Optimization
Avoid the avoidable

Luca Tornatore - I.N.A.F.

DATA SCIENCE & ARTIFICIAL INTELLIGENCE

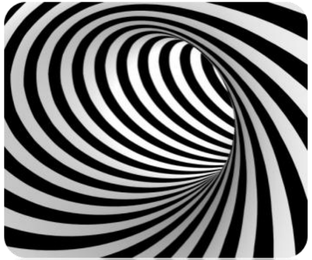
SCIENTIFIC & DATA-INTENSIVE COMPUTING

2024-2025 @ Università di Trieste

Outline

First things first

Cache & Memory



Loops

Branches

Pipelines

Outline

Avoid the avoidable inefficiencies

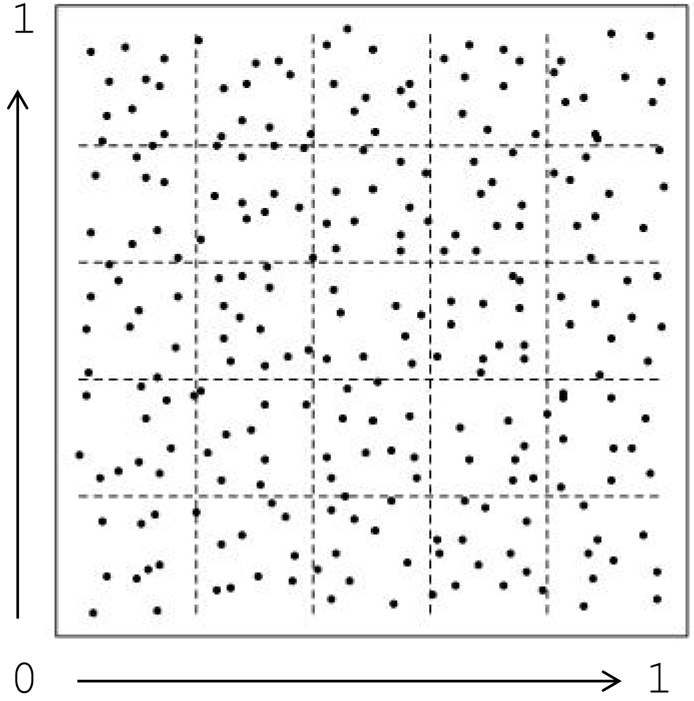
Branches

Pipelines

Loops

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

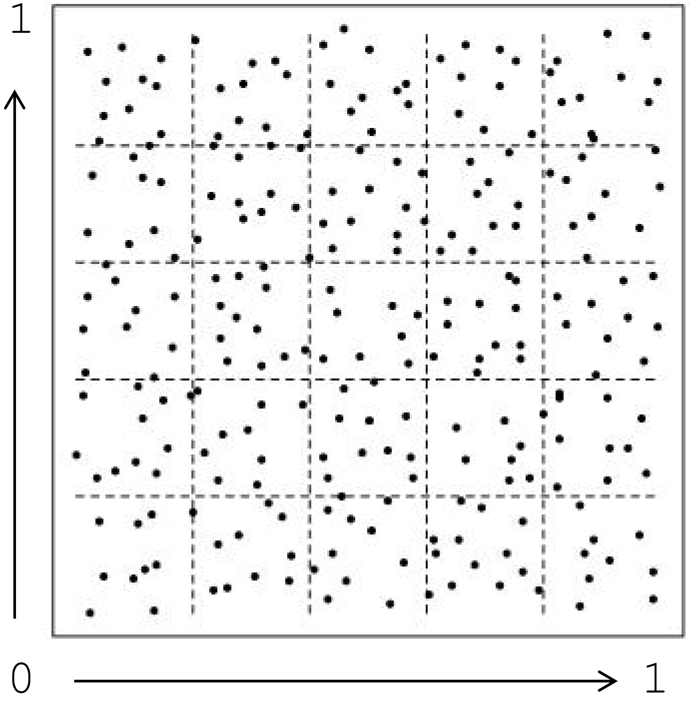
1) we have a distribution of random data points on a 2D plane which we subdivide in sub-regions using a grid.



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.

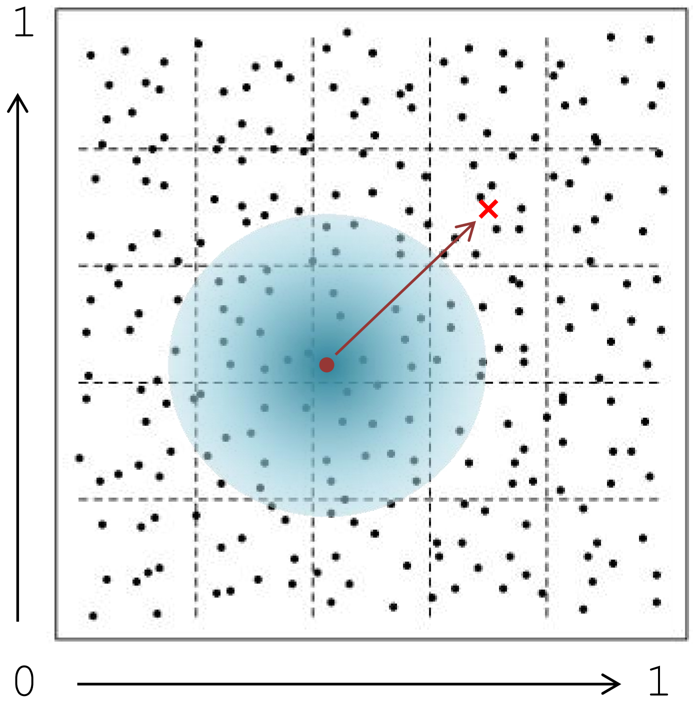
2) for each point *p*, we want to select all the grid cells whose center is closer to *p* than a given radius *r*, and to perform some operations accordingly to our search result.



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

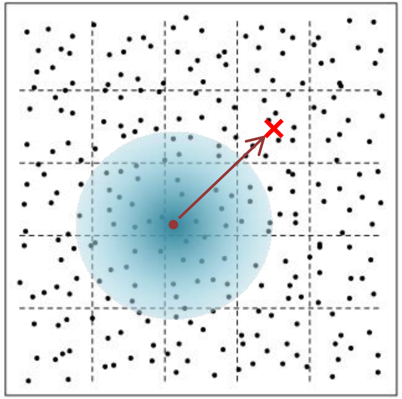
1) we have a distribution of random data points on a 2D plane which we subdivide in sub-regions using a grid.

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 < 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;
          }
```

SCO/avoid_the_avoidable/loop.0.c

(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;
          }
```

SCO/avoid_the_avoidable/loop.1.c

(1) Avoid expensive function calls

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

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 - 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;
          }
```

SCO/avoid_the_avoidable/loop.2.c

(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);
          }
```

SCO/avoid_the_avoidable/loop.3.c

| (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

`(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(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_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);  } } }
```

SCO/avoid_the_avoidable/loop.4.c

(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);  } } }
```

SCO/avoid_the_avoidable/loop.6.c

(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

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 < 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);  } } }
```

SCO/avoid_the_avoidable/loop.5.c

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.
However also the stack, which can be wide, is better to be clearly 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 they were all defined at the begin of a long procedure 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 compiler cares for it all ?

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.

Note: the importance of being earnest

Your compiler is able to take care of most of the aspect we have seen above (but for one, obvisouly: the usage of expensive functions calls, like pow and sqrt).

We'll see that better when talking about loops and branches.

However, that is not a good reason not to write a decent code from the beginning.

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:

These sum up to 0.01

```
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
1.00  =
1.01
```

```
1.00  +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 +
0.001 =
1.00
```

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 `./AOB/kahan_summation`

Associative math

Every compiler allows the users to relax the rules for IEEE FP arithmetics.
Many of these rules ensure the correct treatment of under-normal numbers, `0+` and `0-`, `Inf` and `NaN`. As such, relaxing the checks and the branches that deal with those cases, may incur in some un-correct result.

Explore two resources to have a better comprehension of this

https://simonbyrne.github.io/notes/fastmath/
https://kristerw.github.io/2021/10/19/fast-math/

Appreciate that also explicit tests as **`isinf(x)`** or **`isnan(x)`** will be disabled. As such, to be confident in deactivating those switches, you must be sure that your code is not incurring in those cases. However, by definition, the tests performed without those flags are not definitive because once the operations are re-shuffled, which is due exactly to those flags, the results may be different.

(5) Don't repeat unnecessary checks

Do you expect any great performance from this code ?

If not, why ?

```c
char * find_char_in_string( char *string, char c )
{
    int i = 0;
    while ( i < strlen(string) )
       if( string[i] == c )
         break;
       else
         i++;

    if( i < strlen(string) )
       return &string[i];
    else
       return NULL;
}
```

(5) Don't repeat unnecessary checks

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?
I guess no, but the compiler does not know it and has no way to understand that by code analysis.
Moreover, the memory pointed by string could be modified somewhere else between two iterations.

```
char * find_char_in_string( char *string, char c )
{
    int i = 0;
    while ( i < strlen(string) )
       if( string[i] == c )
         break;
       else
         i++;

    if( i < strlen(string) )
       return &string[i];
    else
       return NULL;
}
```

(5) Don’t repeat unnecessary checks

This very simple change will save you a lot of CPE

```
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) )
       return &string[i];
    else
       return NULL;
 }
```

(5) Don’t repeat unnecessary checks

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;
 }
```

(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
  cmp   rax, rcx
  jne   .L3
```

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

(6) Avoid unnecessary memory references

Introducing a separated, local accumulator will save memory accesses

(asm obtained with -O1)

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

```
.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)
```