${\rm HPC~4MA~2021/2022}$

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1 OpenMP

1.1 Optimization techniques

1.1.1 Naive dot

We first mention here the original naive_dot function. This function serves as an anchor (or base case) for performance comparision as well as for making sure we have the right result when using other techniques.

```
for (i = 0; i < M; i++)
  for (j = 0; j < N; j++)
  for (k = 0; k < K; k++) C[i + ldc * j] += A[i + lda * k] * B[k + ldb * j];</pre>
```

Below is the output of naive_dot for M = 1, K = 2 and N = 2:

```
## ( 1.00 1.50 )
##
## ( 1.00 1.50 )
## ( 1.50 2.00 )
##
## Frobenius Norm = 5.550901
## Total time naive = 0.000001
## Gflops = 0.013333
##
## ( 3.25 4.50 )
```

As

$$\begin{pmatrix} 1 & 1,5 \end{pmatrix} \begin{pmatrix} 1 & 1,5 \\ 1,5 & 2 \end{pmatrix} = \begin{pmatrix} 3,25 & 4,5 \end{pmatrix}$$

The result of this function is correct. We move on to the next technique.

1.1.2 Spatial locality

Spatial locality refers to the following scenario: if a particular storage location is referenced at a particular time, then it is likely that nearby memory locations will be referenced in the near future. In order to take advantages of this property, we notice that:

- In memory, A, B, C are stored in contiguous memory block.
- When using the index order i, j, k, we access B consecutively (as we access B by B[k + ldb * j]), but not A and C.
- Data from A, B, C are loaded in a memory block consisting of severals consecutive elements to cache. Thus, we could make use of spatial locality when reading data continously.

From 3 points above, we decide to switch the index order to k, j, i. Now we see that both reading and writing operations on C are in cache, this brings us a critical gain in performance. In addition, reading operations on A are in cache too but those on B are not.

```
for (k = 0; k < K; k++)
  for (j = 0; j < N; j++)
  for (i = 0; i < M; i++) C[i + ldc * j] += A[i + lda * k] * B[k + ldb * j];</pre>
```

For comparision, we have a table below with M = 4, K = 8 and N = 4.

We have the frobenius norm of both techniques are 3,461352 which indicate we have the right computation result. In addition, calculating time is already significantly small (≈ 0 second in both methods) and the difference between these two can therefore be ommitted.

Table 1: naive vs saxpy when M, N, K is small

algo	time	norm	gflops
naive saxpy	$0.000002 \\ 0.000001$	3.461352 3.461352	$0.111304 \\ 0.182857$

However, if we set M=2048, K=2048 and N=2048, there will be a huge performance gain as in the table shown below. In addition, from now, for an easier comparision between results, we will consider the default value of M, K and N is M=2048, K=2048 and N=2048 if not explicitly mentioned.

Table 2: naive vs saxpy when M, N, K is big

algo	time	norm	gflops
naive	149.30573	2.323362	$\begin{array}{c} 0.115065 \\ 0.276891 \end{array}$
saxpy	62.04563	2.323362	

Here, the naive_dot function is approximately 2,41 times slower than the saxpy_dot function.

1.1.3 OpenMP parallelization

In this section, we will analyse the main technique of this chapter: OpenMP. First, we show how we enable it on each function. We add a directive above each loop we want to parallelize whose general form is as below:

- Variables inside private are tied to one specific thread (each thread has their own copies of those variables).
- SCHEDULE_HPC is replaced by the schedule we want.
- NUM_THREADS_HPC is corresponding to the number of threads to use for parallel regions.

```
#pragma omp parallel for schedule(SCHEDULE_HPC) default(shared) private(i, j) \
    num_threads(NUM_THREADS_HPC)
```

In addition, inside norm function, we add a reduction clause reduction(+ : norm) as we want to sum up every norm from each thread to one final norm and taking square of that final sum. Finally, we have to add #pragma omp atomic above each line that updating the result matrix (C). It is because that matrix is shared among threads, atomic makes sure that there is only one += operation (which is essentially reading and writing) on one specific pair of indices at a given time. Note that norm does not need atomicity thank to reduction.

Here, we show a comparision between with and without OpenMP. Default OpenMP options will be SCHEDULE_HPC = static and NUM_THREADS_HPC = 4.

Table 3: naive vs saxpy with OpenMP

algo	time	norm	gflops	omp
naive	45.08355	2.323362	0.381067	X
naive	149.30573	2.323362	0.115065	
saxpy	15.29221	2.323362	1.123440	x
saxpy	62.04563	2.323362	0.276891	

Thank to OpenMP, naive approach is faster than 0,3 times while the saxpy_dot took less 0,25 times than before. Both approachs performance are significantly improved.

 $^{^{1}}$ https://www.openmp.org/spec-html/5.0/openmpse49.html#x288-20520006.1

1.1.4 Cache blocking (Tiled)

The main idea of the cache blocking technique (or tiled) is breaking the whole matrices into smaller sub-matrices so the data needed for one multiplication operation could fit into the cache, therefore leads to a much faster calculation. Furthermore, if we enable OpenMP, the computation would be even faster as each sub-matrice is processed by a separate thread. However, if we set BLOCK size too small, the benefit of dividing matrix is overshadowed by the additional loops and operations. Meanwhile, a too large BLOCK size leads to an overfitting (data for one operation can not be fitted into the cache), and therefore a slower operation. The principal source code is shown below:

The above code will work only if M, N and K are divisible by BLOCK. A more generic version could be found in full source-code.

We have a table comparision between all techniques we are discussing so far below. Also, we set the default size of BLOCK = 4.

algo	$_{ m time}$	norm	gflops	omp
naive naive	$45.08355 \\ 149.30573$	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$\begin{array}{c} 0.381067 \\ 0.115065 \end{array}$	х
saxpy saxpy	$15.29221 \\ 62.04563$	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$\begin{array}{c} 1.123440 \\ 0.276891 \end{array}$	x
$\begin{array}{c} \text{tiled} \\ \text{tiled} \end{array}$	$17.01662 \\ 17.14018$	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$1.009594 \\ 1.002316$	X

Table 4: naive vs saxpy vs tiled

In the table above, cache blocking technique is already fast enough. However, OpenMP does not help speeding it up as the default BLOCK size is not optimized in this case.

1.1.5 BLAS

One last technique that is used in our code is calling the cblas_dgemm function which use the optimized BLAS implementation. This function is the fastest method even if other methods are "cheated" (by using OpenMP) as their implementation is optimized based on many factors: algorithms, software and hardware.

1.2 Benchmarks

1.2.1 Sequential

In this section, we fix NUM_THREADS_HPC = 1 and vary the matrix size. Instead of using environmental variables, we use a script for generating code with the hard-coded configurations we want as reading environmental variables is an expensive operation.

For the sake of simplicity, we first consider the case where M and K and N are all equal and equal to a 2^s where s = 2 to s = 11. In addition, we have included a non OpenMP result (which is also sequential) for studying how the overhead time of OpenMP impacts the overall performance.

Table 5: all techniques with default options

algo	time	norm	gflops	omp
naive naive	45.083546 149.305728	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$\begin{array}{c} 0.381067 \\ 0.115065 \end{array}$	Х
saxpy saxpy	$15.292206 \\ 62.045634$	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$\begin{array}{c} 1.123440 \\ 0.276891 \end{array}$	x
$\begin{array}{c} \text{tiled} \\ \text{tiled} \end{array}$	17.016616 17.140176	$\begin{array}{c} 2.323362 \\ 2.323362 \end{array}$	$1.009594 \\ 1.002316$	X
blas	6.140073	2.323362	2.797991	

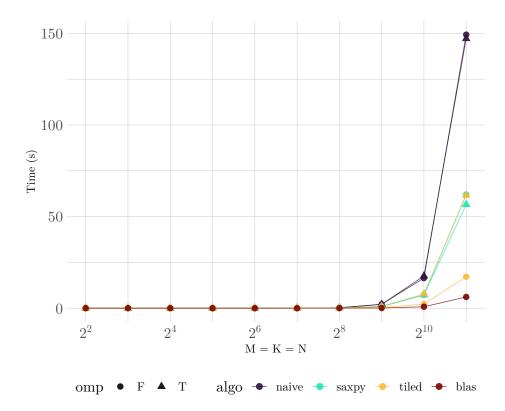


Figure 1: Computational time in function of matrix size

Table 6: Computation time when M=N=K=2048

algo	time	omp
naive naive	147.139047 149.305728	X
saxpy saxpy	56.581041 62.045634	x
$\begin{array}{c} \text{tiled} \\ \text{tiled} \end{array}$	61.600396 17.140176	x
blas	6.140073	

In the graph below, we see that the fastest method is no doubt blas method, followed by tiled, saxpy and

the slowest is naive. This is aligned with what we see in the section 1. In addition, the time for calculating matrices whose size is less than $2^{10} = 1024$ is around 5s for all methods. This could be explained by the fact that these matrices could be fitted entirely into the cache, which leads to a significant drop in computation time.

Another property that could be interesting is the version with OpenMP is close or even faster than the non OpenMP version regardless the overhead of parallelization. This could be explained by many factors ² ³, but the most significant one is As OpenMP is just API specification and C compilers are free to implement it in any way they want as long as they respect the specification, many compilers (notably modern gcc and clang) are smart enough to treat OpenMP version of only 1 thread the same as the sequential version. Therefore, we only see a small difference between each run. If we run both versions enough times, the difference in average time of each will be the smaller.

1.2.2 Threading

Right now, we will be able to see the true power of parallelism, we will keep increasing the number of threads in form of 2^s where s = 1 to s = 7.

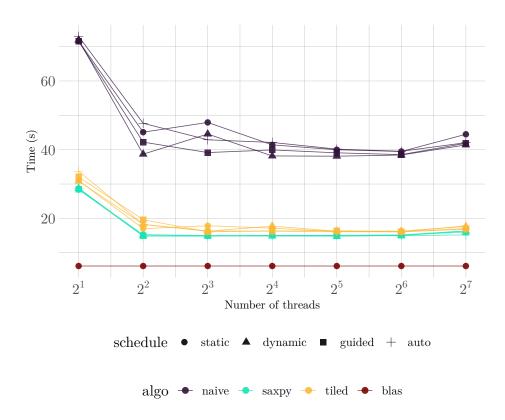


Figure 2: Computational time in function of number of threads and schedule

We see that BLAS method is still the fastest regardless the number of threads and schedule (since it isn't affected by OpenMP options). It shows that in order to achieve high speed computation, we have to not only parallelize, but also make improvements on multiplication algorithms, memory accesses and even use assembly instructions.

²https://stackoverflow.com/questions/22927973/openmp-with-single-thread-versus-without-openmp

 $^{^3}$ https://stackoverflow.com/questions/2915390/openmp-num-threads1-executes-faster-than-no-openmp

In addition, the 4 schedule cuvres of each technique are overlapping each others and there are only very small difference in term of computational time. The phenomenon happened because our problem (matrix multiplication) has a nearly the same workload at each iterations. That means the first iteration will take almost the same as the last iteration or any other iterations. For each schedule:

- static evenly-divides the total workloads into each threads, which is the best schedule for our problem.
- dynamic and guided are designed for different situation, where each iteration takes different amount of time to finish their work. There is overhead compared to static, however, it does not have big effect on overall performance as our matrices are not too big.
- auto lets the compiler choose how to schedule and divide work among threads, so it is compiler-specific. For example, gcc maps auto to static ⁴, at a consequence, we see a similar pattern with static.

Finally, more threads **doesn't** always mean better performance. After we increased thread to 4, time taking for one multiplication fluctuates but does not have any real decline. The reason is there is only a limit number of physical cores inside each computer, when the number of threads goes up too high, the overhead in creating and synchronize threads will overshadowed any benefits we gain.

1.2.3 Blocking

In the last section, we will concentrate ourselves on the impact of BLOCK size to overall performance. We will vary the BLOCK size in a power of 2, from s = 0 to s = 10

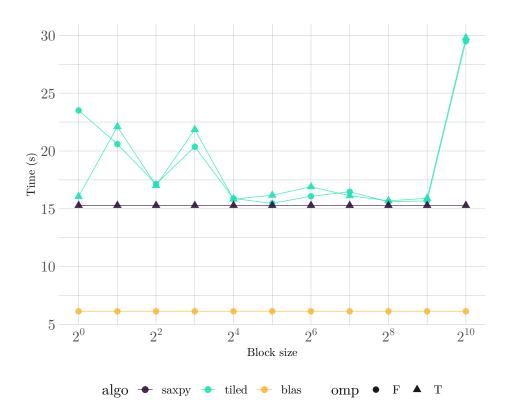


Figure 3: Computational time in function of BLOCK size

 $^{^{4}} https://github.com/gcc-mirror/gcc/blob/61e53698a08dc1d9a54d785218af687a6751c1b3/libgomp/loop.c\#L195-L1981c1b3/libgomp/loop.c#L195-L1981c1b3/libgomp/loop.ch1961c1b3/libgomp/loop.ch1961c1b3/libgomp/loop.ch1961c1b3/libgomp/loop.ch1961c1b3/lib$

We see clearly that as BLOCK size grows, the performance generally becomes better but get worse after BLOCK size grows to approximately 2^{10} . As explained in the section 1, BLOCK should not be too small and neither too large.