CS5220 – Communication in Exact Exchange

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Abstract

The essence of this project is an algorithm problem in graph theory. I expect my group members to have intensive interests in graph theory and math, that can think deeply and provide idea to solve the problem. In this project, we have access to US supercomputer center Argonne, we can run our calculation on thousands of node and tens of thousands of processors.

1 Description

US government want to carry out a study about regional language difference. In each state, several cities in the state's central area, usually 3 to 5, are selected as samples to participate in this study, which gives us a total of 150 to 250 cities. Each city has its own record of local language dictionary in its city library, and each city has established a research team to work on this research project.

To finish this project, the regional language difference report of each pair of "nearby" city has to be generated. The standard of "nearby" is very simple:

- If the distance between the second city and the first city is within a certain threshold, then it is considered nearby to the first city.

To compared the language difference between two cities, one copy of the local language dictionary of the first city and that of its nearby city has to be sent to the same place for a research group to study.

To simplify this problem, we can make a few assumptions:

- The research teams of different cities has the same process power.

  > research team → MPI rank

- Each language dictionary has the same amount of information, as a result the difference between each pair of dictionaries can be studied within the same amount of time.

  > dictionary → data to be sent

- We assume periodic boundary conditions of the states, which means California is connected to Virginia, and North Dakota is connected to Texas.

After all job has been finished and report been generated, all those report are sent to one place, say, NYC.

> Sending Dictionaries .vs. Comparing $\implies$ Communication .vs. Computation

Our mission is to reduce the communication in this algorithm. If you think you can solve this problem or have some idea, you are already perfect for this project. If you are not sure, then keep reading.

2 Our mission

Our mission is to create an algorithm that minimize the communication (number of sending dictionaries) while keeping the computational load balanced.

The most naive algorithm is to ask every MPI rank to compare its own dictionary (local data) with half of its nearby cities, and sending the result to NYC in the end. This is our current implementation and lead to a huge communication fraction (more than half).

I already have another idea of doing this, which can cut 40% communication , means this project would never fail. However, I hope we can talk it over discussion if you are interested in this project.

In fact, this project is a part of theoretical physics package Quantum Expresso, a package for scientific calculation. The model I described is exactly the model we are using for sharing data.

3 My expectation

I hope my team members are familiar with graph theory, or very good at thinking. I will be happy as long as you can provide ideas to solve the problem. If you want to dig into the code and do the profiling and tuning with me, you will be very welcomed and we can learn coding, math and physics together.
If you are interest in joining me, send me an email to jj585@cornell.edu.
If you are not sure and want to hear more about this project, send me an email to jj585@cornell.edu