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High-Performance Computing Lab

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Solution for Project 1

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1. Explaining Memory Hierarchies

(25 Points)

1.1. Memory Hierarchy Parameters of the Cluster

By invoking likwid-topology for the cache topology and free -g for the amount of primary memory, the following memory hierarchy parameters are found:

Main memory 62 GB
L3 cache 25 MB per socket
L2 cache 256 kB per core
L1 cache 32 kB per core

All values are reported using base 2 IEC byte units. The cluster has 2 sockets and a total of 20 cores (10 per socket). The cache topology diagram reported by likwid-topology -g is shown in Figure 1.

Socket 0:

0	1	2	3	4	5	6	7	8	9
32 kB									
$256~\mathrm{kB}$									
25 MB									

Socket 1:

10	11	12	13	14	15	16	17	18	19
32 kB	32 kB	32 kB	32 kB	32 kB	32 kB	32 kB	32 kB	32 kB	32 kB
256 kB	$256~\mathrm{kB}$	256 kB	$256~\mathrm{kB}$	$256~\mathrm{kB}$	256 kB	$256~\mathrm{kB}$	$256~\mathrm{kB}$	$256~\mathrm{kB}$	$256~\mathrm{kB}$
25 MB									

Figure 1: Cache topology diagram as outputted by likwid-topology -g. Byte sizes all in IEC units.

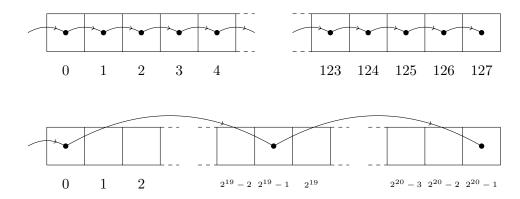


Figure 2: Memory access patterns of memberch.c for csize = 128 and stride = 1 (above) and for csize = 2^{20} and stride = 2^{19} (below)

1.2. Memory Access Pattern of membench.c

The benchmark memberch.c measures the average time of repeated read and write overations across a set of indices of a stack-allocated array of 32-bit signed integers. The indices vary according to the access pattern used, which in turn is defined by two variables, csize and stride. csize is an upper bound on the index value, i.e. (one more of) the highest index used to access the array in the pattern. stride determines the difference between array indexes over access iterations, i.e. a stride of 1 will access every array index, a stride of 2 will skip every other index, a stride of 4 will access one index then skip 3 and so on and so forth.

Therefore, for csize = 128 and stride = 1 the array will access all indexes between 0 and 127 sequentially, and for csize = 2^{20} and stride = 2^{19} the benchmark will access index 0, then index $2^{19} - 1$, and finally index $2^{20} - 1$. The access patterns for these two configurations are shown visually in Figure 2.

1.3. Analyzing Benchmark Results

The members.c benchmark results for my personal laptop (Macbook Pro 2018 with a Core i7-8750H CPU) and the cluster are shown in figure 3.

The memory access graph for the cluster's benchmark results shows that temporal locality is best for small array sizes and for small stride values. In particular, for array memory sizes of 16MB or lower (csize of $4 \cdot 2^{20}$ or lower) and stride values of 2048 or lower the mean read+write time is less than 10 nanoseconds. Temporal locality is worst for large sizes and strides, although the

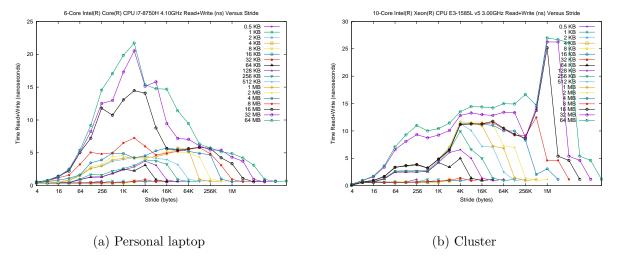


Figure 3: Results of the memberch.c benchmark for both my personal laptop (in Figure 3a) and the cluster (in Figure 3b).

largest values of stride for each size (like csize / 2 and csize / 4) achieve better mean times due to the few elements accessed in the pattern (this observation is also valid for the largest strides of each size series shown in the graph).

2. Optimize Square Matrix-Matrix Multiplication (60 Points)

The file matmult/dgemm-blocked.c contains a C implementation of the blocked matrix multiplication algorithm presented in the project. A pseudocode listing of the implementation is provided in Figure 4.

In order to achieve a correct and fast execution, my implementation:

- Handles the edge cases related to the "remainders" in the matrix block division, i.e. when the division between the size of the matrix and the block size yields a remainder. Assuming only squared matrices are multiplied through the algorithm (as in the test suite provided) the block division could yield rectangular matrix blocks located in the last rows and columns of each matrix, and the bottom-right corner of the matrix will be contained in a square matrix block of the size of the remainder. The result of this process is shown in Figure 5;
- Converts matrix A into row major format. As shown in Figure 6, by having A in row major format and B in column major format, iterations across matrix block in the inner most loop of the algorithm (the one calling *naivemm*) cache hits are maximised by achieving space locality between the blocks used. This achieved approximately an increase of performance of two percentage points in terms of CPU utilization (i.e. from a baseline of 4% to 6%),
- Caches the result of each innermost iteration into a temporary matrix of block size before storing it into matrix C. This achieves better space locality when *naivemm* needs to store values in matrix C. The block size temporary matrix has virtually no stride and thus cache hits are maximised. The copy operation is implemented with bulk copy memcpy calls. This optimization achieves an extra half of a percentage point in terms of CPU utilization (i.e. from the 6% discussed above to a final 6.5%).

The chosen matrix block size for running the benchmark on the cluster is

```
INPUT: A (n by n), B (n by n), n
OUTPUT: C (n by n)
s := 26 # block dimension
A_row := <matrix A converted in row major form>
C_temp := <empty s by s matrix>
for i := 0 to n by s:
    i_next := min(i + s, n)
    for j := 0 to n by s:
        j_next := min(j + s, n)
        <set all cells in C_temp to 0>
        for k := 0 to n by s:
            k_next := min(k + s, n)
            # Perform naive matrix multiplication, incrementing cells of C_temp
            # with each multiplication result
            naivemm(A_row[i, k][i_next, k_next], B[k, j][k_next, j_next],
                    C_temp[0, 0][i_next - i, j_next - j])
        end for
        C[i, j][i_next, j_next] = C_temp[0, 0][i_next - i, j_next - j]
    end for
end for
```

Figure 4: Pseudocode listing of my blocked matrix multiplication implementation. Matrix indices start from 0 (i.e. row 0 and column 0 denotes the top-left-most cell in a matrix). M[a, b][c, d] denotes a rectangular region of the matrix M whose top-left-most cell is the cell in M at row a and column b and whose bottom-right-most cell is the cell in M at row c-1 and column d-1.

as shown in the pseudocode. This value has been obtained by running an empirical binary search on the value using the benchmark as a metric, i.e. by running ./run_matrixmult.sh several times with different values. For square blocks (i.e. the worst case) the total size for the matrix A and B sub-block and the C_temp temporary matrix block for C is:

Bytes = cellSize
$$*s^2 * 3 = 8 * 26^2 * 3 = 16224$$

given that a double-precision floating point number, the data type used for matrix cells in the scope of this project, is 8 bytes long. The obtained total bytes size is fairly close to the L1 cache size of the processor used in the cluster (32Kb = 32768 bytes), which is expected given that the algorithm needs to exploit fast memory as much as possible. The reason the empirically best value results in a theoretical cache allocation that is only half of the complete cache size is due to some real-life factors. For example, cache misses tipically result in aligned page loads which may load unnecessary data.

A potential way to exploit the different cache levels is to apply the blocked matrix algorithm iteratively multiple times. For example, OpenBLAS implements DGEMM by having two levels of matrix blocks to better exploit the L2 and L3 caches found on most processors.

The results of the matrix multiplication benchmark for the naive, blocked, and BLAS implemen-

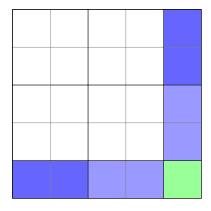


Figure 5: Result of the block division process of a square matrix of size 5 using a block size of 2. The 2-by-1 and 1-by-2 rectangular remainders are shown in blue and the square matrix of remainder size (i.e. 1) is shown in green.

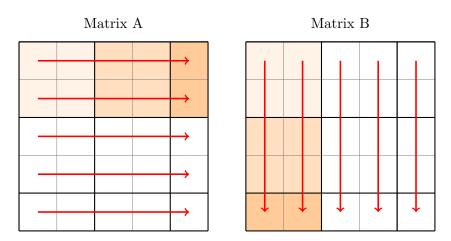


Figure 6: Inner most loop iteration of the blocked GEMM algorithm across matrices A and B. The red lines represent the "majorness" of each matrix (A is converted by the algorithm in row-major form, while B is given and used in column-major form). The shades of orange represent the blocks used in each iteration.

tations are shown in Figure 7 as a graph of GFlop/s over matrix size or in Figure 8 as a table. The blocked implementation achieves on average 50% more FLOPS than the naive implementation thanks to the optimisations in space and temporal cache locality described. However, the blocked implementation achieves less than a tenth of FLOPS compared to Intel MKL BLAS based one due to the microarchitecture optimization the latter one is able to exploit.

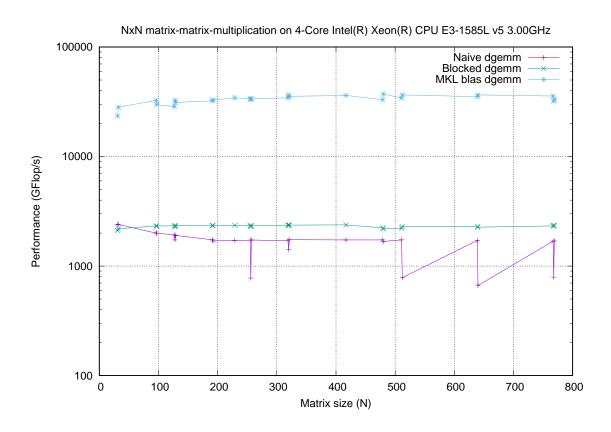


Figure 7: GFlop/s per matrix size of the matrix multiplication benchmark for the naive, blocked, and BLAS implementations. The Y-axis is log-scaled.

	Nai	ve	Block	ked	BLAS		
Size	MFLOPS	% CPU	MFLOPS	% CPU	MFLOPS	% CPU	
31	2393.33	6.50	2112.63	5.74	23449.20	63.72	
32	2400.13	6.52	2187.44	5.94	28198.90	76.63	
96	1998.74	5.43	2325.39	6.32	32542.30	88.43	
97	1996.01	5.42	2322.81	6.31	29801.30	80.98	
127	1923.81	5.23	2330.30	6.33	28557.80	77.60	
128	1731.98	4.71	2282.93	6.20	32643.30	88.70	
129	1903.31	5.17	2334.25	6.34	31198.20	84.78	
191	1736.78	4.72	2345.91	6.37	32247.30	87.63	
192	1694.44	4.60	2345.38	6.37	32830.60	89.21	
229	1715.10	4.66	2351.01	6.39	34360.90	93.37	
255	1720.39	4.67	2335.21	6.35	33477.70	90.97	
256	777.65	2.11	2306.48	6.27	33473.90	90.96	
257	1729.27	4.70	2330.68	6.33	33686.50	91.54	
319	1704.80	4.63	2360.03	6.41	34335.20	93.30	
320	1414.84	3.84	2364.53	6.43	36438.10	99.02	
321	1741.30	4.73	2366.38	6.43	35433.70	96.29	
417	1733.00	4.71	2378.34	6.46	36133.70	98.19	
479	1731.17	4.70	2233.05	6.07	32951.40	89.54	
480	1678.77	4.56	2187.87	5.95	37260.00	101.25	
511	1733.60	4.71	2224.61	6.05	34128.00	92.74	
512	782.96	2.13	2284.85	6.21	36526.40	99.26	
639	1714.42	4.66	2292.78	6.23	35249.20	95.79	
640	663.42	1.80	2264.70	6.15	36538.70	99.29	
767	1690.82	4.59	2324.83	6.32	35718.50	97.06	
768	792.04	2.15	2363.92	6.42	32116.80	87.27	
769	1696.95	4.61	2321.31	6.31	33033.90	89.77	

Figure 8: MFlop/s and CPU utlisation per matrix size of the matrix multiplication benchmark for the naive, blocked, and BLAS implementations.