MPI Assignment: N-body Simulations

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1 The N-body problem

The N-body problem consists of the prediction of the individual motions of N celestial objects (bodies) with some properties (mass, initial velocity, radius, ...). This is done by measuring the force that they exert on each other (Coulomb gravity,...) and as a result, a simulation of the behavior of the system over time is obtained.

2 The sequential algorithm

The Listing 1 shows the simplified structure of the sequential algorithm.

```
for each timestep do
        Compute forces between all bodies
        Compute new positions and velocities
```

Listing 1: general sequential algorithm

As first thing, the time is discretized, so that the application knows what to do at certain time steps. After that, for each step, the algorithm computes the force between the bodies. With the result, the new velocity and position of all the bodies are updated.

2.1 Force computation

This step of the algorithm is the most expensive and defines its complexity. The force that bodies exert on each other has to be calculated once per pair of bodies (Listing 2).

```
for (b=0; b<bodyCt; ++b) {
                for (c=b+1; c<bodyCt; ++c) {
                        ...
```

Listing 2: loop for the force calculation

With N bodies, there are *(N-1)+(N-2)+(N-3)+...+1* pairs, so that $O(N^2)$ force computations for every time step.

3 Parallel N-body algorithm

An efficient parallelization of this algorithm is not trivial because for every step the updated information from all the bodies that are part of our system is needed in order to calculate the correct velocities and positions. The next paragraph was introduced to explain the technology used to develop the parallel implementation.

3.1 MPI

For this project was used the Message Passing Interface (MPI), a message passing library that is developed and maintained by a consortium of academic, research, and industry partners, that can be added to sequential languages (C, Fortran) to program multiple nodes. Using this library, to set up a point-to-point or collective communication is simplified. In addition to High performance, network and process

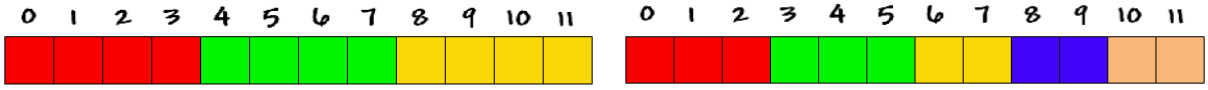
fault tolerance is provided, making this library optimal for the parallel programming. For the collective commmunication, lots of useful functions are provided, like the *MPI_ Bcast* to send data to all processes, the *MPI_ Gather* to gather data from all processes, the *MPI_ Scatter* to scatter data to all processes and others.

3.2 Work distribution

One of the major problems of the parallel algorithms is the load imbalance. If the work is not fairly distributed among the machines involved in the computation, there will be some machines idle while the others will still work. This problem affects a lot the performance of an application because the overall execution time depends on the last machine that terminate the computation. Looking at this specific case, there were two possible ways to follow: a fair distribution of the bodies or a fair distribution of the forces to compute. The major differences between this 2 approaches were encountered when the amount of work to distribute was not perfectly divisible by the number of machines. Using a simple *for* construct (Listing 3), it is possible to calculate the chunks of forces/bodies to assign to each computational node. The Figure 1 shows two examples of repartition.

```
int sum = 0;
int rem = workAmount % numProcs;
for (i = 0; i < numprocs; i++) {
    work_per_proc[i] = workAmount / numProcs;
    if (rem > 0) {
        work_per_proc[i]++;
        rem--;
    }
    displs[i] = sum;
    sum += work_per_proc[i];
}
```

Listing 3: fair distribution of work



(a) 3 computational nodes

(b) 5 computational nodes

Figure 1: Repartition of 12 forces/bodies

A comparison of the two approaches was reported on the next paragraphs in order to clarify the made decisions.

3.2.1 Approach 1 - Bodies repartition

The total amount of bodies (known at the beginning) is distributed as fairly as possible among the MPI processes as shown in the Listing 3. Then, to avoid a duplication of work, given a pair of bodies chunks, half of the forces are calculated by one MPI node, and half by the other. The repartition is clarified in the Figures 2, 3 and 4.

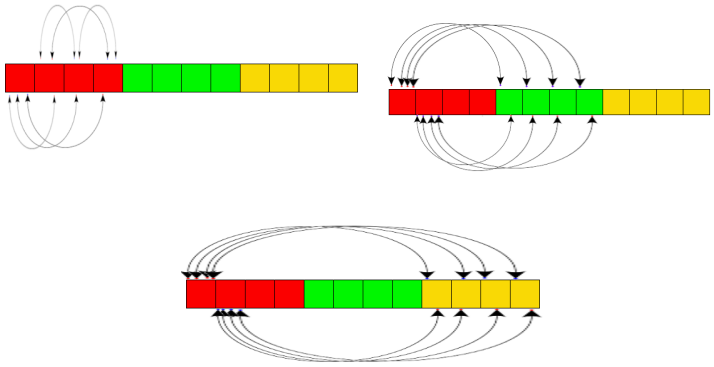


Figure 2: Forces computed by Node 0 (6+8+8=22)

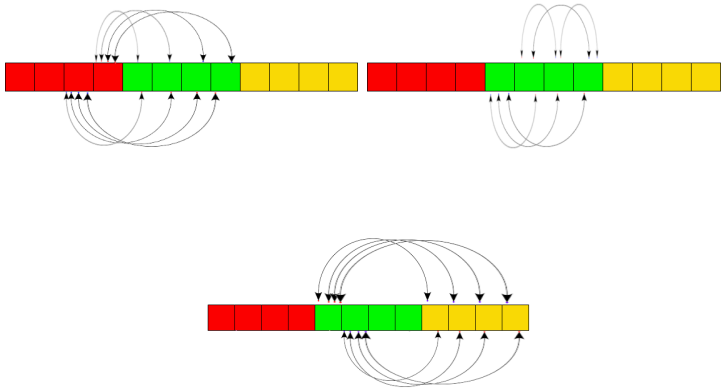


Figure 3: Forces computed by Node 1 (8+6+8=22)

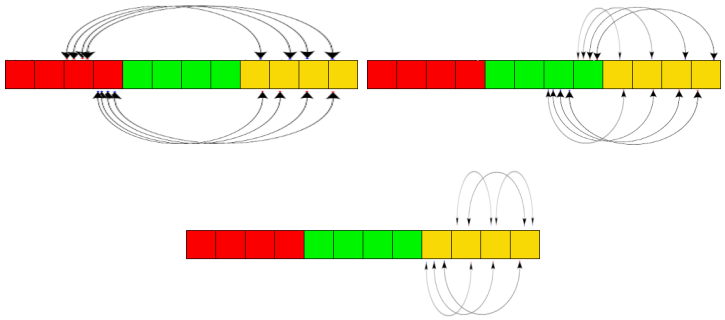


Figure 4: Forces computed by Node 2 (8+8+6=22)

Proceeding in this way, the forces between all pairs of bodies are calculated only one time per step. Each node computes the forces of 22 pairs. There are 3 nodes, so 3 times 22 is 66 that correspond to the number of possible pairs. No useful work is done. The approximated computational time is shown in the Equation 1. The first O represents the computation of the forces between the assigned chunk's bodies and the bodies of other chunks, while the second O represents the computation of the forces among the assigned chunk's bodies.

$$Complexity = O(\lceil\frac{N}{P}\rceil * (\lceil\frac{N}{P}\rceil * \frac{1}{2}) * (P-1)) + O(\sum_{i=1}^{\lceil\frac{N}{P}\rceil}(\lceil\frac{N}{P}\rceil - i)) \quad (1)$$

3.2.2 Approach 2 - Forces repartition

With this approach, the bodies are not taken into consideration, but only the forces to compute, resulting in a more simple and intuitive way to proceed. After calculating the total amount of forces to compute per step (Listing 4), these can be simply distributed as shown in Listing 3. The approximated computational time is shown in the Equation 2.

```
int forceCt = 0;
    for(i = 0; i < bodyCt; i++) {
        forceCt += i;
    }
```

Listing 4: total amount of forces

$$Complexity = O(\lceil \frac{N^2}{P} \rceil) \tag{2}$$

3.2.3 Load imbalance

As mentioned before, the load imbalance is a painful aspect of the parallel programming. If the total amount of work is perfectly divisible by the number of MPI processes, the two approaches are not so different, in fact, the number of forces calculated per machine is the same. The problems come out, when the work (bodies or forces) is not equally distributed. With the second approach, the inequity is simply reduced at the minimum. The maximum work difference between 2 nodes is of one force, that means less than 1% of load imbalance if the assigned forces per machine are more than 100. To reach this bound with 16 MPI nodes, for example, 58 bodies (1653 forces) are sufficient. With the First approach is more difficult to balance the work, because the assigned number of bodies is different, and from one body the forces that exerts on all the others has to be calculated, that means a load imbalance of *O(N)*. For this reason the second approach appeared more simple and efficient, so that it is adopted.

3.3 The final solution

3.3.1 Communication VS Computation

The communication is a common bottleneck of lots of parallel implementations. The data exchange between nodes should be reduced at the minimum in order to obtain good performances. The problem with the N body algorithm is that at every step the updated information (positions, velocities) of all other bodies of the system is needed in order to correctly compute the forces of the assigned chunk.. To gain performances, a good compromise between the data exchange and the work to do on each node has to be found. In particular, the ratio *computation/communication* should be maximized.

3.3.2 Approach one

Due to the fact that the force computation is the most expensive part of the algorithm and that as less data as possible should be exchanged, a good compromise is the following. The force (x, y) applied to a certain body is separated from the structure Body type, so at the beginning there are an array of N bodies and an array of N forces. As first thing, the bodies are broadcasted to all the nodes (*MPI_Bcast* Figure 5). After that, at each step, each node calculates the assigned forces, then with an *MPI_Allreduce* operation, all calculated arrays of N forces are summed (Figure 6) and as the last thing the velocities and positions for all the bodies are computed. Proceeding in this way, only an array of N elements containing the calculated forces is exchanged with the other nodes. The major problem with this approach, is that the positions and velocities of all the bodies are calculated in every node, that represents a duplication of work. An approximation of the complexity of a loop iteration and of the total amount of data exchanged per step is presented in Equations 3 and 4. In the first equation, the first *O* represents the force computation step, the second the velocities computation and the third the positions computation. In the second equation, the *2* represents the (x, y) values of the force.

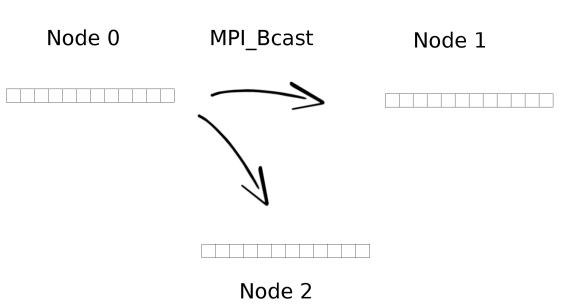


Figure 5: Broadcast the N bodies to all the nodes

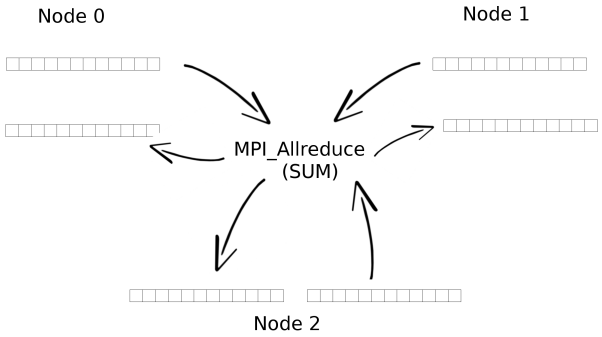


Figure 6: The N forces reduction

$$Complexity(perstep) = O(\lceil \frac{N^2}{P} \rceil)) + O(N) + O(N) \tag{3}$$

$$Communication(perstep) = O(2 * N) * sizeof(double) \tag{4}$$

3.3.3 Approach two

The aim of this approach, is to avoid the work duplication during the positions and velocities computation step. To calculate the force that two bodies exert on each other, at each step their mass, radius and position are needed. As first thing, the position (x, y) and the force of each body are separated from the structure Body type, so at the beginning there are an array of N bodies, an array of N positions and an array of N forces. The bodies and the positions are broadcasted to all the nodes and, after the calculation of the range of bodies and positions to assign to each node (with the method of Listing 3), they are Scattered (Figure 7). The force calculation step is the same as the one of the previous approach (calculation and *MPI_ Allreduce*), afterwards the assigned positions and bodies are updated. Before starting another iteration, with an *MPI_ Allgatherv* operation (Figure 8) the positions are gathered from all the nodes to all the nodes in order to have all the needed updated information for the next step. At the end, with an *MPI_ Allgatherv* operation the final bodies are gathered from all the nodes to the "master" node that prints the results. An approximation of the complexity of a loop iteration and of the total amount of data exchanged per step is presented in Equations 5 and 6. In the first equation, the first O represents the force computation step, the second the velocity computation and the third the position computation. In the second equation, the 4 represents the (x, y) values of the force and the (x, y) values of the position.

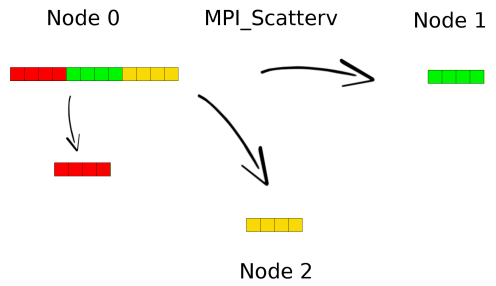


Figure 7: Distribute the N bodies to the nodes

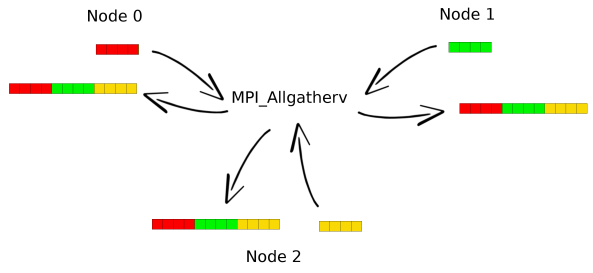


Figure 8: Collect updated positions from all the nodes

$$Complexity(perstep) = O(\lceil \frac{N^2}{P} \rceil)) + O(\lceil \frac{N}{P} \rceil) + O(\lceil \frac{N}{P} \rceil) \tag{5}$$

$$Communication(perstep) = O(4 * N) * sizeof(double) \tag{6}$$

3.3.4 Solutions comparison

After a comparison of the two solutions for different size of inputs (steps and number of bodies), the second approach appears quite better, especially when the number of bodies is big, so that the cost of exchange more data is well covered. In Tables 1 and 2 (corresponding graphs in Figure 9) and in Tables 3 and 4 (corresponding graphs in Figure 10) are shown the execution times and speedups of the 2 approaches for different problem sizes. The lines in the graphs are almost overlapping, so that are not really clear the differences between the two approaches. Looking at the data in the tables, it is easy to understand that the second solution is better, especially when the size of the problem is big (10000 bodies) and for this reason it is the one adopted.

nodes/approaches	1	2
1	474.974	474.974
2	241.078	240.339
4	123.869	123.335
8	65.733	65.470
16	37.264	37.427

Table 1: 256 bodies and 100000 iterations - Execution times

nodes/approaches	1	2
2	1.97	1.97
4	3.83	3.85
8	7.22	7.25
16	12.74	12.69

Table 2: 256 bodies and 100000 iterations - Speedups

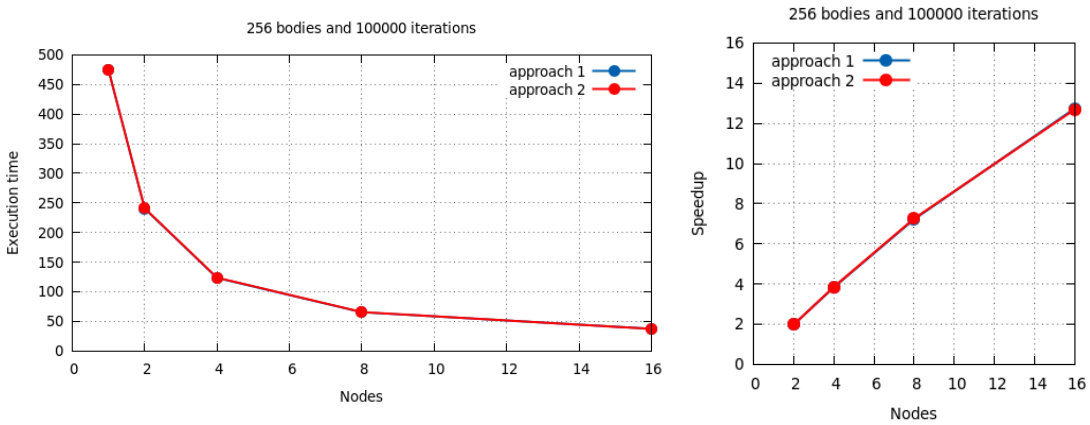


Figure 9: Execution Time and Speedups of the two approaches with 256 bodies and 100000 iterations

nodes/approaches	1	2
1	725.597	725.597
2	362.751	361,145
4	181.514	180.754
8	90.954	90.637
16	45.921	45.520

Table 3: 10000 bodies and 100 iterations - Execution times

nodes/approaches	1	2
2	2.0002	2.009
4	3.997	4.014
8	7.977	8.005
16	15.80	15.94

Table 4: 10000 bodies and 100 iterations - Speedups

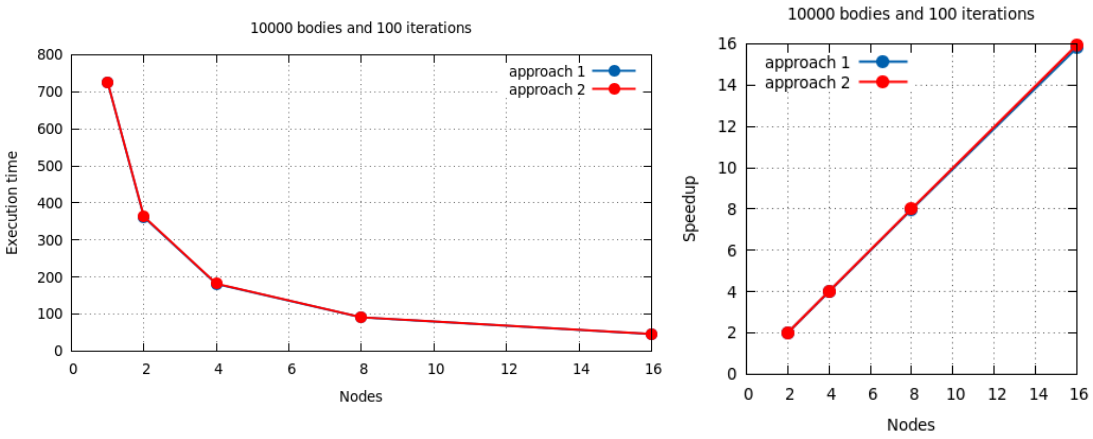


Figure 10: Execution Time and Speedups of the two approaches with 10000 bodies and 100 iterations

3.3.5 Results

In this section the most interesting obtained results are reported. In Figure 11 and Tables 5, 6 we have an example with a big number of iterations (fixed) and different numbers of bodies (small). In Figure 12 and Tables 7, 8 we have an example with a small number of iterations (fixed) and different numbers of bodies (big). As we can see, the more we increase the size of the problem (number of bodies) and the more the implementation obtains good speedups. An interesting aspect is that in some cases, the speedup is superlinear (Figure 12, Table 8, 1000 and 10000 bodies), due to the more cache and memory resources available on parallel systems. On a single machine, in fact, if the memory is not enough, there will be a lot of swapping and trashing, actions that are reduced having bigger available resources. The aim of parallel programming is to deal with big size problems, so this implementation is good because the more we increase the number of bodies, the more the speedup is close to be linear.

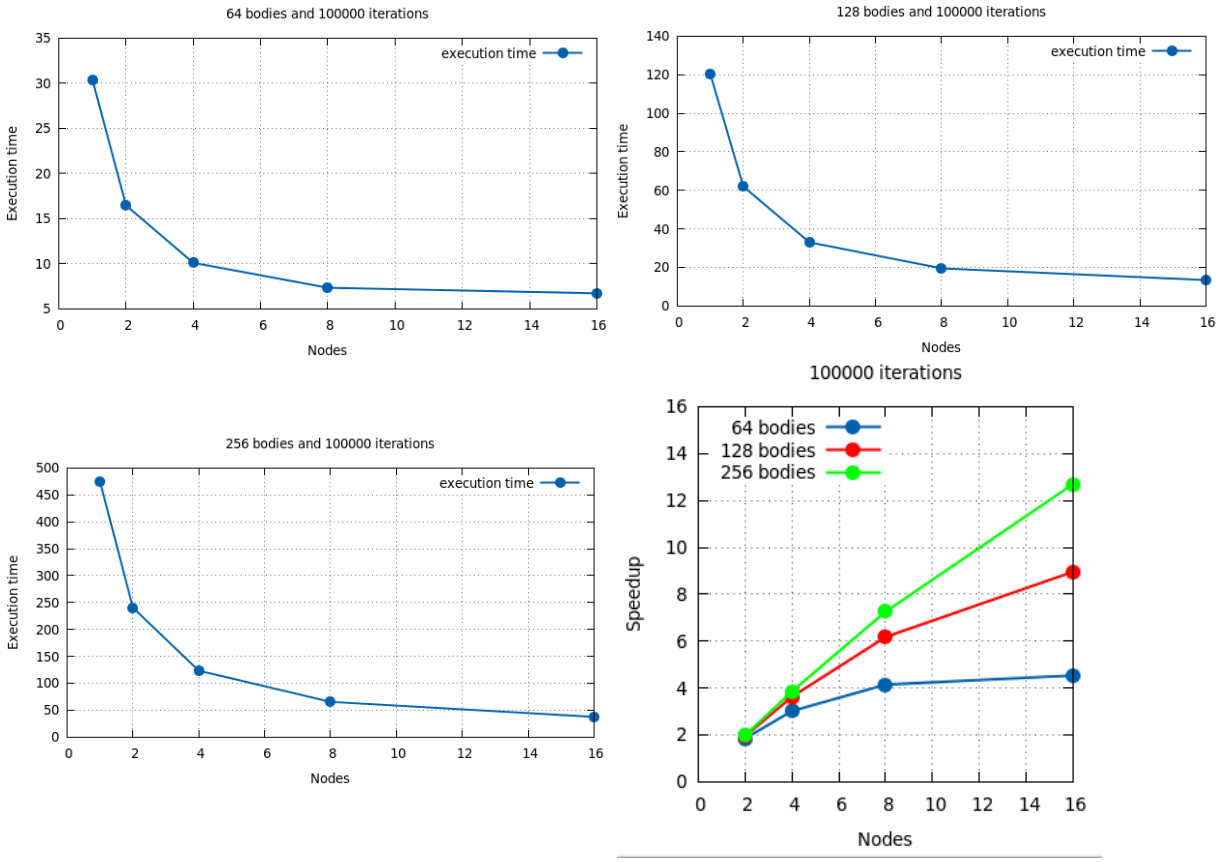


Figure 11: Execution Time and Speedups, 100000 iterations

nodes/bodies	**64**	**128**	**256**
1	30.414	120.347	474.974
2	16.463	61.939	240.339
4	10.095	33,231	123.335
8	7.336	19.477	65.470
16	6.708	13.44	37.427

Table 5: 100000 iterations - Exec. times

nodes/bodies	**64**	**128**	**256**
2	1.84	1.94	1.97
4	3.012	3.62	3.85
8	4.14	6.17	7.25
16	4.53	8.95	12.69

Table 6: 100000 iterations - Speedups

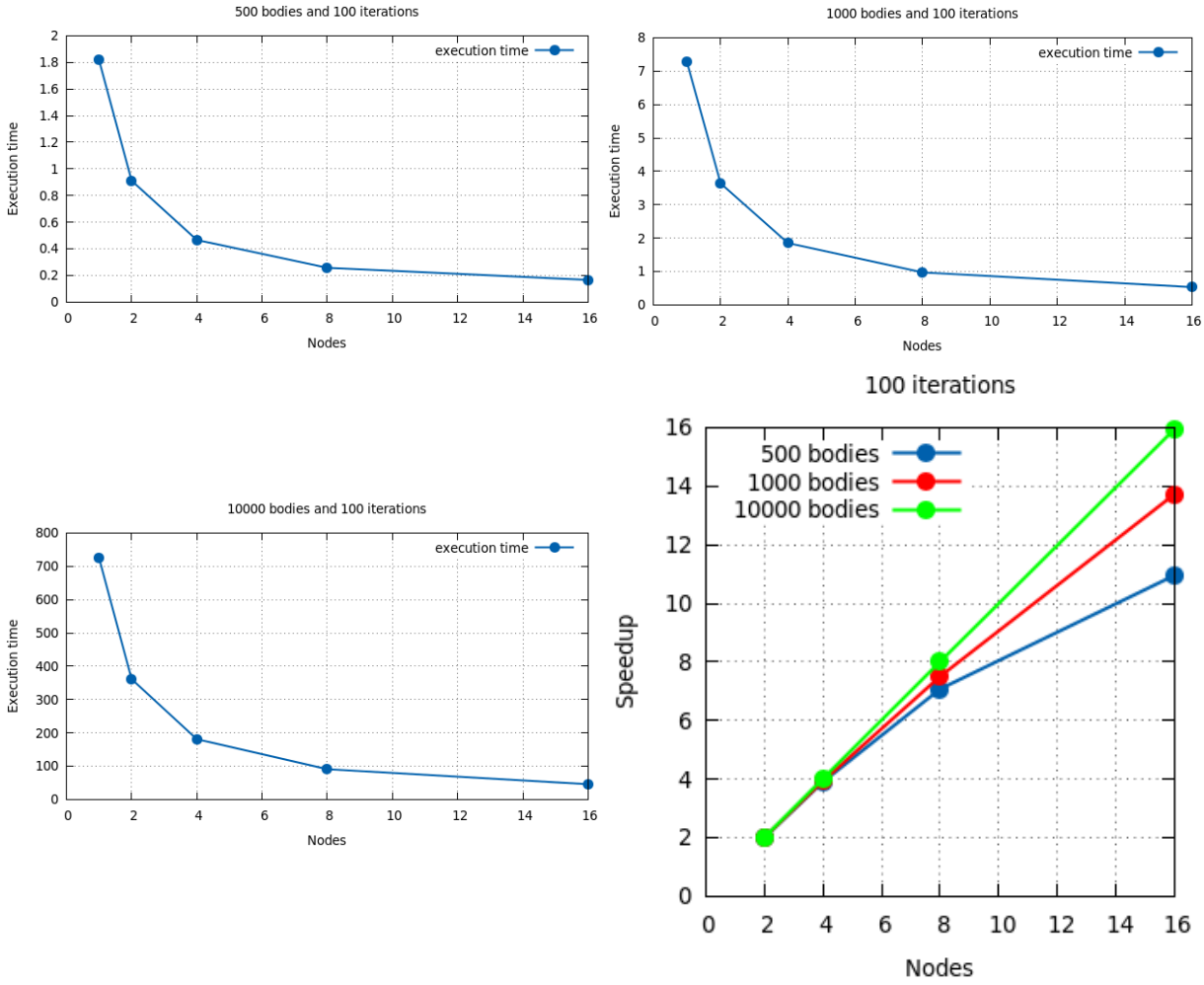


Figure 12: Execution Time and Speedups, 100 iterations

nodes/bodies	500	1000	10000
1	1.818	7.275	725.597
2	0.911	3.636	361,145
4	0.466	1.849	180.754
8	0.257	0.969	90.637
16	0.166	0.530	45.520

Table 7: 100 iterations - Exec. times

nodes/bodies	500	1000	10000
2	1.99	2.0008	2.009
4	3.90	3.93	4.014
8	7.07	7.50	8.005
16	10.95	13.72	15.94

Table 8: 100 iterations - Speedups

With the same number of bodies, but different number of iterations, the obtained speedup was more or less the same (Figure 13 and Tables 9, 10). However, this is not surprising, because, for the same amount of bodies, there is the same work to do, but this is repeated for a different number of times.

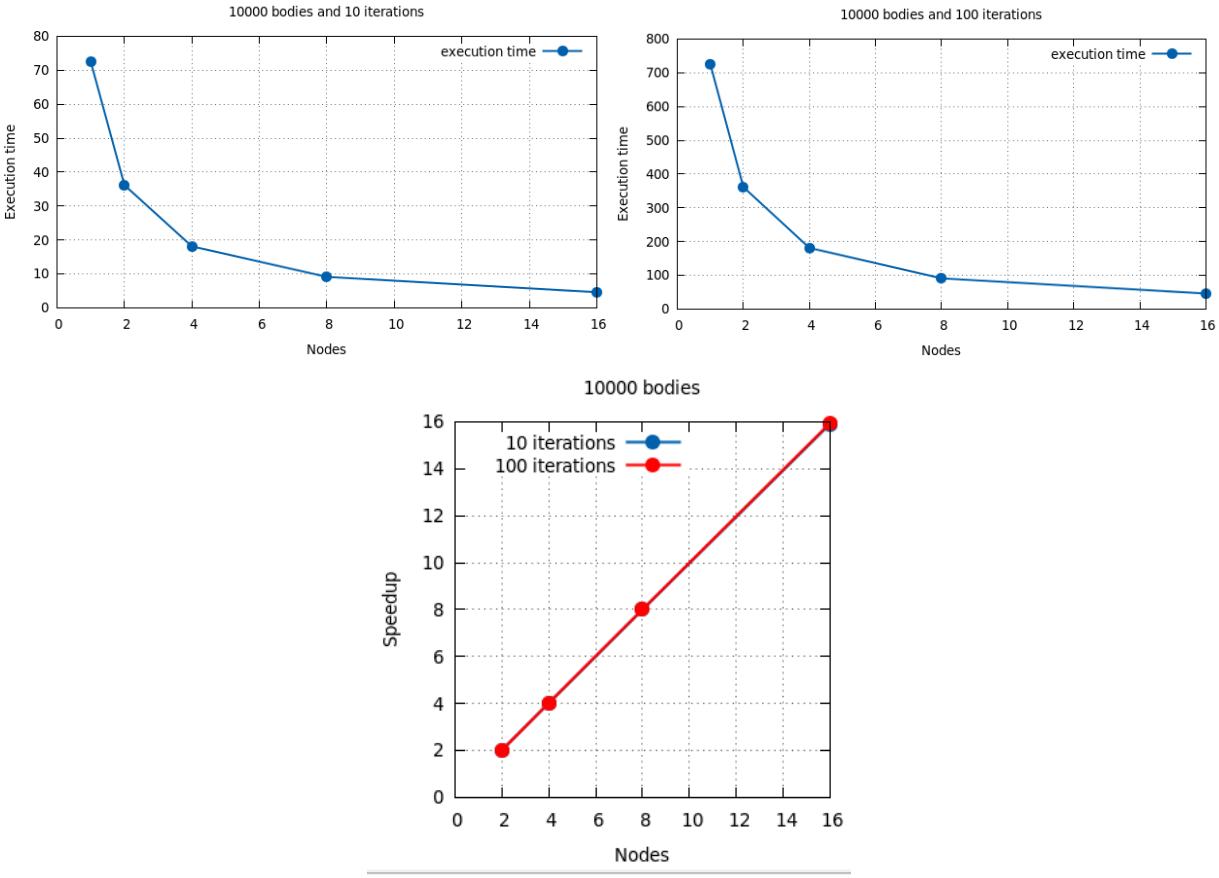


Figure 13: Execution Time and Speedups, 1000 bodies

nodes/iterations	10	100
1	72.539	725.597
2	36.111	361,145
4	18.076	180.754
8	9.076	90.637
16	4.562	45.520

Table 9: 10000 bodies - Execution times

nodes/iterations	10	100
2	2.008	2.009
4	4.013	4.014
8	7.99	8.005
16	15.90	15.94

Table 10: 10000 bodies - Speedups

All the tests were performed on the Delft University of Technology (TUD) cluster (fs3.das4.tudelft.nl) and the execution times were measured using the "wall clock time". The data distribution and the data gathering, as being part of the application initialisation and de-initialisation, were not considered measuring the performance.

4 Conclusions and Personal considerations

With the realized implementation, the speedups are close to be linear for big size problems and that means that is a good implementation. The MPI programming model dimonstrated to be optimal for this kind of works. At the beginning this model could appear hard to understand, especially for the MPI operations (e.g. MPI_Allgatherv, MPI_Scatterv), but after a short period of training it reveals all its power. Another interesting fact, is that programming using this library it could be useful, like in this particular project case, to have more than one implementation in order to compare the results and outline any weaknesses.