Assignment 2 - Scientific Computing SC9505

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All code was compiled inside an Ubunutu WSL environment on an AMD 3900X with 32GB of RAM. All timing and performance data was run with dense, randomly generated arrays and vectors. A full repository containing all of my code can be found at https://github.com/JaredWogan/SC9505.

1 Matrix Vector Multiplication Using MPI

This program calculates the product of a matrix with a vector. Our task is to determine the benefits (if any) that parallelization provides for this problem. The parallelized code can be confirmed to be working, as seen in Figure 1.

The program has been parallelizaed as follows. First, the main process wil initialize both the matrix and the vector that will be used in the calculations. The main process then broadcasts the vector to all other threads. In order to perform the full calculation, the main process will send each thread a unique row of the matrix, which the thread will then use to calculate the corresponding element of the result vector. These results are collected by the main process, which will subsequently send the threads a new row, if there is more work to be done.

```
• (base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MV$ make clean rm -rf 15-matrix-vector.o 16-serial.o
• (base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MV$ make all mpiCC -02 -o 16-serial.o 11-serial-matrix-vector.cpp mpiCC -02 -o 16-serial.o 11-serial-matrix-vector.cpp
• (base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MV$ mpirun -n 4 ./15-matrix-vector.o 1 10 10 Average calculation time = 0.0000002603
Total time = 0.0001655470
( 0, 1, 2, 3, 4, 5, 6, 7, 8, 9)
• (base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MV$ mpirun -n 8 ./15-matrix-vector.o 1 20 20 Average calculation time = 0.0000002964
Total time = 0.0003846000
( 0, 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19)
• (base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MV$
```

Figure 1: Demonstration of the code working. Here the matrix is taken to be the identity, and the vector is filled with consecutive integers.

The scaling when the program is run on 4 threads as a function of the number of rows/columns was determined to be $\mathcal{O}(N^{1.5})$, see Figure 2. This is less than is expected for matrix vector multiplication,

which is typically an $\mathcal{O}(N^2)$ operation. The serial code I used to compare the parallel code with scaled roughly as $\mathcal{O}(N^{2.2})$.

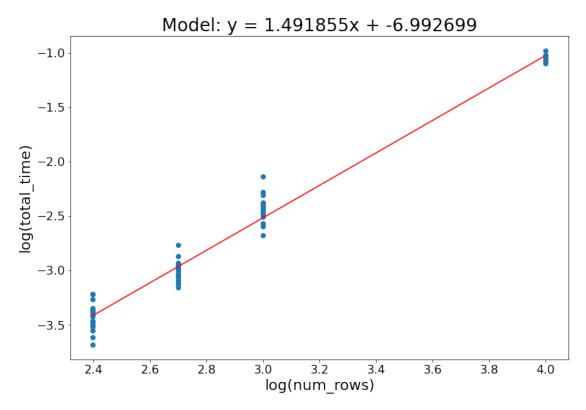


Figure 2: Plotting the runtime of the program as a function of the number of rows N (on a log-log scale), we find that the total runtime scales as $\mathcal{O}(N^{1.5})$, which is less than the expected $\mathcal{O}(N^2)$. Note the plot is generated with data for a constant amount of threads, which in this case is 4.

Looking at the scaling instead for a constant number of rows (here we are using 10000), we find there is no real scaling. Ideally we would like to see the total runtime decrease as we increase the number of threads, but this is not the case for the algorithm being used here.

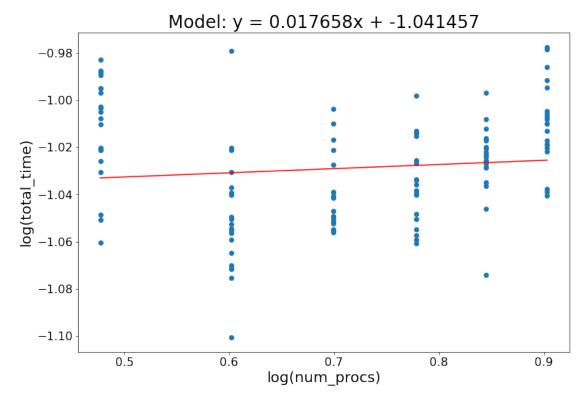


Figure 3: Plotting the runtime of the program as a function of the number of threads *P* (on a log-log scale). The linear fit is not ideal, such that it is fair to conclude that there is no note worthy scaling with the number of processors. Again it is worth noting that the plot has been generated for a constant number of rows which was taken to be 10000.

As discussed in lecture, the efficiency of our algorithm is less than ideal, which is supported by the calculations in Table 1 (see Appendix A for details on how these values were calculated). We see that running the code across 3 threads yields superlinear scaling, and our program is more efficient than the serial code. However, as the number of threads increase, we start seeing diminishing returns in terms of the speedup, and so our efficiency starts dropping dramatically. At 8 concurrent threads, our code is less than half as efficient as the serial code, and it is actually slower than the case with only 3 threads (in reality they are approximataly equal in runtime, but the linear model predicted it would be slower).

If we wanted to write a program to do matrix vector multiplication in parallel more efficiently, it would be best to have a shared pool of memory that each process can read and write to at the same time. This could be done by adding a single line to the serial code and using OpenMP.

Number of Threads	Speedup	Scaling Factor a	Efficiency
3	3.92	1.31	1.31
4	3.76	0.94	0.94
5	3.61	0.72	0.72
6	3.47	0.58	0.58
7	3.33	0.48	0.48
8	3.19	0.40	0.40

Table 1: Summary of the speedup and efficiency of our matrix vector multiplication code. These values are taken for a constant number of rows N = 10000.

```
// Matrix-vector multiplication code Ab=c //
    // Note that I will index arrays from 0 to n-1.
    // Here workers do all the work and boss just handles collating results
    // and sending info about A.
    // include, definitions, globals etc here
   #include <iostream>
11
   #include <fstream>
   #include <iomanip>
13
    #include <random>
   #include "boost/multi_array.hpp"
14
    #include "mpi.h"
15
16
17
    using namespace std;
18
    class MPI_Obj
19
20
    public:
21
22
        int size;
23
        int rank;
24
        MPI_Obj(int &argc, char **&argv)
25
26
            MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &size);
27
28
            MPI_Comm_rank (MPI_COMM_WORLD, &rank);
29
30
31
        ~MPI_Obj()
32
33
       {
            MPI_Finalize();
34
35
36
    };
37
    void GetArraySize(int &output, int &nrows, int &ncols, MPI_Obj &the_mpi, int argc, char **argv)
38
39
40
             // Accept input parameters from the command line, otherwise ask the user
41
        if (the_mpi.rank == 0)
42
43
            if (argc == 4)
44
                 output = atoi(argv[1]);
46
                 nrows = atoi(argv[2]);
                ncols = atoi(argv[3]);
            else
50
                 cout << "Please enter the number of rows -> ";
                 cout << "Please enter the number of columns -> ";
                 cin >> ncols;
        }
        // send everyone nrows, ncols
        int buf[2] = {nrows, ncols};
60
        MPI_Bcast(buf, 2, MPI_INT, 0, MPI_COMM_WORLD);
        if (the_mpi.rank != 0)
```

```
62
              nrows = buf[0];
63
              ncols = buf[1];
64
65
66
67
     void SetupArrays(int nrows, int ncols, boost::multi_array<double, 2> &A, vector<double> &b,
68
     → vector<double> &c, vector<double> &Arow, MPI_Obj &the_mpi)
     {
69
          {\tt uniform\_real\_distribution} < \textcolor{red}{\textbf{double}} > \hspace{0.1cm} \texttt{unif(-1.0, 10);}
70
         default_random_engine re;
71
72
          // Boss part
         if (the_mpi.rank == 0)
73
74
               // Set size of A
75
76
              A.resize(boost::extents[nrows][ncols]);
77
               // Initialize A
78
               for (int i = 0; i < nrows; ++i)</pre>
79
                   for (int j = 0; j < ncols; ++j)</pre>
80
81
82
                        // Identity
                        // if (i == j)
// A[i][j]
83
                                A[i][j] = 1.0;
                        // else
85
                        // A[i][j] = 0.0;
                        // Reverse Identity
// if (i == (ncols - j - 1))
87
                                A[i][j] = 1.0;
89
                        // else
90
                        // A[i
// Random
91
                              A[i][j] = 0.0;
92
93
                        A[i][j] = unif(re);
               // Initialize b
97
               for (int i = 0; i < ncols; ++i)</pre>
                   // b[i] = 1.0;
// b[i] = (double) i;
100
101
                   b[i] = unif(re);
102
103
               // Allocate space for c, the answer
104
              c.reserve(nrows);
              c.resize(nrows);
106
107
          // Worker part
108
109
         else
110
               // Allocate space for 1 row of A
111
              Arow.reserve(ncols);
112
              Arow.resize(ncols);
113
114
115
116
          // send b to every worker process, note b is a vector so b and &b[0] not same
         MPI_Bcast(&b[0], ncols, MPI_DOUBLE, 0, MPI_COMM_WORLD);
117
118
119
     void Output(int output, vector<double> &c, MPI_Obj &the_mpi)
120
121
          if (the_mpi.rank == 0 && output == 1)
122
123
               cout << "( " << c[0];
124
              for (int i = 1; i < c.size(); ++i)
    cout << ", " << c[i];
cout << ")\n";</pre>
125
126
127
128
129
    }
130
     int main(int argc, char **argv)
131
132
133
          // Data File
          // ofstream datafile("/home/jared/Desktop/mv-timings.txt", ios_base::app);
134
         ofstream datafile("mv-timings.txt", ios_base::app);
135
136
137
         // initialize MPI
```

```
138
         MPI_Obj the_mpi(argc, argv);
         if (the mpi.size < 2)</pre>
139
             MPI_Abort (MPI_COMM_WORLD, 1);
140
141
         // determine/distribute size of arrays here
142
         int output = 1, nrows = 0, ncols = 0;
143
144
         GetArraySize(output, nrows, ncols, the_mpi, argc, argv);
         if (the_mpi.size - 1 > nrows)
145
146
             MPI_Abort (MPI_COMM_WORLD, -1);
147
148
149
        boost::multi_array<double, 2> A;
150
         vector<double> b(ncols);
151
         vector<double> c:
152
153
         vector<double> Arow;
         SetupArrays(nrows, ncols, A, b, c, Arow, the_mpi);
154
155
156
         MPI_Status status;
157
         // Timing variables
158
159
         double calc_time = 0, avg_time, total_time;
160
161
         // Boss part
162
         if (the_mpi.rank == 0)
163
164
             total_time = MPI_Wtime();
              // send one row to each worker tagged with row number, assume size<nrows
166
             int rowsent = 0;
167
             for (int i = 1; i < the_mpi.size; i++)</pre>
168
169
                 MPI_Send(&A[rowsent][0], ncols, MPI_DOUBLE, i, rowsent + 1, MPI_COMM_WORLD);
170
172
             for (int i = 0; i < nrows; i++)
174
                  double ans:
                  MPI_Recv(&ans, 1, MPI_DOUBLE, MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
                  int sender = status.MPI_SOURCE;
                  int anstype = status.MPI_TAG; // row number+1
                  c[anstype - 1] = ans;
179
                  if (rowsent < nrows)</pre>
                  { // send new row
                      MPI_Send(&A[rowsent][0], ncols, MPI_DOUBLE, sender, rowsent + 1, MPI_COMM_WORLD);
183
                      rowsent++;
184
185
                  else
                  { // tell sender no more work to do via a 0 TAG
186
                      MPI_Send(MPI_BOTTOM, 0, MPI_DOUBLE, sender, 0, MPI_COMM_WORLD);
187
188
189
190
         else
191
192
              // Get a row of A
193
             MPI_Recv(&Arow[0], ncols, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
while (status.MPI_TAG != 0)
194
195
196
                  // work out Arow.b
197
                 double ans = 0.0;
198
199
                  calc_time -= MPI_Wtime();
200
                  for (int i = 0; i < ncols; i++)</pre>
201
                     ans += Arow[i] * b[i];
202
                  calc_time += MPI_Wtime();
203
204
                  // Send answer of Arow.b back to boss and get another row to work on
205
                  MPI_Send(&ans, 1, MPI_DOUBLE, 0, status.MPI_TAG, MPI_COMM_WORLD);
206
                  MPI_Recv(&Arow[0], ncols, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
207
208
             }
209
         }
210
211
         if (the_mpi.rank == 0)
212
             total_time = MPI_Wtime() - total_time;
213
        MPI_Reduce(&calc_time, &avg_time, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
```

```
215
              if (the_mpi.rank == 0)
216
217
                   avg_time /= (the_mpi.size - 1); // Boss node doesn't do any of the calculations printf("Average calculation time = \$.10f\n", avg_time); printf("Total time = \$.10f\n", total_time);
218
219
220
221
                    datafile << fixed << setprecision(10);
datafile << nrows << " " << ncols << " " << the_mpi.size << " " << avg_time << " " << total_time</pre>
222
223
        \hookrightarrow << endl;
224
225
             // output c here on Boss node
Output(output, c, the_mpi);
226
227
228 }
```

2 Matrix Matrix Multiplication Using MPI

Our second task is to generalize the matrix vector product code to perform matrix matrix products. The modified code can be seen below, while a demonstration that the code works correctly can be seen in Figure 4. The serial code that will be used for comparison was written using the DGEMM_ function from the BLAS library.

The program that computes a matrix matrix produt has been parallelized by first having the main process assemble the two matrices to be used. Each thread is subsequently sent a copy of the second matrix by the main process. To compute the product, each thread is sent a row of the first matrix, which it will then use to compute an entire column of the resulting matrix. Upon completion, the thread will send the completed column to the main process in exchange for a new row (if there are any left).

```
abulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MM$ make all
(base) jared@Nebulaer.../Scientific Computing $53595/Assignment 2 - November 39/MM$ mpirun -n 4 ./15-matrix-matrix.o 1 10 10 10 (base) jared@Nebulaer.../Scientific Computing $C9505/Assignment 2 - November 30/MM$ mpirun -n 4 ./15-matrix-matrix.o 1 10 10 10 Average calculation time = 0.00009256180

Total time = 0.0000256180
 1.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000
0.0000, 2.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000
 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 8.0000, 0.0000, 0.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 9.0000, 0.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 10.0000
(base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MM$ make all
(base) jared@Nebulae:.../Scientific Computing 363505/Assignment 2 - November 36/MM$ mpirun -n 4 ./15-matrix-matrix.o 1 10 10 10 10 10
Average calculation time = 0.0000022110
Total time = 0.0000339140
 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 10.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 9.0000, 0.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 8.0000, 0.0000, 0.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 7.0000, 0.0000, 0.0000, 0.0000
0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 6.0000, 0.0000, 0.0000, 0.0000, 0.0000
                   00, 0.0000, 0.0000, 0.0000, 5.0000, 0.0000, 0.0000, 0.0000, 0.0000
                  00, 0.0000, 0.0000, 4.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000
 0.0000, 0.0000, 3.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000
0.0000, 2.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.00000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.000
(base) jared@Nebulae:.../Scientific Computing SC9505/Assignment 2 - November 30/MM$
```

Figure 4: Demonstration of the code working. In the first example, the first matrix is taken to be the identity and the second has consecutive integers along the main diagonal. In the second example, the first matrix is changed to the reverse identity (1s along the antidiagonal). In both cases, we get the expected result.

The modified code for matrix multiplication scales as $\mathcal{O}(N^{3.3})$, where N is the number of rows as can be seen in Figure 5. This is slightly more than the expected $\mathcal{O}(N^3)$. It should be noted that the serial code scaled as $\mathcal{O}(N^{2.9})$, which is slightly less than expected. It is also interesting that the current world record (as of 2020) for the asymptotic scaling of matrix matrix multiplication has been shown to be of the order $\mathcal{O}(N^{2.3728596})$ by Josh Alman and Virginia Vassilevska Williams (arXiv:2010.05846).

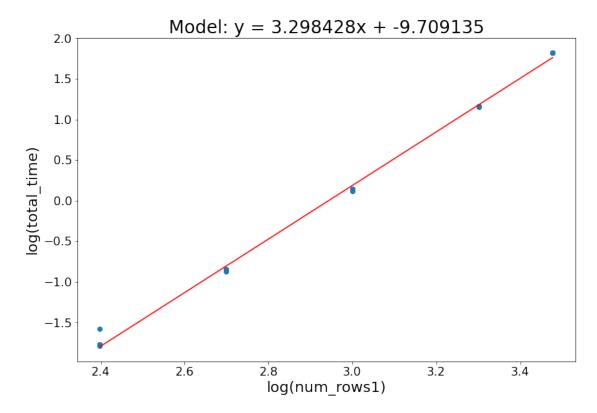


Figure 5: Plotting the runtime of the program as a function of the number of rows N (on a log-log scale), we find that the total runtime scales as $\mathcal{O}(N^{3.3})$, which is slightly more than the expected $\mathcal{O}(N^3)$.

More importantly for our purposes, we find that the total runtime scales as $\mathcal{O}(P^{-1})$, where P is the total number of threads (for a fixed number of rows N). This is the expected result as we discussed in lecture: for large N, we expect the speedup to approach P, which is supported by Figure 6 and Table 2.

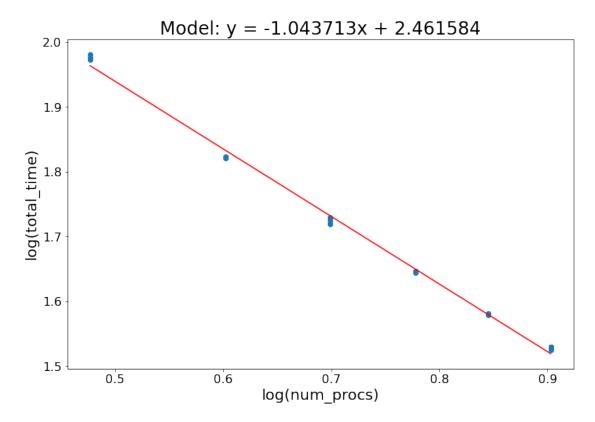


Figure 6: Plotting the runtime of the program as a function of the number of threads P, we find the scaling for a fixed number of rows N (here N=3000) to be of the order $\mathcal{O}(P^{-1})$

Number of Threads	Speedup	Scaling Factor a	Efficiency
3	1.66	0.55	0.55
4	2.24	0.56	0.56
5	2.83	0.57	0.57
6	3.42	0.57	0.57
7	4.02	0.57	0.57
8	4.62	0.58	0.58

Table 2: Summary of the speedup and efficiency of our matrix multiplication code. These values are taken for a constant number of rows N=3000.

```
// Matrix-vector multiplication code Ab=c //
    // Note that I will index arrays from 0 to n-1.
    // Here workers do all the work and boss just handles collating results
    // and sending info about A.
    // include, definitions, globals etc here
    #include <iostream>
10
    #include <fstream>
11
    #include <iomanip>
12
    #include <random>
13
    #include "boost/multi_array.hpp"
#include "mpi.h"
14
15
```

```
17
   using namespace std;
18
    class MPI_Obj
19
20
    public:
21
        int size;
22
23
        int rank:
24
        MPI Obj(int &argc, char **&argv)
25
26
             MPI_Init(&argc, &argv);
MPI_Comm_size(MPI_COMM_WORLD, &size);
27
28
             MPI_Comm_rank (MPI_COMM_WORLD, &rank);
29
30
        }
31
         ~MPI_Obj()
32
33
34
             MPI_Finalize();
35
         }
36
    };
37
    void GetArraySize(int &output, int &nrows, int &ncols, MPI_Obj &the_mpi, int argc, char **argv)
38
39
40
         if (the_mpi.rank == 0)
41
42
             if (argc == 4)
43
44
                 output = atoi(argv[1]);
                 nrows = atoi(argv[2]);
45
                 ncols = atoi(argv[3]);
47
             else
49
                  cout << "Please enter the number of rows -> ";
                  cin >> nrows;
                  cout << "Please enter the number of columns -> ";
53
                  cin >> ncols;
55
        }
57
         // send everyone nrows, ncols
        int buf[2] = {nrows, ncols};
        MPI_Bcast(buf, 2, MPI_INT, 0, MPI_COMM_WORLD);
        if (the_mpi.rank != 0)
        {
             nrows = buf[0];
62
             ncols = buf[1];
63
64
        }
65
    }
66
    void SetupArrays(int nrows, int ncols, boost::multi_array<double, 2> &A, vector<double> &b,
67

    vector < double > &c, vector < double > &Arow, MPI_Obj &the_mpi)

    {
68
         uniform_real_distribution < double > unif(-1.0, 10);
69
        default_random_engine re;
70
71
         // Boss part
        if (the_mpi.rank == 0)
72
73
             // Set size of A
74
             A.resize(boost::extents[nrows][ncols]);
75
76
             // Initialize A
77
             for (int i = 0; i < nrows; ++i)</pre>
78
                 for (int j = 0; j < ncols; ++j)
79
80
                       // Identity
81
                      if (i == j)
    A[i][j] = 1.0;
82
83
                      else
                         A[i][j] = 0.0;
85
                      // Reverse Identity
// if (i == (ncols - j - 1))
87
                             A[i][j] = 1.0;
88
                      // else
89
                            A[i][j] = 0.0;
90
                      // Random
91
92
                      // A[i][j] = unif(re);
```

```
93
                 }
94
              // Initialize b
95
              for (int i = 0; i < ncols; ++i)</pre>
97
                  // b[i] = 1.0;
b[i] = (double) i;
98
99
                  // b[i] = unif(re);
100
101
102
              // Allocate space for c, the answer
103
              c.reserve(nrows);
104
              c.resize(nrows);
105
106
         // Worker part
107
108
         else
109
110
              // Allocate space for 1 row of A
111
              Arow.reserve(ncols);
112
             Arow.resize(ncols);
113
114
          // send b to every worker process, note b is a vector so b and \&b[0] not same
115
116
         MPI_Bcast(&b[0], ncols, MPI_DOUBLE, 0, MPI_COMM_WORLD);
117
118
     void Output(int output, vector<double> &c, MPI_Obj &the_mpi)
119
120
121
         if (the_mpi.rank == 0 && output == 1)
122
              cout << "( " << c[0];
for (int i = 1; i < c.size(); ++i)
    cout << ", " << c[i];</pre>
123
124
125
              cout << ") \n";
127
128
129
    int main(int argc, char **argv)
131
132
133
          // ofstream datafile("/home/jared/Desktop/mv-timings.txt", ios_base::app);
         ofstream datafile("mv-timings.txt", ios_base::app);
134
          // initialize MPI
136
137
         MPI_Obj the_mpi(argc, argv);
         if (the_mpi.size < 2)</pre>
138
              MPI_Abort (MPI_COMM_WORLD, 1);
139
140
          // determine/distribute size of arrays here
141
         int output = 1, nrows = 0, ncols = 0;
142
         GetArraySize(output, nrows, ncols, the_mpi, argc, argv);
if (the_mpi.size - 1 > nrows)
143
144
145
         {
              MPI_Abort (MPI_COMM_WORLD, -1);
146
147
         }
148
         boost::multi_array<double, 2> A;
149
         vector<double> b(ncols);
150
         vector<double> c;
151
         vector<double> Arow;
152
         SetupArrays(nrows, ncols, A, b, c, Arow, the_mpi);
153
154
         MPT Status status:
155
156
          // Timing variables
157
         double calc_time = 0, avg_time, total_time;
158
159
          // Boss part
160
         if (the_mpi.rank == 0)
161
162
              total_time = MPI_Wtime();
163
              // send one row to each worker tagged with row number, assume size<nrows
164
165
              int rowsent = 1;
166
              for (int i = 1; i < the_mpi.size; i++)</pre>
167
                  MPI_Send(&A[rowsent - 1][0], ncols, MPI_DOUBLE, i, rowsent, MPI_COMM_WORLD);
168
                  rowsent++;
```

```
170
             }
171
             for (int i = 0; i < nrows; i++)</pre>
172
173
                  double ans:
174
                 MPI_Recv(&ans, 1, MPI_DOUBLE, MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
175
                 int sender = status.MPI SOURCE;
176
                  int row = status.MPI_TAG - 1;
177
                  c[row] = ans;
178
                  if (rowsent - 1 < nrows)</pre>
179
                  { // send new row
180
                     MPI_Send(&A[rowsent - 1][0], ncols, MPI_DOUBLE, sender, rowsent, MPI_COMM_WORLD);
181
182
                      rowsent++:
183
184
                  else
                  { // tell sender no more work to do via a 0 TAG \,
185
                      MPI_Send(MPI_BOTTOM, 0, MPI_DOUBLE, sender, 0, MPI_COMM_WORLD);
186
187
188
             }
189
190
         else
191
192
              // Get a row of A
193
             MPI_Recv(&Arow[0], ncols, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
194
             while (status.MPI_TAG != 0)
195
196
                  // work out Arow.b
197
                  double ans = 0.0;
198
199
                  calc_time -= MPI_Wtime();
200
                  for (int i = 0; i < ncols; i++)</pre>
                     ans += Arow[i] * b[i];
202
                  calc_time += MPI_Wtime();
204
                  // Send answer of Arow.b back to boss and get another row to work on
                  MPI_Send(&ans, 1, MPI_DOUBLE, 0, status.MPI_TAG, MPI_COMM_WORLD);
206
                  MPI_Recv(&Arow[0], ncols, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
208
         }
210
         if (the_mpi.rank == 0)
             total_time = MPI_Wtime() - total_time;
211
         MPI_Reduce(&calc_time, &avg_time, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
215
         if (the_mpi.rank == 0)
216
             avg_time /= (the_mpi.size - 1); // Boss node doesn't do any of the calculations
             printf("Average calculation time = %.10f\n", avg_time);
218
             printf("Total time = %.10f\n", total_time);
219
220
             datafile << fixed << setprecision(10); datafile << nrows << " " << ncols << " " << the_mpi.size << " " << avg_time << " " << total_time
221
222
     223
        }
224
         // output c here on Boss node
225
226
         Output (output, c, the_mpi);
227
```

3 Matrix Matrix Multiplication Using MPI and BLAS

In this section, we modify the code to compute the matrix matrix porduct from above. The new code is parellelized identically to the non-BLAS code, with the only change being the method each thread uses locally to compute the product of a row with the second matrix. Namely, we use the DDOT_ function provided by the BLAS library. As we did for the previous code, we test the code still works as can be seen in Figure 7.

```
**(base) jarad@Hebulae:../Scientific Computing SC9505/Assignment 2 - November 30/MMblas$ make clean rm =rf 15-matrix=matrix=blas.0 **
(base) jarad@Hebulae:../Scientific Computing SC9505/Assignment 2 - November 30/MMblas$ make all mpiCC -O2 -O 15-matrix=matrix=blas.0 10-matrix=matrix=blas.cpp -lblas -llapack**
(base) jarad@Hebulae:../Scientific Computing SC9505/Assignment 2 - November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=blas.0 1 10 10 November 30/MMblas$ mpirun =n 4 ./15-matrix=matrix=bla
```

Figure 7: Demonstration of the code working. Just as we did for the non-BLAS implementation, the first example takes the first matrix to be the identity while the second has consecutive integers along the main diagonal. In the second example, the first matrix is changed to the reverse identity (1s along the antidiagonal). In both cases, we get the expected result.

The new code using BLAS shows that the total runtime as a function of the number of rows N scales as $\mathcal{O}(N^{3.6})$ as supported by Figure 8. This is peculiar since this means the modified code using BLAS actually scales worse than the non-BLAS code.

Perhaps this is because the BLAS code doesn't actually scale in polynomial time and is instead scaling like $\mathcal{O}(N^{\alpha} \log N)$ for some α , but I am not confident enough to say for certain¹. I would expect the BLAS code to scale better than the non-BLAS code, and given that the linear regression does not fit as nicely as it did for the non-BLAS case, I suspect this may be the case.

¹If there is a more obvious or apparent reason for this behaviour, I'd be interested to know.

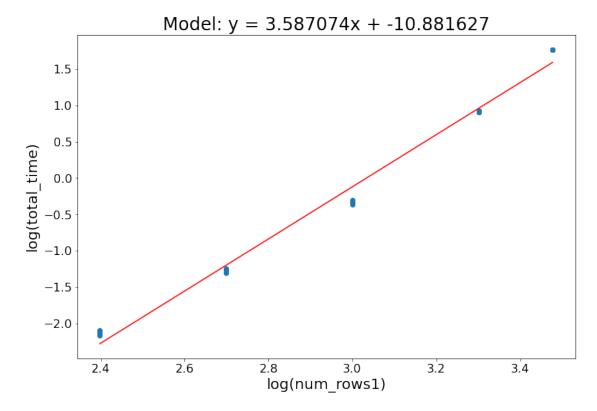


Figure 8: Plotting the runtime of the program as a function of the number of rows N (on a log-log scale), we find that the total runtime scales as $\mathcal{O}(N^{3.6})$, which again is more than the expected $\mathcal{O}(N^3)$, and even worse than the non-BLAS scaling.

Considering now the scaling as a function of the number of threads P, we again find a similar result: that for a fixed number of rows N, the scaling goes as $\mathcal{O}(P^{-1})$, as can be seen in Figure 9. This is once again good news and agrees with what we would expect: the scaling should still be the same as in the non-BLAS case.

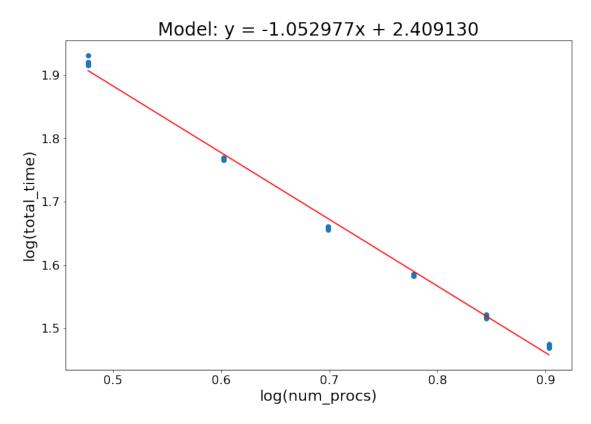


Figure 9: Plotting the runtime of the program as a function of the number of threads P, we find the scaling for a fixed number of rows N (here N=3000) to be of the order $\mathcal{O}(P^{-1})$

Looking at the speedup and efficiency as seen in Table 3, we see that our BLAS code runs faster than the non-BLAS code and is therefore more efficient as well. It also appears that that efficiency of the program increases as we allocate more threads. As a test, I ran the code with N=3000 rows and P=12 threads, and found the efficiency to drop off slightly to 0.59.

Number of Threads	Speedup	Scaling Factor a	Efficiency
3	2.05	0.63	0.63
4	2.65	0.64	0.64
5	3.22	0.65	0.65
6	3.80	0.65	0.65
7	4.35	0.66	0.66
8	4.90	0.66	0.66

Table 3: Summary of the speedup and efficiency of our matrix multiplication code using the BLAS DDOT_ function. These values are taken for a constant number of rows N=3000.

I would expect if we ran the code for say N = 5000, the efficiency would be much higher, since if we look at the efficiency for N = 2000, as in Table 4, we see that the efficiency of the program nearly

doubles going from N = 2000 to N = 3000. As a test, I ran the serial code for N = 5000, which took 1083.20 seconds. The parallel code ran with P = 12 took 128.45 seconds, corresponding to a speedup of 8.43 and an efficiency of 0.70. When run with P = 8 instead, it took 188.57 seconds, giving a speedup of 5.74 and an efficiency of 0.72.

Number of Threads	Speedup	Scaling Factor a	Efficiency
3	1.16	0.39	0.39
4	1.52	0.38	0.38
5	1.87	0.37	0.37
6	2.22	0.37	0.37
7	2.56	0.37	0.37
8	2.90	0.36	0.36

Table 4: Summary of the speedup and efficiency of our matrix multiplication code using the BLAS DDOT_ function. These values are taken for a constant number of rows N = 2000.

```
// Matrix-Matrix multiplication code AB=C //
    // Note that I will index arrays from 0 to n-1.
    // Here workers do all the work and boss just handles collating results
    // and sending infor about A.
    // include, definitions, globals etc here
    #include <iostream>
10
    #include <fstream>
11
   #include <iomanip>
12
   #include <random>
13
    #include "boost/multi_array.hpp"
14
   #include "mpi.h'
15
    extern "C" {
17
        extern double ddot_(int *, double *, int *, double *, int *);
18
19
20
    using namespace std;
21
22
    class MPI_Obj
23
24
    public:
25
        int size;
27
        int rank:
29
        MPI_Obj(int &argc, char **&argv)
30
            MPI_Init(&argc, &argv);
31
            MPI_Comm_size(MPI_COMM_WORLD, &size);
33
            MPI_Comm_rank(MPI_COMM_WORLD, &rank);
35
        ~MPI_Obj()
            MPI_Finalize();
39
    void GetArraySize(
       int &output,
       int &nrows1,
       int &nrowscols12,
       int &ncols2,
       MPI_Obj &the_mpi,
       int argc,
        char **argv
   ) {
```

```
51
         if (the_mpi.rank == 0)
52
              if (argc == 5) {
53
                  output = atoi(argv[1]);
54
                  nrows1 = atoi(arqv[2]);
55
                  nrowscols12 = atoi(argv[3]);
56
                  ncols2 = atoi(argv[4]);
57
58
             } else {
                  cout << "Please enter the number of rows for the first matrix -> ";
59
                  cin >> nrows1;
60
                  cout << "Please enter the number of columns/rows for the first/second matrix-> ";
61
                  cin >> nrowscols12:
62
                  cout << "Please enter the number of columns for the second matrix-> ";
63
                  cin >> ncols2;
64
65
             }
66
        }
67
         //\ {\it send\ everyone\ nrows,\ ncols}
68
         int buf[3] = {nrows1, nrowscols12, ncols2};
69
         MPI_Bcast(buf, 3, MPI_INT, 0, MPI_COMM_WORLD);
70
71
         if (the_mpi.rank != 0)
72
             nrows1 = buf[0];
73
74
             nrowscols12 = buf[1];
75
             ncols2 = buf[2];
76
77
    }
78
79
    void SetupArrays(
         int nrows1,
81
         int nrowscols12,
82
         int ncols2,
83
         boost::multi_array<double, 2> &A,
         boost::multi_array<double, 2> &B,
         boost::multi_array<double, 2> &C,
         vector<double> &Arow,
87
         vector<double> &Crow,
        MPI_Obj &the_mpi
    ) {
         uniform_real_distribution < double > unif (-1.0, 10);
         default_random_engine re;
92
         B.resize(boost::extents[nrowscols12][ncols2]);
93
         Crow.reserve(ncols2); Crow.resize(ncols2); // Main process will need to store the values temporarily
96
         if (the_mpi.rank == 0)
97
              // Set size of A
99
             A.resize(boost::extents[nrows1][nrowscols12]);
100
             C.resize(boost::extents[nrows1][ncols2]);
101
102
              // Initialize A
103
             for (int i = 0; i < nrows1; ++i) {</pre>
104
                  for (int j = 0; j < nrowscols12; ++j) {
    // Identity</pre>
105
106
                      // if (i == j)
107
                             A[i][j] = 1.0;
108
                      // else
109
                          A[i][j] = 0.0;
110
                      // Reverse Identity
// if (i == (nrowscols12 - j - 1))
111
112
                             A[i][j] = 1.0;
113
                      // else
114
                            A[i][j] = 0.0;
115
                      // Random
116
                      A[i][j] = unif(re);
117
                  }
118
             }
119
120
              // Initialize B
121
              for (int i = 0; i < nrowscols12; ++i) {</pre>
122
                  for (int j = 0; j < ncols2; ++j) {</pre>
123
                     // Identity
// if (i == j)
124
125
                      // B[i][j] = 1.0;
126
                      // else
127
```

```
128
                               B[i][j] = 0.0;
                        // Reverse Identity
// if (i == (ncols2 - j - 1))
129
130
                               B[i][j] = 1.0;
131
                        // else
132
                              B[i][j] = 0.0;
133
                        // Random
134
                        // B[i][j] = unif(re);
135
                        // Other
136
                        if (i == j)
137
                            B[i][j] = (double) i + 1;
138
                        else
139
                            B[i][j] = 0;
140
                   }
141
142
143
          } else {
144
               // Worker part
145
               // Allocate space for 1 row of A and 1 row of the answer C
              Arow.reserve(nrowscols12); Arow.resize(nrowscols12);
146
147
          MPI_Bcast(&B[0][0], nrowscols12*ncols2, MPI_DOUBLE, 0, MPI_COMM_WORLD);
148
149
     }
150
151
     void Output(int output, boost::multi_array<double, 2> &array, MPI_Obj &the_mpi)
152
          if (the_mpi.rank == 0 && output) {
   cout << endl << fixed << setprecision(4);</pre>
153
154
155
156
               for (int i = 0; i < array.shape()[0]; i++) {</pre>
157
                   for (int j = 0; j < array.shape()[1]; j++) {</pre>
                        cout << array[i][j];</pre>
158
159
                        if (j < array.shape()[1] - 1) cout << ", ";</pre>
160
                   cout << endl;
162
               cout << endl;
164
               cout << scientific;</pre>
166
168
     int main(int argc, char **argv)
169
170
171
           // ofstream datafile("/home/jared/Desktop/mm-timings.txt", ios_base::app);
         ofstream datafile("mmblas-timings.txt", ios_base::app);
173
174
175
          // initialize MPI
         MPI_Obj the_mpi(argc, argv);
if (the_mpi.size < 2) MPI_Abort(MPI_COMM_WORLD, 1);</pre>
176
177
178
          // determine/distribute size of arrays here
179
          int output = 1, nrows1 = 0, nrowscols12 = 0, ncols2 = 0;
180
         GetArraySize(output, nrows1, nrowscols12, ncols2, the_mpi, argc, argv);
if (the_mpi.size - 1 > nrows1) {
181
182
              MPI_Abort (MPI_COMM_WORLD, -1);
183
184
185
         boost::multi_array<double, 2> A;
boost::multi_array<double, 2> B;
186
187
          boost::multi_array<double, 2> C;
188
          vector<double> Arow;
189
          vector<double> Crow:
190
          SetupArrays(nrows1, nrowscols12, ncols2, A, B, C, Arow, Crow, the_mpi);
191
192
          MPI Status status;
193
194
          // Timing variables
195
          double calc_time = 0, avg_time, total_time;
196
197
          // Boss part
198
          if (the_mpi.rank == 0)
199
200
201
               total_time = MPI_Wtime();
202
               // send one row to each worker tagged with row number, assume size<nrows
203
              int rowsent = 1;
              for (int i = 1; i < the_mpi.size; i++)</pre>
```

```
205
                 MPI_Send(&A[rowsent - 1][0], nrowscols12, MPI_DOUBLE, i, rowsent, MPI_COMM_WORLD);
206
207
                 rowsent++;
             }
208
209
             for (int i = 0; i < nrows1; i++)</pre>
210
211
                 MPI_Recv(&Crow[0], ncols2, MPI_DOUBLE, MPI_ANY_SOURCE, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
212
                 int sender = status.MPI SOURCE;
213
                 int row = status.MPI TAG - 1;
214
                memcpy(&C[row][0], &Crow[0], ncols2 * sizeof(double));
215
216
                 if (rowsent - 1 < nrows1) {</pre>
217
218
                     // send new row
                     MPI_Send(&A[rowsent - 1][0], nrowscols12, MPI_DOUBLE, sender, rowsent, MPI_COMM_WORLD);
219
220
                     rowsent++;
221
                 } else {
                     // tell sender no more work to do via a 0 TAG
222
                     MPI_Send(MPI_BOTTOM, 0, MPI_DOUBLE, sender, 0, MPI_COMM_WORLD);
223
224
225
             }
226
         // Worker part: compute dot products of Arow.b until done message recieved
227
228
        else
229
             // Get a row of A
230
            MPI_Recv(&Arow[0], nrowscols12, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
231
232
             while (status.MPI_TAG != 0)
233
234
                 for (int i = 0; i < ncols2; i++) {</pre>
235
                     // work out Crow = Arow.B
                     calc_time -= MPI_Wtime();
236
237
                     Crow[i] = ddot_(&nrowscols12, &Arow[0], new int(1), &B[0][i], &ncols2);
                     calc_time += MPI_Wtime();
239
                 // Send answer of Arow.B back to boss and get another row to work on
241
                 MPI_Send(&Crow[0], ncols2, MPI_DOUBLE, 0, status.MPI_TAG, MPI_COMM_WORLD);
                 MPI_Recv(&Arow[0], nrowscols12, MPI_DOUBLE, 0, MPI_ANY_TAG, MPI_COMM_WORLD, &status);
        }
246
        if (the_mpi.rank == 0)
             total_time = MPI_Wtime() - total_time;
        MPI_Reduce(&calc_time, &avg_time, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
250
        avg_time /= (the_mpi.size - 1); // Boss node doesn't do any of the calculations
251
        if (the_mpi.rank == 0)
253
254
             printf("Average calculation time = %.10f\n", avg_time);
255
            printf("Total time = %.10f\n", total_time);
256
257
             datafile << fixed << setprecision(10);</pre>
258
            259
260
261
262
         // output c here on Boss node
263
        Output (output, C, the_mpi);
264
    }
265
```

4 Solving Poisson's Equation Using LAPACK

The last part of the assignment is a brief introduction to the LAPACK library. The code being tested solves the Poisson equation $\nabla^2 U(\vec{x}) = f(\vec{x})$. In Figure 10, I have run the provided code and plotted the solution using plotly in Python.

The code works by solving a linear system of equations of the form Ax = b, where A is a matrix, while x and b are vectors. The program is made more efficient by noting for this problem that the matrix A will be a banded, negative-definite matrix, such that we can use the optimized LAPACK functions DPBTRF_ and DPBTRS_ to factor and solve the system.

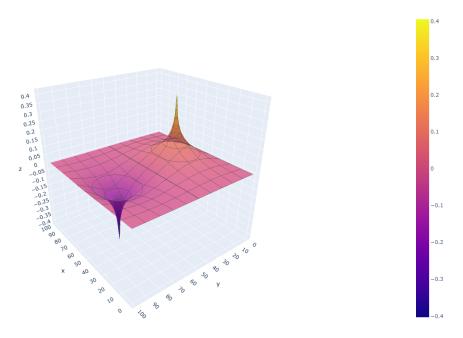


Figure 10: Plot of the solution using N = 100 sites.

Testing the run time of the code as a function of the number of sites N, the scaling is found to be of the order $\mathcal{O}(N^{3.8})$, as can be seen in Figure 11. The scaling can be expected to be $\mathcal{O}(N^4)$, as performing a PLU factoraization scales as $\mathcal{O}(N^3)$, and back-substitution should contribute a factor proportional to $\mathcal{O}(N)$. Given we are using BLAS routines which are optimized for banded and positive definite matrices, it is convincing our scaling should be slightly less than the worst case scenario of $\mathcal{O}(N^4)$.

Using the linear regression model (red line) in the plot, we can estimate that the largest system that can be solved (on my hardware) in 5 minutes to be roughly N = 975. This seems reasonable, since the runtime for a system with N = 1000 was roughly 385 seconds.

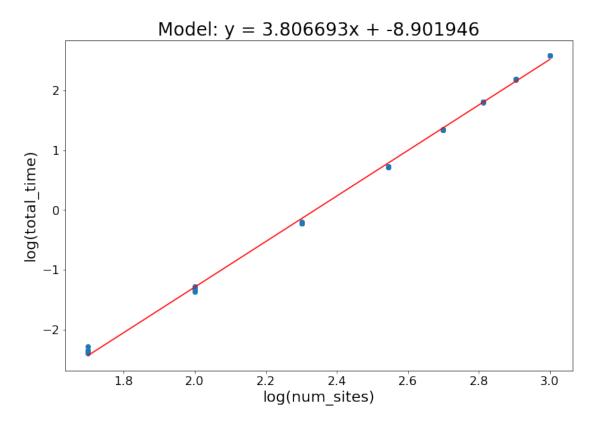


Figure 11: Plotting the runtime of the program as a function of the number of sites N (on a log-log scale), we find that the total runtime scales as $\mathcal{O}(N^{3.8})$.

```
// Program to compute solution to -laplacian u = -F
    // compile with
    // run with mpirun -n 1 <executable> output_cout output_file N
    #include <iostream>
    #include <iomanip>
    #include <fstream>
    #include <mpi.h>
    #include "boost/multi_array.hpp"
10
    // LAPACK library files
extern "C"
11
12
13
         // general band factorize routine
14
        extern int dpbtrf_(char *, int *, int *, double *, int *, int *);
15
16
        // general band solve using factorization routine
17
        extern int dpbtrs_(char *, int *, int *, int *, double *, int *, double *, int *, int *);
18
19
20
    void AbInit(int N, boost::multi_array<double, 2> &Ab)
22
         // Coefficient Matrix: initialize
23
        for (int i = 0; i < N * N; i++)
            for (int j = 0; j < N + 1; j++)</pre>
24
                 Ab[j][i] = 0.0;
                 if (j == 0)
Ab[j][i] = -1.0;
                 if (j == N - 1 && i % N)
                     Ab[j][i] = -1.0;
                 if (j == N)
                     Ab[j][i] = 4.0;
        // std::cout << "Ab initialized \n";
           Printout Ab for testing, small N only
```

```
// for (int i=0; i < N+1; i++) {
36
              std::cout << Ab[i][0];
37
               for (int j=1; j < N*N; j++) {
    std::cout << " " << Ab[i][j];
38
39
40
              std::cout << "\n";
41
42
43
    }
44
     \textbf{void} \ \texttt{RHSInitialize}(\textbf{int} \ \texttt{N}, \ \texttt{std}:: \texttt{vector} < \textbf{double} > \ \&\texttt{F}, \ \textbf{double} \ \texttt{bcx}, \ \textbf{double} \ \texttt{bcy})
45
46
          // RHS: fill in boundary condition values
47
         for (int i = 0; i < N; i++)
48
49
             // bottom boundary
50
51
52
             F[i * N + N - 1] += bcy; // right boundary
53
54
         // std::cout << "RHS initialized\n";</pre>
55
56
          // RHS: fill in actual right-hand side, some "charges", actually h^2*charge
57
         F[N / 4 * N + N / 2] += 0.5;
F[3 * N / 4 * N + N / 2] += -0.5;
58
59
60
    }
62
    int main(int argc, char** argv)
64
         double time = MPI_Wtime();
65
          // ofstream timingfile("/home/jared/Desktop/lp-timings.txt", ios_base::app);
66
         std::ofstream timingfile("lp-timings.txt", std::ios_base::app);
67
         // ofstream datafile("/home/jared/Desktop/lp-data.txt");
68
         std::ofstream datafile("lp-data.txt");
70
          // Coefficient Matrix: declare
72
         int output_cout = 1, output_file = 0;
         int N = 10;
73
         if (argc == 4) {
             output_cout = atoi(argv[1]);
76
              output_file = atoi(argv[2]);
             N = atoi(argv[3]);
77
78
80
         int M = N + 1;
         int ABcols = N * N;
81
82
         boost::multi_array<double, 2> Ab(boost::extents[M][ABcols], boost::fortran_storage_order());
83
         AbInit(N, Ab); // Initialize coefficient matrix
84
85
         // Coefficient Matrix: factorize
86
         char uplo = 'U';
87
         int KD = N;
88
         int info;
89
         dpbtrf_(&uplo, &ABcols, &KD, &Ab[0][0], &M, &info);
90
91
         if (info)
92
         {
              std::cout << "Ab failed to factorize, info = " << info << "\n";
93
              exit(1);
94
95
96
         // RHS: declare
97
         const double bcx = 0.0, bcy = 0.0; // boundary conditions along x and y assume same on both sides
98
         std::vector<double> F(N * N, 0.0);
99
100
         RHSInitialize(N, F, bcx, bcy); // set up boundary conditions and right hand side
101
102
         // Solve system
103
104
         int Bcols = 1;
         dpbtrs_(&uplo, &ABcols, &KD, &Bcols, &Ab[0][0], &M, &F[0], &ABcols, &info);
105
106
         if (info)
107
              std::cout << "System solve failed, info = " << info << "\n";</pre>
108
109
              exit(1);
110
         }
111
         time = MPI_Wtime() - time;
```

```
113
            timingfile << N << " " << time << std::endl;
114
            // Output solution
if (output_cout) {
   for (int i = 0; i < N; i++)</pre>
115
116
117
118
                         std::cout << F[i * N];
for (int j = 1; j < N; j++)
.</pre>
119
120
121
                               std::cout << " " << F[i * N + j];
122
123
                         std::cout << "\n";
124
125
126
            if (output_file) {
    datafile << std::fixed << std::setprecision(10);
    for (int i = 0; i < N; i++)</pre>
127
128
129
130
                         datafile << F[i * N];
for (int j = 1; j < N; j++)</pre>
131
132
133
                               datafile << " " << F[i * N + j];
134
135
                         datafile << "\n";
136
137
138
139
             return 0;
140
141
```

A Jupyter Notebook

Below is an example notebook I have used in order to generate and analyze my timing data. The notebook will compile and run the given program a number of times for various numbers of threads and matrix dimensions. It then creates linear regression models from the data which can be used to determine the speedup and efficiency of parallelization.

plots

November 21, 2022

```
[]: import numpy as np
     from sklearn.linear_model import LinearRegression
     import matplotlib.pyplot as plt
     import pandas as pd
     import subprocess as sp
     import itertools as it
[]: def genData(procs, sizes, data_file, cycles=20, clean=False):
         sp.run(
             "/usr/bin/mpiCC -02 -o 15-matrix-vector.o ./10-matrix-vector.cpp",
             shell=True,
             stdout=sp.DEVNULL,
             stderr=sp.DEVNULL
         )
         if clean:
             sp.run(
                 f'echo "num_rows num_cols num_procs avg_time total_time" >_ 

⟨data_file⟩',
                 shell=True,
                 stdout=sp.DEVNULL,
                 stderr=sp.DEVNULL
             )
         for size, proc in it.product(sizes, procs):
             for _ in range(cycles):
                 sp.run(
                     f"/usr/bin/mpirun -n {proc} ./15-matrix-vector.o 0 {size}_\_

⟨size⟩",
                     shell=True,
                     stdout=sp.DEVNULL,
                     stderr=sp.DEVNULL
             print(f"Finished {size}x{size} with {proc} processes")
     def plotModel(
         data: pd.DataFrame,
         xdata: str,
```

```
ydata: str,
    plot: bool,
    loglog: bool
):
    x = data[xdata].values.reshape(-1, 1)
    y = data[ydata].values.reshape(-1, 1)
    xname = xdata
    yname = ydata
    if loglog:
        x = np.log10(x)
        y = np.log10(y)
        xname = "log(" + xdata + ")"
        yname = "log(" + ydata + ")"
    linear_model = LinearRegression()
    linear_model.fit(x, y)
    model = linear_model.predict(x)
    if plot:
        fig, ax = plt.subplots(figsize=(12,8))
        ax.set_title("Model: y = {:.6f}x + {:.6f}".format(linear_model.

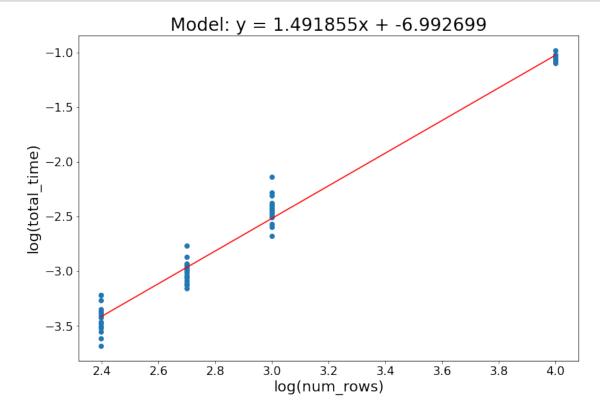
coef_[0][0], linear_model.intercept_[0]), size=24)
        ax.set_xlabel(xname, size=20)
        ax.tick_params(axis='x', labelsize=16)
        ax.set_ylabel(yname, size=20)
        ax.tick_params(axis='y', labelsize=16)
        ax.scatter(x, y)
        ax.plot(x, model, color='red')
        plt.show()
    return linear_model
```

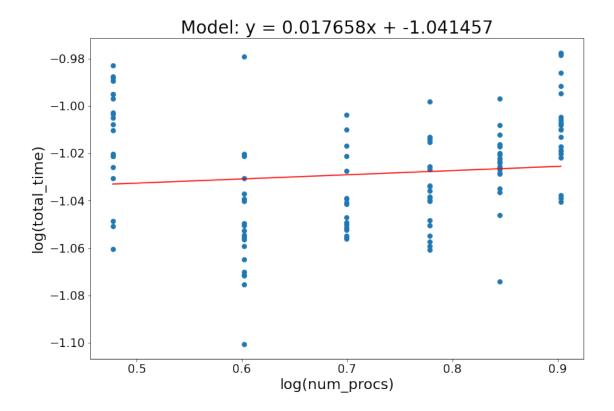
```
[]: # Variables
    # data_file = "/home/jared/Desktop/mv-timings.txt"
    data_file = "./mv-timings.txt"
    procs = np.array([3, 4, 5, 6, 7, 8])
    sizes = np.array([10, 50, 100, 250, 500, 1000, 10000])

# Generate data if needed
    # genData(procs=procs, sizes=sizes, data_file=data_file, clean=True)

# Load the data
    data = pd.read_csv(data_file, delimiter=" ")
```

```
[ ]: num_procs = 4
num_rows = 10000
min_procs = 2
```





```
[ ]: num_rows = 10000
     serial_times = {
         10: 0.0000047090,
         50: 0.0000092870,
         100: 0.0000360770,
         250: 0.0001662810,
         500: 0.0008027130,
         1000: 0.0025987250,
         10000: 0.4020480850,
     }
     prediction = np.array([
         10**val[0] for val in
         reduced_proc_scaling_model.predict(procs.reshape(-1, 1))
     ])
     speedup = serial_times[num_rows] / prediction
     print("speedup = \n", np.array_str(speedup))
     a = speedup / procs
    print("a = \n", np.array_str(a))
```

```
efficiency = speedup / procs
print("efficiency = \n", np.array_str(efficiency))

speedup =
  [3.91524996 3.75924844 3.60946274 3.46564519 3.32755799 3.19497282]
a =
  [1.30508332 0.93981211 0.72189255 0.57760753 0.47536543 0.3993716 ]
```

[1.30508332 0.93981211 0.72189255 0.57760753 0.47536543 0.3993716]

efficiency =