

Optimization Loops & Prefetching

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“Foundation of HPC” course



DATA SCIENCE &
SCIENTIFIC COMPUTING
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Optimization



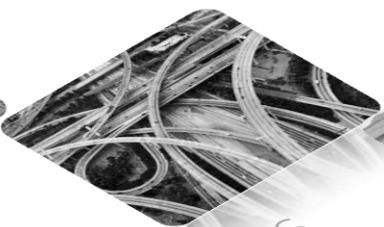
Outline



First
things
first



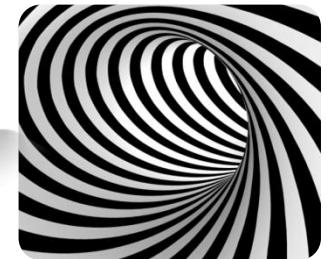
Cache &
Memory



Branches



Pipelines



Loops

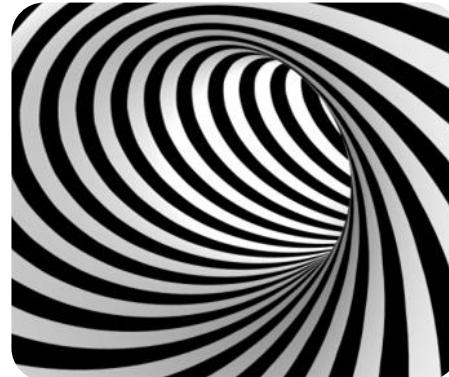
Loops



Outline



Avoid the
avoidable
inefficiencies



Loops
techniques

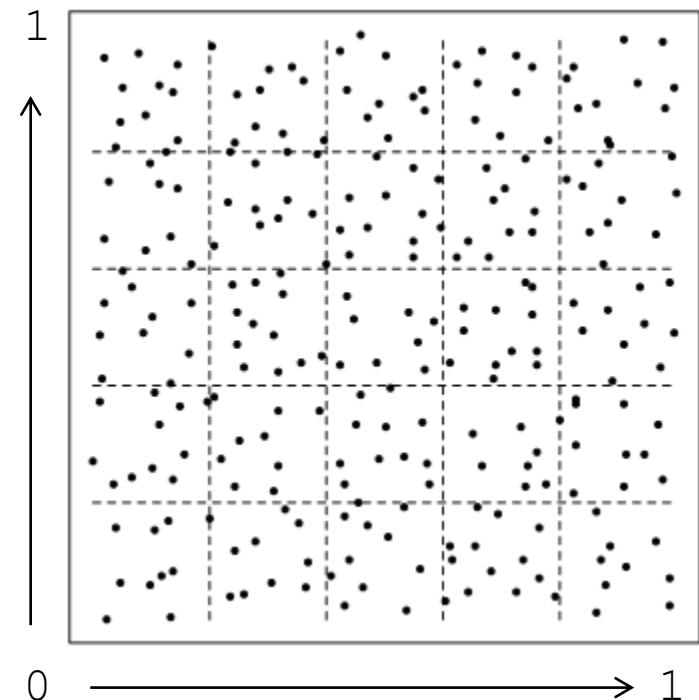


Prefetching

Introducing the example's framework

Let's suppose that

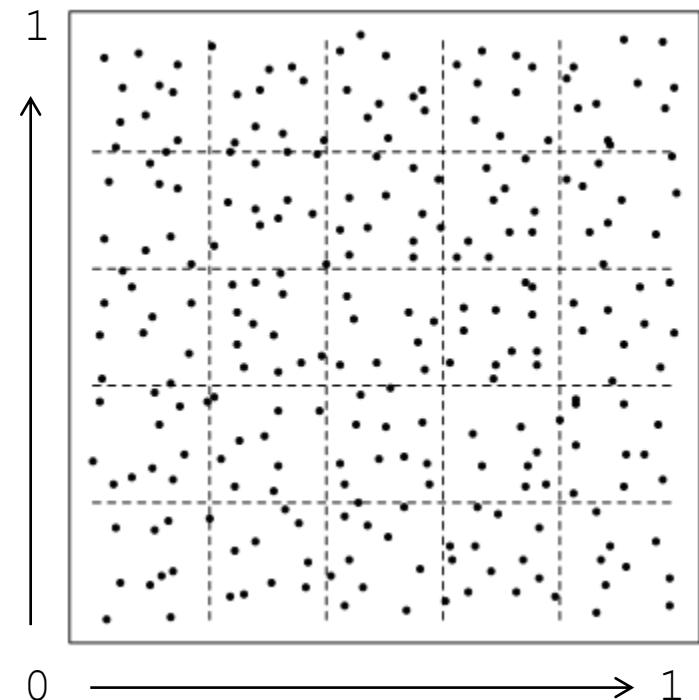
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Introducing the example's framework

Let's suppose that

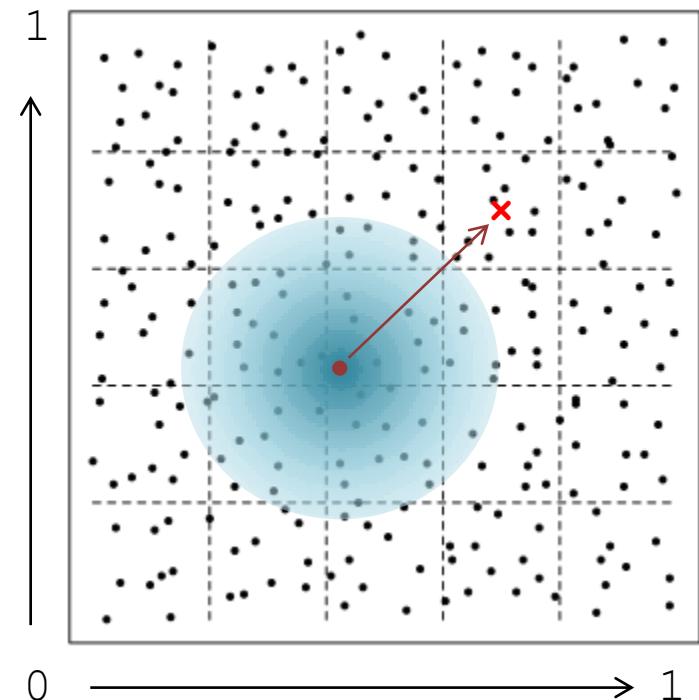
- 1) we have a distribution of random data points on a 2D plane which we subdivide in sub-regions using a grid.
- 2) for each point p , we want to select all the grid cells whose center is closer to p than a given radius r , and to perform some operations accordingly to our search result.



Introducing the example's framework

Let's suppose that

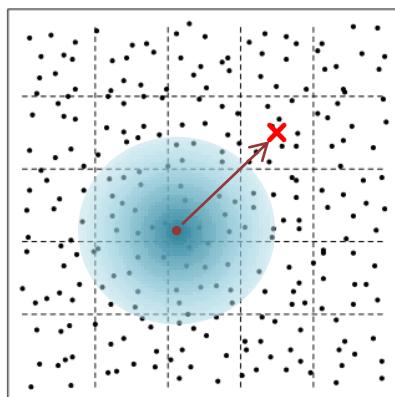
- 1) we have a distribution of random data points on a 2D plane which we subdivide in sub-regions using a grid.
- 2) for each point p , we want to select all the grid cells whose center is closer to p than a given radius r , and to perform some operations accordingly to our search result.



Introducing the example's framework

We may consider to
use a nested loop
like this one →

```
for(p = 0; p < Np; p++)
    for(i = 0; i < Ng; i++)
        for(j = 0; j < Ng; j++)
            for(k = 0; k < Ng; k++)
            {
                dist = sqrt(
                    pow(x[p] - (double)i/Ng - half_size, 2) +
                    pow(y[p] - (double)j/Ng - half_size, 2) +
                    pow(z[p] - (double)k/Ng - half_size, 2));
                if(dist < R)
                    do something;
            }
        }
```



Is there anything
you would change
in this loop?



| (1) Avoid expensive function calls

```
for(p = 0; p < Np; p++)
```

Some function calls are particularly expensive. Those include, among others, `sqrt()`, ...

Try to avoid them *if* possible.

```
for(i = 0; i < Ng; i++)
    for(j = 0; j < Ng; j++)
        for(k = 0; k < Ng; k++)
{
    dist2 = pow(x[p] - (double)i/Ng - half_size, 2) +
            pow(y[p] - (double)j/Ng - half_size, 2) +
            pow(z[p] - (double)k/Ng - half_size, 2));
    if(dist2 < R2)
        do something;
}
```



| (1) Avoid expensive function calls

```
for(p = 0; p < Np; p++)
```

Some function calls are particularly expensive. Those include, among others, `sqrt()`, `pow()`, ...

Try to avoid them *if* possible.

```
for(i = 0; i < Ng; i++)
    for(j = 0; j < Ng; j++)
        for(k = 0; k < Ng; k++)
        {
            dx = x[p] - (double)i/Ng - half_size;
            dy = y[p] - (double)j/Ng - half_size;
            dz = z[p] - (double)k/Ng - half_size;

            dist2 = dx*dx + dy*dy + dz*dz;
            if(dist2 < R2)
                do something;
        }
```



| (1) Avoid expensive function calls

```
for(p = 0; p < Np; p++)
```

Some function calls are particularly expensive. Those include, among others, `sqrt()`, `pow()`, floating point division, .. Try to avoid them if possible.

```
for(i = 0; i < Ng; i++)
    for(j = 0; j < Ng; j++)
        for(k = 0; k < Ng; k++)
        {
            dx = x[p] - (double)i * Ng_inv - half_size;
            dy = y[p] - (double)j * Ng_inv - half_size;
            dz = z[p] - (double)k * Ng_inv - half_size;

            dist2 = dx*dx + dy*dy + dz*dz;
            if(dist2 < R2)
                do something with sqrt(dist2);
        }
```



| (1) Avoid expensive function calls

```
(double)<i,j,k> * Ng_inv + half_size
```

was performed N^3+N^2+N times, always returning the same values.

Hoisting would save

$N(N^2+N^1+1)$ **mul**, **add** and **mem** accesses.

You can do better pre-computing the relevant values:

```
double ijk[Ng];
for(i = 0; i < Ng; i++)
    ijk[i] = i * Ng_inv + half_size
```

```
for(p = 0; p < Np; p++)
    for(i = 0; i < Ng; i++)
        for(j = 0; j < Ng; j++)
            for(k = 0; k < Ng; k++)
            {
                dx = x[p] - (double)i * Ng_inv - half_size;
                dy = y[p] - (double)j * Ng_inv - half_size;
                dz = z[p] - (double)k * Ng_inv - half_size;

                dist2 = dx*dx + dy*dy + dz*dz;
                if(dist2 < R2)
                    do something with sqrt(dist2);
            }
```



| (2) Hoisting of expressions

```
for(i = 0; i < Ng; i++) {  
    dx2 = x[p] - (double)i * Ng_inv - half_size;  
    dx2 = dx2*dx2;  
  
(double)<i,j,k> * Ng_inv + half_size
```

was performed N^3+N^2+N times,
always returning the same values.
Hoisting would save

$N(N^2+N^1+1)$ `mul`, `add` and `mem` accesses.

```
for(j = 0; j < Ng; j++) {  
    dy2 = y[p] - (double)j * Ng_inv - half_size;  
    dy2 = dy2*dy2;  
    dist2_xy = dx2 + dy2;
```

```
for(k = 0; k < Ng; k++) {  
    dz = z[p] - (double)k * Ng_inv - half_size;  
    dist2 = dist2_xy + dz*dz;  
    if(dist2 < Rmax2)  
        do something with sqrt(dist2); } } }
```



| (2) Hoisting of expressions

You could do even better by pre-computing the relevant values:

```
double ijk[Ng];
for(i = 0; i < Ng; i++)
    ijk[i] = i * Ng_inv + half_size
```

```
for(i = 0; i < Ng; i++) {
    dx2 = x[p] - Ng_inv[i] - half_size;
    dx2 = dx2*dx2;

    for(j = 0; j < Ng; j++) {
        dy2 = y[p] - Ng_inv[j] - half_size;
        dist2_xy = dx2 + dy2*dy2;

        for(k = 0; k < Ng; k++) {
            dz = z[p] - Ng_inv[k] - half_size;
            dist2 = dist2_xy + dz*dz;
            if(dist2 < Rmax2)
                do something with sqrt(dist2); } } }
```



| (3) Clarify the variables' scope

All these variables are very local, there's no need for them to have a wider scope.

That will help you in writing the code, and may help the compiler in optimizing the stack and perhaps the registers usage.

```
for(int i = 0; i < Ng; i++) {  
    double dx2 = x[p] - (double)i * Ng_inv - half_size;  
    dx2 *= dx2;  
  
    for(j = 0; j < Ng; j++) {  
        double dy2 = y[p] - (double)j * Ng_inv - half_size;  
        double dist2_xy = dx2 + dy2*dy2;  
  
        for(k = 0; k < Ng; k++) {  
            double dz = z[p] - (double)k * Ng_inv - half_size;  
            double dist2 = dist2_xy + dz*dz;  
  
            if(dist2 < Rmax2)  
                do something with sqrt(dist2); } } }
```



| (4) Suggest what is important

```
double register Ng_inv = 1.0 / Ng;  
for(int i = 0; i < Ng; i++) {  
    double dx2 = x[p] - (double)i * Ng_inv - half_size;  
    dx2 *= dx2;  
  
    for(j = 0; j < Ng; j++) {  
        double dy2 = y[p] - (double)j * Ng_inv - half_size;  
        dy2 *= dy2;  
        double register dist2_xy = dx2 + dy2;  
  
        for(k = 0; k < Ng; k++) {  
            double register dz = z[p] - (double)k * Ng_inv - ...;  
            double register dist2 = dist2_xy + dz*dz;  
  
            if(dist2 < Rmax2)  
                do something with sqrt(dist2); } } }
```

These variables are often calculated and reused subsequently.

Keeping a register dedicated to them may be useful.

Note: *this is a suggestion, the compiler, after analyzing the code, may decide differently*

Note: the importance of being earnest

Paying attention to the scope of the variables and keeping local what *is* local has a twofold importance.

One hand:

all your local variables will reside in the stack, fine.

However, also the stack, which can be wide, must be organized: where each “variable” should be put? Where is the best location for it to be “hot” at the right moment at the right place? Should it stay “together” (i.e. close in memory and hence probably close in cache) with other local variables that will be used at the same time?

for instance, in the previous example: i,j,k,dx2,dy2,dz,dist2_xy,Rmax2 are all used packed together. What if where all defined at the begin of a long procedure with general labels and used for different purposes all around? What would have been the most optimal place to stack all them? (help the poor compiler in taking the best decision..)

Note: the importance of being earnest

Paying attention to the details of C/C++ has a twofold importance.

One hand: all your local variables should be put in one place? Should they be with other local variables? For instance, in C/C++, in together. What is used for different stack all them?

Since many among you asked:
in

```
for(int i = 0; i < Ng; i++) {  
    double dx2 = something; ...; }
```

the definition of **dx2** does not cause any additional “operation”: the variable is just 8 bytes in the stack that have been reserved by the compiler since the beginning.

C/C++ are *compiled* languages, not *interpreted* languages.

variable”
at the right
in cache)

ed packed
ral labels and
al place to

Note: the importance of being earnest

Paying attention to the scope of the variables and keeping local what *is* local has a twofold importance.

One the other hand:

Keep your mind clear and sharp. Think carefully to what you need and where, and make it clear.

That will help you a lot in the next future when you'll have to maintain/debug – or just understand – your code.

That will help you in *not* inserting dependence chains by mistake (for instance, with a variable with a general label “temp” used all around may carry some garbage when it was not intended to).

Being a good programmer is all about thinking clearly and sharply.



CAVEAT !!

Do not suppose that your compiler is *always* able to re-arrange calculations – like avoiding expensive calls or using mathematically-equivalent more convenient expressions – all the time. It may be able to do that for *integer* calculations but it will not do it for *floating-point* calculations.

The reason is simple, and it is related to the fact that on a digital system the math is *not always* as it is on the blackboard:

Integer math (+ and \times) in 2's complement
is commutative and associative.

Floating point math (+ and \times) is
commutative between 2 operands
is never associative.



| CAVEAT !!

In fact, if you study, as you should, the “what every computer scientist should know about floating-point” paper (find it in the `materials/` folder on `github`), you discover that if **a**, **b**, and **c** are FP numbers,

$$(a + b) + c \neq a + (b + c)$$

due to the very nature of floating-point representation in a digital system (with a finite number of digits).

The issue is related to the limited number of digits available to represent the number which, in turn, limits the precision.



CAVEAT !!

Let's suppose that we have 3 digits of precision for the mantissa. For the sake of simplicity, we consider a base 10 (so every single digit ranges in [0..9]).

Then the following hold:

$$1.00 + 0.01 = 1.01$$

$$1.00 + 0.001 = 1.00$$

The last is true because, although we can represent 0.001 (it is 1.00 with a -3 exponent) the summation of 1.00 and 0.001 is beyond our precision: 1.001 would require 4 digits. As a consequence, we are not able to distinguish it from 1.00.



CAVEAT !!

Then again:

These sum up to 0.01

$$\begin{array}{r} \mathbf{0.001} + \\ \mathbf{0.001} = \\ \mathbf{1.01} \end{array}$$

$$\begin{array}{r} \mathbf{1.00} + \\ \mathbf{0.001} = \\ \mathbf{1.00} \end{array}$$

Each of these ops results in 1.00

So, the compiler is NOT free to reshuffle the order of floating-point operations,

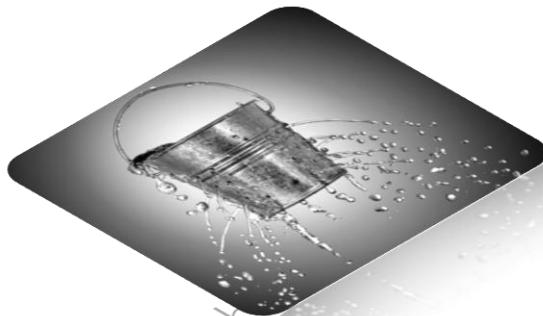
..even if a mathematically-equivalent formulation, different than the one you coded, would be more performant.

see the materials in the github folder
./materials/kahan_summation

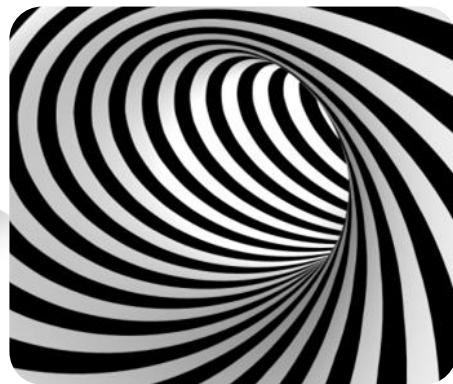
Loops



Outline



Avoid the
avoidable
inefficiencies



Loops
techniques



Prefetching

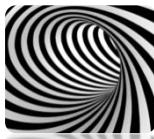


Loop classification

$$A_I = \frac{f(n)}{n}$$

Arithmetic Intensity: the ratio between the number of performed operations and the amount of the data.

1. $O(N) / O(N)$
optimization potential limited
2. $O(N^2) / O(N^2)$
some more opportunities for opt.
3. $O(N^3) / O(N^2)$
significant optimization potential



Cache access in loops: $O(N)/O(N)$

Example

1-level loops: Scalar products, vector additions, sparse matrix-vector multiplication

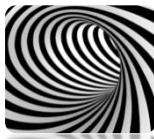
Inevitably memory-bound for very large N ; in general, improvements come from *avoiding unnecessary operations and/or repeated memory accesses, and increasing data reuse*

[check the room for loops fusion]

$O(N) / O(N)$

```
for(int j=0; j<2; j++)           for(int j=0; j<2; j++)  
    A[i] = B[i] × C[i]           {  
                                A[i] = B[i] × C[i]  
                                Q[i] = B[i] + D[i]  
    }  
for(int j=0; j<2; j++)           }  
    Q[i] = B[i] + D[i]
```

Loop fusion: in the version on the right, B is recalled from memory only once.



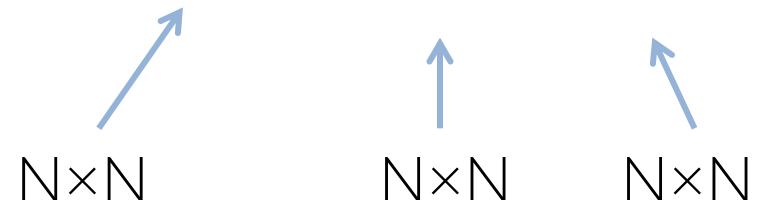
Cache access in loops: $O(N^2)/O(N^2)$

Example

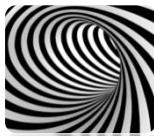
2-levels loops: dense matrix-vector mul, matrix transpos., matrix add, ...

Improvements comes again from increasing *data reuse*, exploiting *locality* and avoiding unnecessary operations and memory accesses.

```
for(int i=0; i < N; i++)  
    for(int j=0; j<N; j++)  
        C[i] += A[i][j] * B[j];
```



→ $3 \times N^2$ memory accesses



Cache access in loops: $O(N^2)/O(N^2)$

Step 1:
Avoid unnecessary loads /stores

```
for(int i=0; i < N; i++)  
    for(int j=0; j<N; j++)  
        C[i] += A[i][j] * B[j];
```



```
for(int i=0; i < N; i++) {  
    c_temp = C[i];  
    for(int j=0; j < N; j++)  
        c_temp += A[i][j] * B[j];  
    C[i] = c_temp; }
```

Now it is clearer for the compiler that **C[i]** need to be loaded and stored only 1 time

→ $2 \times N^2 + N$ memory accesses



Cache access in loops: $O(N^2)/O(N^2)$

Step 2:

Unroll outer loop and fuse in the inner loop; there is potential for vectorisation.

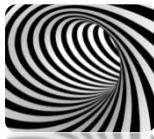
```
for(int i=0; i < N; i++)  
    for(int j=0; j<N; j++)  
        C[i] += A[i][j] * B[j];
```



$$\rightarrow N^2 \times (1 + 1/m) + N$$

```
for(int i=0; i < N; i += m){  
    for(j = 0; j < N; j++){  
        b_temp = B[j];  
        C[i] += A[i][j] * b_temp;  
        C[i+1] += A[i+1][j] * b_temp;  
        ...  
        C[i+m] += A[i+m][j] * b_temp; }  
}
```

$N \times N / m$



Note: unrolling and register spill

Using a too large m in the previous example while the target CPU does not have enough registers to keep all the needed operands results in a “code bloating”.

In this case, the CPU has to spill registers’ content to cache and viceversa, slowing down the computation.

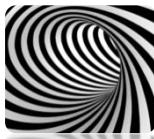
→ learn to inspect the compiler’s *log*

A too much involute and obscure loop body may hamper the compiler to effectively perform *unroll & jam* optimizations targeted to the CPU it runs on.

→ hand code effort to clarify the code

→ hints / directives to the compiler

(directives are generally not portable across different compilers)



Cache access in loops: $O(N^2)/O(N^2)$

Sometimes no magic wand can cure the fact that you have to access N^2 memory locations.

For instance: in matrix transpose you have to access all the source matrix and all the destination matrix once.

Unroll & Jam strategy can bring benefits as long as the cache can hold N lines.

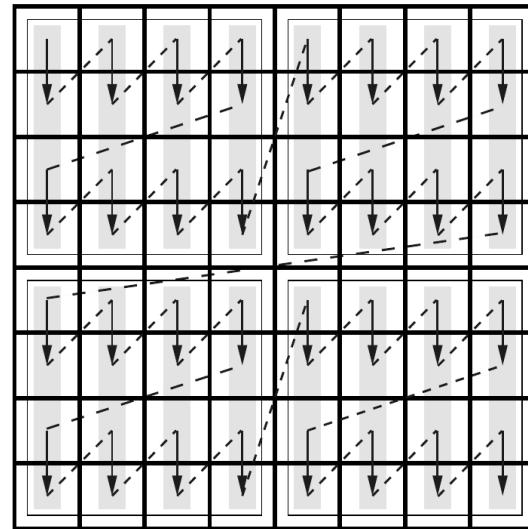
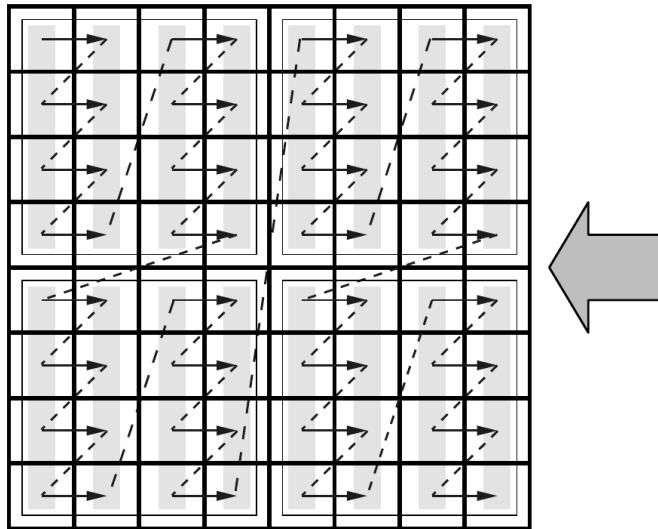
An L_C -way unrolling is too much aggressive and may easily result in register pressure.

Loop tailing (or blocking) is a good strategy that does not save memory loads but increase dramatically the cache hit ratio



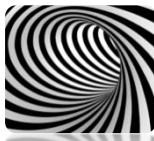
Loops

Cache access in loops: $O(N^2)/O(N^2)$



Step 3:
Fully exploit locality
of referenced data;
cut TLB misses by
accessing 2D arrays
by blocks

Image taken from: introduction to HPC for scientists and engineers



| Loop unrolling

Loop unrolling is a fundamental code transformation which usually helps significantly in improving your code performance:

- It reduces the loop overhead (counter update, branching)
- It exposes *critical data path* and dependencies
- It helps in exploiting ILP, especially in case of memory aliasing

We have already seen this technique in the examples from past lecture, although we did not really focus on it.

Now, let's understand it with some more detail.



Loop unrolling

Let's examine this simple *reduction*:

```
for ( int i=0; j<N; i++ )  
    S += A[i];
```

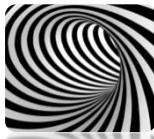
-00

```
.L3:  
# reduction.c:41:    acc = acc OP array[ii];  
    mov    rax, QWORD PTR -24[rbp] # ii  
    lea    rdx, 0[0+rax*8]  
    mov    rax, QWORD PTR -48[rbp] # array  
    add    rax, rdx  
    movsd  xmm0, QWORD PTR [rax]  
    movsd  QWORD PTR -56[rbp], xmm0  
    fld    QWORD PTR -56[rbp]  
  
# reduction.c:41:    acc = acc OP array[ii];  
    fld    TBYTE PTR -16[rbp]      # acc  
    faddp st(1), st  
    fstp   TBYTE PTR -16[rbp]      # acc  
  
# reduction.c:40:    for ( uLint ii = 1; ii < N; ii++ )  
    add    QWORD PTR -24[rbp], 1  # ii,  
.L2:  
# reduction.c:40:    for ( uLint ii = 1; ii < N; ii++ )  
    mov    rax, QWORD PTR -24[rbp] # ii  
    cmp    rax, QWORD PTR -40[rbp] # N  
    jb    .L3
```

-03 -march=native

```
.L3:  
# reduction.c:41:    acc = acc OP array[ii];  
    fadd   QWORD PTR [rax] # array  
    add    rax, 8          #  
# reduction.c:40:    for ( uLint ii = 1; ii < N; ii++ )  
    cmp    rdx, rax        # N  
    jne    .L3  
  
    ret
```

With optimization turned on the compiler manages much better the loop overhead, but does not optimize the FP ops in any way.



Loop unrolling

If we compile exactly the same code but using `int` as data type instead of `double`, we obtain a quite different result:

-00

```
.L3:  
# reduction.c:43:    acc = acc OP array[ii];  
    movq    -8(%rbp), %rax # ii  
    leaq    0(%rax,4), %rdx  
    movq    -32(%rbp), %rax # array  
    addq    %rdx, %rax  
    movl    (%rax), %eax  
    movl    %eax, %eax  
# reduction.c:43:    acc = acc OP array[ii];  
    addq    %rax, -16(%rbp)  
# reduction.c:42:    for ( uLint ii = 1; ii < N; ii++ )  
    addq    $1, -8(%rbp)    #, ii  
.L2:  
# reduction.c:42:    for ( uLint ii = 1; ii < N; ii++ )  
    movq    -8(%rbp), %rax # ii  
    cmpq    -24(%rbp), %rax # N  
    jb     .L3
```

-03 -march=native

```
.L4:  
# reduction.c:43:    acc = acc OP array[ii];  
    vmovdqu 4(%rax), %ymm0  
    addq    $32, %rax  
    vpmovzxdq    %xmm0, %ymm1  
    vextracti128 $0x1, %ymm0, %xmm0  
    vpmovzxdq    %xmm0, %ymm0  
# reduction.c:43:    acc = acc OP array[ii];  
    vpaddq   %ymm0, %ymm1, %ymm0  
    vpaddq   %ymm0, %ymm2, %ymm2  
    cmpq    %rdx, %rax  
    jne     .L4
```

Now the compiler opts for the complete vectorization of the loop, with a very strong impact on performances !!



| Loop unrolling

Why does the compiler choose to optimize the loop when the data are of type **int** and it does not when the data are of type **double** ?

It is due to the fact that, as we [have seen](#) the compiler is NOT free to restructure the code that deals with floating-point numbers.

Since the math with floating point is not associative, changing the exact order of the operations in your code may – from what the compiler may judge at compile time – change the correctness of the calculations at run time.

For instance, in the [example](#) that we have considered, changing the order of the operations obviously impacts on the result. From the point of view of the compiler, you may have chosen a given workflow exactly because you know that it is the most correct with respect to the data it will apply to!

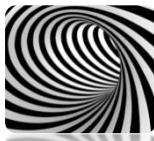


| Loop unrolling

Then, we are left with the responsibility of optimizing this simple code. Since we are traversing it continuously in natural memory order, the cache is not an issue.

Our aim is to re-structure the code so that the compiler could exploit the CPU's ILP.

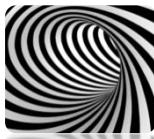
```
for ( int i=0; j<N; i++ )  
    S += A[i];
```



| Step 1: unrolling

Our first attempt is to reduce the loop overhead and expose some parallelism among the data by explicitly processing 2 elements per iteration.

```
for ( int i=0; i<N; i++ )  
    S = S OP A[i];  
  
↓  
  
for ( int i=0; i<N-2; i+=2 )  
    S = (S OP A[i]) OP A[i+1] ;
```



| Step 1: unrolling 2×1

Our first attempt is to reduce the loop overhead and expose some parallelism among the data by explicitly processing 2 elements per iteration.

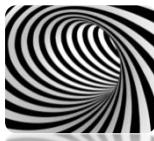
```
for ( int i=0; i<N; i++ )  
    S = S OP A[i];
```



```
for ( int i=0; i<N-2; i+=2 )  
    S = (S OP A[i]) OP A[i+1] ;
```

Note: when unrolling, you always have to care about the final iterations that would be left behind. A common way to do it for an unrolling factor U (usually U ranges in [2..16] of a loop with N iterations is:

```
int N_ = (N/U)*U;           // by construction this is the largest multiple of U  
                           // smaller than N  
for ( int i = 0; i < N_; i += U )  
    iteration_ops;  
  
for ( int i = N_; i < N; i++ )  
    iteration_ops;
```



Step 1: unrolling 2×1

The compiler generates (*)
the following assembly code:

```
.L17:  
    vmovupd ymm1, YMMWORD PTR [rax]  
    add    rax, 32  
    vaddsd xmm0, xmm0, xmm1  
    vunpckhpd xmm2, xmm1, xmm1  
    vextractf128 xmm1, ymm1, 0x1  
    vaddsd xmm0, xmm0, xmm2  
    vaddsd xmm0, xmm0, xmm1  
    vunpckhpd xmm1, xmm1, xmm1  
    vaddsd xmm0, xmm0, xmm1  
.LVL18:  
    cmp    rax, rcx  
    jne    .L17
```

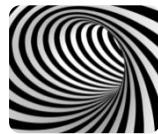
load 32B (4 double) starting from *i*th element.
ymm1 has 256bits.

rax contains the address to the *i*th element of the array, **[rax]** means “the address pointed by *rax*”

registers' reshuffle to move each double at the begin, in order to use **vaddsd**

all these instructions sum with,
and store in, **xmm0**

(*) in the following we will always comment the code generated with `-O3 -march=native`



Step 1: unrolling 2×1

In a (hopefully) simpler view,
the scheme of what happens
is the following

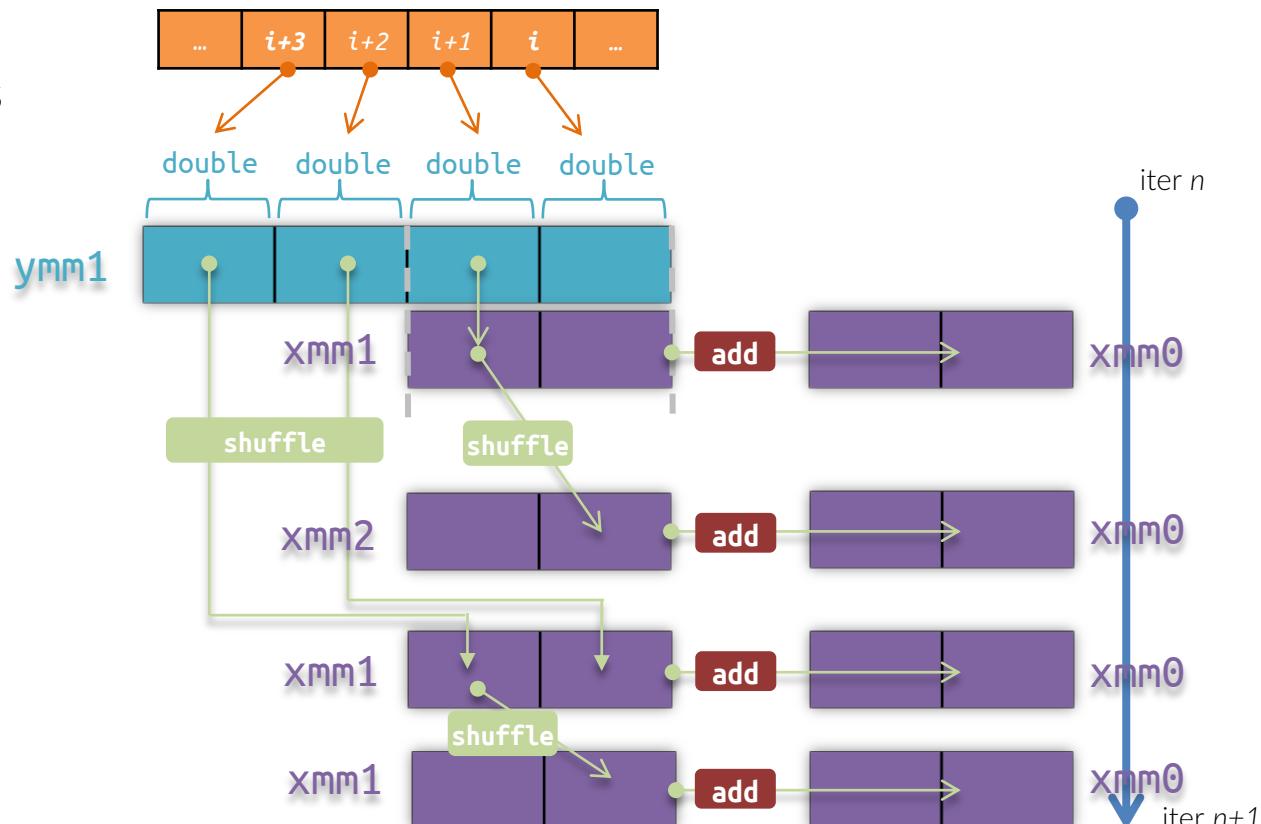


.L17:

```
vmovupd ymm1, YMMWORD PTR [rax]
add    rax, 32
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm2, xmm1, xmm1
vextractf128 xmm1, ymm1, 0x1
vaddsd xmm0, xmm0, xmm2
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm1, xmm1, xmm1
vaddsd xmm0, xmm0, xmm1
```

.LVL18:

```
cmp    rax, rcx
jne    .L17
```





Step 1: unrolling 2×1

Then, we have the following abstraction:

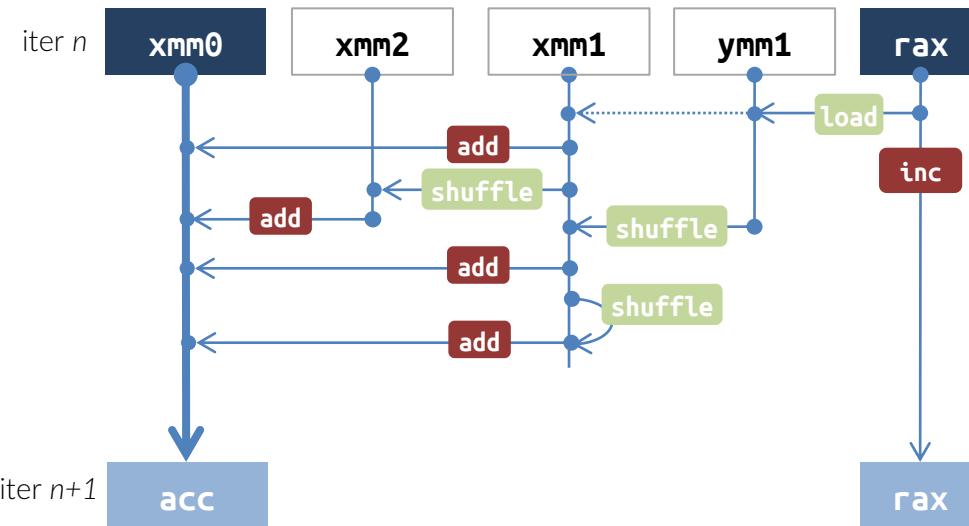
(arrows indicate a dependency)

.L17:

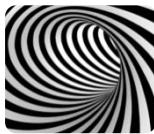
```
vmovupd ymm1, YMMWORD PTR [rax]
add    rax, 32
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm2, xmm1, xmm1
vextractf128 xmm1, ymm1, 0x1
vaddsd xmm0, xmm0, xmm2
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm1, xmm1, xmm1
vaddsd xmm0, xmm0, xmm1
```

.LVL18:

```
cmp    rax, rcx
jne    .L17
```



xmm0 carries a loop dependency because its value is to be used in the next iteration (that is true for **rax** too, but its latency is smaller than that of FP operations)
It forms a *critical path* that limits the efficiency.



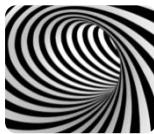
| Step 2: unrolling 2×1 + reshuffle

Let's explore what happens if we apport a semantic change to our code, just using the fact that our OP is associative.

```
for ( int i=0; i<N-2; i+=2 )  
    S = (S OP A[i]) OP A[i+1] ;
```



```
for ( int i=0; i<N-2; i+=2 )  
    S = S OP (A[i] OP A[i+1]) ;
```



Loops

Step 2: unrolling $2 \times 1 +$ reshuffle

```
for ( int i=0; i<N-2; i+=2 )
S = S OP (A[i] OP A[i+1]) ;
```

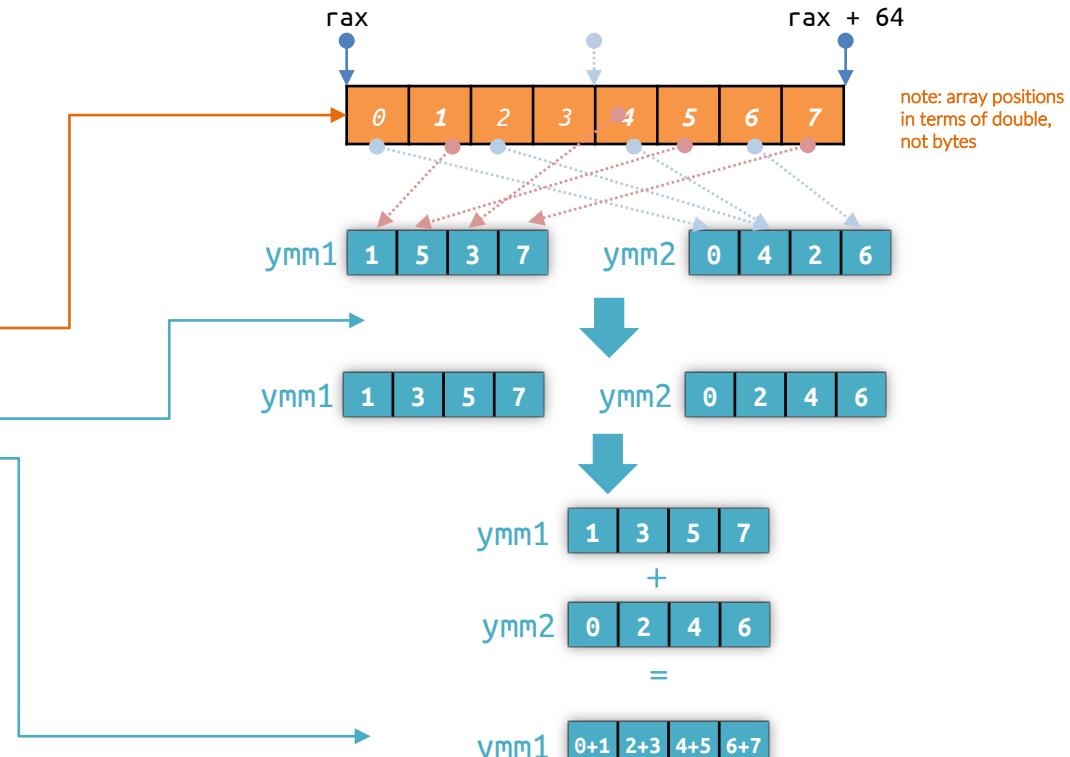


.L33:

```

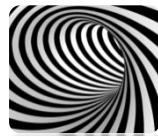
vmovupd ymm4, YMMWORD PTR [rax]
add    rax, 64
vunpcklpd ymm1, ymm4, YMMWORD PTR -32[rax]
vunpckhpd ymm2, ymm4, YMMWORD PTR -32[rax]
vpermpd ymm1, ymm1, 216
vpermpd ymm2, ymm2, 216
vaddpd ymm1, ymm1, ymm2
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm3, xmm1, xmm1
vextractf128 xmm1, ymm1, 0x1
vaddsd xmm0, xmm0, xmm3
vaddsd xmm0, xmm0, xmm1
vunpckhpd xmm1, xmm1, xmm1
vaddsd xmm0, xmm0, xmm1

```



8 doubles are processed per iteration; thanks to the re-association of operations, the compiler can reshuffle operations in a more efficient way

4 summation of subsequent elements in the array!



Step 2: unrolling $2 \times 1 +$ reshuffle

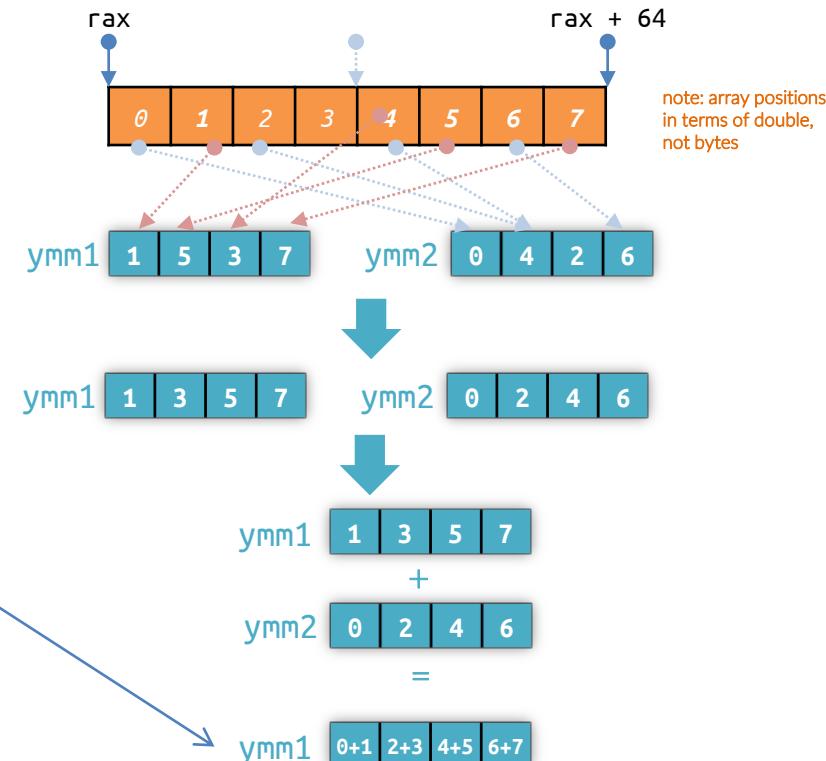
To be clearer: just because we re-associated the math expression in the loop,

from $S = (S \text{ OP } A[i]) \text{ OP } A[i+1] ;$
to $S = S \text{ OP } (A[i] \text{ OP } A[i+1]) ;$

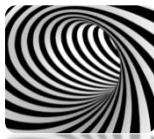
the compiler is entitled to exploit the fact that in
the semantics that now we are giving, the
operation order will be

Sum= ((([0]+[1]) + ([2]+[3])) + ([4]+[5])) +
([6]+[7])...

And the result is what we have just discussed, more
efficient than what we obtained with the previous code



4 summation of subsequent elements in the array!



Step 3: unrolling 2×2

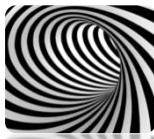
As we have seen, what is the blocking element is the critical path of the accumulator, because we are using a unique place to store the summation.

A logical step is to separate partial results in multiple accumulators.

```
for ( int i=0; i<N; i++ )  
    S = S OP A[i];
```



```
for ( int i=0; i<N-2; i+=2 )  
{  
    s0 = s0 OP A[i];  
    s1 = s1 OP A[i+1];  
}  
return s0 = s0 OP s1;
```



Step 2: unrolling 2×2

```
for ( int i=0; i<N-2; i+=2 ) {  
    s0 = s0 OP A[i];  
    s1 = s1 OP A[i+1]; }
```



```
.L49:  
    vmovupd    ymm4, YMMWORD PTR [rax]  
    vmovupd    ymm3, YMMWORD PTR 32[rax]  
    vmovapd    xmm2, xmm4  
    vaddsd    xmm1, xmm1, xmm4  
    vunpckhpd  xmm2, xmm2, xmm2  
    vaddsd    xmm0, xmm0, xmm2  
    vextractf128  xmm4, ymm4, 0x1  
    vaddsd    xmm1, xmm1, xmm4  
    vunpckhpd  xmm4, xmm4, xmm4  
    vaddsd    xmm0, xmm0, xmm4  
    vmovapd    xmm6, xmm3  
    vaddsd    xmm5, xmm1, xmm3  
    vunpckhpd  xmm6, xmm6, xmm6  
    vaddsd    xmm0, xmm0, xmm6  
    vextractf128  xmm3, ymm3, 0x1  
    vaddsd    xmm1, xmm5, xmm3  
    add       rax, 64  
    vunpckhpd  xmm3, xmm3, xmm3  
    vaddsd    xmm0, xmm0, xmm3  
  
    cmp       rax, rcx  
    jne       .L49
```

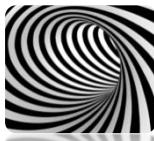
As before (2x1g) the compiler feels free to load 8 doubles per iteration, and then reshuffling them appropriately in order to respect the semantics of our coding, it sums them up using **xmm0** and **xmm1** as separate accumulators.



| Loop unrolling

In the next few slides, before to discuss the results from the different implementation, let's have a look at what happens if the accumulator S is required to be **long double** instead of **double**
(**long double** is not supported by vector registers)

```
for ( int i=0; j<N; i++ )  
    S += A[i];
```



Step 1: unrolling 2×1

Accumulator is long double

The compiler generates (*)
the following assembly
code:

```
.L10:  
fadd    QWORD PTR [rax]  
add     rax, 16  
fadd    QWORD PTR -8[rax]  
  
cmp     rdx, rax  
jne     .L10
```

rdx is equal to N-2, just
check the exit condition

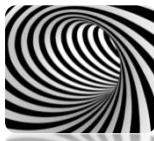
fadd sums the content of the memory
specified by the argument to the first register
of the FPU

rax contains the address to the i th element of
the array, `[rax]` means “the address pointed
by rax”

Now rax points to array's element $i+2$

This sums the array's element $i+1$ to the first
FPU's register, which hold the updated result
of the summation chain

(*) in the following we will always comment the code generated with `-O3 -march=native`



Loops

Step 1: unrolling 2×1

Accumulator is long double

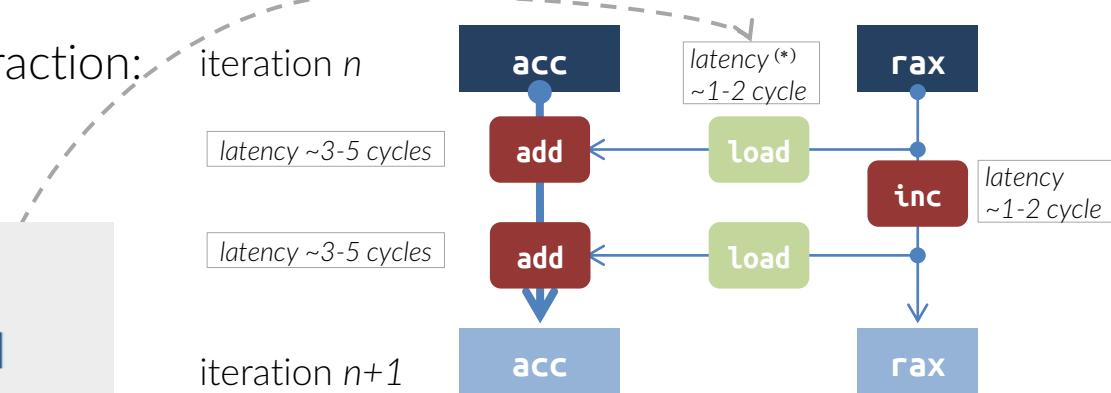
Then, we have the following abstraction:
(arrows indicate a dependency)

.L10:

```
fadd    QWORD PTR [rax]
add     rax, 16
fadd    QWORD PTR -8[rax]

cmp    rdx, rax
jne    .L10
```

(*) obviously depends on whether the data are in L1, L2, L3 or RAM



Both the FPU's register, which we name **acc**, and **rax** carry a *loop dependency* because their result is used – and them waited for – in the subsequent iteration. However, the FP addition has a larger latency (~3-5) than int addition (~1). As such, the left one (in bold) is the *critical path* that limits our efficiency.



Step 2: unrolling 2x1 + reshuffle

Accumulator is
long double

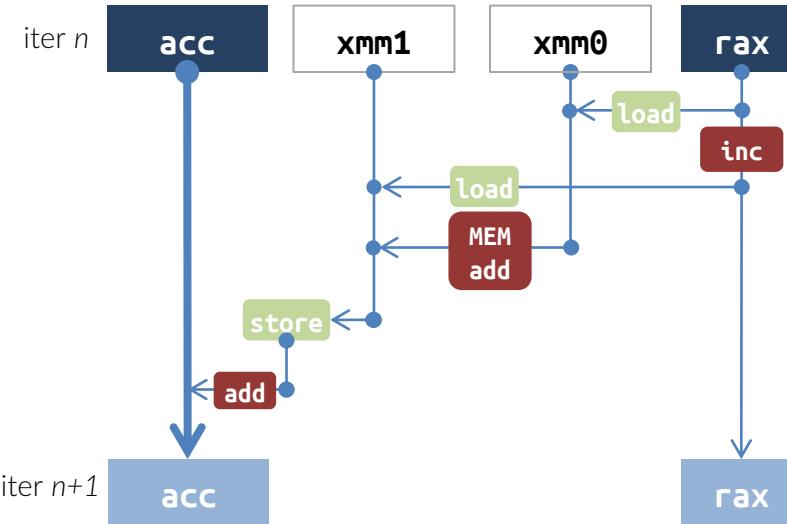
```
for ( int i=0; i<N-2; i+=2 )  
    S = S OP (A[i] OP A[i+1]) ;
```

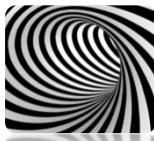


L19

```
vmovsd    xmm0, QWORD PTR [rax]
add       rax, 16
vaddsd    xmm1, xmm0, QWORD PTR -8[rax]
vmovsd    QWORD PTR -16[rsp], xmm1
fadd     QWORD PTR -16[rsp]

cmp      rdx, rax
jne     .L19
```



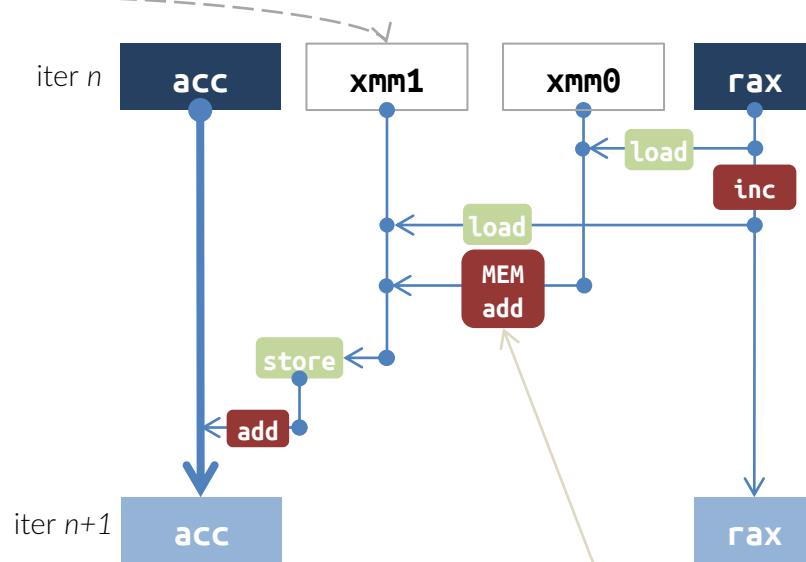


Step 2: unrolling 2×1 + reshuffle

Accumulator is long double

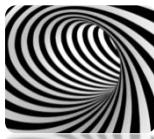
The scenario is somehow different now.
The loop dependency is still carried by **acc** (the latency of **rax** is negligible); however, its latency is now hidden by the operations on **xmm0** and **xmm1**.

We may expect some improvement from this code.



White background means that these regs are *local* to each iterations, i.e. they do not carry any loop dependency

This add is within **xmm0** and the $(i+1)$ -th array's element from memory



Step 3: unrolling 2×2

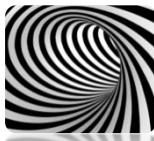
As we have seen, what is the blocking element is the critical path of the accumulator, because we are using a unique place to store the summation.

A logical step is to separate partial results in multiple accumulators.

```
for ( int i=0; i<N; i++ )  
    S = S OP A[i];
```



```
for ( int i=0; i<N-2; i+=2 )  
{  
    s0 = s0 OP A[i];  
    s1 = s1 OP A[i+1];  
}  
return s0 = s0 OP s1;
```



Loops

Step 3: unrolling 2×2

Accumulator is long double

```
for ( int i=0; i<N-2; i+=2 ) {  
    s0 = s0 OP A[i];  
    s1 = s1 OP A[i+1]; }
```

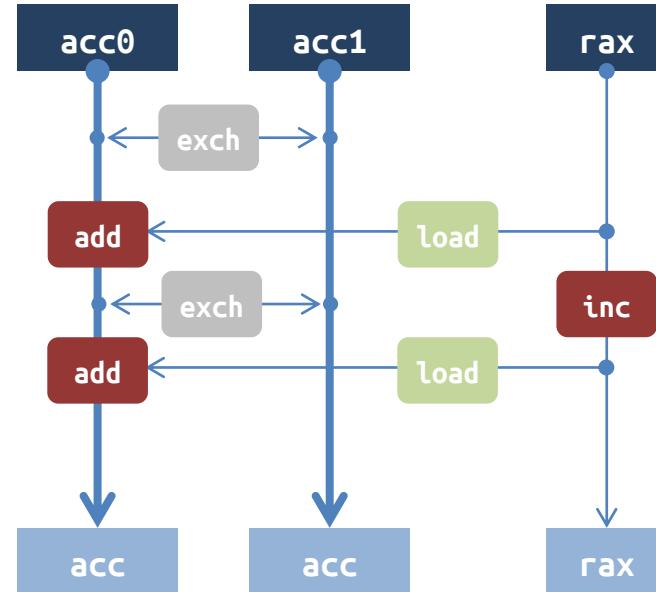


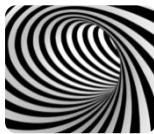
.L34:

```
fxch    st(1)  
fadd    QWORD PTR [rax]  
fxch    st(1)  
add     rax, 16  
fadd    QWORD PTR -8[rax]  
  
cmp    rdx, rax  
jne    .L34
```

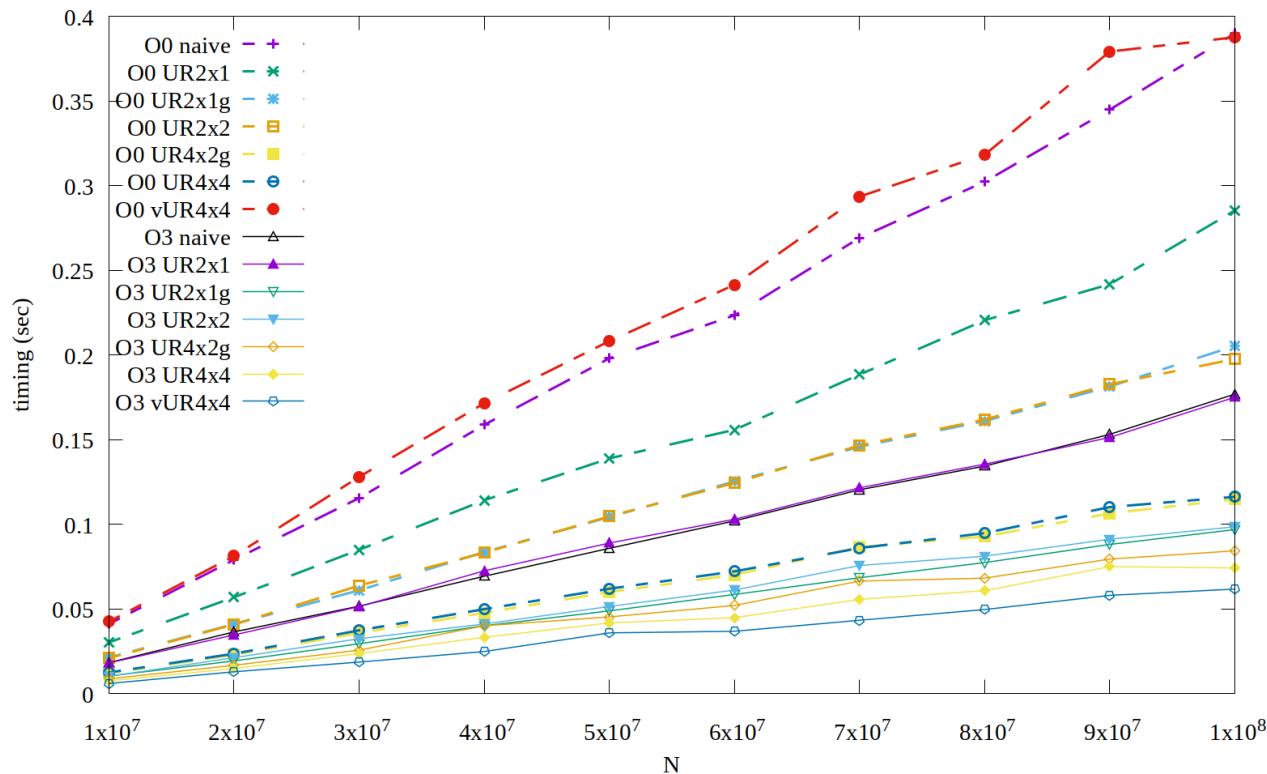
iter n

iter n+1





Reduction: results

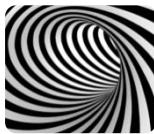


Run time of different implementation with and without compiler's optimization

UR NxM: unrolled N times using M accumulators.

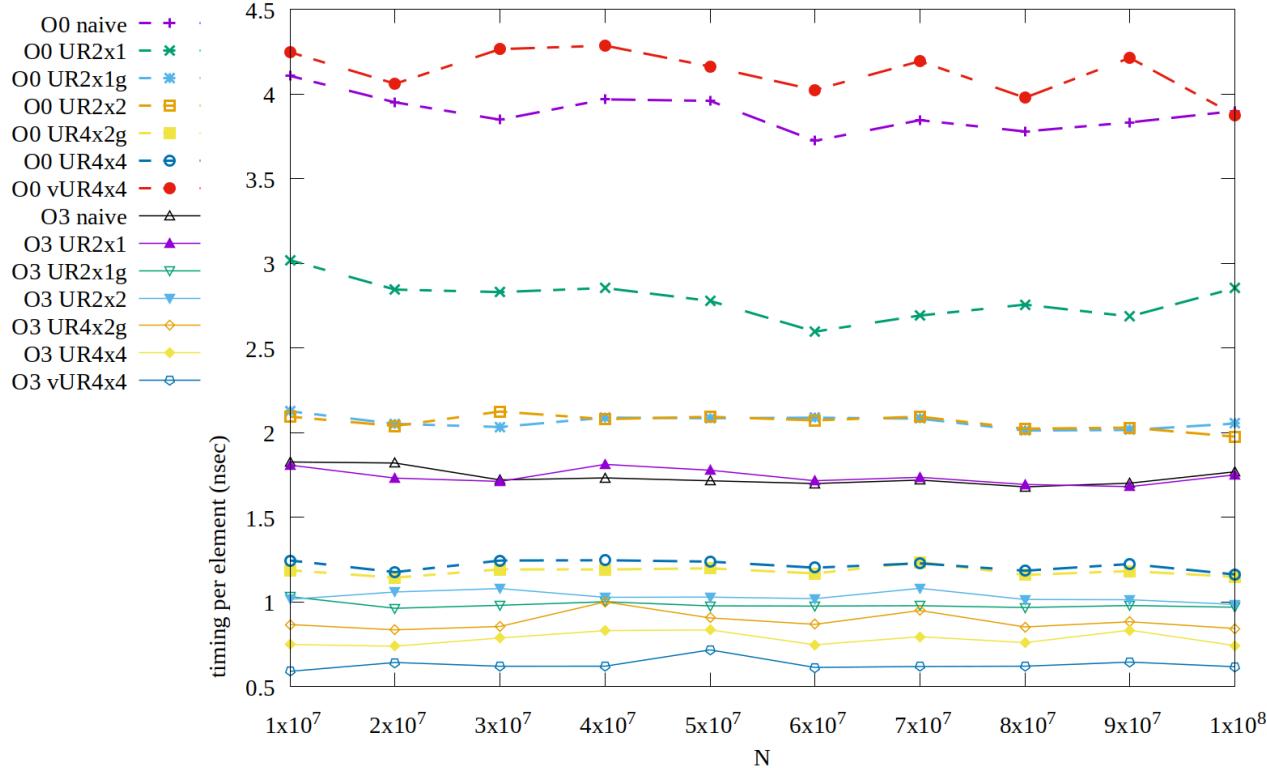
vUR4x4: UR4x4 with explicit vectorization.

In this plot and in the following ones dashed lines are for -O0 and solid line for -O3 -march=native
(only gcc has been used)



Loops

Reduction: results

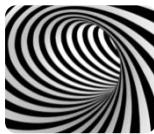


Run time of different implementation with and without compiler's optimization

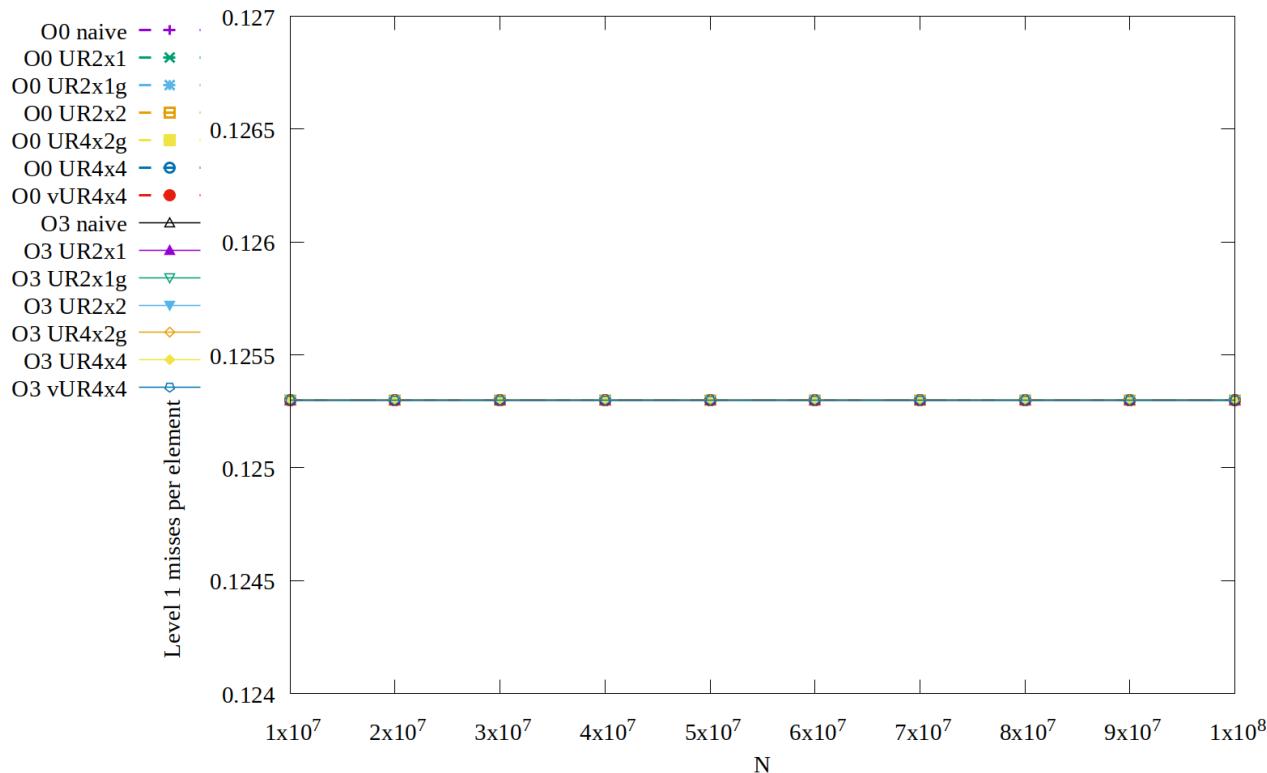
UR NxM: unrolled N times using M accumulators.

vUR4x4: UR4x4 with explicit vectorization.

In this plot and in the following ones dashed lines are for -O0 and solid line for -O3 -march=native
(only gcc has been used)

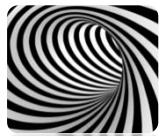


Reduction: results



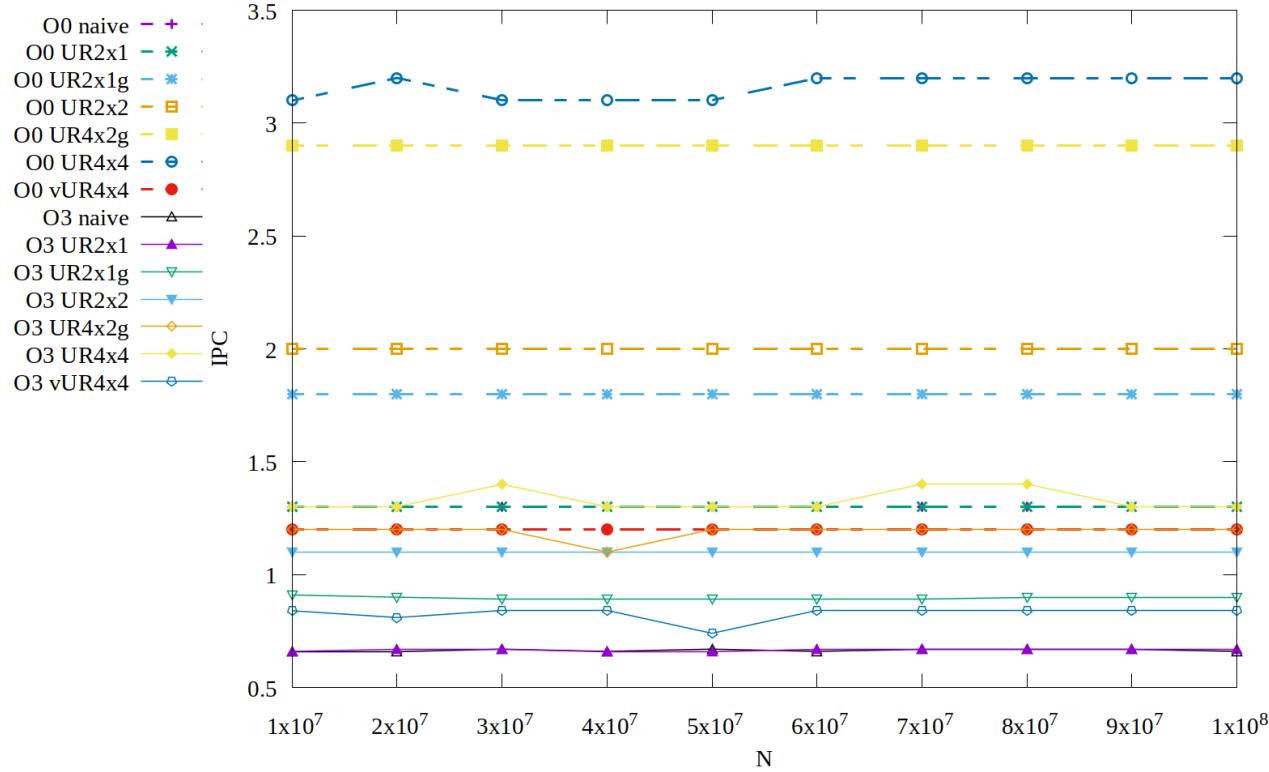
Level 1 Data cache misses

of course, the expected 1/8 since we are processing the array continuously.

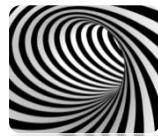


Loops

Reduction: results

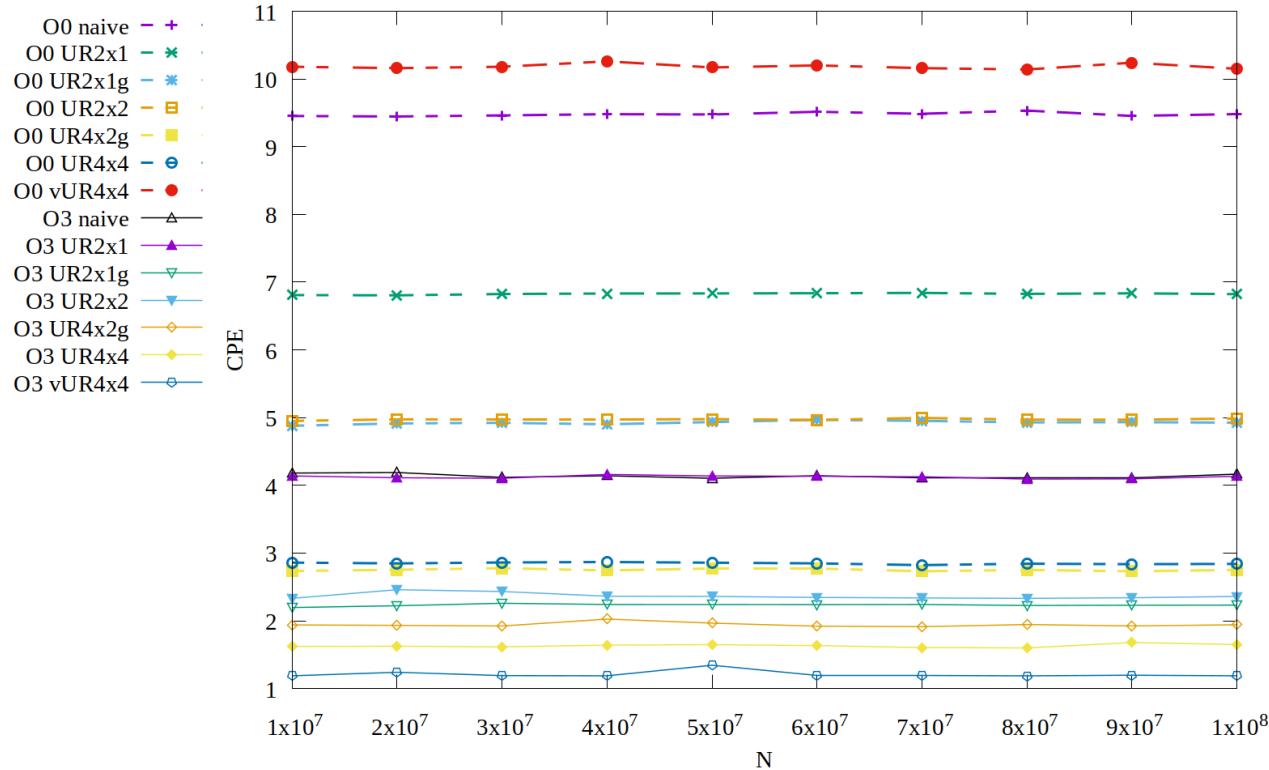


Instructions per cycle

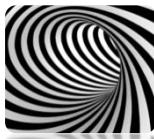


Loops

Reduction: results



Cycles per element

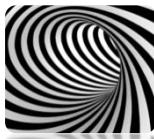


Cache access in loops: $O(N^3)/O(N^2)$

These algorithms (ex: matrix-matrix multiplication or dense matrix diagonalization) are very good candidates for optimizations that lead flop/s performance very close to the theoretical peak (in fact, MMM is at the core of `linpack`).

Tailing, unroll&jam + vectorization of operations, reorganization of ops to exploit CPU's pipelines and out-of-order capability, are all used by extremely specialized libraries.

→ It is a brilliant idea to link those library instead of developing your own algorithm, unless some very special needs must be met.



matrix-matrix multiplication is a very common task in HPC.

Although there are highly optimized library that performs the job, it is a very classical and useful case study to understand the loop tiling and the cache-oblivious algorithms.

Let's start from the definition of the problem.

Given 2 matrices, A and B, having respectively (m, n) and (n, p) rows and columns respectively, their product is defined as the matrix C(m, p)

$$C_{i,j} = \sum_{k=0}^n A_{i,k} \times B_{k,j}$$

| $O(N^3)/O(N^2)$ example

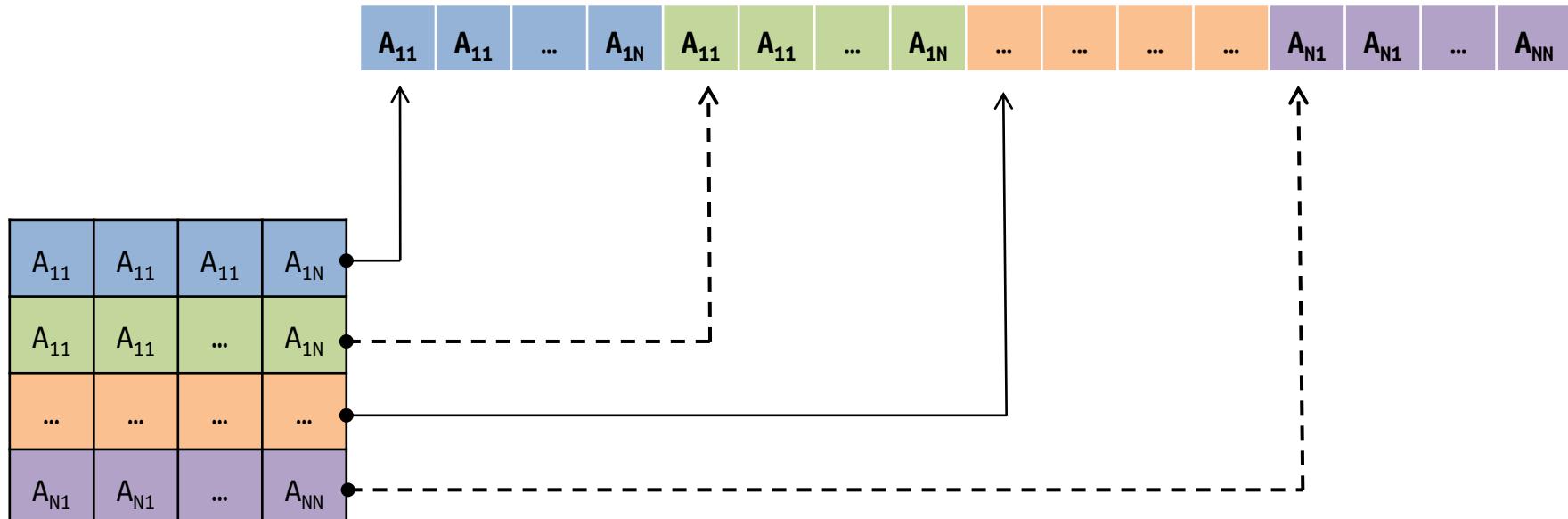
$$C_{i,j} = \sum_{k=0}^n A_{i,k} \times B_{k,j}$$

A possible obvious straightforward implementation of this algorithm is as follows:

```
for ( int i = 0; i < m; i++ )           // traverse the A's (and C's) rows
    for ( int k = 0; k < p; k++ )         // traverse the B's rows ( Ac = Br )
        for ( int j = 0; j < n; j++ )
            C[i][k] += A[i][j] * B[j][k];
```

Note: how a matrix is stored in memory

Remember the obvious fact that your memory is a continuous 1-dimensional stream of bytes.

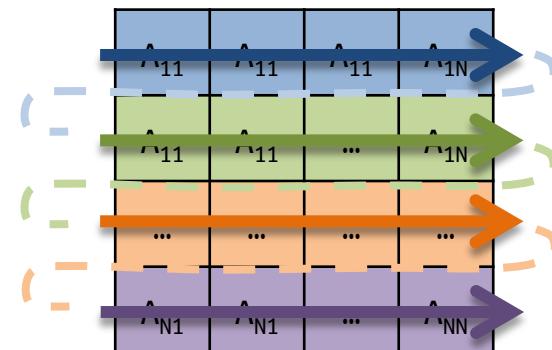


This convention is the C/C++ convention, which is labelled as *row-major order*. Note that the Fortran convention is opposite, with columns being contiguous in memory (*column-major*).

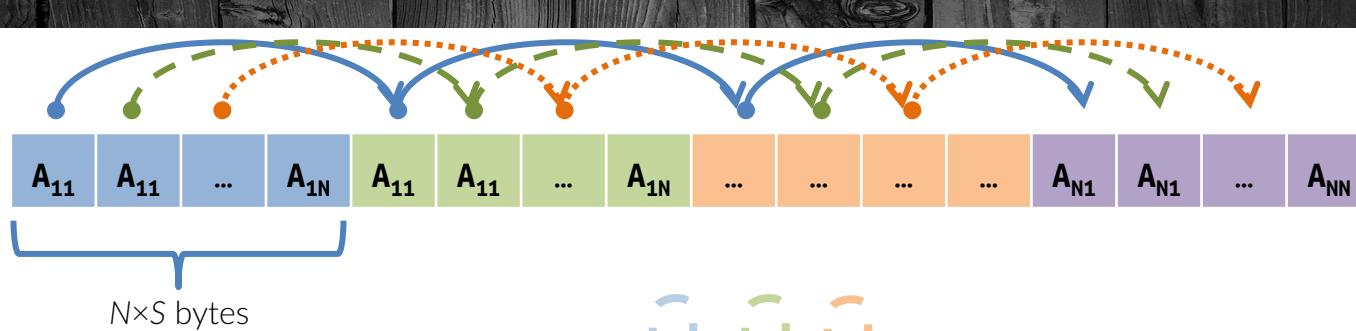
Note: how a matrix is stored in memory



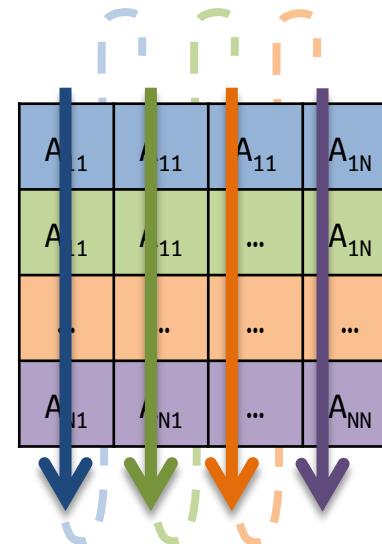
Then, traversing the matrix in the same row-major order amounts to traverse the memory in contiguous order.

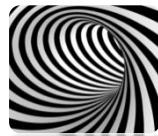


Note: how a matrix is stored in memory



Whereas, traversing the matrix in the opposite column-major order amounts to jump in memory by N positions, i.e. $N \times S$ bytes is S is the size of each element.

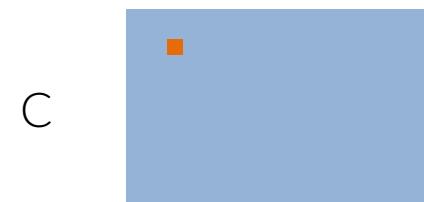




Loops

| $O(N^3)/O(N^2)$ example

Matrix representation



Memory representation



C

=

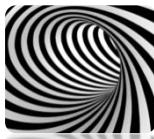
A



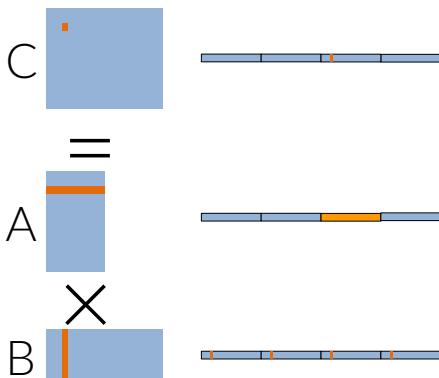
X

B





| $O(N^3)/O(N^2)$ example



The naïve implementation has an obvious issue with data locality for large enough matrixes.

For each C's element, possibly all accesses to B result in a cache miss.

Then, we may have mnp cache misses (if L is the line capacity of the cache in terms of the data type used) only to traverse B.

The total number of expected misses is:

$$\begin{aligned} & mn/L + \\ & mnp/L + \\ & mnp \end{aligned}$$

C is traversed once
A is scanned entirely n times
B is accessed randomly

In fact, the naïve implementation is never used for any large matrix multiplication: since $2mnp$ flop are required, it amounts to have nearly a cache miss per each flop.

How can we fix this problem ?

Transposing the matrix B before entering the loop should alleviate the problem; although the transposition requires some additional work, for large enough matrices there is still a performance gain.



| $O(N^3)/O(N^2)$ example

A different strategy may consist in swapping the two inner loops:

```
for ( int i = 0; i < m; i++ )           // traverse the A's (and C's) rows
    for ( int k = 0; k < p; k++ )         // traverse the B's rows ( Ac = Br )
        for ( int j = 0; j < n; j++ )
            C[i][k] += A[i][j] * B[j][k];
```

```
for ( int i = 0; i < m; i++ )
    for ( int j = 0; j < n; j++ )
        for ( int k = 0; k < p; k++ )
            C[i][k] += A[i][j] * B[j][k];
```

Now we are still having lots of cache misses due to the fact that we are re-loading $C[i][k]$ many times (Ac times).

Now we expect to have

mnp/L + running over C
 mnp/L + running over A
 mnp/L running over B

cache misses. Then, with respect to the previous nesting scheme we expect to have
 $\sim mnp(L - 2)$
less cache misses.

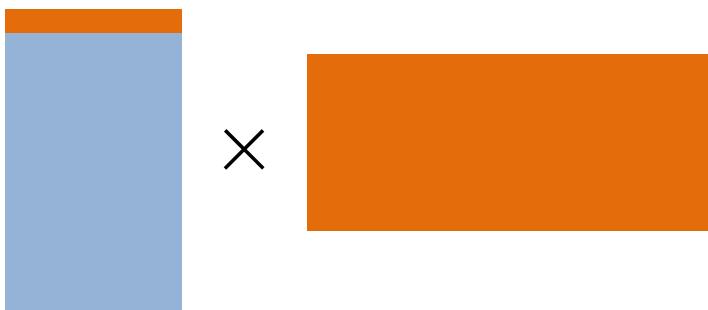


| $O(N^3)/O(N^2)$ example

We can do even better by optimizing both the memory accesses and the data contiguity by *tailing* the loops:



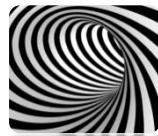
=



To compute a single line in C we need to access the corresponding line in A p times. In the hypothesis that A,B and C can not fit in memory, each time the cache will have been flushed and the A's line will not be there anymore.

This amounts to have n/L compulsory misses per each column if B, i.e. np/L cache misses for each C's line, as we have already calculated.

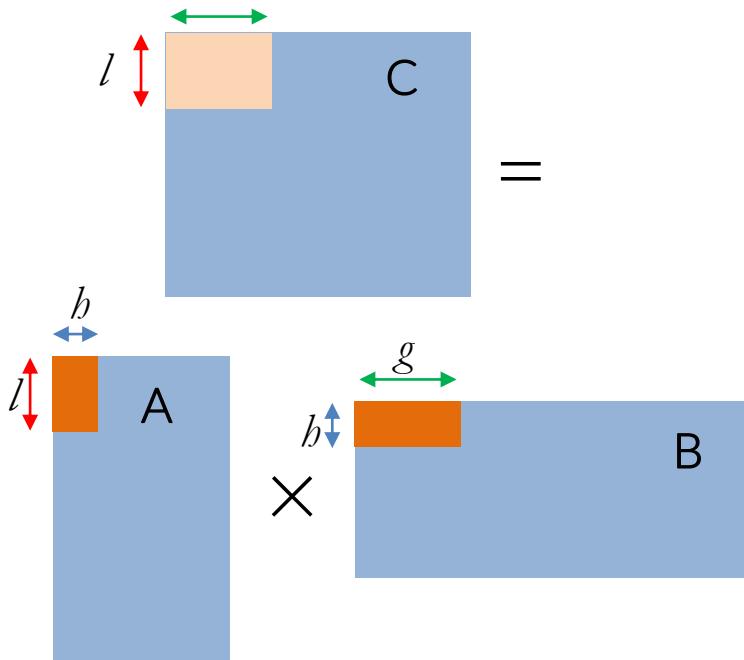
The same holds for the B' s columns and so on...



Loops

| $O(N^3)/O(N^2)$ example

We can do even better by optimizing both the memory accesses and the data contiguity by *tailing* the loops:



If, instead, we keep in the cache a segment of the A's line, re-using it against the columns of B – or, better, against a columns section tall as the line segment is large (blue arrows in the figure) – we could greatly reduce the amount of cache misses per C's element.

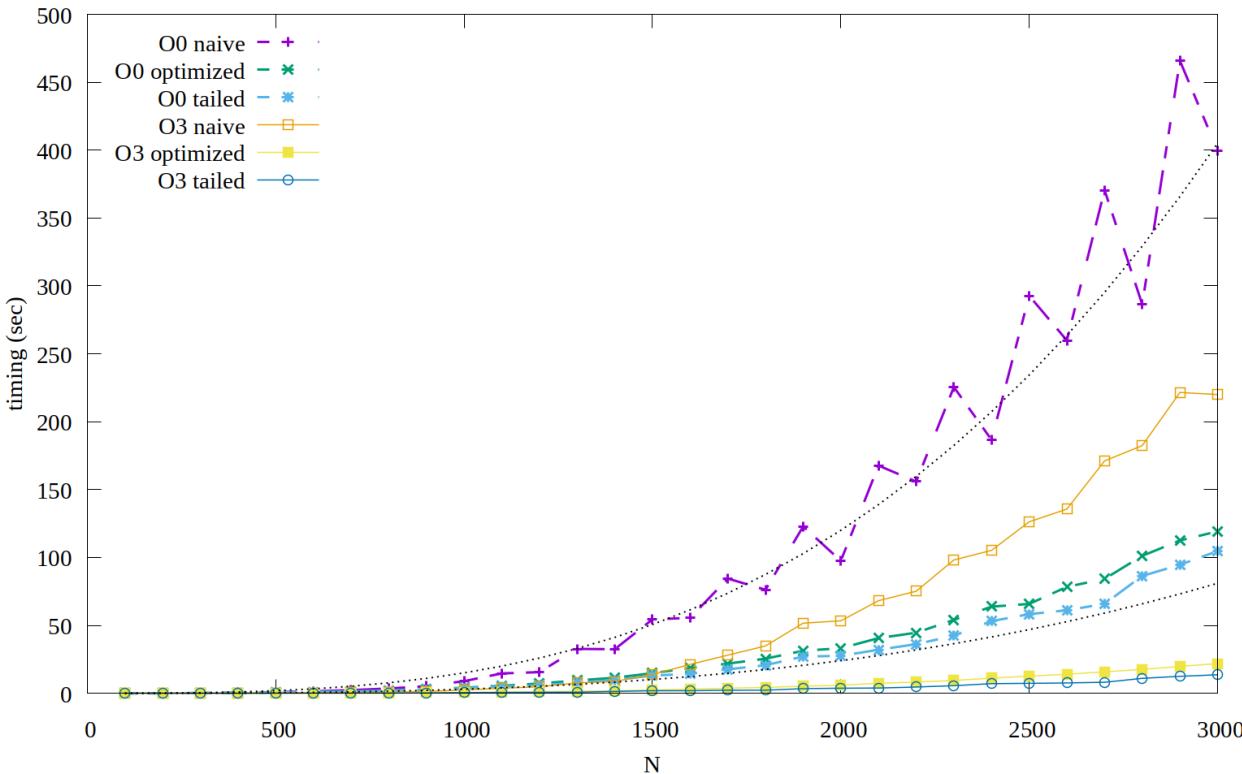
Traversing A and B by *blocks* as in the figure allows to accumulate partial results in the corresponding C's area while decreasing the number of cache misses by a factor

$$L / (l \times b \times g)$$

where L is the cache capacity and are the block factors. With standard value, this figure becomes of the order of 0.001.



Matrix multiplication results



Run time of different implementation with and without compiler's optimization

the results are for the case of 2 square matrix of dimension N

Naïve: the schoolbook's implementation

Optimized: inner loops swapped

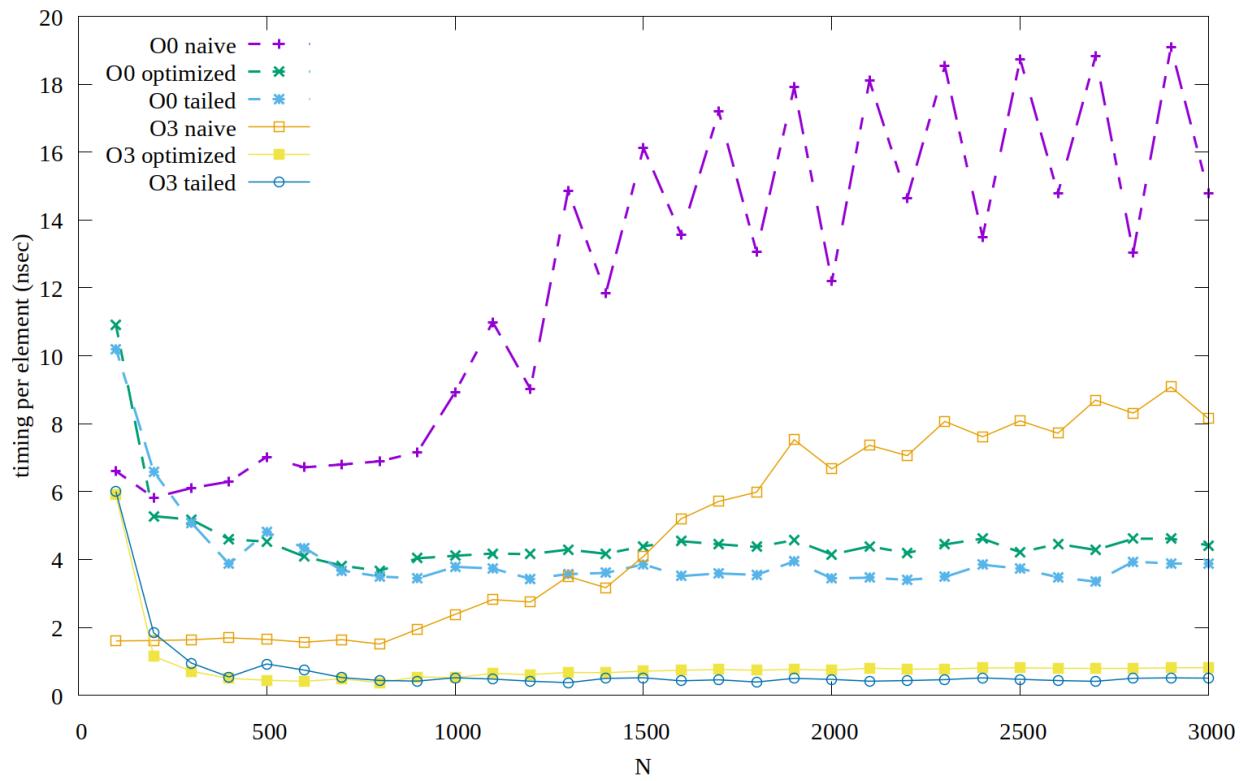
Tailed: M-M by blocks

In this plot and in the following ones dashed lines are for -O0 and solid line for -O3 -march=native
(only gcc has been used)



Loops

Matrix multiplication results

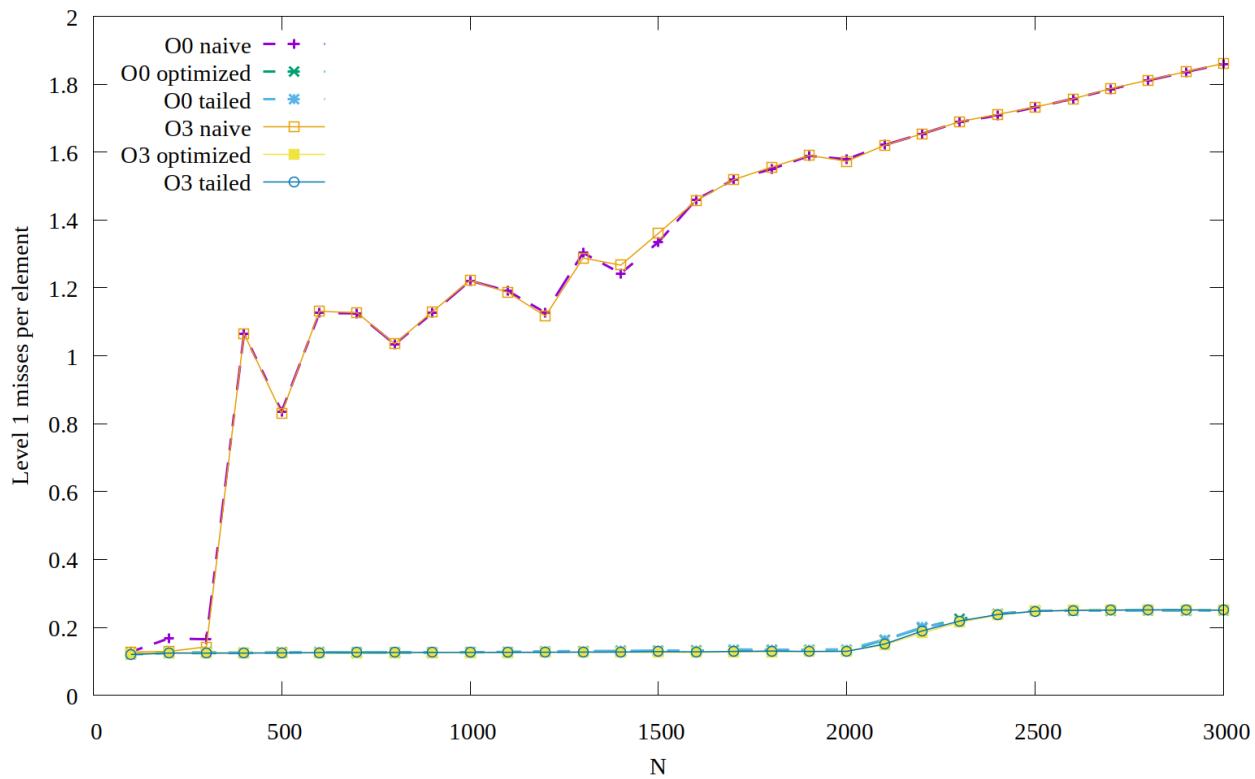


Time per element
accessed (N^3)

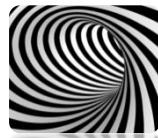


Loops

Matrix multiplication results

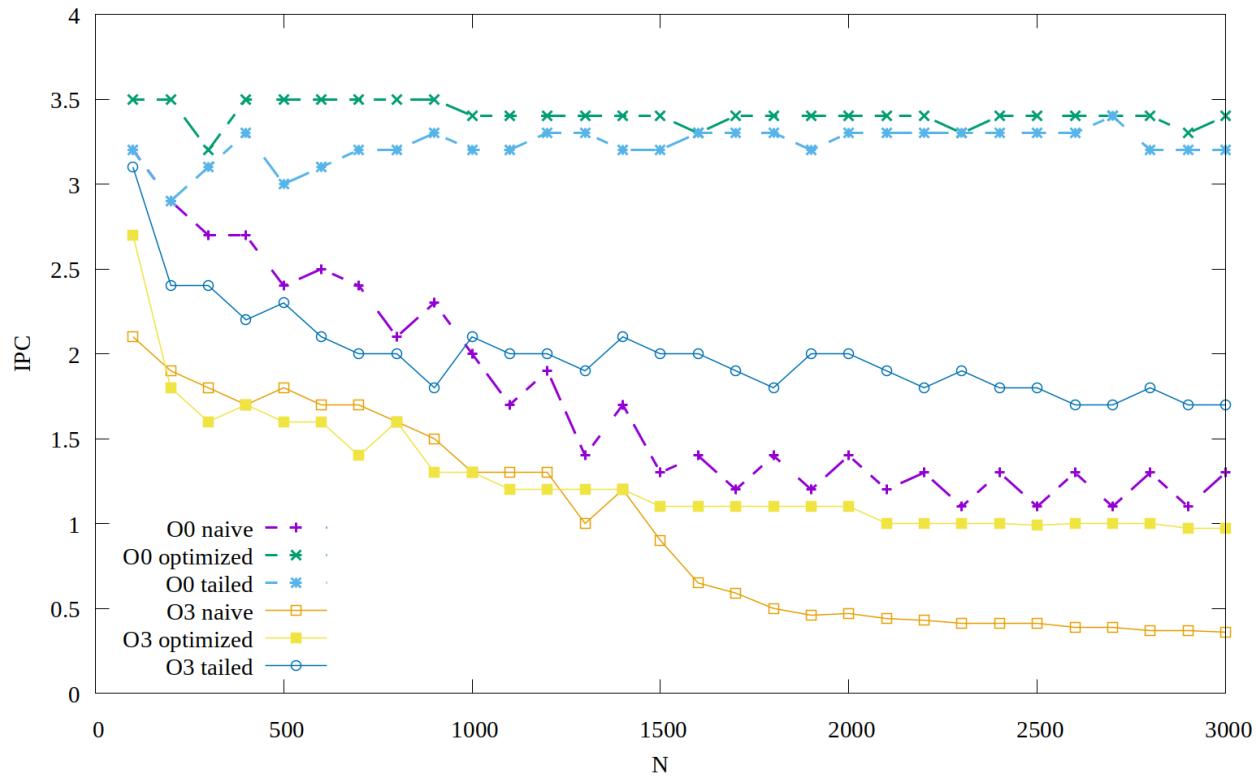


Level 1 Data cache
misses per element



Loops

Matrix multiplication results

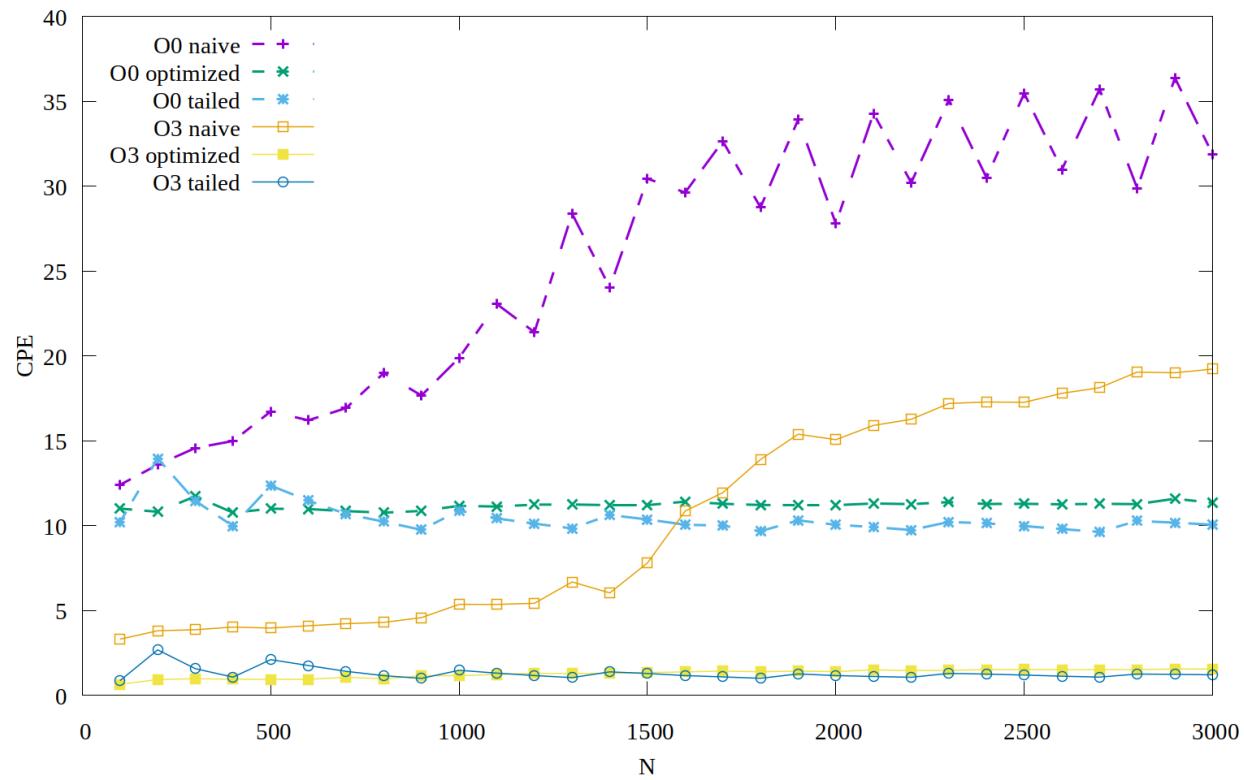


Instructions per cycle



Loops

Matrix multiplication results

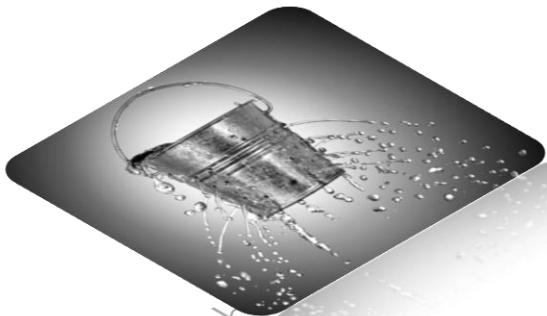


Cycles per element

Loops



Outline



Avoid the
avoidable
inefficiencies



Prefetching



At the right moment, at the right place

We know that waiting for data and instructions is a major performance killer.

Modern CPUs have the capability of pre-emptively bring from memory into cache levels data that **will be needed shortly afterwards**.

They can do that following some speculative algorithm based on the current execution flow and assuming spatial locality and temporal locality.

Both *data* and *instructions* can be pre-fetched.

Pre-fetching may be both hardware-based and software-based (typically the compiler insert pre-fetching instructions at compile-time).



From the point of view of the programmer, there are 2 possible ways to deal with prefetching:

EXPLICIT

you explicitly insert a pre-fetching directive.

Very difficult to be achieved effectively: the directive must be inserted timely but not too early (data eviction) or too late (load latency).

INDUCED

you consciously arrange data layout and execution flow so that to make it obvious to the compiler what to prefetch.



Explicit prefetching

This is a standard binary search implementation.

Find the median element

Define the next search

```
int mysearch(int *data, int N, int Key)
{
    int register low = 0;
    int register high = N;
    int register mid;

    while(low <= high) {
        mid = (low + high) / 2;

        if(data[mid] < Key)
            low = mid + 1;
        else if(data[mid] > Key)
            high = mid-1;
        else
            return mid;
    }
    return -1;
}
```



Explicit prefetching

We can make it better by simply making sure that the element to be compared for (the `mid`) is in the cache when requested

```
int mybsearch(int *data, int N, int Key)
{
    int register low = 0;
    int register high = N;
    int register mid;

    while(low <= high) {
        mid = (low + high) / 2;

        if(data[mid] < Key)
            low = mid + 1;
        else if(data[mid] > Key)
            high = mid-1;
        else
            return mid;
    }
    return -1;
}
```



Explicit prefetching

We can make it better by simply making sure that the element to be compared for (the mid) is in the cache when requested

```
int mybsearch(int *data, int N, int Key)
{
    int register low = 0;
    int register high = N;
    int register mid;

    while(low <= high) {
        mid = (low + high) / 2;
        __builtin_prefetch (&data[(mid + 1 + high)/2], 0, 3);
        __builtin_prefetch (&data[(low + mid - 1)/2], 0, 3);

        if(data[mid] < Key)
            low = mid + 1;
        else if(data[mid] > Key)
            high = mid-1;
        else
            return mid;
    }    return -1; }
```



Explicit prefetching

```
luca@GGG:~/code/HPC_LECTURES/prefetching% ./prefetching off
performing 13421772 lookups on 134217728 data..
set-up data.. set-up lookups..
start cycle.. time elapsed: 20.7534
luca@GGG:~/code/HPC_LECTURES/prefetching% ./prefetching on
performing 13421772 lookups on 134217728 data with prefetching enabled..
set-up data.. set-up lookups..
start cycle.. time elapsed: 12.6204
```



Explicit prefetching

```
Samples: 71K of event 'cpu/mem-loads,ldlat=30/P', Event count (approx.): 13901140
Overhead          Samples  Memory access
```

71,08%	42196	Local RAM hit
24,14%	17022	LFB hit
4,11%	10967	L3 hit
0,63%	1714	L1 hit
0,02%	75	L2 hit
0,01%	15	L3 miss
0,00%	1	Uncached hit

Read perf-report man page on Linux & man 1 perf-report

```
Samples: 61K of event 'cpu/mem-Loads,ldlat=30/P', Event count (approx.): 11720387
```

```
Overhead          Samples  Memory access
```

68,74%	29450	LFB hit
27,04%	28208	L1 hit
2,72%	909	Local RAM hit
1,29%	2983	L3 hit
0,20%	346	L2 hit

Read perf-report man page on Linux & man 1 perf-report



Explicit prefetching

Usage of direct prefetching directive is highly uncertain, since it is difficult to spot the exact point – both in the code and in the execution – where to place them (also because your C code is different than the generated assembly code).

Moreover, the “exact point” is very likely dependent on the system you run on, and then it is susceptible to change significantly.

It is normally much safer to re-organize your code so to have **prefetching by pre-loading**.



Prefetching by moral suasion

Let's discuss together this very simple example before putting the hands on the code you find in the git

```
elem a = elements[0]
for ( i = 0; i < 4*N_4; i+= 4 )
{
    elem e = elem[i+4]; // non-blocking miss
    elem b = elem[i+1]; // possible cache-hit
    elem c = elem[i+2]; // possible cache-hit
    elem d = elem[i+3]; // possible cache-hit
    Elaborate(a);
    Elaborate(b);
    Elaborate(c);
    Elaborate(d);
    a = e;
}
```



You find code snippets with different flavours of prefetching-by-preloading technique on our GitHub, with some comments about compilation.

```
for ( i = 0; i < N; i++ )  
    sum += array[ i ];
```

Compile and run them with different options (and possibly different compilers) and try to understand what happens on your laptop and/or on HPC facility.

that's all, have fun

"So long
and thanks
for all the fish"