j]=b[i][j]+d[i]*e[j];
```

Interchange loops for better performance

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Loop Fusion

```
for (i=0; i<n; i++)
    a[i] = 2 * b[i];
```

```
for (i=0; i<n; i++)
    c[i] = a[i] + d[i];
```

- *Assume that 'n' is large*
- *In the second loop, a[i] will no longer be in the cache*
- *Fusing the loops will ensure a[i] is still in the cache when needed*

Fusion

```
for (i=0; i<n; i++)
{
    a[i] = 2 * b[i];
    c[i] = a[i] + d[i];
}
```

Note that it is possible to apply fusion to loops with (slightly) different boundaries

In such a case, some iterations will have to be 'peeled' off

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Fission and Fusion – Summary

```
for(i=0;i<n;i++)
{
   ... [i] ...
}
```

Fission

```
for(i1=0;i1<n;i1++)
{
   ... [i1] ...
}
```

```
for(i2=0;i2<n;i2++)
{
   ... [i2] ...
}
```

Fusion

```
for(i=0;i<n;i++)
{
   ... [i] ...
}
```

Fission

- ✔ Reduce register pressure
- ✔ Enable loop interchange
- ✔ Isolate dependencies
- ✔ Increase opportunities for optimization (e.g. vectorization of intrinsics)

Fusion

- ✔ Reduce cache reloads
- ✔ Increase Instruction Level Parallelism (ILP)
- ✔ Reduce loop overhead

Inner Loop Unrolling

Through unrolling, the loop overhead ('book keeping') is reduced

```
for (i=0; i<n; i++)
    a[i] = b[i] + c[i];
```

```
Loads      : 2
Stores     : 1
FP Adds    : 1
I=I+1
Test I < N ?
Branch
Addr. incr: 3
```

Work: 4
Overhead: 6

Loop is unrolled with a factor of 4

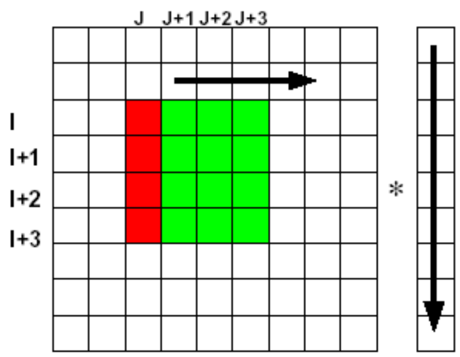
```
for (i=0; i<n; i+=4)
{
   a[i  ] = b[i  ] + c[i  ];
   a[i+1] = b[i+1] + c[i+1];
   a[i+2] = b[i+2] + c[i+2];
   a[i+3] = b[i+3] + c[i+3];
}
<clean-up loop>
```

```
Loads      : 8
Stores     : 4
FP Adds    : 4
I=I+4
Test I < N ?
Branch
Addr. incr: 3
```

Work: 16
Overhead: 6

Note: the amount of addressing needed in reality is less

Outer Loop Unrolling




```
for (i=0; i<m; i++)
  for(j=0; j<n; j++)
  {
    a[i] += b[i][j] * c[j];
  }
```

```
for (i=0; i<m; i+=4)
  for(j=0; j<n; j++)
  {
    a[i  ] += b[i  ][j] * c[j];
    a[i+1] += b[i+1][j] * c[j];
    a[i+2] += b[i+2][j] * c[j];
    a[i+3] += b[i+3][j] * c[j];
  }
<clean-up loop>
```

- ***Advantage:***
  - *c[j] is re-used 3 more times* ***(temporal locality)***
- ***Deeper unrolling, say 8, requires more fp registers (17 instead of 9), but improves re-use of c[j]***

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Outer Loop Unrolling – how to

```
for (i=0; i<m; i++)
  for(j=0; j<n; j++)
    a[i] += b[i][j] * c[j];
```

Outer loop unrolling

```
for (i=0; i<m-m%4; i+=4)
{
  for(j=0; j<n; j++)
    a[i  ] += b[i  ][j] * c[j];
  for(j=0; j<n; j++)
    a[i+1] += b[i+1][j] * c[j];
  for(j=0; j<n; j++)
    a[i+2] += b[i+2][j] * c[j];
  for(j=0; j<n; j++)
    a[i+3] += b[i+3][j] * c[j];
}
for (i=m-m%4; i<m; i++)
  for(j=0; j<n; j++)
    a[i] += b[i][j] * c[j];
```

clean-up loop

Jam the loops together again

Unroll and Jam

```
for (i=0; i<m-m%4; i+=4)
  for(j=0; j<n; j++)
  {
    a[i  ] += b[i  ][j] * c[j];
    a[i+1] += b[i+1][j] * c[j];
    a[i+2] += b[i+2][j] * c[j];
    a[i+3] += b[i+3][j] * c[j];
  }
for (i=m-m%4; i<m; i++)
  for(j=0; j<n; j++)
    a[i] += b[i][j] * c[j];
```

clean-up loop

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Loop unrolling – structure

```
for (i=0; i<n; i++)
{
   ... [i] ...
}
```

```
DO I = 1, N
   ... (I) ...
END DO
```

Loop unroll factor is "unroll"

```
for(i=0;i<n-n%unroll;i+=unroll)
{
   ...[i]   ...
   ...[i+1]...
   ...[i+2]...

   ...[i+unroll-1]...
}
```

```
DO I = 1, N-mod(N,unroll), unroll
   ...(I)   ...
   ...(I+1)...
   ...(I+2)...

   ...(I+unroll-1)...
END DO
```

Unrolled Loop

Cleanup Loop

```
for(i=n-n%unroll;i<n;i++)
{
   ...[i]...
}
```

```
DO I = N-mod(N,unroll)+1,N
   ... (I) ...
END DO
```

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Loop Unrolling – Summary

- More than one iteration per loop pass
- Inner loop unrolling:
  - reduce loop overhead
  - better instruction scheduling
- Outer loop unrolling:
  - improve cache line usage (spatial locality)
  - re-use data (temporal locality)
- Disadvantages:
  - more registers needed, clean-up code required

Loop Unrolling – Compilers

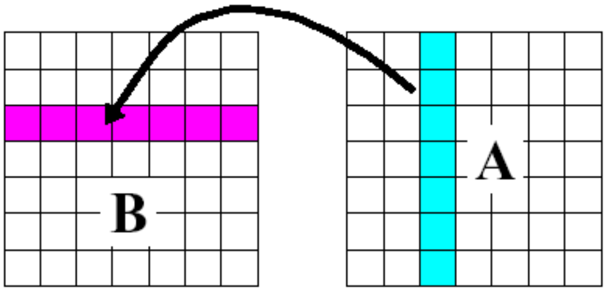
- Compilers do usually a good job in loop unrolling
- there are options to control the unroll depth
  - gcc: -funroll-loops --params max-unroll-times=n
  - suncc: -xunroll=n (1: no unroll, 2..n: unroll n times)
  - Intel: -unroll[n] (0: disable loop unrolling)

Application Tuning

Loop Blocking – 1

Transposing a matrix

```
for (j=0; j<n; j++)
    for (i=0; i<n; i++)
        b[j][i] = a[i][j];
```



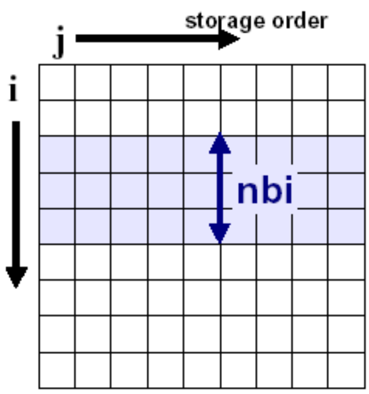
- *Loop interchange will not help here:*
  - *Role of 'a' and 'b' will only be interchanged*
- *Change of programming language won't help either*
- *Unrolling the i-loop can be beneficial, but requires more registers and doesn't address TLB-misses*
- *Loop blocking achieves good memory performance, without the need for additional registers*

Application Tuning

Loop Blocking – 2

Blocking and interchanging the I-loop

```
for(i1=0; i1<n; i1+=nbi)
  for (j=0; j<n; j++)
     for (i2=0;i2<MIN(n-i1,nbi);i2++)
        b[j][i1+i2] = a[i1+i2][j];
```



- *Parameter 'nbi' is the blocking size*
- *Should be chosen as large as possible*
- *Actual value depends on the cache to block for:*
  - ✔ *L1-cache*
  - ✔ *L2-cache*
  - ✔ *TLB*
  - ✔ *....*

Fortran

```
do i = 1, n
```

```
do i1 = 1, n, nbi
  do i2 = 0,min(n-i1+1,nbi)-1
```

Loop Blocking – Summary

- Powerful technique to improve:
  - memory access (spatial locality)
  - data re-use (temporal locality)
- Preserves portability – but blocking size depends on:
  - cache type/level/capacity
  - data requirements

Loop Blocking – Summary

Application Tuning

Recommendations:

- choose blocking size as large as possible
- leave space for other data
- parameterize cache characteristics, especially size

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Tricked by the compiler

Fortran code example: long and bulky loop

```
DO I1=1,NAT(IMT)
  IA1=IM1+(I1-1)*3
  DO I2=1,NAT(JMT)
    IA2=IM2+(I2-1)*3
        ... statements removed ...
    DX(1)=XNOW(IMT,IA1+1)-XNOW(JMT,IA2+1)
    DX(2)=XNOW(IMT,IA1+2)-XNOW(JMT,IA2+2)
    DX(3)=XNOW(IMT,IA1+3)-XNOW(JMT,IA2+3)
    CX(1)=CM1(1)-CM2(1)
    CX(2)=CM1(2)-CM2(2)
    CX(3)=CM1(3)-CM2(3)
        ... statements removed ...
  ENDDO
ENDDO
```

Independent of loop indices!!!

Moved the 3 lines above the DO loops – no improvement!
Compiler had done this already!

Application Tuning

Only the programmer knows ...

```
subroutine do_calc(...)

real(8),dimension(N,M,O,P):

!---- data initialization
r = 0.0d0; s = 0.0d0; t = 0

select case(calc_type)
   case(most_of_the_time)
     ...
     r(i,j,k,l) = r(i,j,k,l
     s(i,j,k,l) = s(i,j,k,l
     ...

   case(rare_event)
     ...
     r(i,j,k,l) = r(i,j,k,l
     s(i,j,k,l) = s(i,j,k,l
     t(i,j,k,l) = t(i,j,k,l
     ...
end select
```

```
subroutine do_calc(...)

real(8),dimension(N,M,O,P):: r,s,t

!---- data initialization
r = 0.0d0; s = 0.0d0

select case(calc_type)
   case(most_of_the_time)
     ...
     r(i,j,k,l) = r(i,j,k,l) + ...
     s(i,j,k,l) = s(i,j,k,l) + ...
     ...

   case(rare_event)
     t = 0.0d0
     ...
     r(i,j,k,l) = r(i,j,k,l) + ...
     s(i,j,k,l) = s(i,j,k,l) + ...
     t(i,j,k,l) = t(i,j,k,l) + ...
     ...
end select
```

Application Tuning

Data structure design

Access your data in the right way

Application Tuning

Data structure design

- "Good advice" from a HPC tutorial: Use data structures to avoid too many index calculations
- Example: particle simulation in 3D with x, y, z coordinates and some other information about each particle, e.g. distance to origin, particle type
  - `x[i], y[i], z[i], dist[i], ptype[i]`
  - turn this into a data structure ...

Application Tuning

Data structure design

- Particle data structure

```
typedef struct particle {
    double x, y, z;
    char ptype;
    double dist;
} particle_t;
```

- Is this a good idea?

Application Tuning

Data structure design

- Answer: It depends ...
  - ... on problem size
  - ... how you access the data
    - ... and how often
  - ... cache, CPU, etc.
- Example: program with 2 functions/routines
  - calc() - accesses all parts of particle_t
  - re-use() - accesses particle.dist only
  - usage ratio of both functions is 1:1

Application Tuning

Data structure design

Advantages of the data structure:

- `particle_t *p;` (and then allocate N)
- easy to pass data in function calls
  - `func(p, N);`
  - ... vs `func(x, y, z, ptype, dist, N);`
- flexible: I can add new elements to particle_t, without having to change the function interfaces/prototypes

Application Tuning

Data structure design

Downside of the data structure:

- memory access is no longer optimal
  - neighbouring elements of the same type, e.g. ‘x’ are no longer ‘stride 1’:
  - `x[i] -> x[i+1]` : stride 1
  - `p[i].x -> p[i+1].x` : ~stride 5 (in this example)
  - no good cache line usage
- compiler cannot optimize loops

Application Tuning

Data structure design

Get the best of both worlds!

- instead of using an “array of struct” (AOS),
- we can create a “struct of arrays” (SOA):

```
typedef struct particle {
     double *x, *y, *z;
     char   *ptype;
     double *dist;
} particle_t;
```


Application Tuning

Data structure design

Downside of the SOA:

- memory allocation is more complicated
  - one call to malloc() for each element
- need to change code:
  - `p[i].x -> p.x[i]`
  - ... and function prototypes: `f(*p,N) -> f(p,N)`
- but that’s a ‘one time effort’

Application Tuning

Data structure design

Advantages of SOA outweigh this by far:

- memory access is optimal again
- neighbouring elements of the same type, e.g. ‘x’ are again ‘stride 1’:
  - `p.x[i] -> p.x[i+1]` : stride 1
  - better cache line usage
  - access to single components, e.g. `p.dist`, do not need to load ‘all the rest’
- compiler can optimize loops better

Application Tuning

Data structure design

- Example: program with 2 functions/routines
  - calc() - accesses all parts of particle_t
  - re-use() - accesses particle.dist only
  - usage ratio of both functions is 1:1

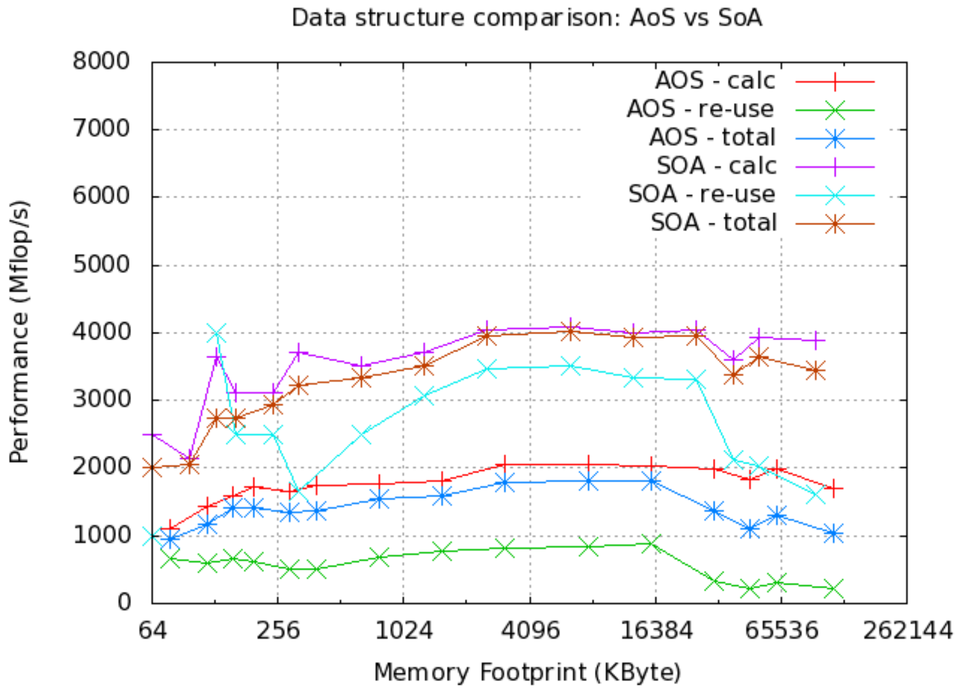
Data structure design

Comparison – two versions:

- *aos* – use 'array of struct'
- *soa* – use 'struct of arrays'

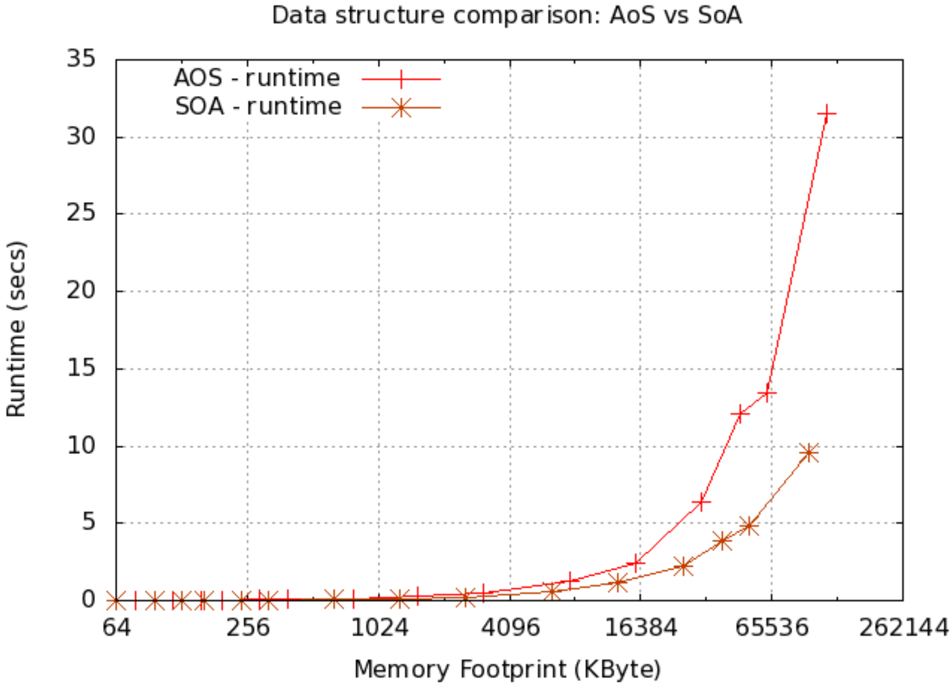
- different problem sizes:
  - number of particles

Data structure design



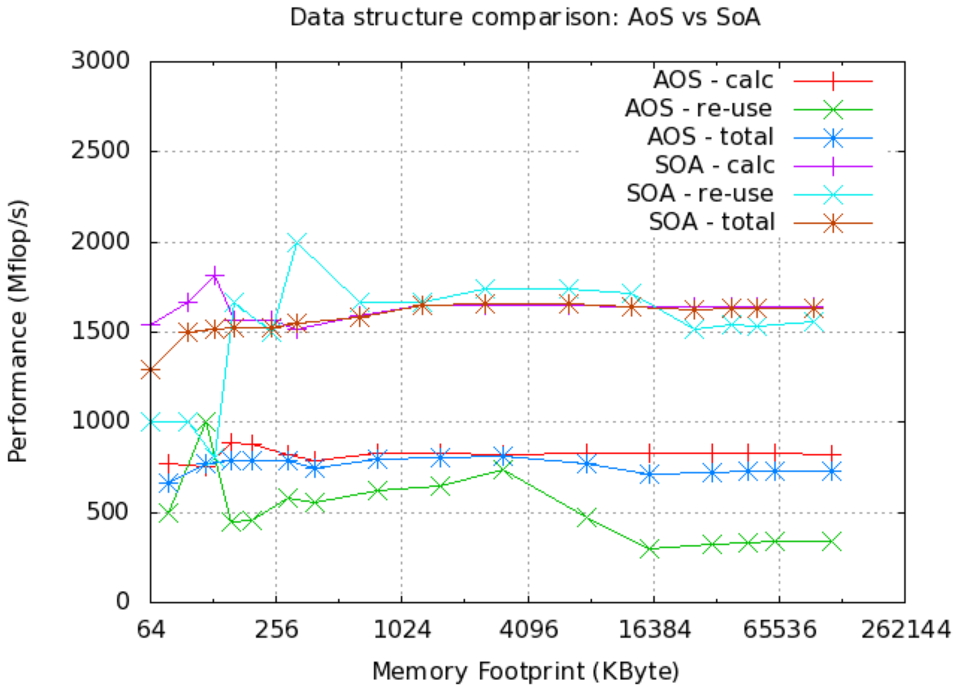
XeonE5-2660v3 25MB L3 cache

Data structure design



XeonE5-2660v3 25MB L3 cache

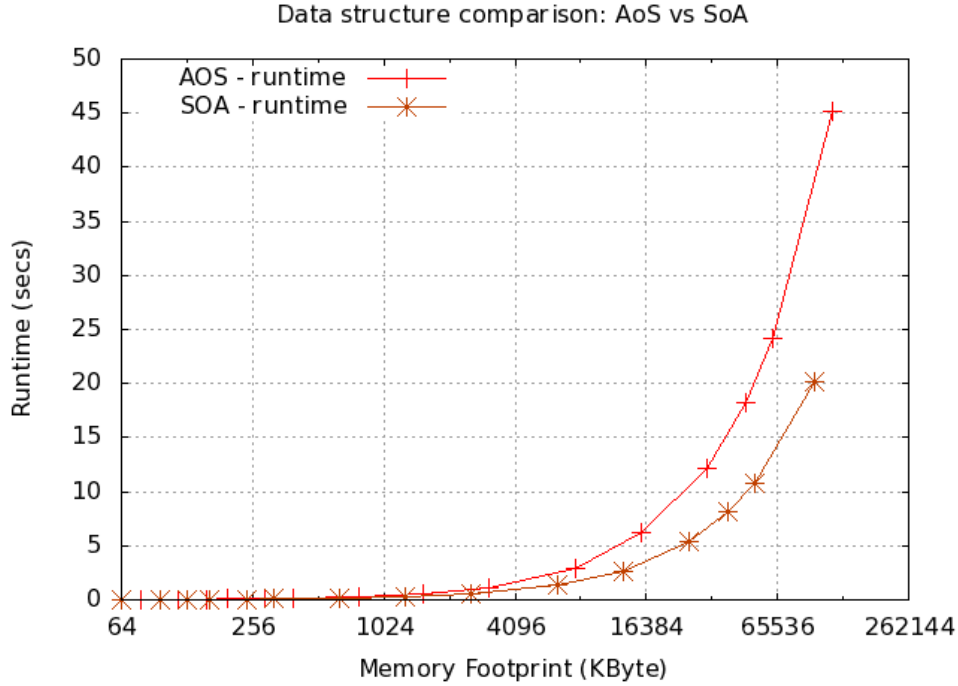
Data structure design



XeonX5550 8MB L3 cache

Application Tuning

Data structure design



XeonX5550 8MB L3 cache

Application Tuning

Data structure lab (aka tune_labs)

- download the ZIP file from DTU Inside
- read the instructions
  - do parts I and II now
  - part III needs more information (after lunch)
- Goals:
  - design and do performance experiments
  - extract the relevant data – and plot it