Department of Applied Mathematics and Computer Science



Getting good performance from your application

Tuning techniques for serial programs on cache-based computer systems

Overview

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





Moore's Law

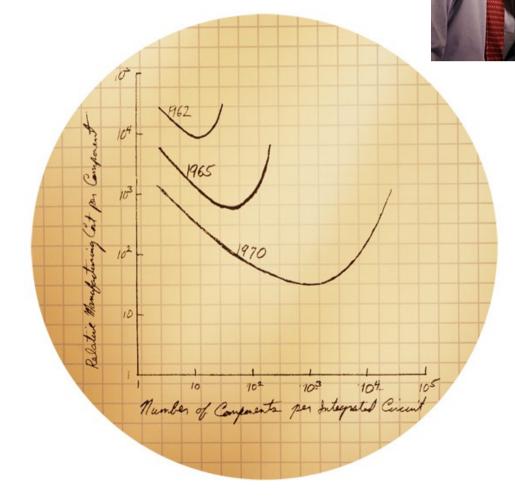
- Popular version:
 - "CPU speed usually doubles every 18 months."
- More correct version:
 - "The number of transistors per integrated circuit will double every 18 months."



Gordon Moore – co-founder of Intel

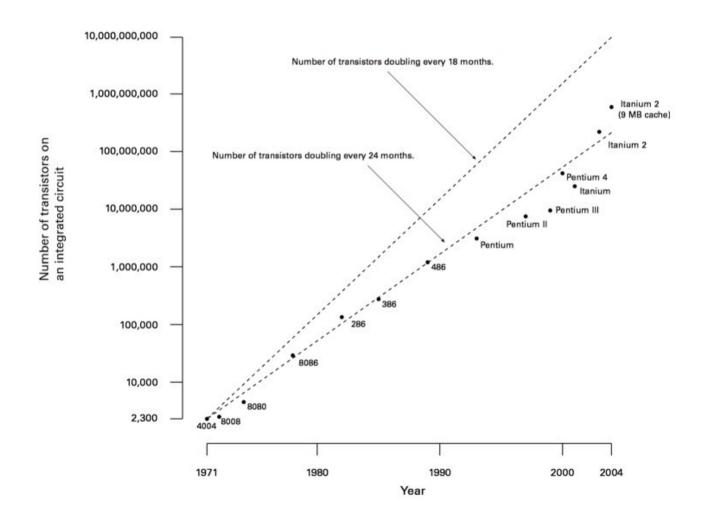
"I never said 18 months. I said one year, and then two years ... Moore's Law has been the name given to everything that changes exponentially. ... If Gore invented the Internet, I invented the exponential."

- Gordon Moore in an interview (2000)



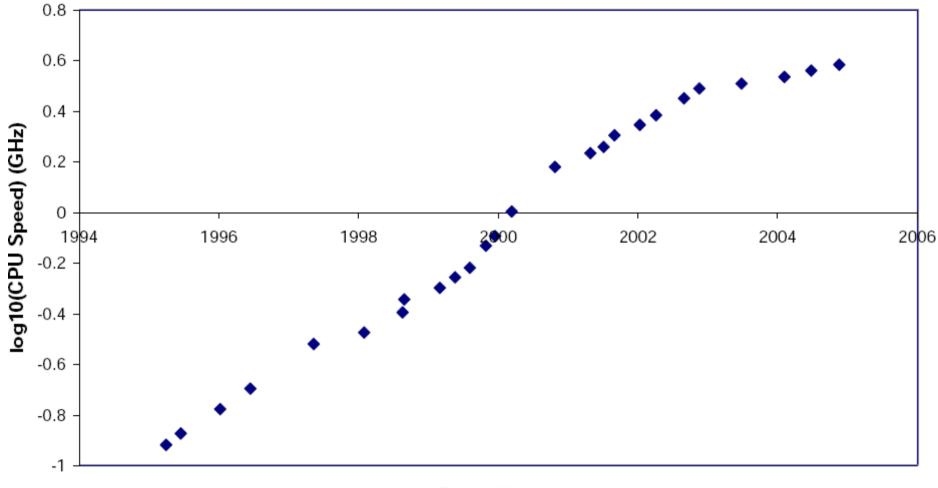


Moore's Law



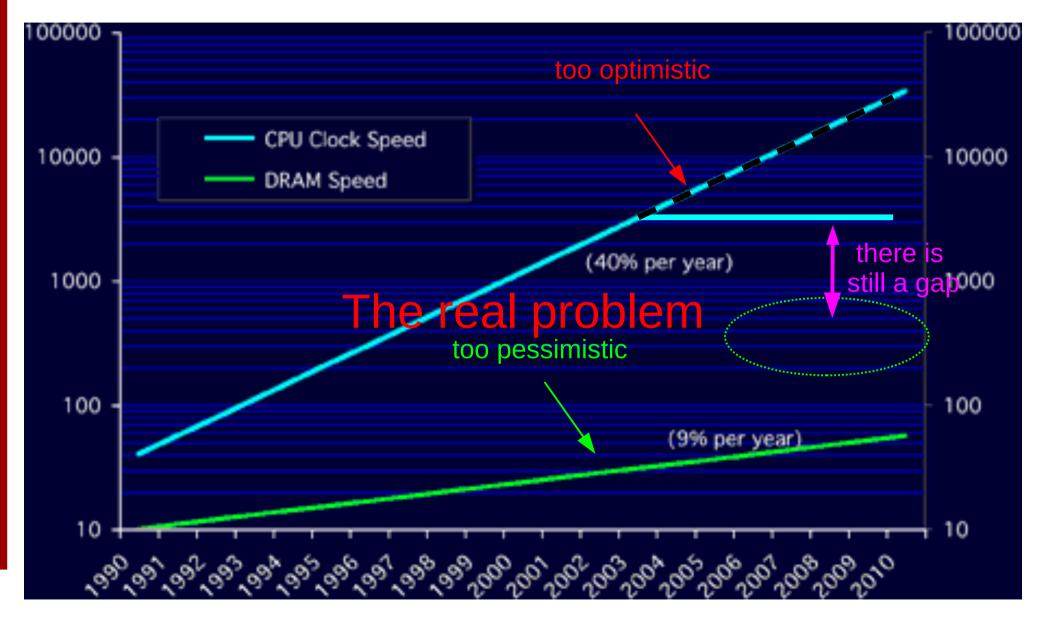


Maximum Intel CPU Speed (IA-32) vs Time Public domain, 2005-11-13





Time (Years)





- 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 (~ 4-6 years!).
- Memory speeds catch up but also have to serve more cores!
- New memory technologies do help (e.g. HBM)
- Something you should have in mind when designing your program!

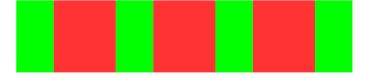


Motivation for Application Tuning

time flow in a computational task (simplified picture):



new hardware:



ideal: 2x faster computer



reality: 2x faster CPU



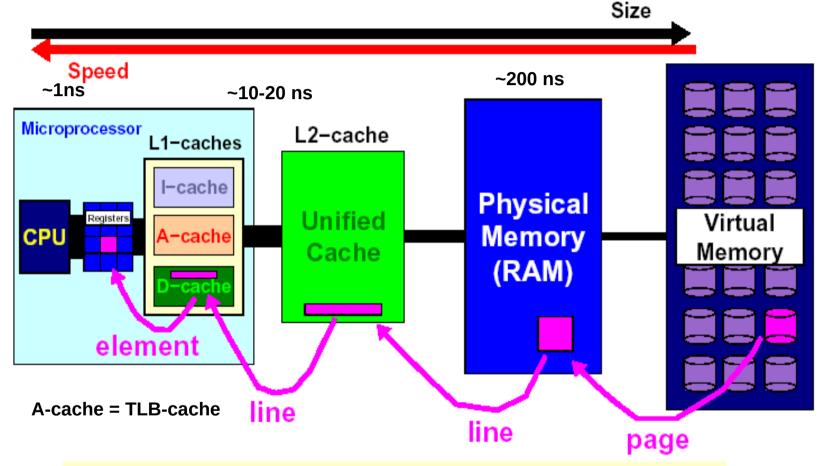




Intuitive Performance Graph:



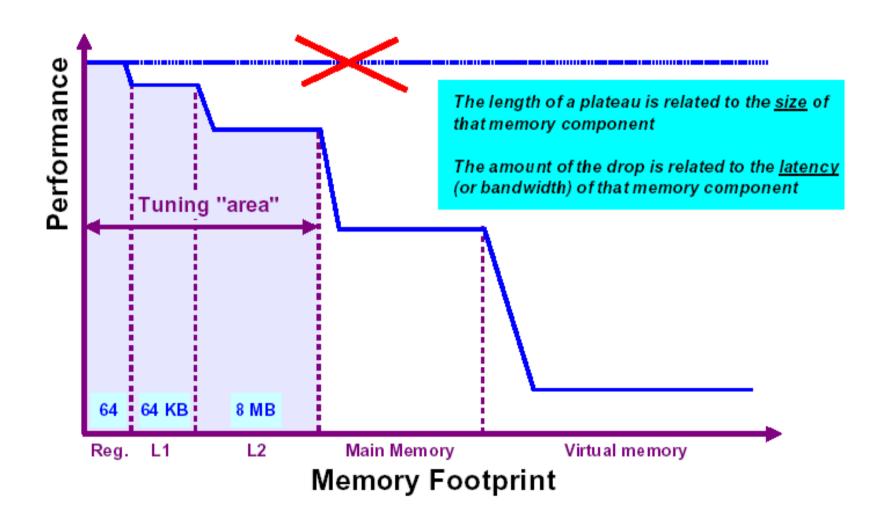




Memory Optimization: Keep frequently used data close to the processor

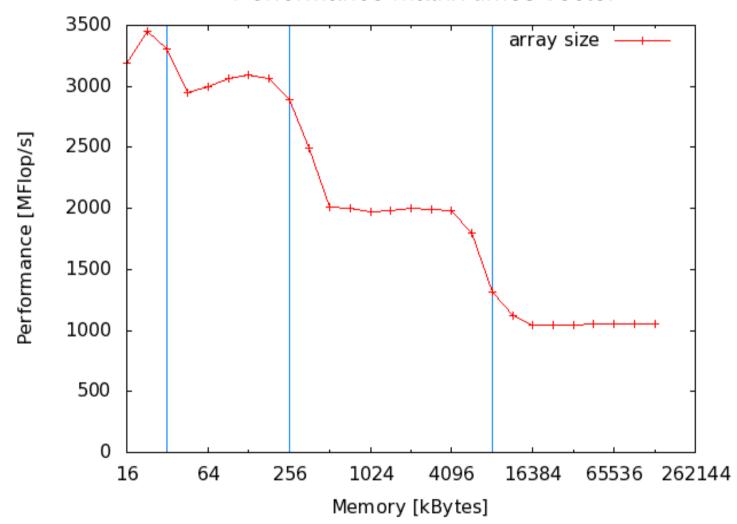


Performance is not uniform:





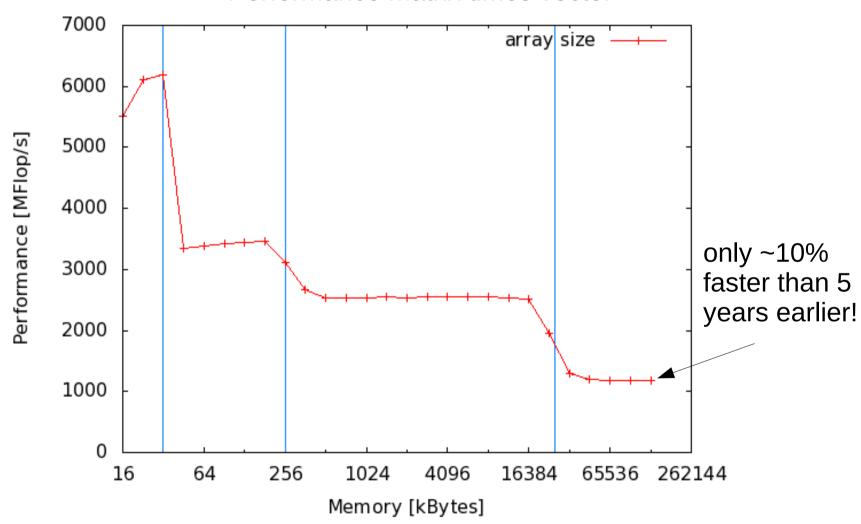
Performance matrix times vector





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

Performance matrix times vector





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

- 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



Caches – and all that ...

How do those caches work?



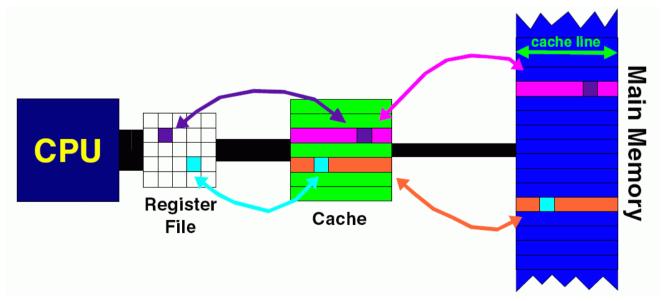
Caches

- 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



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





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



Cache Organisation

Fully Associative:

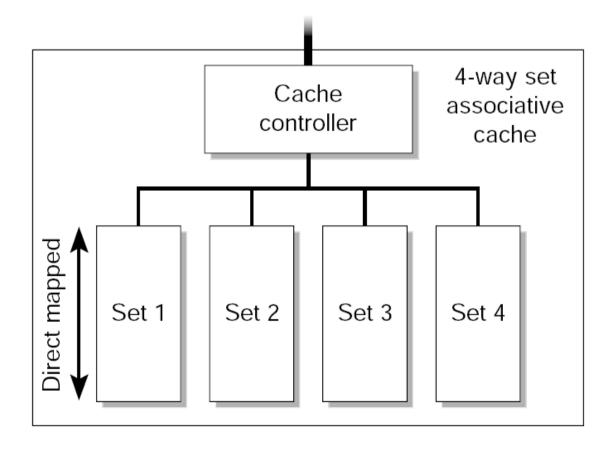
- Every memory address can be mapped anywhere in cache
- Need to track usage of cache lines
- Requires a replacement policy, e.g.
 - least recent used (LRU),
 - least frequent used (LFU),
 - random, etc
- Doesn't scale well to large sizes
- Costly design



Cache Organisation

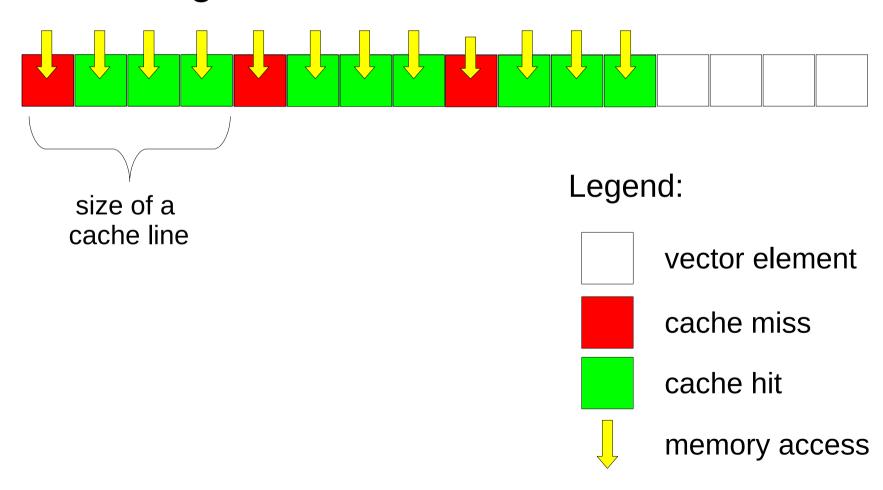
N-way Set Associative:

Sets of direct mapped caches:



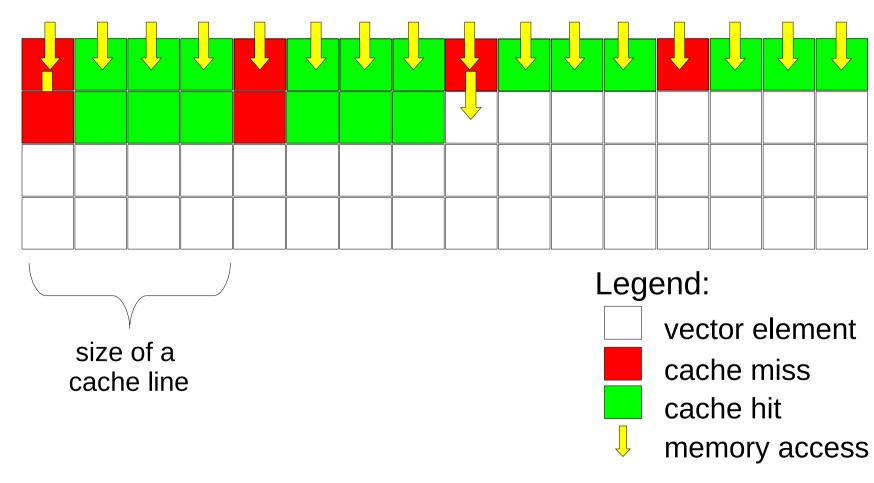


- Memory has a 1-dimensional linear structure
- Accessing vector elements:



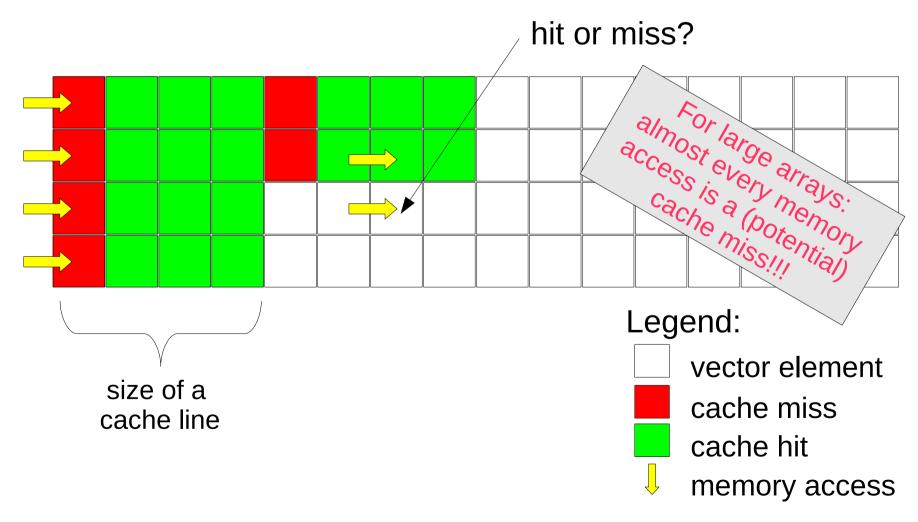


Accessing 2d arrays in C – row wise:





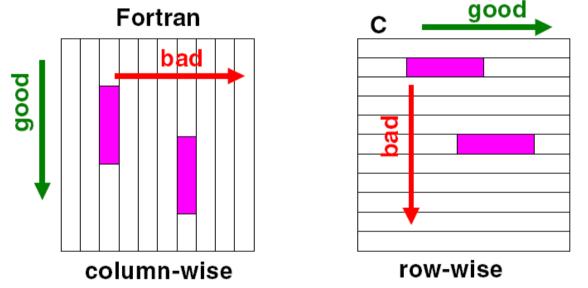
Accessing 2d arrays in C – column wise:

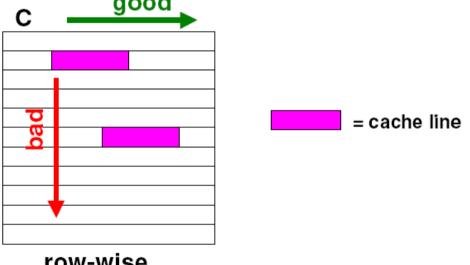




January 2025

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





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

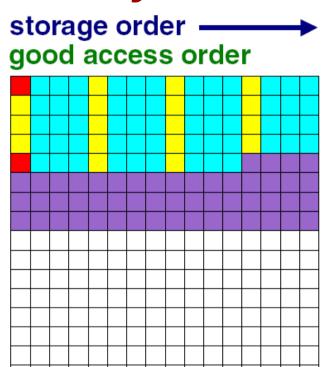


The TLB cache

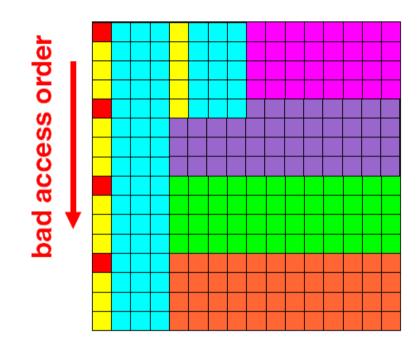
- the Translation Lookaside Buffer (TLB) translates virtual memory addresses (in your application) to physical addresses
- also called 'address cache'
- unit: page typical size 4kB
- creation of lookup table is an expensive operation
- □ cost: 10 100 clock cycles/miss
- modern CPUs are having advanced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



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 <u>does</u> matter both data cache and TLB misses



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



Cache Line Utilization

Two key rules: Maximize ...

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



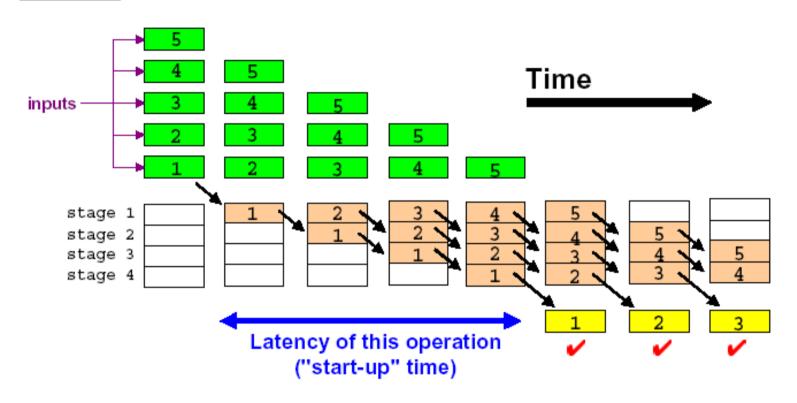
Some Terminology



Terminology: Pipelining

stage 1 stage 2 stage 3 stage 4

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

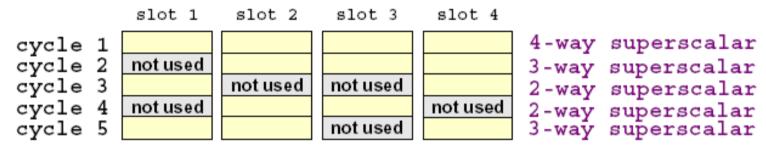


Rule of thumb: keep the pipeline filled for good performance!



Terminology: Superscalar (or ILP)

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



- 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: FMA

One variant of ILP for floating point operations:

- FMA Fused Multiply Add
- special instruction, that calculates

$$a + (b * c)$$

in one operation, with a single rounding

- □ faster
- ... but the result might slightly differ, due to the single rounding!



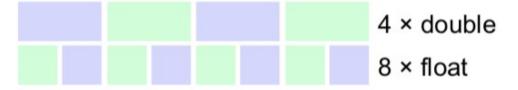
Terminology: Vectorization (SIMD)

- □ 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.

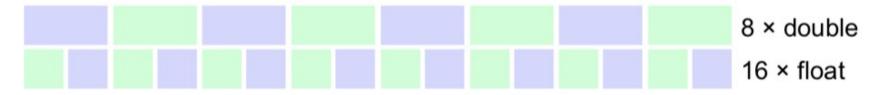


Terminology: Vectorization (SIMD)

- Vector types
 - 128 bit: SSE = Streaming SIMD Extension (1999)
 - 2 × double 4 × float
 - 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



General Optimization Techniques



Optimization Techniques - Overview

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



Optimization Techniques - Overview

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



Loop based optimizations



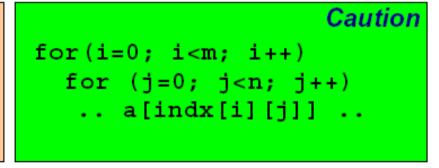
Coding style: array indexing

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

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

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





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

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



Loop Fission

```
for (j=0; j< n; j++)
                                      Access on arrays 'a'
                                        and 'b' is bad
   c[j] = exp(j/n);
                                      We can not simply
   for (i=0; i< m; i++)
       a[i][j]=b[i][j]+d[i]*e[j];
                                        interchange the loops
                                      Fission/splitting is the
                          Fission
                                        solution
                           for (j=0; j< n; j++)
 This loop can now
                                                New loop created
                              c[i] = exp(j/n);
 also be vectorized
                           for (j=0; j< n; j++)
Interchange loops for
                              for (i=0; i<m; i++)
better performance
                                 a[i][j]=b[i][j]+d[i]*e[j];
```



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

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

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



Fission and Fusion – Summary

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];
            Loop is unrolled
            with a factor of 4
for (i=0; i< n; i+=4)
       ] = 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 : 2
Stores : 1
FP Adds : 1
I=I+1
Test I < N ?
Branch
Addr. incr: 3
```

```
Work: 4
Overhead: 6
```

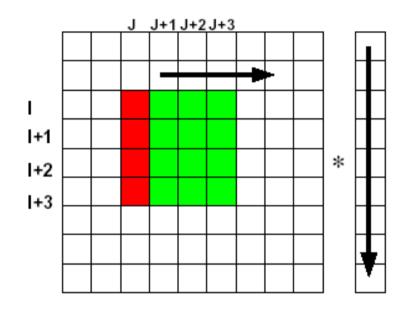
```
Loads : 8
Stores : 4
FP Adds : 4
I=I+4
Test I < N ?
Branch
Addr. incr: 3
```

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];
}</pre>
```

```
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]



Outer Loop Unrolling – how to

```
for (1=0; 1< m-m%4; 1+=4)
for (i=0; i<m; i++)
  for (j=0; j< n; j++)
                                    for(j=0; j< n; j++)
   a[i] += b[i][j] * c[j];
                                      a[i] += b[i][j] * c[j];
                                    for (j=0; j< n; j++)
                  Outer loop
                                      a[i+1] += b[i+1][j] * c[j];
                   unrolling
                                    for (1=0; 1< n; 1++)
                                      a[1+2] += b[1+2][1] * c[1];
                                    for (j=0; j< n; j++)
Unroll and Jam
                                      a[i+3] += b[i+3][j] * c[j];
                                  for (1=m-m%4; 1<m; 1++) clean-up loop
                                    for (1=0; 1< n; 1++)
for (i=0; i< m-m%4; i+=4)
                                      a[i] += b[i][i] * c[i];
  for(j=0; j<n; j++)
                                                     Jam the loops
    a[i] += b[i][j] * c[j];
                                                     together again
    a[i+1] += b[i+1][j] * c[j];
    a[i+2] += b[i+2][i] * c[i];
    a[i+3] += b[i+3][i] * c[i];
for (i=m-m%4; i<m; i++)
                            clean-up loop
  for(j=0; j<n; j++)
    a[i] += b[i][i] * c[i];
```



Loop unrolling – structure

```
(i=0; i< n; i++)
                                        DO I = 1, N
                                             ... (I) ...
       ... [i] ...
                                         END DO
                         Loop unroll factor
                             is "unroll"
for(i=0;i<n-n%unroll;i+=unroll)</pre>
                                    DO I = 1, N-mod(N, unroll), unroll
                                        ...(I) ...
   ...[1] ...
                                        ...(I+1)...
   ...[1+1]...
                                        ...(I+2)...
   ...[1+2]...
                           Unrolled Loop
                                        ...(I+unroll-1)...
   ...[i+unroll-1]...
                                    END DO
                           Cleanup Loop
for(1=n-n%unroll;1<n;1++)
                                    DO I = N-mod(N, unroll)+1, N
                                        ... (I) ...
   ...[1]...
                                    END DO
```



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

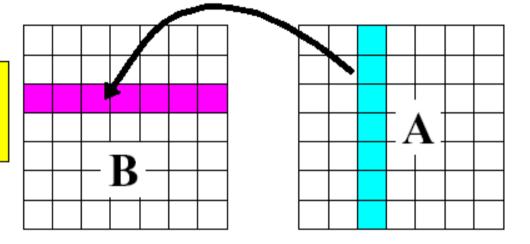
- compilers do (usually) a good job in loop unrolling – leave it to the compiler
- some compiler need to be told to do loop unrolling – not part of standard optimization, always check if in doubt
- there are options to control the unroll depth
 - gcc: -funroll-loops --params max-unroll-times=n
 - clang: -funroll-loops --unroll-count=n
 - Intel: -unroll[n] (0: disable loop unrolling)
- or compiler specific pragmas (see docs)



Loop Blocking – 1

Transposing a matrix

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



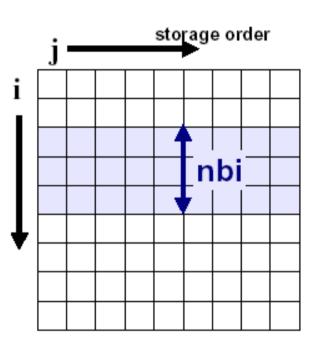
- Loop interchange will not help here:
 - Role of 'a' and 'b' will only be interchanged
- Change of programming language won't help either
- Unrolling the i-loop can be beneficial, but requires more registers and doesn't address TLB-misses
- Loop blocking achieves good memory performance, without the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



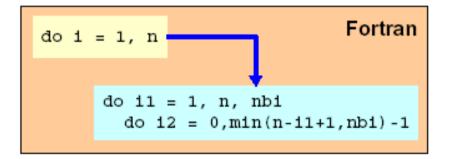
Loop Blocking – 2

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];</pre>
```



- ◆ 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
 - ·





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 (hardware)
 - data requirements



Loop Blocking – Summary

Recommendations:

- choose blocking size as large as possible
- leave space for other data
- parameterize cache characteristics, especially size
- How many loops should I block?
 - depends on the data access pattern, i.e. look for load and store operations



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)
                                      Independent of loop indices!!!
    CX(2) = CM1(2) - CM2(2)
    CX(3) = CM1(3) - CM2(3)
          ... statements removed ...
  ENDDO
ENDDO
```

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



Only the programmer knows ...

```
subroutine do calc(...)
subroutine do calc(...)
                            real(8), dimension(N, M, O, P):: r, s, t
real(8), dimension(N, M, O, P):
                            !--- data initialization
!--- data initialization
                            r = 0.0d0; s = 0.0d0
r = 0.0d0; s = 0.0d0; t = 0
                            select case (calc type)
select case (calc type)
                               case (most of the time)
   case(most of the time)
                                 r(i,j,k,l) = r(i,j,k,l) + ...
     r(i,j,k,l) = r(i,j,k,l)
                                 s(i,j,k,l) = s(i,j,k,l) + ...
     s(i,j,k,l) = s(i,j,k,l)
                               case(rare event)
   case(rare event)
                                 t = 0.0d0
     r(i,j,k,l) = r(i,j,k,l)
                                 r(i,j,k,l) = r(i,j,k,l) + ...
     s(i,j,k,l) = s(i,j,k,l)
                                 s(i,j,k,l) = s(i,j,k,l) + ...
     t(i,j,k,l) = t(i,j,k,l)
                                 t(i,j,k,l) = t(i,j,k,l) + ...
end select
                            end select
```



Access your data in the right way



- "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 ...



Particle data structure

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

Is this a good idea?



- 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



Advantages of the data structure:

- particle_t *p; (and then allocate N)
- easy to pass data in function calls

```
\square func(p, N);
```

```
\square ... VS func(x, y, z, ptype, dist, N);
```

Ilexible: I can add new elements to particle_t, without having to change the function interfaces/prototypes



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



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;
```



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]
 - \square ... and function prototypes: $f(*p,N) \rightarrow f(p,N)$
- but that's a 'one time effort'



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



- 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

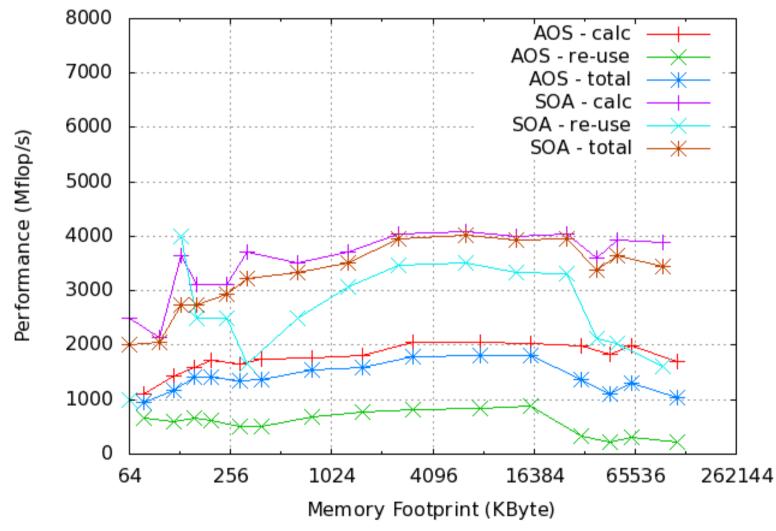


Comparison – two versions:

- aos use 'array of struct'
- soa use 'struct of arrays'
- different problem sizes:
 - number of particles



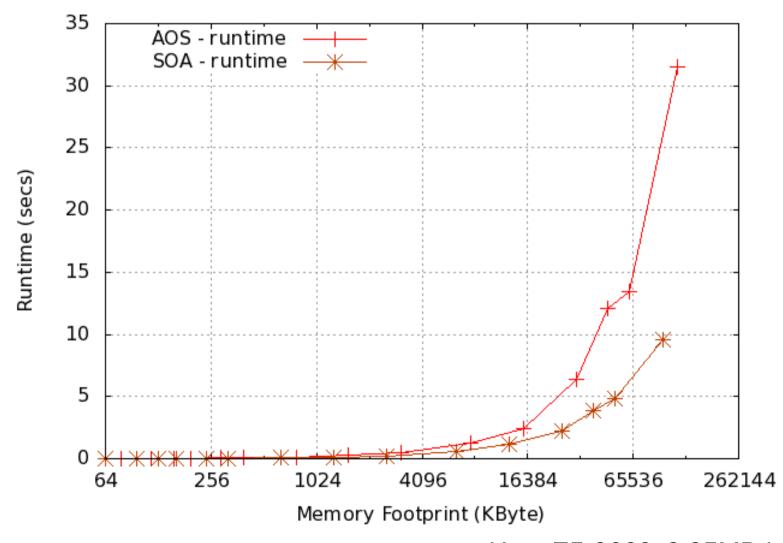
Data structure comparison: AoS vs SoA





XeonE5-2660v3 25MB L3 cache

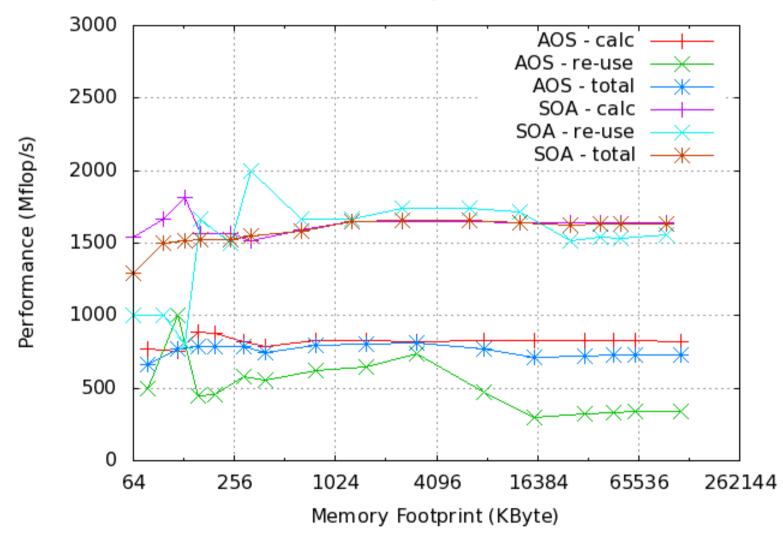
Data structure comparison: AoS vs SoA





XeonE5-2660v3 25MB L3 cache

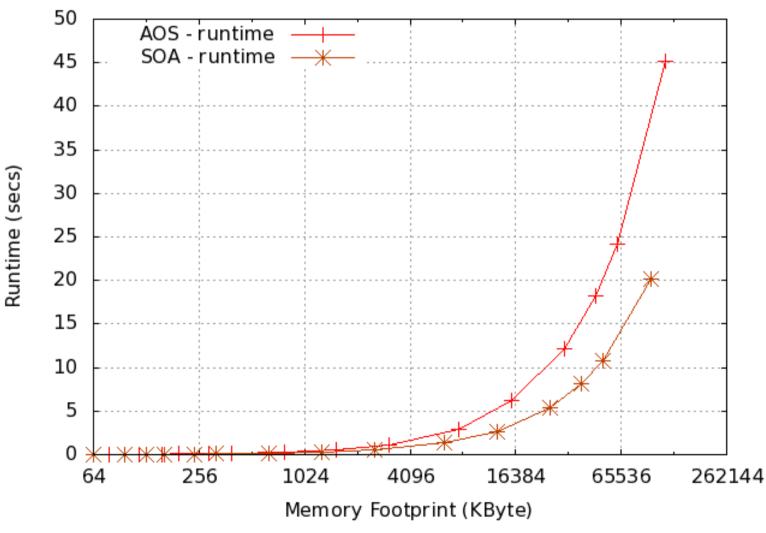
Data structure comparison: AoS vs SoA





XeonX5550 8MB L3 cache

Data structure comparison: AoS vs SoA





XeonX5550 8MB L3 cache

Data structure lab (aka tune_labs)

- download the ZIP file from DTU Learn
- 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



Think about the 'design' of your experiment!

- What can I measure directly?
 - Almost always: time!
 - Time is not always a "good" quantity
- Adding 'a priori' knowledge: for a given problem size we typically know the ...
 - number of iterations
 - number of operations (flops, loads, stores)
- allows us to calculate Mflop/s, iter/s, bandwidth, ...

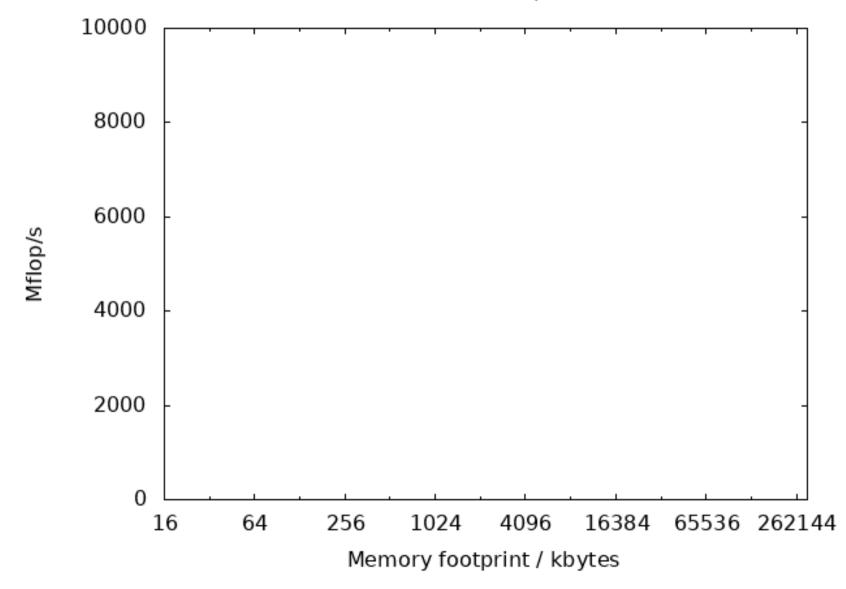


Think about the 'design' of your experiment!

- "Where" should I measure?
 - your measurement should support a model (or an 'idea'), e.g. 'performance vs memory footprint'
 - make use of prior knowledge, e.g. the memory layout of the hardware (L1,...,L3 cache sizes, and latencies/bandwidths)
 - choose your measuring points, e.g. memory footprint, to map the "interesting areas" in the "performance landscape"

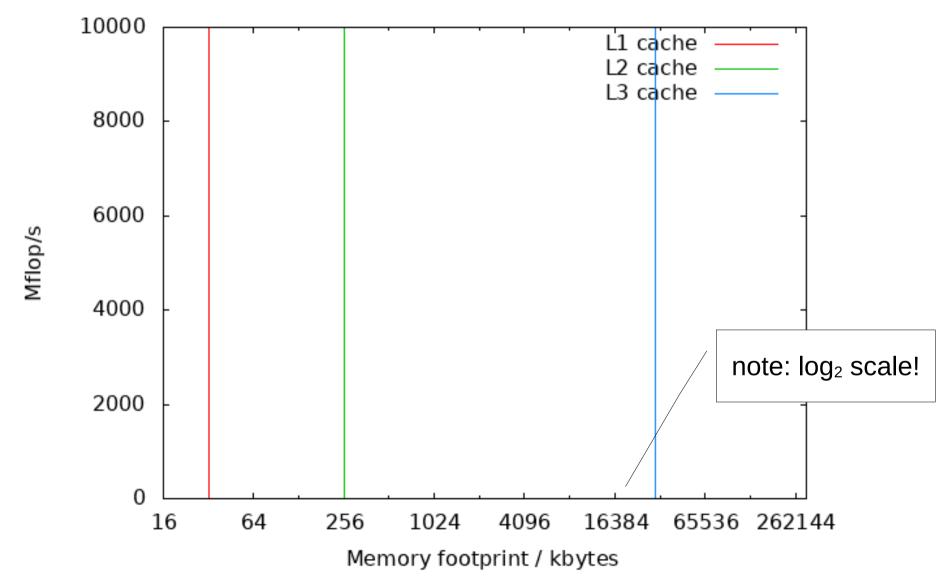


Performance plot





Performance plot





Best practice:

- isolate the "kernel" you want to benchmark (e.g. in a function)
- do a pre-measurement call ("warm up")
- □ repeat the measurements to get a "reasonable" run time (e.g. 2-3 secs), take the average
- make sure to use the same system (CPU type), to get comparable results
- □ reduce the "system noise", i.e. other processes, users, etc use the batch system



End of lecture 1

