CSE 6220 Introduction to High Performance Computing
Spring 2020
Programming Assignment 3

Jacobi's Method

Jacobi's method is an iterative, numerical method for solving a system of linear equations. Formally, given a full rank $n \times n$ matrix $A \in \mathbb{R}^{n \times n}$ and a vector $b \in \mathbb{R}^n$, *Jacobi's method* iteratively approximates $x \in \mathbb{R}^n$ for:

$$Ax = b$$

Given the matrix A,

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

we first separate A into its diagonal elements D and the remaining elements R such that $A = D + R$ with:

$$D = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}, \qquad R = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ a_{21} & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}$$

Jacobi's method then follows the following steps till convergence or termination:

1. Initialize x: $x \leftarrow \begin{bmatrix} 0 & 0 & \ldots & 0 \end{bmatrix}$

2. $D = diag(A)$

3. $R = A - D$

4. **while** $||Ax - b|| > l$ **do**

    (a) update $x \leftarrow D^{-1}(b - Rx)$

where $||x||$ is the L2-norm, and l is a parameter for the termination accuracy.

A matrix A is *diagonally dominant*, if its diagonal elements are larger than the sum of absolutes of the remaining elements in the corresponding rows, i.e., iff:

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}|.$$

It can be shown that for *diagonally dominant* matrices, *Jacobi's method* is guaranteed to converge. The goal of this assignment is to develop a parallel algorithm for *Jacobi's method*.

Parallel Algorithm

Data distribution   We use a 2-dimensional grid/mesh as the communication network for this problem. We assume that the number of processors is a perfect square: $p = q \times q$ with $q = \sqrt{p}$, arranged into a mesh of size $q \times q$. The inputs are distributed on the grid as follows:

- The n-by-n matrix A is block distributed onto the grid. The rows of A are distributed onto the rows of the processor-grid such that either $\lceil \frac{n}{q} \rceil$ or $\lfloor \frac{n}{q} \rfloor$ rows of A are distributed onto each row of the grid. More specifically, the first $(n \mod q)$ rows of the grid contain $\lceil \frac{n}{q} \rceil$ rows of A, and the remaining rows of the grid contain $\lfloor \frac{n}{q} \rfloor$ rows of A. The same applies to the distribution of columns. A processor with coordinates (i, j) thus has the following size local matrix:

$$\begin{cases} \lceil \frac{n}{q} \rceil^2 & \text{if } i < (n \mod q) \text{ and } j < (n \mod q) \\ \lceil \frac{n}{q} \rceil \times \lfloor \frac{n}{q} \rfloor & \text{if } i < (n \mod q) \text{ and } j \geq (n \mod q) \\ \lfloor \frac{n}{q} \rfloor \times \lceil \frac{n}{q} \rceil & \text{if } i \geq (n \mod q) \text{ and } j < (n \mod q) \\ \lfloor \frac{n}{q} \rfloor^2 & \text{if } i \geq (n \mod q) \text{ and } j \geq (n \mod q) \end{cases}$$

- The size n vectors b and x are equally block distributed only along the first column of the processor-grid, i.e., only among processors with indexes $(i, 0)$. Processor $(i, 0)$ will thus have the following local size:

$$\begin{cases} \lceil \frac{n}{q} \rceil & \text{if } i < (n \mod q) \\ \lfloor \frac{n}{q} \rfloor & \text{if } i \geq (n \mod q) \end{cases}$$

Parallel Matrix-Vector Multiplication   Let A be a n-by-n matrix and let x and y be n dimensional vectors. We wish to compute $y = Ax$. Assume that the square matrix A and the vector x are distributed on the processor grid as explained above. The answer y will again be distributed in the same fashion as the vector x. To do so, we will first "transpose" the vector x on the grid, such that a processor with index (i, j) will end up with the elements that were on processor $(j, 0)$ according to the above distribution. We do this by first sending the elements from a processor $(i, 0)$ to its corresponding diagonal processor (i, i), using a single `MPI_Send` and the sub-communicator for the row of processors. We then broadcast the received elements from (i, i) along each column of the grid using a sub-communicator for the column of processors.

Now, each processor has the elements it needs for its local matrix-vector multiplication. We multiply the local vector with the local matrix and then use a parallel reduction to sum up the resulting vectors along the rows of the grid back onto the processors of the first column. The final result of the multiplication thus ends up distributed among the first column in the same way that the input x was.

Parallel Jacobi   For parallelizing *Jacobi's method*, we distribute A and R as described above and use parallel matrix-vector multiplication for calculating Rx. The vectors x, and b, are distributed among the first column of the processor grid. The diagonal elements D of A need to be collected

along the first column of the processor grid. We can thus update x by $x_i \leftarrow \frac{1}{d_i}(b_i - (Rx)_i)$ using only local operations.

In order to detect termination, we calculate Ax using parallel matrix-vector multiplication, and then subtract b locally on the first column of processors (where the result of the multiplication and b are located). Next, we calculate the L2-norm $||Ax - b||$ by first calculating the sum of squares locally and then performing a parallel reduction along the first column of processors. We can now determine whether to terminate or not by checking the L2-norm against the termination criteria and then broadcasting the result along rows. Now, every processor knows whether or not to continue with further iterations. In your implementation, you should not only check for the termination criteria, but also terminate after a pre-set maximum number of iterations.

Task

In this assignment, you will implement *Jacobi's* method using MPI. A framework is provided with this programming assignment, which declares all functions that you should implement.

Guidelines/Rules

- Your code should be written in C or C++ language

- **Compilation and execution should work out of the box at Pace-ICE cluster.** You may modify the `Makefile` if necessary, but make sure you submit your modified Makefile. In any case, we must be able to compile and run your code out of the box with the modules `gcc` and `mvapich2/2.2` on Pace-ICE.

- Expected output format (taken care of by the code framework) should be strictly adhered since the grading for this is automated and additional output (eg: debug print statements you've forgotten to remove) will prevent you from getting full points.

- **You are not to discuss the solutions** for the assignment openly on Piazza. However you may discuss strategies to collectively work on how to solve a particular issue you may face.

- If you have done the Programming Assignments 1 and 2, we are fairly certain you should be able to complete this assignment with similar knowledge and effort in C/C++ programming language + MPI framework without any additional help from the TAs or the Instructors. However we are happy to help you should you have any problems.

Code Framework

You are required to implement your solution within the provided framework in the attached zip file. In the event that we have to update the framework, we will publish the updates and notify the class via Canvas.The framework comes with some pre-implemented unit tests. You are encouraged to add more test cases to make sure that your implementation works as expected.

First, you should implement matrix-vector multiplication and *Jacobi's* method sequentially. You will later use this as the comparison for measuring speedup and as reference implementation for testing your parallel code.

Implement the sequential code in the file `jacobi.cpp` according to the function declarations in `jacobi.h`. Unit tests for the sequential code are implemented in `seq_tests.cpp`. Add your own test cases in this file. To compile and run the tests, run `make test` either locally on your own machine, or in an interactive job. Do NOT run the tests on the login node of the cluster.

Next, you should implement the parallel algorithm as described above. For this, you'll have to implement functions to distribute the data among the grid of processors and gather results back to the processor with rank $(0, 0)$. Then, implement the parallel algorithms for matrix-vector multiplication and Jacobi's method. Implement your parallel code in the file `mpi_jacobi.cpp` according to the function declarations in `mpi_jacobi.h`. A few test cases are already provided in the file `mpi_tests.cpp`. You may also want to add your own test cases in this file as well. Some utility functions for block distributions are provided in `utils.h` and `utils.cpp`. You can make use of these function, and implement your own utility functions in these files.

Finally, test the performance of your parallel implementation against your sequential implementation for various input sizes. Use the executable `jacobi` for this and generate the input on-the-fly via the `-n` and `-d` (difficulty) parameters. Report your achieved speedups for different input sizes and difficulties. Increasing difficulty increases the number of iterations needed for *Jacobi's Method* to converge.

Testing

You may implement, run and test your solutions in your local machine (see the references section to see how), but you MUST test your code in the Pace-ICE cluster for the following.

1. Compilation should be done via the `Makefile`. You should call the compilation and execution through scheduling a pbs job or via an interactive node.

2. Use the modules `gcc` and `mvapich2/2.2` for compilation and execution.

3. Fresh copy of your solution should compile out of the box without any changes to the `Makefile` you have provided.

4. Generate input files for small matrices and vectors A and b and verify that your parallel solution gives correct results. You may do this manually or by comparing against your serial implementation. For your convenience we have also introduced unit testing for both your serial and parallel implementations. You are welcome to add your own unit tests to these files. Refer the `README.md` on how to build and execute the unit tests.

5. Your solution should execute and give correct results for very large matrices (By "very large", we mean $n \geq 10000$) and using as many nodes as allowed from the cluster. **Your largest p should be at least as large as** 64**.**

6. You may assume $n^2 \geq p$.

7. Resources in Pace-ICE cluster is limited. And this class has around 105 students. **To avoid lack of resource, we highly suggest that you start early and finish testing the code at least 3 days before the deadline. Also, do not acquire more resources than you need. For example, you should not ask for 64 processors when you only need to use 4 of them.**

Team

You can form a team up to three members. No matter how you decide to share the work between yourselves, each student is expected to have full knowledge of the submitted program. **And only one member from each team should submit the required deliverables on Canvas.**

Grading [20pt]

- The highest score you can get for this assignment is 20pt

- Your submission will be graded based on,

  - Correct submission format (including comments on the code)
  - Successful compilation of the submitted code in Pace-ICE cluster
  - Efficient parallel implementation
  - Successful execution in Pace-ICE cluster and correctness in final results
  - Report

- A submission made by a team will receive the same grade for all members of the team.

Submission Policies
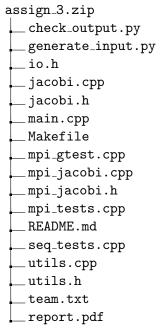
Submission Content

The submission must be a single zip file named `assign_3.zip` with the following named contents:

1. **team.txt**: A text file containing the names of all team members.

2. **[Source files]**: You should use good programming style and comment your program so that it is easy to read and understand. Make sure that your implementation does not rely on any extra files or functions implemented outside of the provided source files. (please exclude the `gtest/` directory from your submission)

3. **report.pdf**: A PDF report containing the following

   - The names of all team members.

- Short design description of your algorithm(s)

- Runtime and speedup plots by varying problem size and difficulty, when using different numbers of processors. Give observations on how your algorithm behaves on varying the parameters. Show the results of your experiments, and the conclusions along with the evidence that led you to reach the conclusions.

- Explain any ideas or optimizations of your own that you might have applied and how they might have affected the performance.

The program will be graded on correctness and use of the appropriate parallel programming features.

Your archive submission MUST look like the following:
```
assign_3.zip
├── check_output.py
├── generate_input.py
├── io.h
├── jacobi.cpp
├── jacobi.h
├── main.cpp
├── Makefile
├── mpi_gtest.cpp
├── mpi_jacobi.cpp
├── mpi_jacobi.h
├── mpi_tests.cpp
├── README.md
├── seq_tests.cpp
├── utils.cpp
├── utils.h
├── team.txt
└── report.pdf
```

Notes

We will enforce the specified polices strictly. You will risk losing points if you do not adhere to them. We will check all submissions for plagiarism. Any cases of plagiarism will be taken seriously, and dealt in accordance with the GT academic honor code (honor.gatech.edu).