Code Optimization
Hands-On

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Outline

Examples to play with:

- Memory access
- Conditional branches
- Exploiting everything in loops

How it works

Examples

- Every example code aims at clarifying a topic discussed in the lecture.
- We re-focus, and we get through the example together.
- Usually the example illustrates several ways in which you can code, from the naīve to a much better, so that you can understand it and verify.
- At the beginning, you can verify just by the shrinking of the run-time; we'll teach you how to look at different metrics

How it works

Exercise

- We give you a problem to solve
- Tipically, we’ll start from a (semi-complete) serial code and we’ll ask you to parallelise it

How it works

Start on your laptop, by compiling and executing some tests.

Then, bring the code to the cluster, get a core, or a node, compile and execute.

If you can not use your laptop

If you can't use your laptop, for instance because

- you're on a pure Windows box
- you're on a MAC, and you did not install the compiler

you need to go to the cluster

btw: there are reasons for the fact that all the HPC platforms run Linux..

If you can not use your laptop

1) login to the logn node: ssh ....

```
Last login: Mon Sep 22 15:57:15 2025 from 192.168.1.184
===================================================================
=                                                                 =
=      ___ _    ___ ___   _   ___ ___    ___   _   ___ _____     =
=     | _ \ |  | __|_ _| /_\ |   \_ _|__/ _ \ /_\ / __|_   _|    =
=     |  _/ |__| _| | | / _ \| |) | |___| (_) / _ \ (__  | |     =
=     |_| |____|___|___/_/ \_\___/___|  \___/_/ \_\___| |_|     =
=                                                                 =
=                                                                 =
===================================================================
[hpcschool46@pleiadi ~]$ sinfo
PARTITION  AVAIL  TIMELIMIT  NODES  STATE NODELIST
hpc_school    up 3-12:00:00     16   idle r35c5s[01-07,11-12],r35c6s[01,04-08,10]
128g          up 3-12:00:00      1  down* r35c3s07
128g          up 3-12:00:00     17  alloc r35c2s[01-04],r35c3s[01,03-05,09-10],r35c4s[03-09]
128g          up 3-12:00:00      2   idle r35c4s[01-02]
256g*         up 3-12:00:00      1    mix r35c2s10
256g*         up 3-12:00:00     17  alloc r35c1s[01-12],r35c2s[05-09]
[hpcschool46@pleiadi ~]$
```

If you can not use your laptop

2) get a core on a node, addressing the hpc_school partition

```
[hpcschool46@pleiadi ~]$ sinfo
PARTITION  AVAIL  TIMELIMIT  NODES  STATE NODELIST
hpc_school    up 3-12:00:00     16   idle r35c5s[01-07,11-12],r35c6s[01,04-08,10]
128g          up 3-12:00:00      1  down* r35c3s07
128g          up 3-12:00:00     17  alloc r35c2s[01-04],r35c3s[01,03-05,09-10],r35c4s[03-09]
128g          up 3-12:00:00      2   idle r35c4s[01-02]
256g*         up 3-12:00:00      1    mix r35c2s10
256g*         up 3-12:00:00     17  alloc r35c1s[01-12],r35c2s[05-09]
[hpcschool46@pleiadi ~]$ srun -N1 -n1 --cpus-per-task=1 -A hpc_school -p hpc_school --pty /bin/bash
srun: job 395453 queued and waiting for resources
srun: job 395453 has been allocated resources
[hpcschool46@r35c5s11 ~]$
```

If you can not use your laptop

3) anatomy of a srun

```
srun -N1 -n1 --cpus-per-task=1 -A hpc_school -p hpc_school --pty /bin/bash
```

how many nodes you want (in this case, 1)

how many tasks per node (in this case, 1)

how many cores per task (in this case, 1)

The budget account

The cluster partition to be used

If you can not use your laptop

4) inspect what compilers are available

```
[hpcschool46@r35c5s11 ~]$ module av
----------------------------------------- /opt/Modules/compilers/gcc ------------------------------------
gcc-9.4.0  gcc-10.3.0  gcc-11.2.0

---------------------------------------- /opt/Modules/compilers/intel ------------------------------------
intel_xe_2020_update4

---------------------------------------- /opt/Modules/compilers/nvidia -----------------------------------
nvhpc_2022_221/gcc-9.4.0  nvhpc_2022_221/gcc-10.3.0  nvhpc_2022_221/gcc-11.2.0  nvhpc_2022_221/nvhpc_

--------------------------------------- /opt/Modules/compilers/openmpi -----------------------------------
```

If you can not use your laptop

5) load the corresponding module by

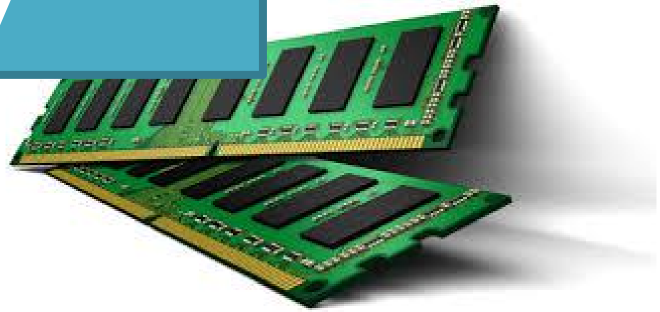
```
module load $module_name
```

How it works

All of us will be available to discuss, answer questions, solve technical problems and solve doubts.

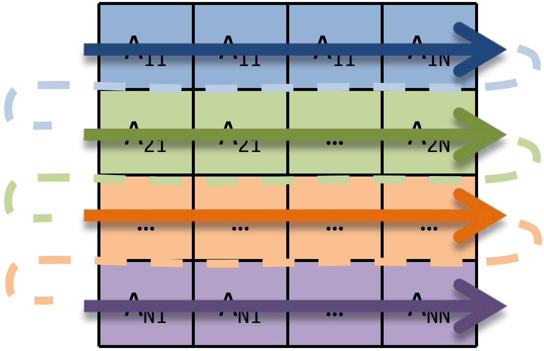
Please, rise your hand and call us at any moment.

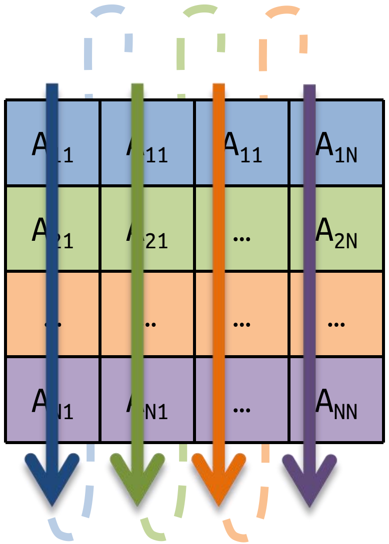
Accessing the Memory



Array traversal

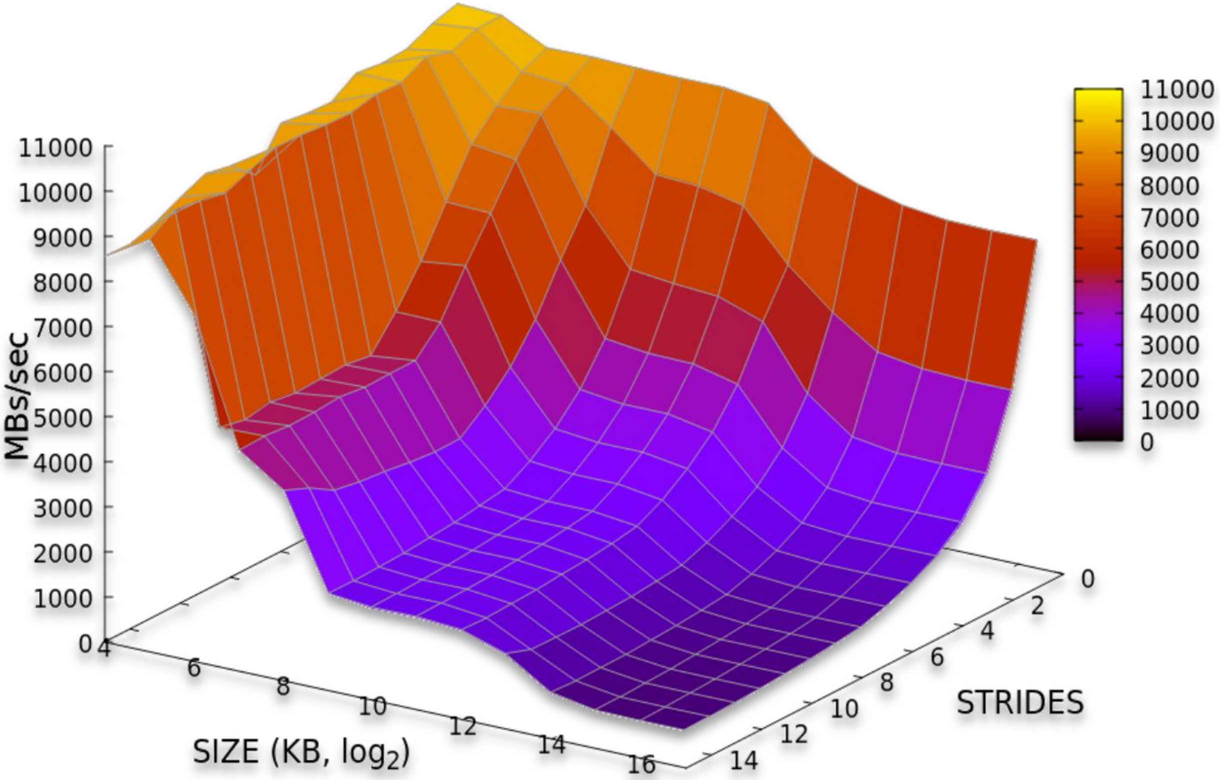
After having built a 2D array(*), let's assess what is the impact of accessing it by contiguous locations or by strided locations.
That is the very first step to sense how the cache works.



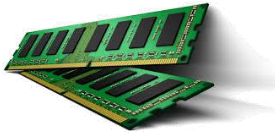


(*) how do you "build" a 2D array on an intrinsically 1D object like the RAM ?)

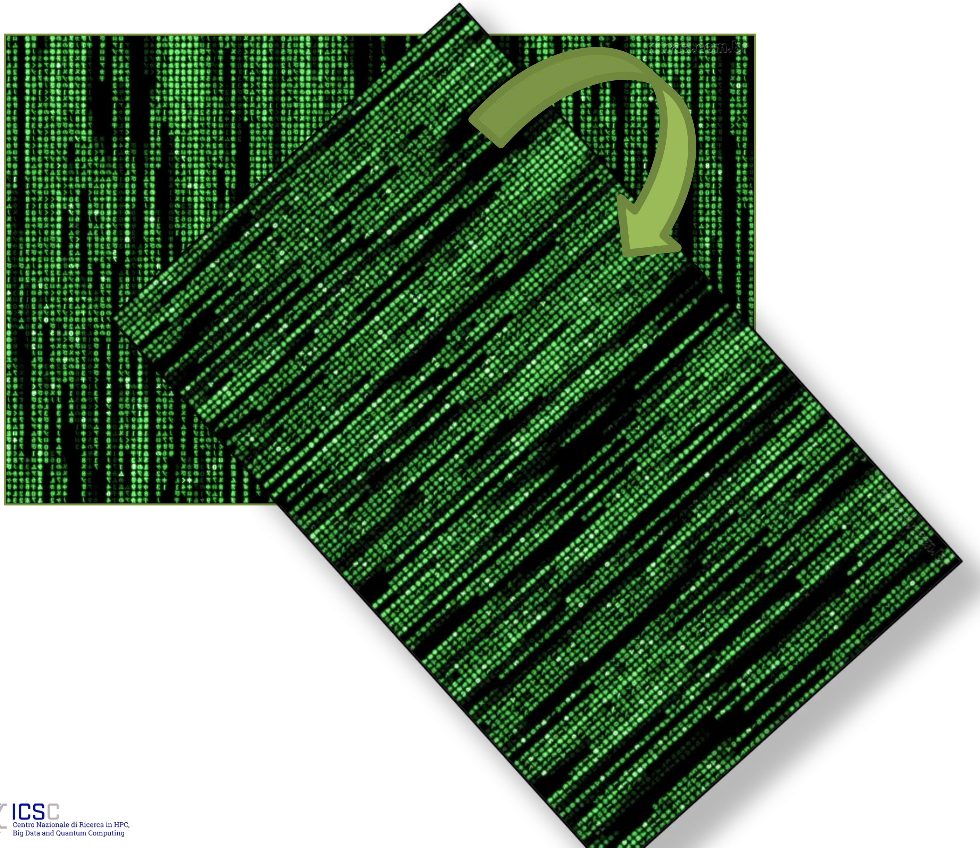
The memory mountain



That is basically the extension of the previous exercise.
Let’s dig more, and get the mountain from your own laptop



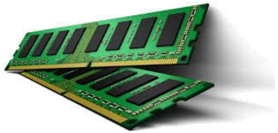
Transpose a 2D Matrix



In this problem it is unavoidable to either write or read with a stride.

```
   for ( int i = 0; i < Nrows; i++ )
      for ( int j = 0; j < Ncols; j++ )
strided write → At[j][i] = A[i][j]
strided read  → At[i][j] = A[j][i]
```

Which one is better ?
Is there any way to be more cache friendly?



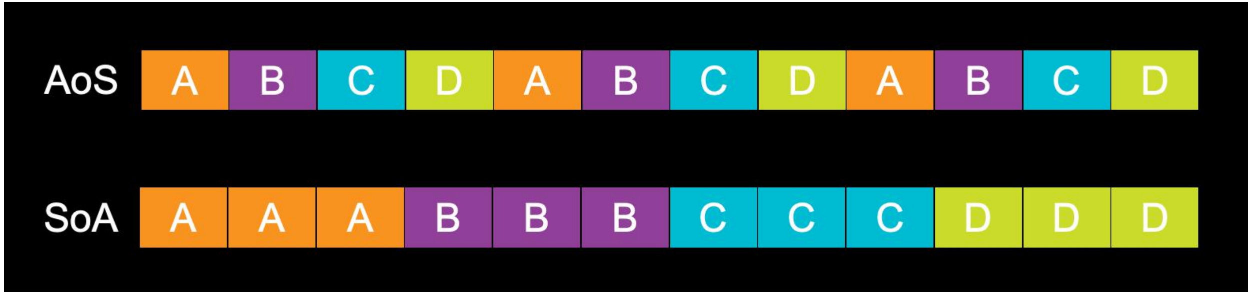
Hot and Cold fields

We use a much known data structure, the “linked list”, at its worst

(which is pretty easy, though.
Actually, we covertly aim at convince you *not to use* linked lists).

Why **conveying big data structures** around is a **bad idea** if you’re using only a tiny fraction of them *very often* - for instance, to retrieve the data to be processed - and most of them only once, or very few times?

AoS vs SoA



Which is the “best” data layout?
Well, it depends.

But let’s test AoS and SoA in a simple case, and in a the same case rendered slightly less simple.

Conditional Branches

| Unpredictable stream

Branch predictors are surprisingly good… when there is something to predict.
If This Then That.

How do you do when the unpredictable jumps in?

Unpredictable streams

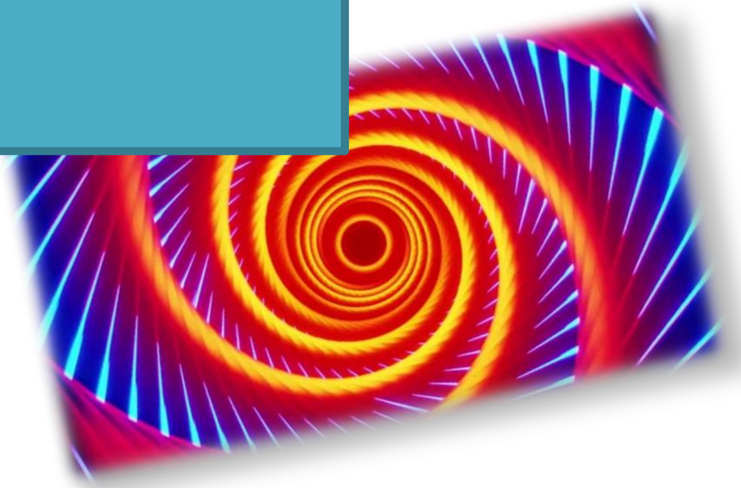
We will explore two cases:

1) scanning an array to process only a subset of its values

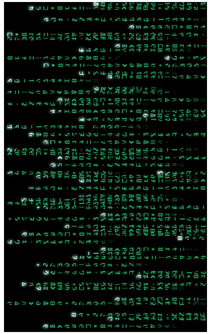
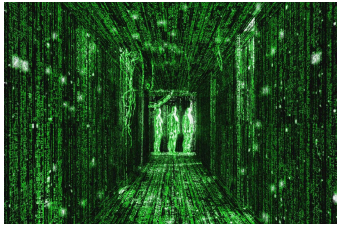
2) element-wise sorting two arrays so that

$$A_i \geq B_i \ \ \forall i$$

Loops



Matrix Multiplication


x

=


A great classic, we couldn't miss it.
This problem, whose arithmetic intensity grows with the problem's size, is used to rank supercomputers world-wide.

It is also among the bricks of AI.

Exploiting superscalarity

that’s all, have fun