

INAF HPC School 2025 Catania, Sep. 22nd - 26th







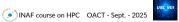
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Introduction

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Outline



Avoid the avoidable inefficiencies



Cache & Memory



Loops



Branches



Pipelines



Unleash the Compiler



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Avoid the avoidable inefficiencies



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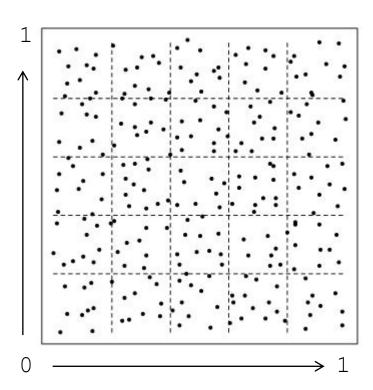


Unleash the Compiler



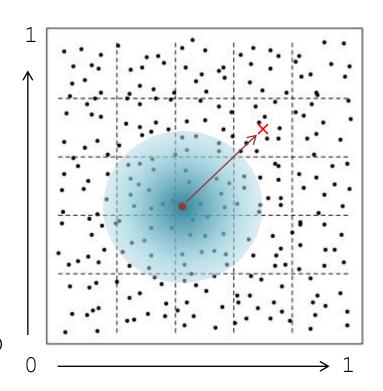
For the purpose of setting-up an example, let's suppose that

1) we have a distribution of random data points on a 2D plane which we subdivide in sub-regions using a grid.



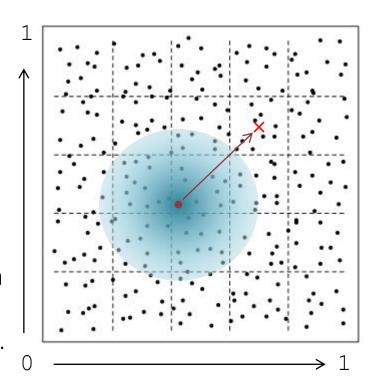
For the purpose of setting-up an example, let's suppose that

- 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 (i) select all the grid cells whose center is closer to p than a given radius r; (ii) perform some operations accordingly to our search result.



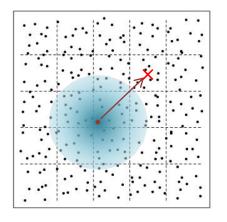
For the purpose of setting-up an example, let's suppose that

- 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.



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

Is there anything you would change?



```
for(p = 0; p < Np; p++)
    for(i = 0; i < Ng; i++)
      for(j = 0; j < Nq; j++)
        for(k = 0; k < Nq; 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;
```







(1) Avoid expensive function calls

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

Try to avoid them if possible.

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



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

```
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



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

was performed N³+N²+N times, always returning the same values.

Hoisting would save $N(N^2+N^1+1)$ mul, add and mem accesses.

```
for(i = 0; i < Ng; i++) {
  dx2 = x[p] - (double)i * Ng inv - half size;
   dx2 = dx2*dx2:
      for(j = 0; j < Ng; j++) {
         dy2 = y[p] - (double)j * Ng inv - half size;
         dy2 = dy2*dy2;
         dist2 xv = dx2 + dv2;
         for(k = 0; k < Nq; k++) {
            dz = z[p] - (double)k * Ng inv - half size;
            dist2 = dist2 xy + dz*dz;
            if(dist2 < Rmax2)
               do something with sqrt(dist2); } } }
```



(1) Avoid expensive function calls



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

was performed N³+N²+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</pre>
```







(2) *Hoisting* of expressions



You could do even better by precomputing the relevant values:

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





(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;
 \int dx2 = dx2:
      for(j = 0; j < Ng; j++) {
      >> double dy2 = y[p] - (double)j * Ng inv - half size;
      \rightarrow 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)</pre>
               do something with sqrt(dist2); } } }
```



(4) Suggest what is important



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

```
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 < Nq; 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); } } }
SCO/avoid the avoidable/loop.5.c
```



Do you expect any great performance from this code?

If not, why?

```
char * find char in string( char *string, char c )
    int i = 0;
    while ( i < strlen(string) )</pre>
       if( string[i] == c )
         break;
       else
         i++;
    if( i < strlen(string) )</pre>
       return &string[i];
    else
       return NULL;
```





There are several details that dump the performance, i.e. the CPE, of this loop.

The one I want to draw your attention to is the repeated call to the strlen() function.

Do you expect the string to change while you are scanning it? No, but the compiler does not know that and has no way to understand that by code analysis. Moreover, the memory pointed by string could be modified

somewhere else between iterations.

```
char * find char in string( char *string, char c )
    int i = 0;
    while ( i <istrlen(string) )
       if(string[i] == c )
         break;
       else
         i++:
    if( i < strlen(string) )</pre>
       return &string[i];
    else
       return NULL;
```





This very simple change will save you a lot of CPE

CPE = Cycles Per Element

```
char * find char in string( char *string, char c )
    int i = 0;
    int len = strlen(string);
    while ( i < len )
       if( string[i] == c )
         break;
       else
         i++;
    if( i < strlen(string) )</pre>
       return &string[i];
    else
       return NULL;
```





For a number of reasons, this version is even more efficient than the previous one.

Can you tell why?

```
char * find_char_in_string( char *string, char c )
{
   char *pos = string;
   while( ( *pos != '\0' ) && ( *pos != c ) )
       pos++;

   return ( *pos == '\0' ? NULL : pos );
}
```







(6) Avoid unnecessary memory references

This simple loop for a reduction of an array accumulates the partial results de-referencing the pointer sum at each iteration.

```
void reduce_vector( int n, double *array, double *sum )
{
   for ( int i = 0; i < n; i++ )
      *sum += array[i];
   return;
}</pre>
```



(6) Avoid unnecessary memory references

This simple loop for a reduction of an array accumulates the partial results de-referencing the pointer sum multiple times.

(asm obtained with -O1)

```
void reduce vector( int n, double *array, double *sum )
    for ( int i = 0; i < n; i++ )
          *sum += array[i];
    return;
```

```
.L3:
 movsd xmm0, QWORD PTR [rdx]
 addsd xmm0, QWORD PTR [rax]
 movsd QWORD PTR [rdx], xmm0
 add
       rax, 8
       rax, rcx
 CMD
 ine
        .L3
```

```
movsd xmm0, value of *sum
addsd xmm0, value of *array
movsd address of sum, xmm0
add
      rax, 8
                   ( array++ )
      rax, n
CMD
```





(6) Avoid unnecessary memory references

Introducing a separated, local accumulator will save memory accesses

(asm obtained with -O1)

NOTE

Try to get the point..
example simple enough in
introductory lectures has the
cons that they may be too
simple for the compiler
In very simple cases as this
one, the compiler is able to
do the job for you most of
the time.

```
void reduce_vector( int n, double *array, double *sum )
{
   double cum = 0;
   for ( int i = 0; i < n; i++ ) cum += array[i];
   *sum = cum;
   return;
}</pre>
```

```
.L11:
addsd xmm0, QWORD PTR [rax]
add rax, 8
cmp rax, rdx
jne .L11
```

```
addsd xmm0, value of *array;
add rax, 8 (array++)
cmp rax, rdx (array with end-of-array)
```





The compiler is smart..

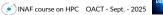


.. but it is also **constrained**.

A compiler is

a program that translates a program from a sourcelanguage into an <u>equivalent</u> program in a targetlanguage







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 ×) in 2's complement is commutative and associative.

Floating point math (+ and ×) is commutative between 2 operands is *never* associatve.







CAVEAT!!

In fact, if you study, as you should, the "what every computer scientist should know about floating-point" paper (find it in the sco/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.

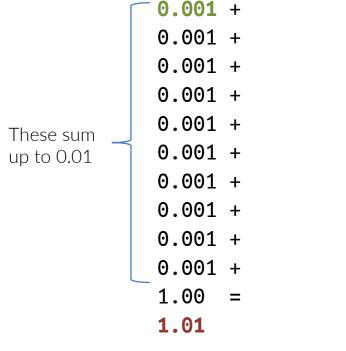






CAVEAT !!

Then again:



1.00 +0.001 +0.001 +0.001 +0.001 +Fach of 0.001 +these ops results in 0.001 +1.00 0.001 +0.001 +0.001 +0.001 =1.00

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

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

We'll see the impact of that in the next slides.



that's all, have fun

