APMA 2822b Homework 2

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Code is attached in the email. I have included a CMakeLists.txt file which can be used to compile the code on the CCV. The MPI module must be loaded. Note that there is a hard coded path to the OpenBLAS library because CMake did not automatically find the library. I also added the SLURM scripts I used. There are 3 executables in the project, one which tests the code, one which times the matrix multiplication, and one which times MPI message passing.

Algorithm and Implementation

I used a grid data decomposition across all matrices. Any grid dimensions can work, but if the dimensions are closer to being equivalent the algorithm will be more efficient. As such, the closest integer factors of the MPI world size are used. The code doesn't handle the case where a matrix dimension isn't divisible by the corresponding grid dimension, but this would be simple to implement use padding and would have a negligible effect on performance. Figures 1 and 2 show the decomposition for different grid dimensions. The approach of the algorithm is to loop over the blocks in the dimension shared between A and B. At each step, each process adds to its section of matrix C the product of the sections of A and B which it currently possesses. Then, each row of matrix A rotates and each column of matrix B rotates. This allows each process to only send data to the same two other processes each step. Because matrix multiplication is performed at each step, 3 level blocking techniques can be used to improve cache utilization. The intuition behind this algorithm is that the value of the top left block of C is computed by multiplying the first row of A by the first column of B. This operation can be decomposed into the multiplication of the top left block of A and the top left block of B as well as every remaining block in the top row of A with its corresponding block in the left most column of B. A similar decomposition can be done for every block in C. Note that the data in row and columns other than the first must start rotated in order for the data to be multiplied by the correct other block at each step. The grid pattern will not always be square, so it is potentially necessary further divide the shorter dimension. In my implementation, there are always more column blocks. Multiple approaches can be used for further dividing the data. I assigned the additional divisions as blocks in matrix B (they are always in matrix B because there are always more column blocks) that some process contains but aren't used in that iteration. This can be seen in figure 2. Note these blocks require extra rotations of the next row in A. This can be seen in the bottom row of A in figure 2. This approach has the advantage of being simple and computationally light, but it does result in a slightly uneven distribution of data.

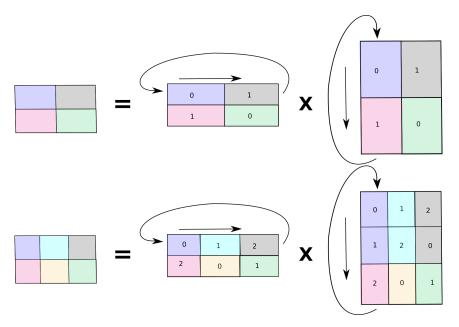


Figure 1: Examples of the data decomposition. Each color represents a different process. The numbers indicate the initial data placement in terms of which block along the shared dimension the data is from. For instance, if the numbers in a column in matrix B are 2, 0, 1, the column has been rotated once.

I evaluated this algorithm with OpenBLAS as well as the matrix multiplication implementation that I did for the last homework. This is so the efficacy of the distributed matrix multiplication algorithm can be assessed independently from the shared memory matrix multiplication algorithm used. I attempted to use MKL, but I had issues with linking, MKL using threads, and icc substantially slowed down my shared memory matrix multiplication. I used only the non-blocking MPI functions for both send and receive. Both are started before the matrix multiplication each step, and the wait for completion happens after the multiplication. Additional memory is required to do this. In the case where there is just one process in the data communication ring, I still use MPI to communication with itself. This case could be further optimized at the cost of some simplicity.

2 Analysis

The roof-line model will be evaluated for square grids of processes for simplicity though the analysis will generally apply to other cases. The total number of FLOPs used by this algorithm is the same as the number of FLOPs used in standard shared memory matrix multiplication. The number of times the data is passed between processes is $\sqrt{d}-1$ if d is the number of processes. The total memory bandwidth will be the number of times data is passed between processes multiplied by the combined size size of matrices A and B and the memory bandwidth for standard matrix multiplication. This counts memory bandwidth associated with MPI communication. If the dimension of A is $n \times n$, the dimension of B is $n \times n$, and the bigger of the two previous block dimensions is d, the total

number of FLOPs used is $2n^3$ and the total memory that must be transfered in bytes is $8*3*(\sqrt{d}-1)*n^2+8*3*n^2=24*\sqrt{d}*n^2$. The arithmetic intensity is $\frac{2n^3}{24*\sqrt{d}*n^2}=\frac{n}{12*\sqrt{d}}$. The CPUs used in the CCV are Intel Xeon model number 6126. According to the Intel specification found here: the CPU has 652.8 peak GFLOPS. The peak memory bandwidth should be about 100 gigabytes per second based on the memory bandwidth of other similar CPUs. As such, the ratio of peak FLOPS to peak memory bandwidth is approximately $(\frac{652.8}{100}=6.528)$. So long as $\frac{n}{12*(d+1)}$ is greater than 6.528, the computation will ideally be FLOP limited. For values of n in the range 2,048 to 16,384 and d between 1 and 64, the computation should be FLOP limited.

This previous computation doesn't factor in that MPI message passing bandwidth will be substantially lower than the peak memory bandwidth. The total MPI memory bandwidth is $24*(\sqrt{d}-1)*n^2$. I attempted to test the between process memory bandwidth, but the bandwidth seems too low (around 4 GB/s). If this is assumed to be accurate, then the computation has an effective MPI ratio of peak FLOPS to peak memory bandwidth of $(\frac{652.8}{4}=163.2)$ The effective MPI arithmetic intensity is $\frac{n}{12*(\sqrt{d}-1)}$, so MPI communication will be limiting for some values of n and d within the scope of this computation. For instance, the computation will theoretically be MPI bandwidth limited for n=2048 and d=9 and n=4096 and d=16.

3 Results

A table with data from all runs can be found in the appendix.

All testing was done on the CCV. The distributed matrix multiplication was evaluated using the code I wrote for the last project and using BLAS (OpenBLAS specifically). The performance is far better using BLAS. I am not entirely sure why my code of shared memory matrix multiplication is so much worse. A variety of experiments were conducted, but the figures show the result of using 16 threads and different numbers of nodes and 1 thread and different numbers of processes. Note that 16 processes corresponds to 1 node, 32 processes corresponds to 2 nodes and 64 processes corresponds to 4 nodes. I was unable to get SLURM to allocate threads which run on different cores and processes on a single node at the same time. Note that the BLAS matrix multiplication gets substantially faster with increases in the matrix size. As such, adding more processes is problematic even without considering the overhead of the message passing. Note that square grids were more effective than none square grids. The distributed matrix multiplication scales quite well. 4 nodes with 16 threads is just less than 4 times faster than 1 node with 4 threads. The optimal model seems to be using 1 MPI rank per CPU and a thread for each core. The maximum FLOP rate I achieved with 4 nodes was 865 GFLOPS using BLAS and 194 GFLOPS using my shared memory matrix multiplication implementation. Strong scaling can be seen in the plots which display node/process count vs GFLOPS.

A Additional data

The full data can be seen in the below two tables. The column used refers to which shared memory matrix multiplication algorithm was used. The setup, wait, copy, and dgemm

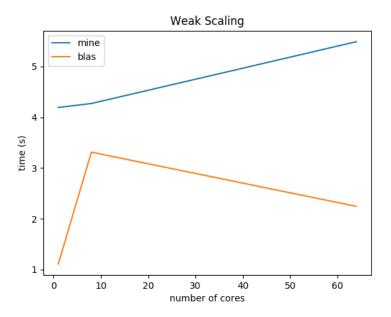
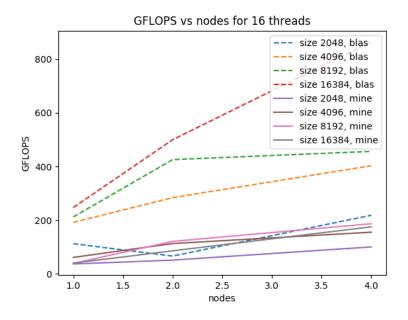
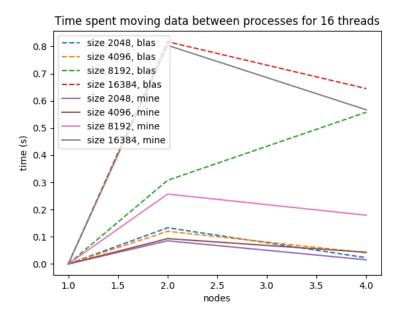
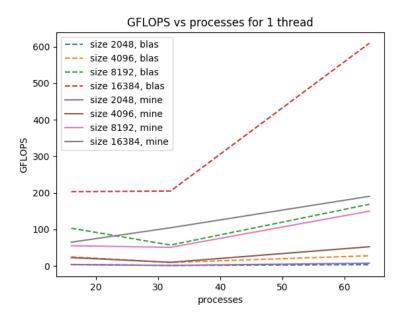


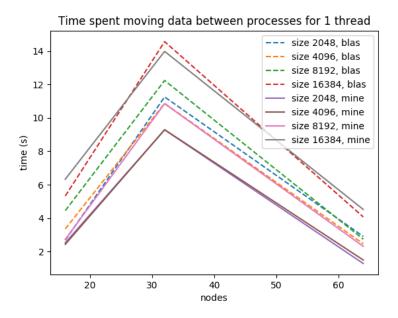
Figure 2: The first, second, and third values use 1 thread and 1 node, 8 threads and 1 nodes, and 8 threads and 4 nodes respectively. To keep the problem size per core constant, the cores must increase by a factor of 8 for every factor of 2 the total data size increases.



columns refer to the total spent doing each of those tasks.







| threads | processes | nodes | n | used | gflops | setup | wait | copy | dgemm |
|---------|-----------|-------|-------|------|---------|------------|-----------|------------|-----------|
| 8 | 1 | 1 | 2048 | blas | 47.7667 | 0 | 0 | 0 | 0.278573 |
| 8 | 1 | 1 | 2048 | mine | 26.7809 | 0 | 0 | 0 | 0.506932 |
| 8 | 1 | 1 | 4096 | blas | 38.6369 | 0 | 0 | 0 | 3.09188 |
| 8 | 1 | 1 | 4096 | mine | 29.9626 | 0 | 0 | 0 | 4.05046 |
| 8 | 1 | 1 | 8192 | blas | 44.9202 | 0 | 0 | 0 | 21.914 |
| 8 | 1 | 1 | 8192 | mine | 19.9453 | 0 | 0 | 0 | 50.4504 |
| 8 | 1 | 1 | 16384 | blas | 72.9442 | 0 | 0 | 0 | 108.798 |
| 8 | 1 | 1 | 16384 | mine | 20.7888 | 0 | 0 | 0 | 390.516 |
| 16 | 1 | 1 | 2048 | blas | 112.098 | 0 | 0 | 0 | 0.0883248 |
| 16 | 1 | 1 | 2048 | mine | 36.4969 | 0 | 0 | 0 | 0.383815 |
| 16 | 1 | 1 | 4096 | blas | 191.71 | 0 | 0 | 0 | 0.458686 |
| 16 | 1 | 1 | 4096 | mine | 60.9018 | 0 | 0 | 0 | 1.89523 |
| 16 | 1 | 1 | 8192 | blas | 211.796 | 0 | 0 | 0 | 4.03631 |
| 16 | 1 | 1 | 8192 | mine | 38.566 | 0 | 0 | 0 | 25.7391 |
| 16 | 1 | 1 | 16384 | blas | 246.826 | 0 | 0 | 0 | 29.9783 |
| 16 | 1 | 1 | 16384 | mine | 39.8028 | 0 | 0 | 0 | 202.615 |
| 8 | 2 | 2 | 2048 | blas | 45.9791 | 0.00413686 | 0.0906128 | 0.0353779 | 0.0695233 |
| 8 | 2 | 2 | 2048 | mine | 50.8592 | 0.00405215 | 0.0533599 | 0.00123115 | 0.227584 |
| 8 | 2 | 2 | 4096 | blas | 125.556 | 0.0152528 | 0.258129 | 0.0046053 | 0.504755 |
| 8 | 2 | 2 | 4096 | mine | 61.3704 | 0.0158789 | 0.137663 | 0.00471361 | 1.81844 |
| 8 | 2 | 2 | 8192 | blas | 216.728 | 0.126833 | 0.0931871 | 0.0211473 | 3.75363 |
| 8 | 2 | 2 | 8192 | mine | 61.1919 | 0.0629568 | 0.123547 | 0.0192578 | 16.0993 |
| 8 | 2 | 2 | 16384 | blas | 260.433 | 0.499814 | 0.196414 | 0.0772465 | 28.9567 |
| 8 | 2 | 2 | 16384 | mine | 40.922 | 0.50382 | 0.196392 | 0.0780313 | 197.686 |
| 16 | 2 | 2 | 2048 | blas | 65.9625 | 0.00929961 | 0.0203101 | 0.103526 | 0.0688881 |
| 16 | 2 | 2 | 2048 | mine | 50.7611 | 0.00404378 | 0.0162771 | 0.0648065 | 0.201195 |
| 16 | 2 | 2 | 4096 | blas | 283.817 | 0.0164215 | 0.0536486 | 0.0499838 | 0.216928 |
| 16 | 2 | 2 | 4096 | mine | 112.667 | 0.0150878 | 0.0471517 | 0.0309087 | 0.937368 |
| 16 | 2 | 2 | 8192 | blas | 425.66 | 0.0576426 | 0.229659 | 0.0202813 | 1.57966 |
| 16 | 2 | 2 | 8192 | mine | 120.798 | 0.0578863 | 0.116619 | 0.0824271 | 7.82413 |
| 16 | 2 | 2 | 16384 | blas | 499.753 | 0.252816 | 0.45899 | 0.105163 | 13.9953 |
| 16 | 2 | 2 | 16384 | mine | 85.4951 | 0.231671 | 0.470755 | 0.101114 | 93.4414 |

| threads | processes | nodes | n | used | gflops | setup | wait | copy | dgemm |
|---------|-----------|-------|-------|------|---------|-------------|------------|-------------|-----------|
| 1 | 16 | 1 | 2048 | blas | 3.58378 | 4.1418e-05 | 1.16057 | 1.52322 | 1.03319 |
| 1 | 16 | 1 | 2048 | mine | 3.86192 | 2.5566e-05 | 1.1372 | 1.3869 | 0.96981 |
| 1 | 16 | 1 | 4096 | blas | 24.7603 | 6.93e-05 | 1.39897 | 1.95591 | 1.32715 |
| 1 | 16 | 1 | 4096 | mine | 22.8327 | 4.0539e-05 | 0.537606 | 1.89522 | 2.84192 |
| 1 | 16 | 1 | 8192 | blas | 103.192 | 4.1638e-05 | 2.54013 | 1.91146 | 5.2546 |
| 1 | 16 | 1 | 8192 | mine | 55.2286 | 5.2436e-05 | 1.67128 | 1.05411 | 14.9515 |
| 1 | 16 | 1 | 16384 | blas | 203.11 | 5.3044e-05 | 4.20376 | 1.12288 | 31.5746 |
| 1 | 16 | 1 | 16384 | mine | 64.8972 | 4.9335e-05 | 5.31518 | 1.01614 | 118.633 |
| 4 | 16 | 4 | 2048 | blas | 24.0798 | 0.00023221 | 0.362493 | 0.05429 | 0.0778591 |
| 4 | 16 | 4 | 2048 | mine | 50.1262 | 0.000216744 | 0.115041 | 0.000680538 | 0.0671567 |
| 4 | 16 | 4 | 4096 | blas | 175.215 | 0.000530238 | 0.341215 | 0.00414194 | 0.181162 |
| 4 | 16 | 4 | 4096 | mine | 157.914 | 0.000567374 | 0.150019 | 0.00368773 | 0.543925 |
| 4 | 16 | 4 | 8192 | blas | 531.028 | 0.0185465 | 0.429401 | 0.0159047 | 1.10177 |
| 4 | 16 | 4 | 8192 | mine | 189.281 | 0.00274346 | 0.342857 | 0.0156812 | 4.8044 |
| 4 | 16 | 4 | 16384 | blas | 886.162 | 0.0397578 | 0.977789 | 0.0632309 | 7.4089 |
| 4 | 16 | 4 | 16384 | mine | 194.061 | 0.0397732 | 2.71324 | 0.058316 | 38.1079 |
| 1 | 32 | 2 | 2048 | blas | 1.22459 | 0.00143051 | 3.93324 | 7.31769 | 1.30482 |
| 1 | 32 | 2 | 2048 | mine | 1.28475 | 0.000284275 | 3.48279 | 5.80199 | 1.86865 |
| 1 | 32 | 2 | 4096 | blas | 9.55717 | 0.000400333 | 5.09728 | 5.76809 | 1.90973 |
| 1 | 32 | 2 | 4096 | mine | 9.87654 | 0.014119 | 3.7044 | 5.57485 | 2.33138 |
| 1 | 32 | 2 | 8192 | blas | 57.0062 | 0.000258864 | 1.35948 | 10.8778 | 5.33454 |
| 1 | 32 | 2 | 8192 | mine | 50.8025 | 0.0558136 | 3.37863 | 7.41753 | 8.34072 |
| 1 | 32 | 2 | 16384 | blas | 204.967 | 0.000396412 | 7.66612 | 6.89602 | 23.6195 |
| 1 | 32 | 2 | 16384 | mine | 104.449 | 0.000522341 | 4.08164 | 9.89758 | 64.145 |
| 16 | 4 | 4 | 2048 | blas | 218.194 | 0.0049528 | 0.00305767 | 0.0149129 | 0.0301758 |
| 16 | 4 | 4 | 2048 | mine | 100.085 | 0.000552069 | 0.0137194 | 0.000945043 | 0.12254 |
| 16 | 4 | 4 | 4096 | blas | 402.94 | 0.0105919 | 0.0173653 | 0.0130606 | 0.209621 |
| 16 | 4 | 4 | 4096 | mine | 155.047 | 0.0102802 | 0.0246147 | 0.00821585 | 0.624417 |
| 16 | 4 | 4 | 8192 | blas | 456.375 | 0.0731058 | 0.456121 | 0.0285154 | 0.832948 |
| 16 | 4 | 4 | 8192 | mine | 186.511 | 0.0442442 | 0.107235 | 0.0276274 | 5.0225 |
| 16 | 4 | 4 | 16384 | blas | 865.319 | 0.175643 | 0.364849 | 0.10408 | 6.50175 |
| 16 | 4 | 4 | 16384 | mine | 174.993 | 0.0401204 | 0.450364 | 0.076162 | 45.3777 |
| 8 | 4 | 4 | 2048 | blas | 68.0084 | 0.0037108 | 0.0722899 | 0.0314687 | 0.0666243 |
| 8 | 4 | 4 | 2048 | mine | 74.3238 | 0.00282934 | 0.0384147 | 0.000488909 | 0.112573 |
| 8 | 4 | 4 | 4096 | blas | 284.548 | 0.00294532 | 0.105617 | 0.00232854 | 0.218599 |
| 8 | 4 | 4 | 4096 | mine | 115.627 | 0.00287362 | 0.057027 | 0.00240996 | 0.922932 |
| 8 | 4 | 4 | 8192 | blas | 375.233 | 0.0102069 | 0.552328 | 0.0091469 | 1.81112 |
| 8 | 4 | 4 | 8192 | mine | 126.912 | 0.0111452 | 0.234846 | 0.00908523 | 7.45041 |
| 8 | 4 | 4 | 16384 | blas | 525.905 | 0.0437044 | 1.03468 | 0.0372861 | 11.8671 |
| 8 | 4 | 4 | 16384 | mine | 78.7252 | 0.043419 | 0.427618 | 0.0370708 | 83.3374 |
| 1 | 64 | 4 | 2048 | blas | 3.44022 | 0.000858813 | 2.02787 | 0.874364 | 1.63681 |
| 1 | 64 | 4 | 2048 | mine | 7.50764 | 0.0452747 | 0.476482 | 0.761887 | 0.299881 |
| 1 | 64 | 4 | 4096 | blas | 27.7975 | 0.000193663 | 1.46668 | 0.993756 | 1.63706 |
| 1 | 64 | 4 | 4096 | mine | 52.4181 | 0.000315995 | 0.294509 | 1.19871 | 0.718232 |
| 1 | 64 | 4 | 8192 | blas | 168.74 | 0.000170699 | 1.8775 | 0.861384 | 2.49915 |
| 1 | 64 | 4 | 8192 | mine | 149.795 | 0.000183126 | 1.77825 | 0.531122 | 3.81381 |
| 1 | 64 | 4 | 16384 | blas | 609.544 | 0.000256883 | 3.16026 | 0.91117 | 8.81494 |
| 1 | 64 | 4 | 16384 | mine | 190.45 | 0.000364729 | 3.5987 | 0.920173 | 37.6115 |
| 8 | 8 | 4 | 2048 | blas | 44.3405 | 0.00325842 | 0.0878071 | 0.15857 | 0.0633794 |
| 8 | 8 | 4 | 2048 | mine | 65.1491 | 0.00102803 | 0.0770617 | 0.026423 | 0.0654919 |
| 8 | 8 | 4 | 4096 | blas | 234.351 | 0.000413269 | 0.0301224 | 0.248752 | 0.23706 |
| 8 | 8 | 4 | 4096 | mine | 152.592 | 0.00261909 | 0.0449692 | 0.0849738 | 0.590471 |
| 8 | 8 | 4 | 8192 | blas | 457.655 | 0.000947662 | 0.482697 | 0.0959676 | 1.37528 |
| 8 | 8 | 4 | 8192 | mine | 171.819 | 0.000945103 | 0.328512 | 0.0548389 | 5.34775 |
| 8 | 8 | 4 | 16384 | blas | 535.082 | 0.0752286 | 0.546276 | 0.151114 | 13.0185 |
| 8 | 8 | 4 | 16384 | mine | 173.633 | 0.0423695 | 2.96215 | 0.183347 | 43.419 |
| 1 | 1 | 1 | 2048 | blas | 14.442 | 0.0423033 | 0 | 0.103347 | 1.00556 |
| 1 | 1 | 1 | 2048 | mine | 3.81504 | 0 | 0 | 0 | 4.01677 |
| | 1 | 1 | 2040 | пппе | 0.01004 | l v | L | V | 4.01011 |