High Performance Computing Assignment 2022/2023

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1 Exercise 1

1.1 Introduction

1.1.1 Rules of the Game of Life (GOL)

Each cell can be either "alive" or "dead" depending on the conditions of the neighboring cells:

- a cell becomes, or remains, alive if 2 to 3 cells in its neighborhood are alive;
- a cell dies, or do not generate new life, if either less than 2 cells or more than 3 cells in its neighborh are alive (under-population or over-population conditions, respetitively) way, the evolution of the system is completely determined by the initial conditions and by the rules adopted to decide the update of the cells' status.

1.1.2 Notations

This report aims to describe the algorithms chosen for running the Game of Life and their performances, according to the "size" of the problemstly, we define precisely what are the inputs of the problem and what are the outputs.

The main inputs are:

- matrix size, that is a rectangular grid isize x jsize (in the experiments we will focus just on square matrices);
- number *n* of steps to be calculated;
- the type of evolutiostatic or ordered;
- the frequency *s* of screenshot requested during the run.

Considering the hardware point of vitimere are other important inputs such as the number of MPI processes (nMPI) and OMP threads (nOMP).

The outputs are the final snapshot after *n* steps and the time measured during the run of the algorithm which is crucial for the scalability analysis (we will focus on it later).

1.1.3 Methodology

The general setting of this work is organised into the maiand two source fileswrite_pgm_images.c and game_functions.cThe main actually record all the inputs and chooses to run the static or the ordered algorithm. In write_pgm_images.c there are the read and write functions for pgm images (this is taken from github repository assignment), game_functions.c contains alwe need to run the game, particular there are:

- void initialize_game(int isize, int jsize, const char *image_name, double prob) just creates a isize × jsize matrix with every cell alive with probability prob and it saves it in a file with name image name.
- void run_game(int isize, int jsize, const char *image_name, int total_steps, int step_for_snap, int evolution_type) gets the initial matrix from image_namthen run the static (or ordered introduction_type == 0) for total_steps number of steps.
- unsigned char upgrade_cell(unsigned char **pixels, int i, int j, int isize, int jsize) is the nucleus of the algorithin returns a char value ('b'alive,'255'if dead) that represents the new status of the cell (i, j), given the 2d array pixels. function follows the rule of the game, and note that it just needs a "local" information of the neighbourhood of (i, j) to give an output, not the all matrix.

The key part of run_game algorithm is the nested 'flood with the upgrade_cell function. This for loop can be parallelized using OMP pragmas, this is the main and unique point in which we used openMP tools. The entire run_game function is built in order to exploit a possible increasing number of MPI processes in the following way:

$$q + 1, q + 1, \ldots, q + 1, q, \ldots, q$$

with exactly r times the number q +Hence every MPI process performs its task only on its own slice. It is now obvious that at the beginning every iteration we need an MPI_Scatterv ctdl distribute the slices at the end of the iteration an MPI_Gatherv to rebuild the entire image (see **Conclusions** section from improvements on this part).

1.2 Implementation

1.2.1 upgrade cell function

We start from the simple function upgrade_cellIt doesn't exploit any OMP threadization nor MPI processes, because the operations done are very simple **The tarty** possible problem is the presence of the boundariesout it is easily overcome by using some basic modular arithmetic, we store the coordinates of the neighbours, in the following way:

```
inti_mod[3] = { (isize+i -1) %isize, i %isize, (isize+i +1) %isize };
intj_mod[3] = { (jsize+j -1) %jsize, j %jsize, (jsize+j +1) %jsize };
```

Then we evaluate the sum of the number stored in the neighbours, and check if it is equal to 255 \cdot 5 or 2 (in this case the cell (i, j) becomes alive, that is '0').

1.2.2 run game function

The codes of this function are logically divided into two **pacts** irst concerning the ordered evolution, the other the static evolution.

Ordered evolution This code exploit only OMP threadizations, cause it is intrinsically serial, the core of this function is the following:

```
#pragma omp parallelfor shared(isize, jsize, pixeod)apse(2)
for(inti = 0; i < isize; i++) {
    for(intj = 0; j < jsize; j++) {
        pixels[]i[j] = upgrade_cell(isize, jsize, pixe)l;s, i
    }
}</pre>
```

The previous nested 'for' cycle is inside a big 'for' cycle that iterates on the number of steps (time_steril is the variable that counts the stelps) ide there is also:

```
if ( time_ste phote processes the printf(snapshot_stribute printf(
```

Static evolutionIn the static evolution we exploit MPI and OMP features, as generally explained in the section before features the call MPI_Comm_rank(MPI_COMM_WORLD, &rank), we split the 2d array pixels into nMPI "slices":

```
MPI Comm rank(MPI COMM WORLD, &rank);
  MPI Comm size(MPI COMM WORLD, &size);
4 // Here we splittheimage alongthey axis
5 int sub_isizæisize / size;
6 intrest = isize% size;
8 // In the followin way we can sharepart of the image in piece sof subisized subisize
      +1
9 int rank minor rest = (rank < rest);</pre>
int start= rank * sub_isize(rank) * (rank_minor_rest);
int end = (rank + 1)
                     * s u b _ i s i z e ( rank +1) * ( rank_minor_rest );
12
13 //we need this becaustene previou as ssignme fnotma certainpoint adds only zeros
if (! rank minor rest) {
15
        start+=rest;
         end += rest;
16
17 }
```

Then, we need to create two array of integers for the calls of MPI_Scatterv and MPI_Gat/hech, are respectively senddispls and recvdisplehe entry *i* of such arrays specifies the displacement (relative to sendbuf or recvbuffer) from which to take the outgoing data to process *i*.

Other two necessary arrays, one for MPI_Scatterv one for MPI_Gatherv, are sendcounts and recvcount Their scope is to specify the number of elements to send (or receive) to (from) each@cotheseris the code and then an explanation:

```
int sum = 0;
int double_jsi ≠ ② * jsize;
for (int i = 0; i < size; i++){
    recvcounts ⊨ (sub_isize (i < rest)) * jsize;
    sendcounts ⊨ i [ecvcounts[i] + double_jsize;
    recvdispls[±]sum;
    senddispls[±]sum-jsize;
    sum += recvcount § [i]
}</pre>
```

Concerning the MPI_Gatherv ca(so, recvcounts and recvdispls) we just need to create the slices as explained in the **Methodology** section, that is $q \times$ jsize or $(q + 1) \times$ jsize depending on the rest.

For the MPI_Scatterv call, we want to update a slice of dimensions $k \times j$ size that begins at wew i. need at least a slice of $(k+2) \times j$ size that begins at row i-1 (then the function upgrade_Trails works). is what exactly we are doing in the previous code for senddispls and senddownedser, the reasoning do not work with the first and the last slices because we would use rows indexes of -1 and isize, that are not definedSo, we fix this problem by sending each time all the 2d array, that is the aim of the following code.

```
senddispls[=00];
senddispls[size=-0];
sendcounts+03ize * jsize;
sendcounts[size+3]ze * jsize;
```

Clearly, this is unoptimized version because we send each time all "central" datas of the array, which pointless for the first and the last slikeany case, all other slices receive just the information they need, so there are no obvious optimizations in this showe the core of the static evolution function is almost straightforward fter the allocations of the arrays data_image and sub_image, the following code is inside a 'for' loop that iterates over the number of steps.

The variable end_minus_start is an integer (different for each MPI process) that represents the numbe of rows contained in data_imagAlso temp_init is a variable defined outside the glotter loop, and represents the row index data_image that corresponds to the (ell) that has to be updated. The methods for snapshots creation is the same of the ordered case.

As we can read from the previous analysis, twe have done is a domain decomposition among MPI tasks, and threads are used only with the nested for low pat follows is a scalability analysis for both OMP and MPI features.

1.3 Results & discussion

Recallthat Amdahl's law states that "the overpaliformance improvement gained by optimizing a single part of a system is limited by the fraction of time that the improved part is actually issed he key point we wish to underline of experiments improvable part is not always the slowest part of the code.

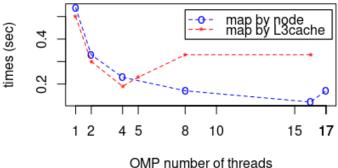
The section is divided into a OMP and MPI scalability analysis, for each case we provide some meaning examples and relative comme\(\text{Wise} \) we talk about "the time of the nested 'for' loops" we refers to the time measured to execute the lines 5 to \(\text{1the} \) for previous code\(\text{All} \) datasets are present in the GitHub repository, in the 'statistics' folder.

1.3.1 OpenMP scalability

Example 1:Here are reported the inputs data of our first experiment

Size:1000 \times 1000, n = 100, s = 50, ndofesYC, MPI processes = 8, OMP_PLACES=cores, OMP_PROC_BIND=close

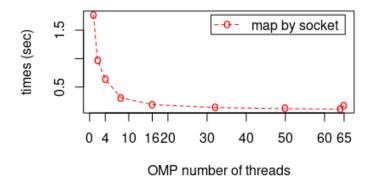
The results are shown in the following plot:



Note that a map by L3cache increase performance until the number of threads is 4, then it increases t time needed his is simply explained by the fact that a L3cache is divided among 4 cores and then at mos 4 threads (since SMT = 1 in this case) can be exploited for each MPI Three reasoning holds for map by node optionindeed, when we consider 8 MPI processes and 16 threads for each process, then 128 cores are sufficient toweverby the option -map-by node MIPI processes are spread among the 3 node we have requested.

Something strange happenswift try to use the -map-by socket option with nMPI = 8 (not shown in figure): the time taken is approximately indipendent with respect to OMP threads and it is 12.6 \pm 0.5 seconds. Note that we have requested 3 EPYC nodes, we have theorically at most 6 sockets (with 64 cores each), hence when we use more than 6 socket the slurm has some troubles in finding the appropria location for each MPI processIsually, I know how many sockets I can use, I will ask for less let us decrease *nM P I* for testing properly the -map-by socket option.

Same as before but with MPI processes = 2.



Note that in the datasets (in GitHub) the time measured for a MPI_Scatterv (idem for MPI_Gatherv) starts from the calbf MPI_Barrier to the end of MPI_Scatterv. Every MPI call takes a time of the order of 10⁴ secondswhich is really fast compared to the updating for loop whichforkesery single iteration with just one threadpproximately 10 seconds. By Amdahl's law, we can make the process faster, increasing the number of OMP threads (also increasing the number of MPI processes, but we will s later).

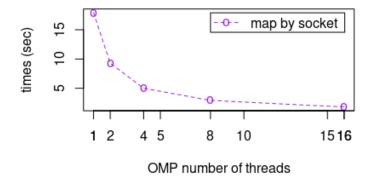
Note that when we consider 65 threads for both MPI processes, then we have to consider 2 distinct no because one node contains 128 cores (less then 65 · 2This 30)t makes the MPI calls a little slower and it is the reason of the strange red right tail of the plot.

We also repeated Example 1 with a fixed nMPI = 8 with a -map-by numawhattion got (consul the GitHub repository) is a very smooth scalability when we increase nOM P.

Finally, we have tried to change binding policies (between 'spread' and 'close') and also places (choos' threads'). The times measured are identibeliever when we have chosen 'threads' aces and 'close' as binding, the time is 2% less, we think because the shared memory among threads is the nearest poss and this reduces time when threads search for data_image.

Example 2: We try now to increase the size of the matWe use 2 MPI processes it a map by socket option (from experiments I've seen that the discussion above about the number and location of M processes is still valid).

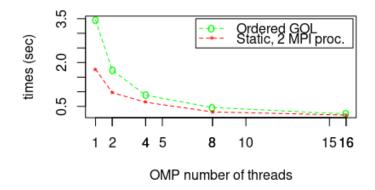
Size:10000 \times 10000, n = 10, s = 5, n3oEFSYC, MPI processes = 2, OMP_PLACES=cores, OMP_PROC_BIND=close



We can see from the plot above that if we double the number of threads, then the time alimitist halves. is possible because MPI_Scatterv and MPI_Gatherv calls take about 0.02 seconds, while the two nested 'f loops take 0.8 seconds.this caseby Amdahl's lawincreasing the number of OMP threads is the right choice because the improvable time is a large fraction of the total.

If we change threads polity instance we set OMP_PROC_BIND as 'spread' then the times we measure are very similar to the 'close' case, MPI_Gatherv call is slightly slower, 'for' loops and MPI_Scatte remain constante have also tried to set OMP_PLACES as 'threads' with both 'close' and 'spread' policies, and results are similar Only with 'spreadthe times are slightly increased becauster for loops are slower in accessing shared memory as they are far from each other within the same socket with 'cores' places this effect was not measurable).

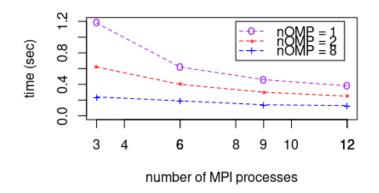
Ordered Game of Life (GOL): The final OMP scalability test it is for the ordered Game of Life, that is intrisincally serials only a OMP scalability analysis is meaningfule input datas are the same of Example 1From the plot below we can see that time almost halves when we double the number of thread however, the static game with 2 MPI processes almost halves the times (as expected).



1.3.2 Strong MPI scalability

Example 1:

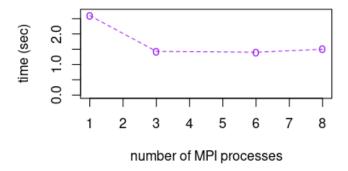
Size: 1000×1000 , = 100, s = 50, nodes: 3 EPYC, map by numaQMP_PLACES=cores, OMP_PROC_BIND=close



The description of the plot above starts from the times recorded with one single MPI process with one single thread: an overaltime of 3.55 seconds (with nMPI = 1, nOMPnet1shown in figure) with $3 \cdot 10^5$ for every MPI calls and $3.5 \cdot 10$ seconds the nested 'for op. The improvable part is a fraction 99.8%, so we can increase both the number of MPI processes and threads for each peocess are pretty clear, and we also know when to stop increasing nMPI or nlow ed, when we increase nMPI also MPI calls are a bit slower when we reach when we choose nMPI = 12 and nOMP = 8 is thoughtor' take $3 \cdot 10^6$ seconds each, and also MPI calls $4^4 \cdot 10^6 \cdot 10^6$ seconds Amdahl's law tells us that at this point it's difficult to obtain better performance because the improvable part now is not the largest one.

Example 2:

Size: 10000×10000 ,= 10, s = 5, nodes:3 EPYC, map by numaQMP_PLACES=cores, OMP PROC BIND=close, OMP NUM THREADS=16



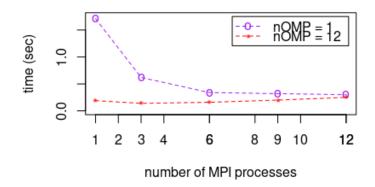
This experiment shows that a high number of MPI processes could be of ldwdetiditywhen nMPI = 1 a single nested 'for' loop takes approximately 0.2 seconds, while an MPI calls 0.0 However, deven with nMPI = 8 the time of the 'for' decrease to 0.04 seconds and MPI calls increase to 0.04 deconds each this situation the improvable time is half of the total, however, the gain in time due to the increase of nM is balanced by the loss caused by slower MPI calls.

Note that in the dataset is also present the experiment on the same with width, a -map by socket and nOMP = 64, nMPI = 2. It takes a total of 1.1 seconds which is better than 1.5 seconds with the same amount of cores (i.e.ap-by numa, nOMP = 16 and nMPI = 8) This is a natural consequence of a decrease in the number of MPI calls, and it's the best way of doing the experiment.

Example 3:

Size: $100 \times 1007 = 5000$, s = 2500, nodes: 3 EPYC, map by numaOMP_PLACES=cores, OMP_PROC_BIND=close

This time the 2d array is very tiny but it is updated for a long/tithea single MPI process, the nested 'for' loops take 10 seconds for every iteration, increasing nMPI gives us better performance until 'for' loops take the same time as MPI calles stationary time is 0.34 seconds (with nMPIHe0ce, we can scale with respect to MPI processes.



With nOMP = 12 we see nice performahoexeverwe come across a danger when we try to increase nMPI. The reason is simple nested 'for' loops are so fast that if we increase nMPI the delay due to slowe MPI calls is not recovered by a faster 'for' loop.

1.3.3 Weak MPI scalability

The goal now iggiven an initial size, show to run-time behaviour when you scale up from 1 socket (saturat with OpenMP threads) up to as many sockets you can keeping fixed the workload per MPI task.

In order to maintain fixed the MPlworkload,we use severahcreasing input images dfmensions $\{(500, 500), (500, 1000), (1000, 1000), (1000, 1500)\}$ with respectively nMPI = 1, 2, 4, The places for MPI processes are socket (of three different EPYC nodes), so we are going to use nOMP = 64.

All the statistics for the experiment are precisely state in Weak_MPI_scalability.csv in the statistics folder. However, the significant conclusion is that even MBIIprocesses has the same amount of work, the overaltime increases principally becausthe fincreased number messages that we need to send. Indeed, every MPI_Gatherv and MPI_Scatterv become a bit slower when we increase the size of the input images (and also nMPI).

Given the previous image dimensions and nMPI size, we set n = 500 and n = 400 times vary from 0.14 sec of the (500, 500) case up to 1 sec of the (1000, 1500) at set ake a look to the specific time, we note that the 'for' loop time remains more or less constant for every test, while MPI calls becomup to 10 times slower as we increase the size of the input array.

1.4 Conclusions

This report concludes that increasing the number of MPI processes is not always the right office: happen, the bottleneck is due to communication provides degree you have to consider that increasing nMPI usually slows the calls of MPI_Scatterv and MPI_Gatherand sometimes specially when the 2d array is very big (time depends mainly on the bandwidth) or very tiny (message latency becomes a bottleneck could nullify the gain in time for the 'for' lob paddition, increasing nMPI is useful when the improvable part is a consistent fraction of the totalrk (as Amdahl's law suggests) e have not seen a significant disadvantage in increasing nOMP.

1.4.1 Further improvement

The code we implemented could be optimized pricular the MPI calls. Indeed, the first and the last slices receive every time the whole 2darray, and this could slow down a little bit the combanications. possible improvements are the following:

- We can use better MPI calls just for adjacent slices, instead of building the image after every iteration
- In principle, it should also be possible to decrease the memory occupied by the image, encoding it w boolvalues Indeed we have only two states (alive or delamperations should use the boolues and the translation from bools to pgm file should be effective only if snapshots are required.
- we can compress-decompress the sparse matrix for the communication messages if bandwidth is "to low" respect to matrix sizes.

2 Exercise 2

2.1 Introduction

This assignment aims to understand, test and show the performance of dense matrix product (provided MKL and OBLAS libraries) running over some nodes (Fife). In particular, the benchmark includes an analysis of the scalability in two ways:

- Measuring time and Gflops of executions increasing the size of the matrix at a fixed number of cores
 (64 for EPYC and 12 for THIN) for single and double precision free threads allocation policies
 were also tested.
- Measuring time and Gflops of executions increasing the number of cores at a fixed matrix size for bosingle and double precision.

The algorithm used is called gemm (general matrix multiplication) and is tested only with squared ma with both float (32 bits) and double (64 bits) precision.

2.2 EPYC and THIN node details

The scalability studies are performed for *THIN* and *EPYC* notes that the technical information obtained through the command Iscpu:

- EPYC-01:it has two sockets ach equipped with an AMD Epyc 7h12 (a 64 core CEDA)ch socket is divided in 4 numa region CPUs max MHz is 2600 and min MHz is 150 The sum of all cache memory (both sockets) is the followind is 4MiB; L1i is 4MiB, L2 is 64MiB and L3 is 512 MiB (only 32 instances instead of 13B) nultaneous multi thread is disabled.
- THIN-007:it has 2 sockets, each equipped with an Intel Xeon Gold 6126 (a 12 core CPU). Each socket contains just one numa region have max 3700 MHz and min 1000 MHze sum of all cache memory (both sockets) is the following:is 768 KiB, L1i is 768 KiB, L2 is 24 MiB, L3 is 38.5 MiB (2 instances instead of 29) multaneous multi thread is disabled.

We want to point out that on /sys/devices/system/cpu/smt ofhe THIN node there was the file control with 'on' writtent means that SMT is supported by the CPU and enabledogical CPUs can be onlined and offlined without restrictions.

The theoretical peak performance is given by:

Number of cores: Frequency × Floating operations per clock cycle.

There exist different values to evaluate the cpu frequency, for the purpose of theoretical peak performance we decided to use the maximum value since we want to estimate an upper we late found some discrepancy between web dated those reported with Iscplin particular, for the THIN node case, the direct inspection provides 3.7GHz as max and 1GHz as min frequency while on web we founded 2.6GHz as with a boost up to 3.3GHz.

The number of floating operations per clock cycle is hard to evaluate since depends on different facto. We estimated it based on a web researchespeak performance amounts to:

- EPYC: 64 × 2.6GHz × 16(float) = 2662 Gflops.
- THIN: 12×3.3 GHz $\times 64$ (float) = 2534 Gflops.

We'll see later that the peak performance of the EPYC node is almost reached while the peak performance of the THIN nodes is way above, probably caused by an overestimation of the upper bound.

2.3 Slurm job

In the following we report an example of slurm job file that we used to submit on Orfeo.

 $^{^1} https://www.intel.it/content/www/it/it/products/sku/120483/intel-xeon-gold-6126-processor-19-25 m-cache-2-60-ghz/specifications.html$

https://www.amd.com/en/products/cpu/amd-epyc-7h12

```
#!/ b i n / bash
#SBATCH --no-requeue
#SBATCH -- job-name=" Curaba_test "
#SBATCH --partition=EPYC
#SBATCH --nodes=1
#SBATCH --exclusive
#SBATCH --time =2:00:00
module I o a darchitecture/AMD
module I o a dmkl
module I o a dopenBLAS/0.3.21 - omp
exportcode=/u/dssc/ccurab00/scratch/Foundations of HPC 2022/ Assignment/exerci
exporOtMP NUM THREADS=64
cd $code
make clean
make cpu
g c c-fopenmp 00 where I am . c -o 00 where I am . x
rm where I am . c sv
./00 where I am .x >> where I am .csv
fori in {0..20}
        letsize=\$((2000+2000*\$i))
do
        forj in {1..3}
        do
               echo $size
                ./gemm mkl. $size$size$size>> 1 double mkl EPYC.csv
                ./gemm oblas.x$size$size$size>> 1 double oblas EPYC.csv
        done
done
```

The executable 00_where_I_am.x is a simple code that writes on the where_I_am.csv file where (which core) each thread is executed;ust for checking purpose.

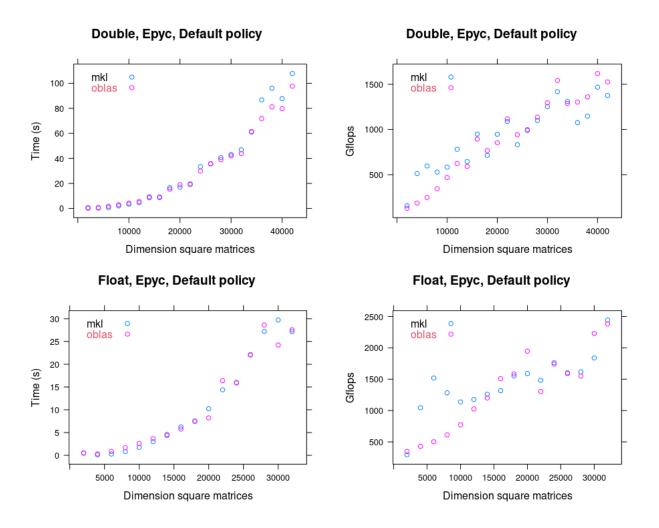
We also highlight that, for each matrix dimension, we executed 3 test and calculate the mean so we of get a more robust estimate of time and gflop scalability.

2.4 Results

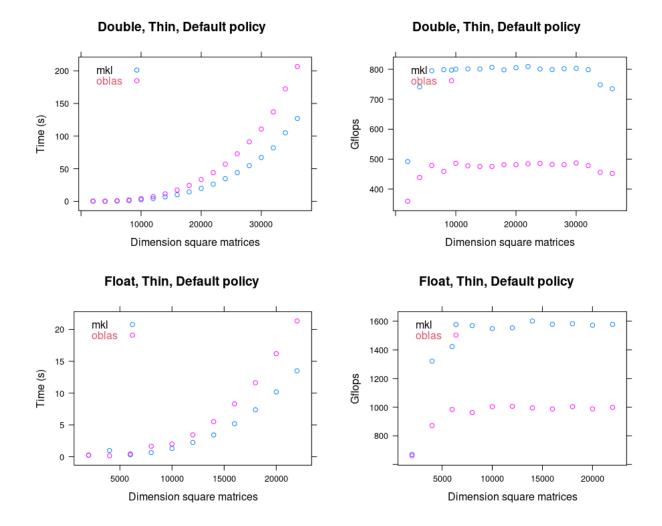
It follows some consideration we provided looking at the graphs:

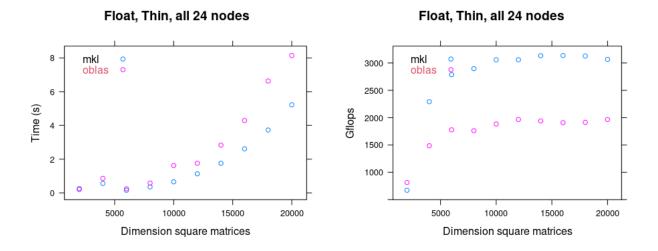
- There are some 'spikes' on the number of gflops graph for EPYC node with mtd tibdens tand it with certainty we would need to go deep into the code and hardward the tail sthough make some guesses probably the dimension is used in the code to exploit the capacity of the cache mountain trying to avoiding cache misses wing this dimension can produce a loth of e cache misses.
- There's a huge different in the performance of the two libraries for THIN nodeWastiscarded various hypothesis to explain such a differemost ofthem where based on the fact that the node could contain non-homogeneous CPU's (some faster than other) but we have observed the same difference also when the THIN node is used. Even if, as stated before the mkl library can take advantage of SMTthis doesn't seem to be enough to explain such difference ally on intensive and optimized computational task such as matrix multiplicationally hypothesis we formulated (that we haven't discarded) to explain such behaviour is the fostom the mkl library code produces a favorable vectorization of data that exploite abmputation appacity of the CPUs. It's like performing twice the operations per clock.
- The number of float operations per second is approximately twice the double operations per second as expectedThis rule doesn't seem to fit rigorously on *EPYC* node:fact float operations per seconds tend to per even less then double operations per setting due to technical hardware details which can be complicated and we don't handle in this report.

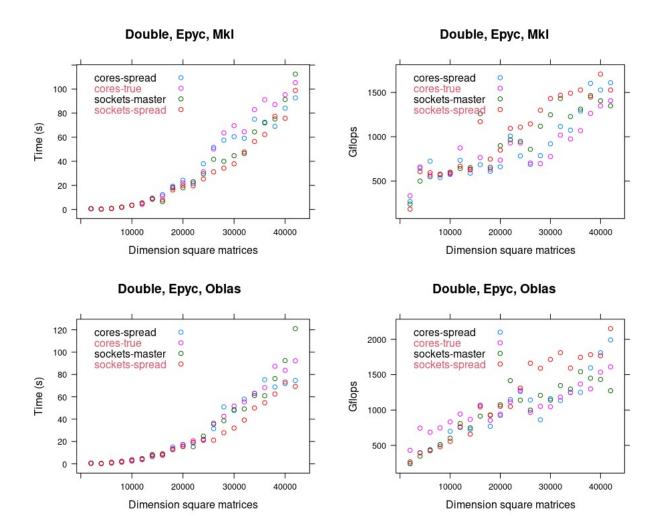
• Since for *EPYC* node the number of gflops tends to increase linearly respect to the square dimensior (we remember that the number of operations require by the task increases approximately as a cubi function respect to the matrix dimension) we observe that time increases approximately as a quadr function. On the other hand the *THIN* node reaches the plateackly and his time seems to grow up as a cubic function as expected.



²maximum number of floating operation per second

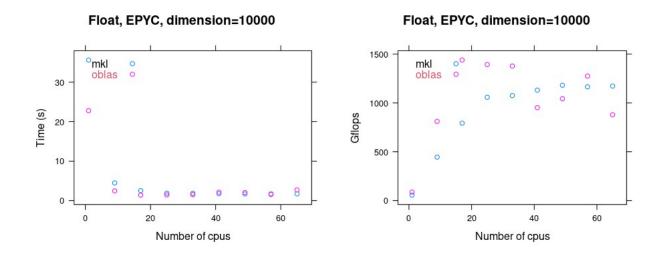






Giving a look at the different thread affinity policy chosen we can deduce that:

- All policies assign each of the 64 threads at a different core (there aren't constrained policies like compaster) sosince the task is computational expensive and doesn't move muchtimey purpor nearly the same.
- The policy sockets-master constrain the threads to use just one node, so it's using less L3 cache me and less dram (only 4/8 NUMA regions usæd)s produce a bit worse performance on average.
- The policy cores-true forbids the migration of the the description doesn't allow the operative system to optimize the computation and results in a bit worse performance.
- The spread policies (cores-spread and sockets-spread) are nearly the same uses all NUMA regions available and indeed they perform basically the same.



Looking at the last figures (in particular the gflops graph) we can see that the strong scalability propri is greatly satisfied until it reaches about 16 cpus (clearly this plateau is case <code>bliephemothentmatrices</code> dimension - higher is the maximum number of CPUs that we can use to minimize the computational time