Syddansk Universitet

DM818 Assignment 2

# Parallel Particle Simulation

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# Chapter 1

# Introduction

This reports documents the second mandatory assignment for the course DM818 Parallel Computing. In this assignment we were given a particle simulation which runs in $O(n^2)$ time, and were asked to code the following:

1. Change the implementation such that it runs in $O(n)$ time.
2. Parallelize the changed code using either OpenMP, PThreads, or MPI.

In order to measure proper performance gain, we need to optimize the serial algorithm first, and then parallelize it such that the comparison stays fair. It would be easy to show a massive performance gain if the algorithm for the parallel implementation is vastly superior to the one used for linear.

## 1.2 Work Load

The distribution of the workload has been equal, and pair programming in the IMADA terminal room have been the preferred method throughout this project.

# Chapter 2

# A Linear Algorithm

## 2.1 The Base Algorithm

The given algorithm for the serial implementation (and the parallel versions) are as follows, clearly running in $O(n^2)$ runtime. This was unacceptable and thus a new algorithm has been developed.

```
for(int i = 0; i < n; i++) {
  particles[i].ax = particles[i].ay = 0;
  for (int j = 0; j < n; j++) {
    apply_force(particles[i], particles[j]);
  }
}
```

The problem with this algorithm is that it applies forces between all pairs of particles, while the rules for the particle simulation states that any particle may only be affected by nearby particles.

## 2.2 The new algorithm

The range for interaction for the particles was reduced to a smaller value, denoted as the "cutoff" value. This cutoff value was showcased as a grey border on a particle in the assignment.

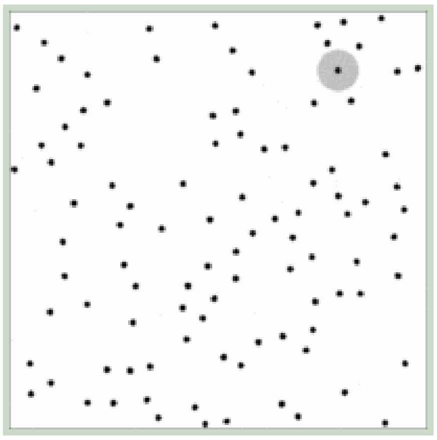


Figure 2.1: Snapshot of the GIF from the assignment showcasing the influence ring.

Having a reduced area of interaction, allows us to reduce the amount of particles influencing the amount of force needed to be applied to a given particle, thus we can reduce the inner for-loop greatly.

In order to reduce the loop it is necessary to know which particles are within (or at least close by) the particle we want to apply the force. To do this we needed to develop a data structure, to keep track of where the particles are positioned.

In order to track the location of the particles, the coordinate system is divided into a grid of cells. Each cell holds some number of particles within a sub-grid of the entire universe. The sizes of the cells are chosen to match the “cutoff” value, such that we only need to check the neighboring cells for collisions with a particle.

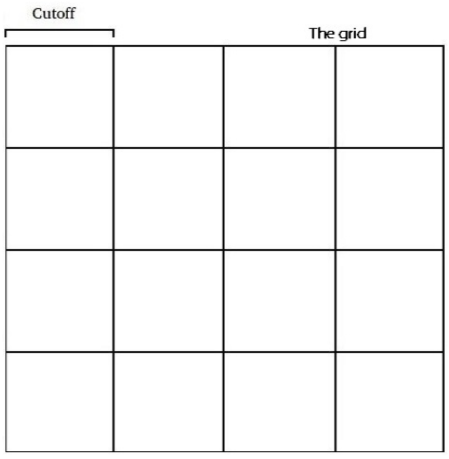


Figure 2.2: The grid structure, showcasing the size of a single position equals the cutoff size.

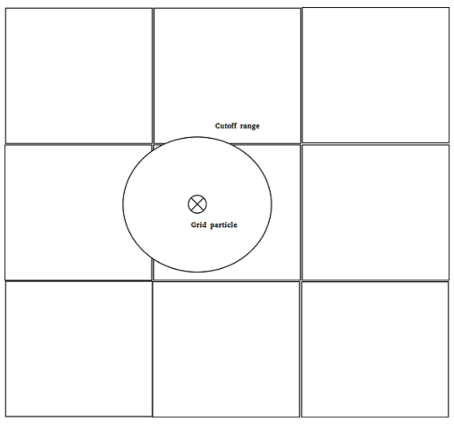


Figure 2.3: A particle located inside a grid positions, and its influence range.

Initially all particles are added to the grid. When updates are performed on a particle, it will be moved to the appropriate cell as well.

## 2.3 Implementing the Grid Approach

The implementation uses a separate file named `grid.cpp` and `grid.h`. These files holds the data structure and a series of helper methods that allows us to add, get and remove particles to the grid.

The grid itself is a vector of vectors with particles.

```
std::vector<std::vector<particle_t *> > grid;
```

The coordinate positions consists of doubles, while the grid positions are mapped to integers. To overcome this the coordinate positions are simply converted using the following formula, which simply moves the decimal two places to the right and casting to an integer. Thereby giving us a consistent mapping of doubles to integers:

$$\frac{\text{double value}}{0.01}$$

Whenever we move a particle, we simply remove the particle from the grid completely, and then add it back in. This way the old position is removed, and the new position is calculated from the particles new position when added again.

This method assumes the particle always switches position in the grid, it could be calculated whether this actually is the case, but this was not done. Consequence to this method is that some unnecessary calculations might be performed whenever a particle do not move, since it would be removed and added back to the same grid position. The correctness of the algorithm is however not affected.

## 2.4 Performance of the New Algorithm

Below is a graph plotted for different times (see appendix A) showcasing how the $O(n^2)$ and $O(n)$ algorithms do versus each other. It is easy to see that the $O(n)$ is indeed linear. Note that bigger sizes did not terminate in reasonable time for the $O(n^2)$ algorithm.

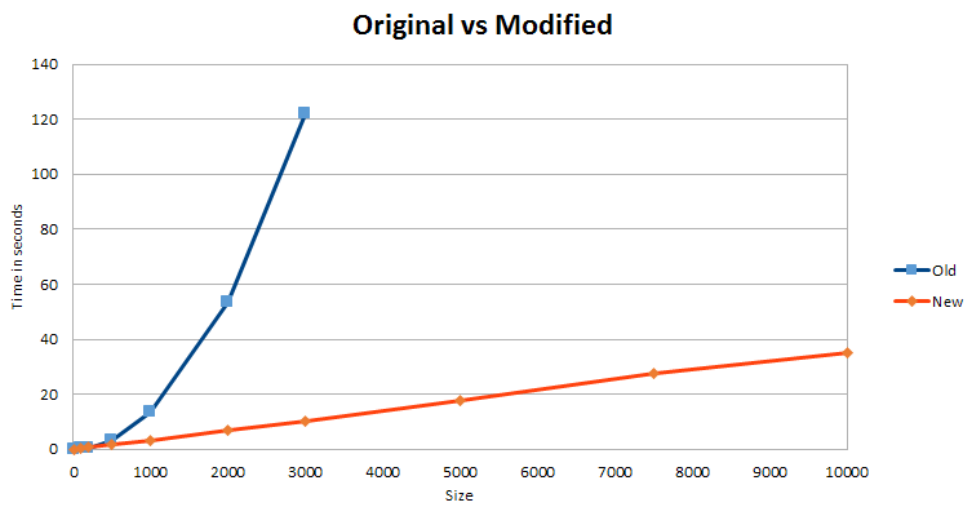


Figure 2.4: The original $O(n^2)$ algorithm (blue) versus the new $O(n)$ algorithm (red).

# Chapter 3

# Parallelization using OpenMPI

Throughout this chapter we will discuss how our serial implementation was parallelized. The parallelization was done using OpenMPI, and we will be referring to concept found in this library whenever relevant.

## 3.1 Model for Communication

We would like to share the work onto multiple processors, to parallelize our serial implementation. Looking at our implementation it seems obvious to give each processor a set of cells to be responsible for, instead of giving each processor a set of particles to be responsible for. By letting each processor be responsible for a zone, it can perform most of the work completely locally, since each cell can only contain particles that will be affected by particles in neighboring zones. This means that only particles lying in a cell at the border of the zone, may be affected by a cell not owned by the local processor.

There are several ways in which the grid may be divided into zones for the processors. For the sake of simplicity each processor is given some number of rows in the grid, for which they are responsible. This means that any processor will have at most two neighboring processors, the one responsible for the rows above, and the one for the rows below.

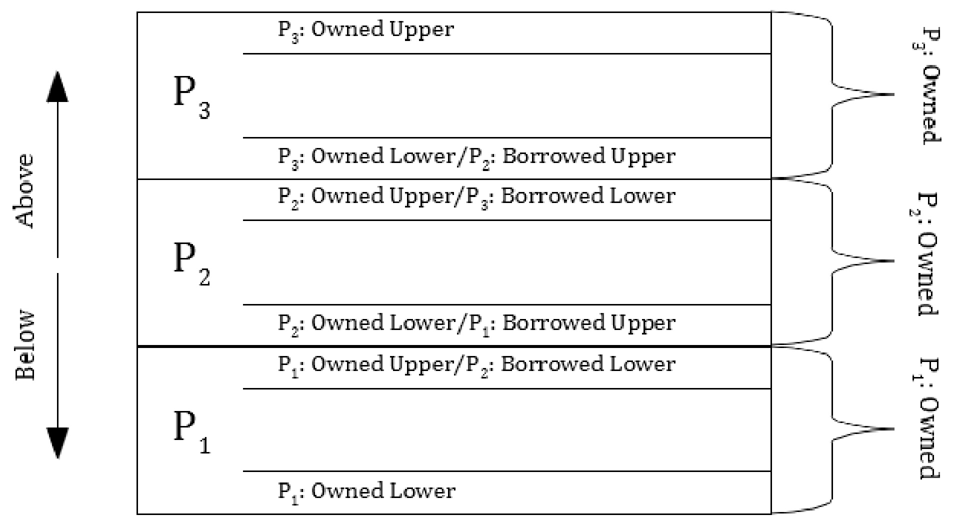

P3: Owned Upper
P3
P3: Owned Lower/P2: Borrowed Upper
P2: Owned Upper/P3: Borrowed Lower
P2
P2: Owned Lower/P1: Borrowed Upper
P1: Owned Upper/P2: Borrowed Lower
P1
P1: Owned Lower
Above
Below
P3: Owned
P2: Owned
P1: Owned

Figure 3.1: Splitting the grid into zones.

To deal with the problems of the zones lying at the border of a zone, we've introduced the concept of borrowed and owned zones as shown in figure 3.1. These zones are exactly correspond to exactly one row in the grid. Each processor will contain up-to-date "borrowed" copies of these zones. The figure how each processor identifies the different zones. Each processor will have to communicate with its neighbors to keep these zones in sync.

## 3.2 Synchronization of Nodes

As discussed in the previous section, each processor will need to keep synchronized copies of zones that they borrow from each other. Since we in every iteration may make a change to these zones, we will need to perform this synchronization step in every single iteration as well. The synchronization process is two-fold, first we gather up-to- date information, and then we merge our information to get a correct picture of the system.

**Step 1: Synchronize Processors**

At the beginning of every iteration, we will need to synchronize all processors, such that they are all ready for the next iteration. Once they are ready for the next iteration, we may begin exchanging information. This synchronization can be done using the `MPI_Barrier` procedure.

**Step 2: Prepare for Exchange with Neighbors**

A processors' neighboring processes will expect a complete image of how the zone it is borrowing looks. This message needs to be prepared, such that we can transmit it, this process consists solely of packing all the particle into a single buffer.

Before beginning the exchange, we will also clear out any particles that reside inside of the borrowed zones. This is done since we will receive a completely new zone from our neighbors.

**Step 3: Exchange Message with Neighbors**

Once the messages are ready, we may exchange data with our neighbors. For efficiency reasons we use `MPI_SendRecv`, which allows for simultaneously sending and receiving data between two nodes. MPI requires that both parties involved in the transfer, call this function with each other as arguments. For this reason, the following pattern has been established: processors with an even rank communicate with the processor above it first, while processors with an odd rank will communicate with the processor below first. The exchange process between two processors go like this:

1. Exchange sizes (in particles) of zones
2. Exchange the particles, this exchange requires the knowledge of how many particles we will receive
3. Exchange sizes of local insertions into borrowed zones
4. Exchange particles involved in local insertions into borrowed zones

It should also be noted that this means that the synchronization process for the system as a whole, will only take the time of communicating with each neighbor, since these are all done in parallel.

**Step 4: Update the World**

We have already discussed that we share our owned zones with our neighbors. The reason for this fairly simple, we're the ones responsible for updating these zones, hence we are the ones capable of telling our neighbors about updates made in it.

However, it is also possible for particles to migrate from one processor to another. Hence we need to track whenever we perform an insertions of particles from our owned zone into a borrowed zone. These particles are all tracked in a separate buffer, and exchanged with the neighbor in step 3.

The insertions that we receive from our neighbors are then merged together with our own local view to give a completely up-to-date view of the system.

**Step 5: Cleanup**

Finally we clear out our local insertions from an owned zone into a borrowed zone. Such that we're ready for the next iteration.

## 3.3 Implementation Details

1. What we do when we actually work (This hasn't changed)

## 3.4 Load Balancing

1. How do we distribute particles? Limitations and potential changes
2. The current implementation has a severe limitation on how many nodes can be used. This could be changed by balancing the load differently

## 3.5 Performance

1. Overall performance
2. Breakdown of time used in a single run

## 3.6 Testing

1. (Should also be added to serial)
2. Testing stuff

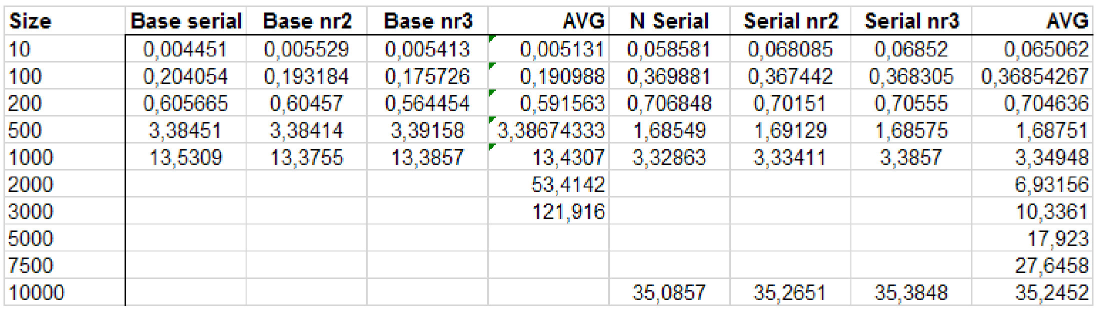
# Chapter 4

# Conclusion

# Chapter 5

# Appendix

## 5.1 Serial algorithm plotting data



| Size | Base serial | Base nr2 | Base nr3 | AVG | N Serial | Serial nr2 | Serial nr3 | AVG |
|---|---|---|---|---|---|---|---|---|
| 10 | 0,004451 | 0,005529 | 0,005413 | 0,005131 | 0,058581 | 0,068085 | 0,06852 | 0,065062 |
| 100 | 0,204054 | 0,193184 | 0,175726 | 0,190988 | 0,369881 | 0,367442 | 0,368305 | 0,36854267 |
| 200 | 0,605665 | 0,60457 | 0,564454 | 0,591563 | 0,706848 | 0,70151 | 0,70555 | 0,704636 |
| 500 | 3,38451 | 3,38414 | 3,39158 | 3,38674333 | 1,68549 | 1,69129 | 1,68575 | 1,68751 |
| 1000 | 13,5309 | 13,3755 | 13,3857 | 13,4307 | 3,32863 | 3,33411 | 3,3857 | 3,34948 |
| 2000 | | | | 53,4142 | | | | 6,93156 |
| 3000 | | | | 121,916 | | | | 10,3361 |
| 5000 | | | | | | | | 17,923 |
| 7500 | | | | | | | | 27,6458 |
| 10000 | | | | | 35,0857 | 35,2651 | 35,3848 | 35,2452 |

Figure 5.1: Plotting data for the linear runtimes.