Parallelization on PC clusters - Experimental evidence of the Collatz conjecture

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Contents

The problem

In this chapter we will explain the problem we are trying to solve.

The Syracuse recurrence

Before we can define the problem we are facing we need to define some mathematical vocabulary.

The Syracuse recurrence is a recurrence relation on positive integers. It is defined this way :

$$R(x) = \begin{cases} \frac{n}{2} & \text{if n is even} \\ 3n+1 & \text{if n is odd} \end{cases}$$

The Syracuse series

Now that we have defined the Syracuse recurrence we can define a Syracuse series. There are as many series as positive integers. We can define the k^{th} Syracuse series this way:

$$S_k(n) = \begin{cases} k & \text{if } n = 0 \\ R\left(S_k(n-1)\right) & \text{otherwise} \end{cases}$$

Examples

- The 4^{th} series: 4, 2, 1, 4, 2, 1, ...
- The 7^{th} series: 7, 22, 11, 34, 17, 52, 26, 13, 40, 20, 10, 5, 16, 8, 4, 2, 1, ...
- the 8^{th} series: 8, 4, 2, 1, 4, 2, 1, ...

The Collatz/Syracuse conjecture

As you might already have noticed, the series are infinite and more interesting it seems they always eventually reach 1. We can now define the Collatz conjecture in different ways (they are both equivalent):

- Every Syracuse series eventually reach 1
- Every Syracuse series only contain the trivial cycle (1, 4, 2)

There are other ways to define this conjecture but we will not use them so it was not useful to include them in this document.

The aim of the project

The aim of this project is to check that the Collatz conjecture is true for as many series as possible (starting at 2). We will try to find an efficient algorithm and make it parallel in order to be able to run it on the EPFL deneb cluster.

Algorithms and strategies

Naive algorithm

Sequential implementation

This is the naive sequential algorithm:

```
for(i = 2; i < T; i++) {
  j = i
  l = 0; //the length of the serie
  while (j != 1) {
    if (j%2 == 0) {
      j = j/2
    } else {
      j = 3*j + 1
    }
    l++;
  }
}
```

If this piece of code does stop. Then the Collatz conjecture is verified for all Syracuses series up to T.In Any real world application we would like to add a cycle detection algorithm but here we are more interested in the parallelization of this algorithm.

Complexity analysis Before we can do a proper analysis, we need to do some empirical tests. Indeed, for each starting point, we don't know in advance how many iterations of the Syracuse recurrence it will take before we reach 1. So we cannot really determine the complexity of the algorithm in advance. For this analysis we will use the naive sequential approach to determine the number of steps. For example to reach 1 starting from 3 it take 7 steps to reach 1 :

```
3 -> 10 -> 5 -> 16 -> 8 -> 4 -> 2 -> 1
```

Using the very naive approach we compute the average number of iterations to reach 1 for each starting point from 2 to T. We did it for each $T \in \{10^x | x \in [1; 8]\}$. Let's note $f(x)$ the average number of steps per integer to compute from 2 to 10^x. For example $f(1) = 7.44$ because as you can see in the example we gave before, the average of the values is 7.44. Here are the values we found for $f(1)$ to $f(8)$ (It takes too much time on a single machine to compute more).

```
7.4444444444444
31.737373737374
59.601601601602
84.975097509751
107.53947539475
131.43455543456
155.27249862725
179.23493762235
```

As you might remark, the values are almost perfectly linear. It was not expected but it will be very convenient for our analysis. As we are in exponential scale, we can deduce that the number of steps for each starting point is logarithmic. To be more precise here is the approximate formula :

$$f(x) \simeq 7.44 + 24.6(x - 1)$$

We now have the number of steps of the naive algorithm :

$$T \times f(\log_{10}(T)) = \mathcal{O}(T \log(T))$$

Parallel implementation

As you can see there are no dependencies between all instances of the for loop. This means this algorithm can be parallelized by spreading all i's among nodes. We can expect a prefect linear speedup. But only if we spread the i's randomly because there are some series more expensive than the others. Parallelizing this algorithm is so simple it's not worth it to detail it here.

The heuristic

Description of the heuristic

A simple (yet powerful) heuristic for this problem is to apply a time-memory trade-off. We can save for each starting point we already computed the number of iterations before reaching 1.

For example we compute the number of steps to go from 5 to 1 it take 5 steps, we memorize it. When we want to compute starting at 10. We apply the recurrence once and we find 5 (because $10/2 = 5$) we can deduce that the number of steps from 10 to 1 is $1 + 5 = 6$. And it took only 2 iterations instead of 6 for the naive algorithm.

Sequential implementation

Here is the algorithm:

```
memory = new Hashmap();
for (i = 2; i < T; i++) {
  j = i
  l = 0 // the length of the serie
  while (j > 1) {
    if (memory[j] != undefined) {
      l = memory[j]
    } else {
      if (j%2 == 0) {
        j = j/2
      } else {
        j = 3*j + 1
      }
      l++;
    }
  }
  memory[i] = l;
}
```

In the practical implementation of this algorithm I used a tail recursive function instead of the while loop in order to save all steps to the `memory` hash map.

Complexity analysis The problem to evaluate this new algorithm is that we cannot predict how many iterations it will take before we reach a value we already know (i.e. already in the hashmap). We can't even predict **if** we will be using the hashmap for a given series.

To overcome this we also did an empirical approach to estimate this value. We note $g(x)$ the number of **iterations** it took with this new algorithm. x goes also from 1 to 8.

```
4
9.1010101010101
6.3833833833834
6.1842184218422
6.2091520915209
6.2262642262642
6.2359355235936
6.2389850023899
```

As we can see it seems that the values of $g(x)$ are converging to a value near 6.24. This is great because we can assume that with this algorithm the amortized complexity for each integer is constant. We now have the complexity for the new algorithm:

$$T \times g(log_{10}(T)) = \mathcal{O}(T)$$

Parallel implementation

Here is the strategy we will be using to parallelize this algorithm: We will divide T (the number of series we want to test) into N equal rounds. We will also divide each round among all nodes. Each round will consist in two stages:

1. **Computation stage**: each node compute its sub-interval of T (and uses his precomputed values table which is initially empty)
2. **Sharing stage**: nodes share their new precomputed values between each others (only the ones they learnt during the last computation stage.

The algorithm is described visually in the figure 1.

Theoretical Analysis

The naive algorithm is very easy to parallelize because there is no shared state between the iteration. On the other side, in the improved algorithm we memorize the previous values. The problem is that nodes cannot share all their memory. If we distribute the algorithm, at some point precomputed values will not be available when needed. We had to evaluate the how the algorithm behaves when only part of memorized values are available.

Here are the number of **iterations** needed to compute the values from 10^1 to 10^8 if only 50% of the precomputed values are available

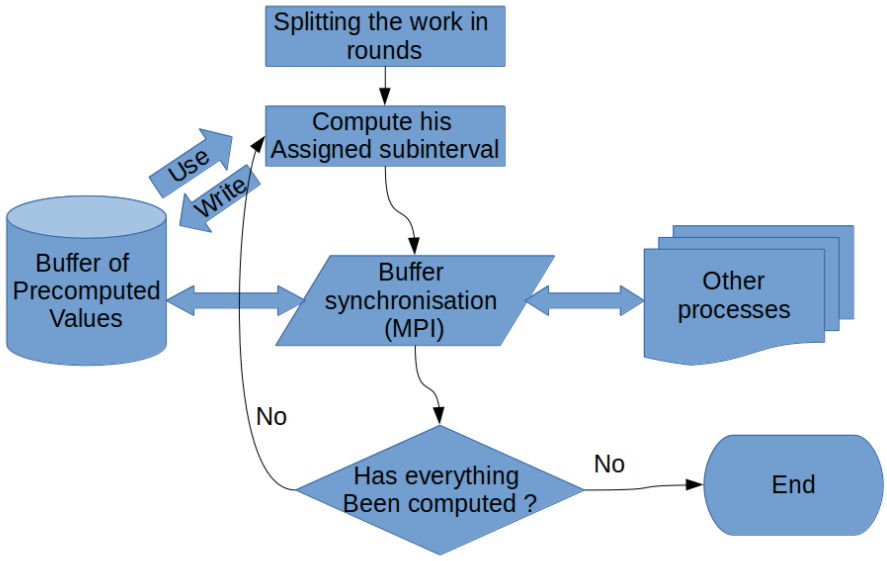

Figure 1: Algorithm

```
7.6666666666667
11.058823529412
7.7884231536926
8.0161967606479
8.1495170096598
8.1739256521487
8.1845663630867
8.1816952563661
```

And here are the result if only 1% of the values are available:

```
7.4444444444444
31.737373737374
54.368314833502
40.619634380366
41.315612973606
41.427014720187
42.121434533188
42.143153897544
```

As the experiment shows, it seems that the value is still constant. This is great

for us because it means we still have a linear algorithm even if all the memory is not shared between nodes.

Now we know that the overall complexity stays linear even if we don't have all precomputed values we can do a proper analysis.

Upper bound speedup

If we choose to have only one round of computation there is no communication between nodes. Moreover there are no initialization phase. That means, thanks to Amdahl's law, we can reach an infinite speedup with an infinite number of nodes. The problem is if we have only one round (no sharing) the algorithm is very slow, so even if we can parallelize it on multiple nodes easily it has a very bad efficiency.

I order to have a better estimation we will need a detailed speedup formula.

Detailed analysis

Timing Diagram

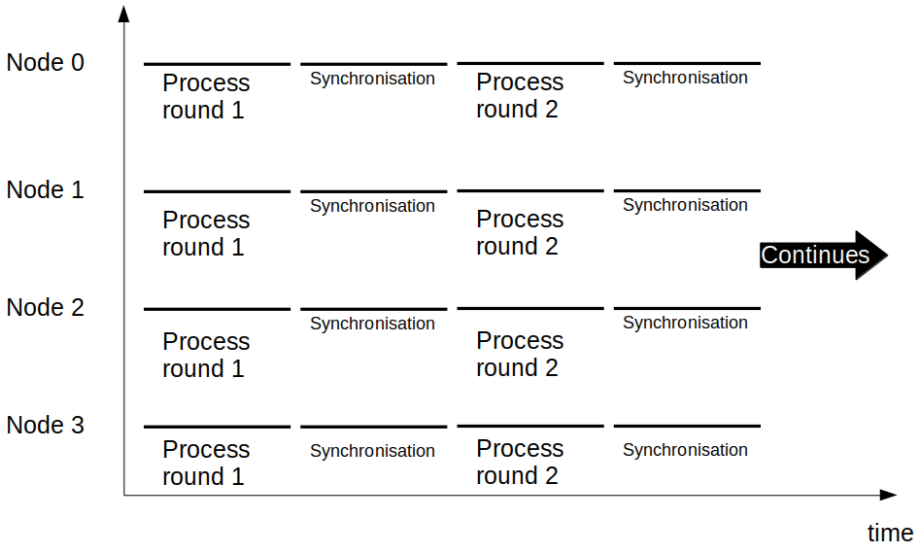

Figure 2: Timing Diagram (4 nodes)

The critical path is always a straight line on the node that has the longest last processing round. This comes from the fact that there is no master node. In our model we assume all processing round take the same amount of time. With this assumption all paths are critical paths.

Theoretical analysis

Let's define the 3 parameters of our model:

N : The number of computation nodes

M : The number of rounds

T : The target (The number of series we want to compute)

We will cut the interval we want to compute into $M \times N$ sub-intervals named τ_1 to $\tau_{M \times N}$. In our model, we will assume the work associated to a sub-intervals do not deviate too much from the average case. We will note $t = \frac{T}{N \times M}$ the number of series to compute in a given sub-interval.

In round r each node (of id n), we compute $\tau_{n+r \times N}$. And between each computation round, each node broadcast the new values he found so the others can use it in order to shorten their computation time.

As we can see on the timing diagram, the critical path is clearly a straight line on node 1.

We will now try to estimate the speedup using this model. The time to solve the problem with the optimized sequential algorithm is $W_{seq} = C_1 \times T$ for some C_1

The time to solve a sub-interval(red block in the timing diagram) assuming we have enough precomputed values available is $W_{si} = C_2 \times t$. In average we have $C_2 > C_1$.

In the communication part, each node has to send the new values it precomputed during the previous round to all other nodes. We know we can't have more new values than the number of the iterations of the algorithm. QWe know each broadcast can be done in $C_3 \times \log(N) \times t$ for some C_3. We need to do this for each node so the communication part can be done in $W_{com} = C_3 \times N \log(N) \times t$.

In the last part (yellow in the timing diagram), each node has to send his results. But it does not need to send it all because most of it was already sent during the previous communication rounds. It only has to send exactly t values. It can be done in time $C_4 \times t$ for some C_4. The whole merging phase can be done in $W_{merge} = C_4 N t$.

We can now compute the length of the critical path (W_{cp}).

$$\begin{aligned} W_{cp} &= M \times W_{si} + (M-1)W_{com} + W_{merge} \\ &= MC_2 t + (M-1)tN\log(N)C_3 + NtC_4 \\ &= MC_2 \frac{T}{NM} + (M-1)\frac{T}{NM}N\log(N)C_3 + N\frac{T}{NM}C_4 \\ &= \frac{C_2 T}{N} + (M-1)\frac{T}{M}\log(N)C_3 + \frac{T}{M}C_4 \end{aligned}$$

To simplify our understanding, instead of computing W_{cp} we will compute an upper bound for it. Let's consider $C_5 = \max(C_3, C_4)$

$$\begin{aligned}
W_{cp} &< \frac{C_2 T}{N} + \frac{T}{M}\left((M-1)\log(N)C_5 + C_5\right) \\
&< \frac{C_2 T}{N} + \frac{T}{M}\left((M-1)\log(N)C_5 + C_5\log(N)\right) \text{because } N \geq 1 \\
&= \frac{C_2 T}{N} + \frac{T}{M} M\log(N)C_5 \\
&= \frac{C_2 T}{N} + T\log(N)C_5 \\
&= T\left(\frac{C_2}{N} + \log(N)C_5\right)
\end{aligned}$$

Let's compute the speedup:

$$\begin{aligned}
S_p &= \frac{W_{seq}}{W_{cp}} \\
&> \frac{TC_1}{T\left(\frac{C_2}{N} + \log(N)C_5\right)} \\
&= \frac{C_1}{\frac{C_2}{N} + \log(N)C_5} \\
&= \frac{NC_1}{C_2 + N\log(N)C_5}
\end{aligned}$$

As we can see, the limit of our speedup when N reach ∞ is 0. But for some values of the constant we can get a positive speedup for some values of N. We can split our analysis into 3 cases.

- $C_5 \sim C_2$: The speedup is always decreasing, and less than 1.
- $C_5 < C_2$: The speedup grows until it reach a global maximum and the decrease to 0.
- $C_5 \ll C_2$: The speedup is almost linear and the slope of the line is C_1/C_2

You can see the 3 cases on Figure 3

Estimating the values of the constants

In order to predict if there will be a speedup in real life we need to have an rough idea of C_1, C_2 and C_5.
From experiments on the sequential program we found that $C_1 \simeq C_2 \simeq 3 \times 10^{-8}$

If we suppose we have an Intel 40Gb/s QDR IB network, according to the mellanox website we would have a throughput of 3.2GB/s. C_5 roughly represent

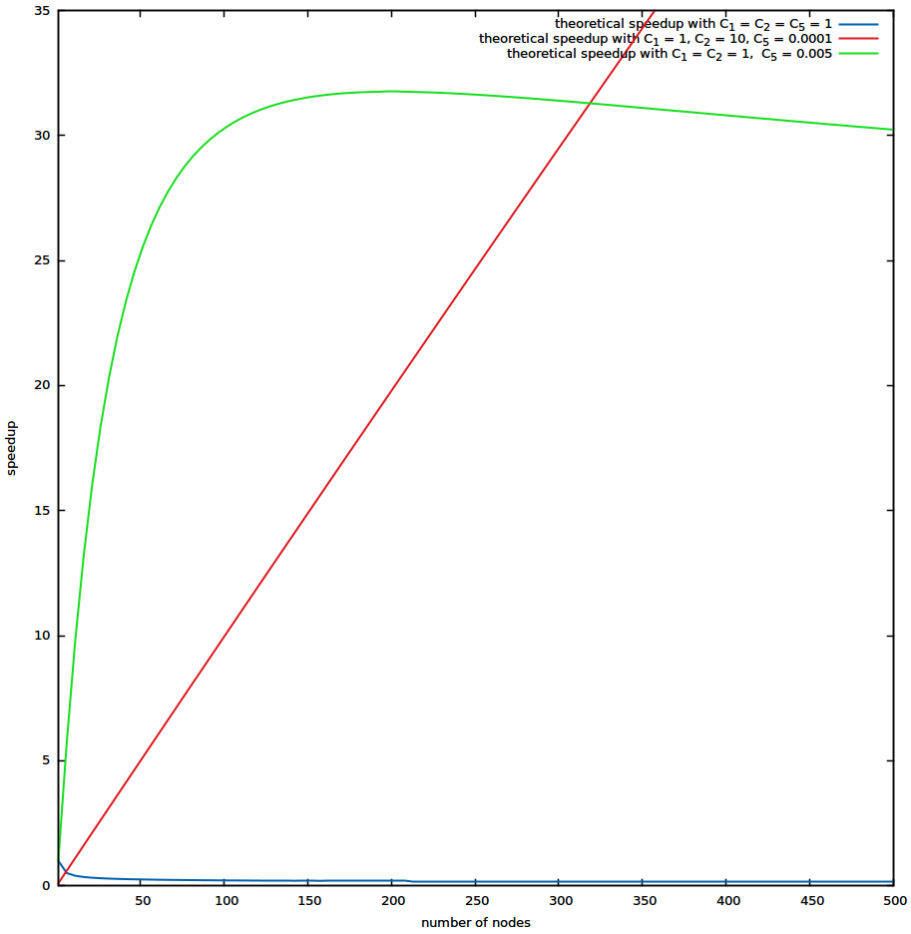

Figure 3: Theoretical simulations of the speedup

the time required to send an integer. Our integers are encoded with 32bits. We can estimate $C_5 \sim \frac{32}{3.2 \times 2^{30}} = 9.3 \times 10^{-9}$

With this constants the best speedup we could achieve is 1.5 with 3 nodes.

Results

All results were obtained with an implementation using OpenMPI and OpenMP. The tests were run on the Deneb cluster.

In charts you will see different timings, here are the explanations:

- **init**: this is the time spent during initialization phase. In the theoretical analysis this aspect was neglected because I didn't thought allocating memory would take that long.
- **compute**: this is the time spent computing. When there are multiple thread this value is the time spent computing by 1 thread. All the threads should have a similar compute time because we are using a dynamic OpenMP scheduler.
- **pack**: this is the time spent preparing the MPI packet
- **communicate**: this is the time spent synchronizing hints among nodes
- **total**: this is the time from the beginning to the end of the program (except the MPI finalization)

Impact of the input size

First we would like to know how increasing the number of series we want to compute (input size) impact the required time to do the computation.

Explanation

As we already know from our theoretical analysis, the complexity of the optimized algorithm is linear on the number of series to compute. From Figure 4 we can see we are getting a nice straight line (please note that the two axis are in log scale. The theoretical was consequently correct.

Impact of the number of rounds

We can evaluate its impact on figure 5

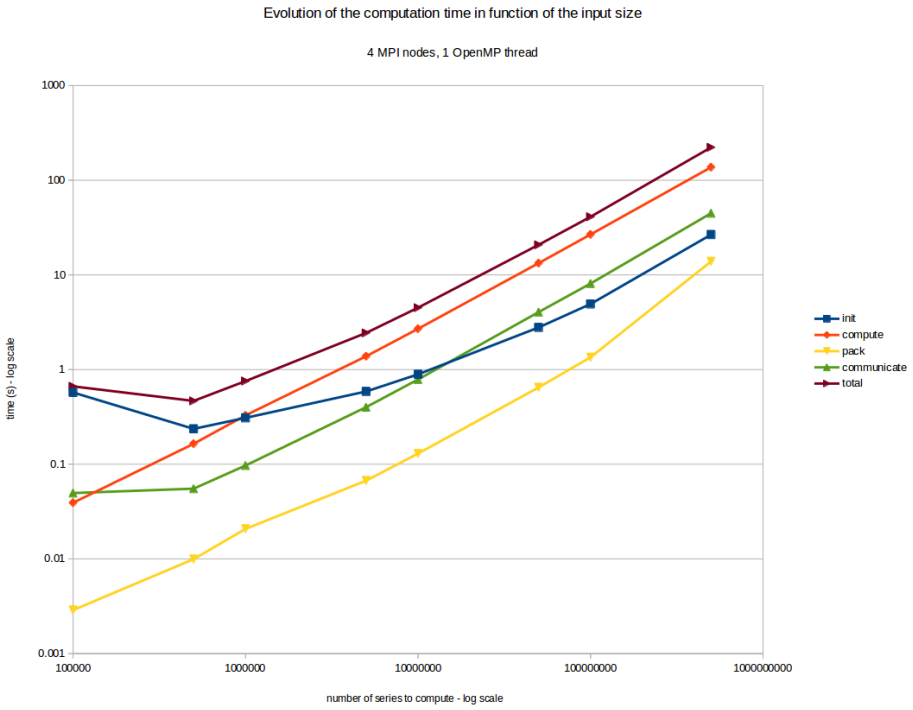

Figure 4: Evolution of the time in function of the input size

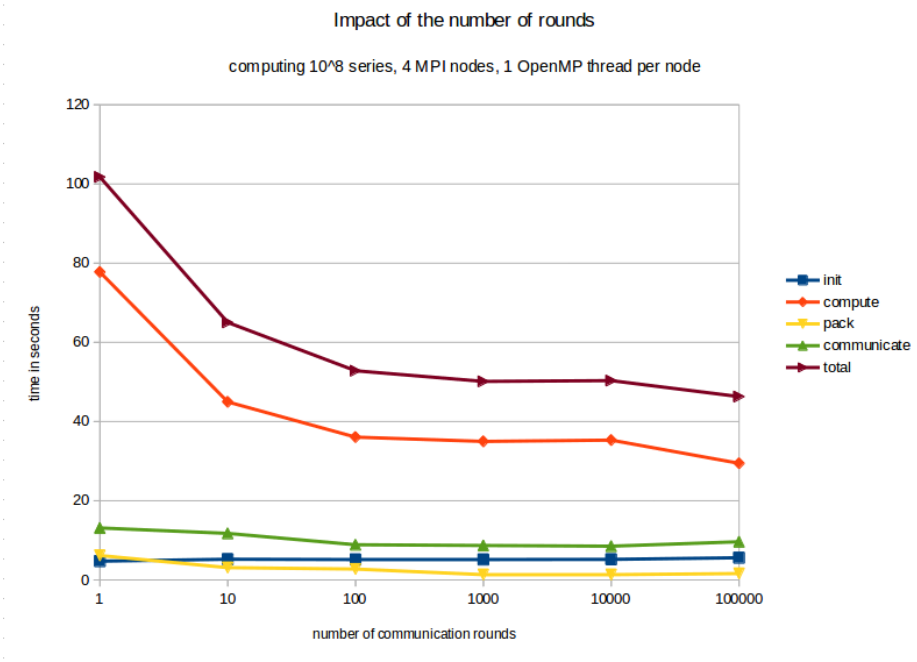

Figure 5: Impact of the number of rounds, 4 nodes, 1 thread per node

Explanation If we increase the number of rounds, nodes are sharing their hints more often. It helps their peers in their computations. Increasing the number of rounds should therefore reduce the computation time and increase the communication time.

As we can see on figure 6, with 4 OpenMP threads, we are getting the same computation time as 4 MPI processes with 100000 communication rounds. Having more rounds will not reduce the computation time because we already have the same speed as shared memory.

Scaling

Increasing the number of threads

Our implementation uses both MPI and OpenMP. We will first see how the program scales when we increase the number of threads (on the same node)

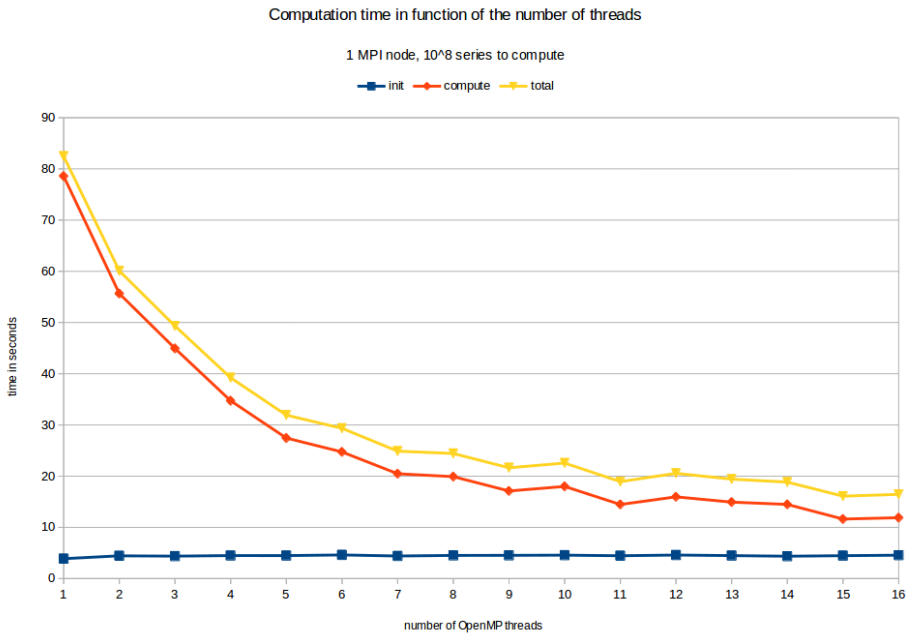

Figure 6: Evolution of the computation time in function of the number of OpenMP threads

Explanation If we stay on one node, there is no communication (and no packing). Thus the total time should decrease linearly. But as we can see on figure it decrease in a logarithmic way. There are multiple reason to this.

- We neglected the initialization time. Here, for 10^8 series it is about 4.5 seconds (about 5% of the sequential time). Now with Amdahl's law we can conclude that the best theoretical speedup we can get is: $\frac{1}{5\%} = 20$
- Here we are only getting a speedup of $\simeq 5$. There must be an explanation. Even if there is no MPI communication. Threads are sharing the same array. The cache coherence algorithm will take time. And sharing data from a processor to another on the same board will also take time, especially in NUMA architecture. This is why we are not getting the expected speedup.

Increasing the number of nodes

MPI only As we can see on figures on figures 7 and 8. The global speedup seems to tend to 4.0. The computation speedup seems to grow linearly.

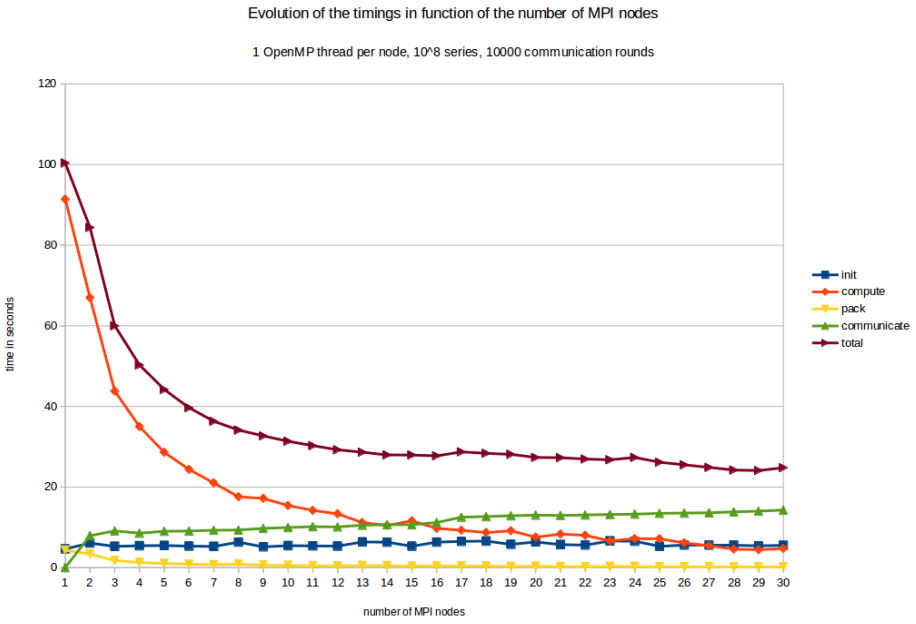

Figure 7: Time in function of the number of MPI nodes

Explanation What we can see here is exactly what was predicated. Only the estimation of the constants were a little off. Here the speedup of the computation is linear, which is normal as the computation is entirely parallel. The communication time is growing and is not parallel. The communication time are equal for 14 nodes. After that point the communication time is exceeding the computation time.

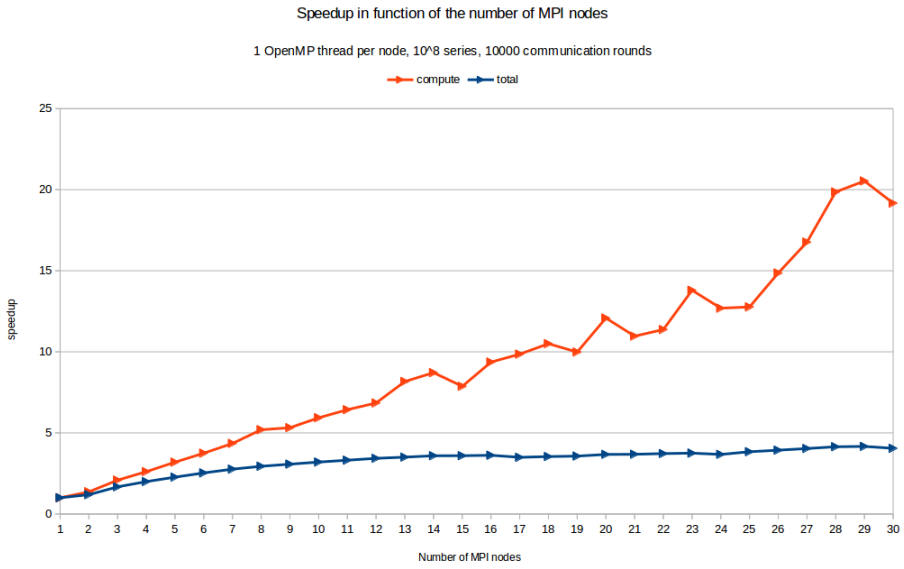

Figure 8: Speedup with 1 OpenMP thread per node

We can also remark that the packing time is decreasing. It makes sense because if there are more nodes, each node compute less values, hence the number of values to send to the peers is less.

MPI and OpenMP

Explanation As we can see on figures 9 and 10. The moment when the communication start taking more time that the computation comes earlier than when we only have 1 OpenMP thread per node. It helps us understanding the problem. In fact the bottleneck comes from the network bandwidth and not from the latency. Here, the communication line and the computation line cross between 1 and 2 nodes. In the previous case (1 OpenMP thread), they cross around 15 nodes. Here, we have 16 threads per node. In both cases the two lines cross when the network has to transmit the values of more than 15 workers (MPI or OpenMP).

Therefore we took the good decision when we ignored the latency in our model.

We can also see that the speedup is constantly decreasing. Here we are in the case where:

- $C_5 \sim C_2$: The speedup is always decreasing, and less than 1.

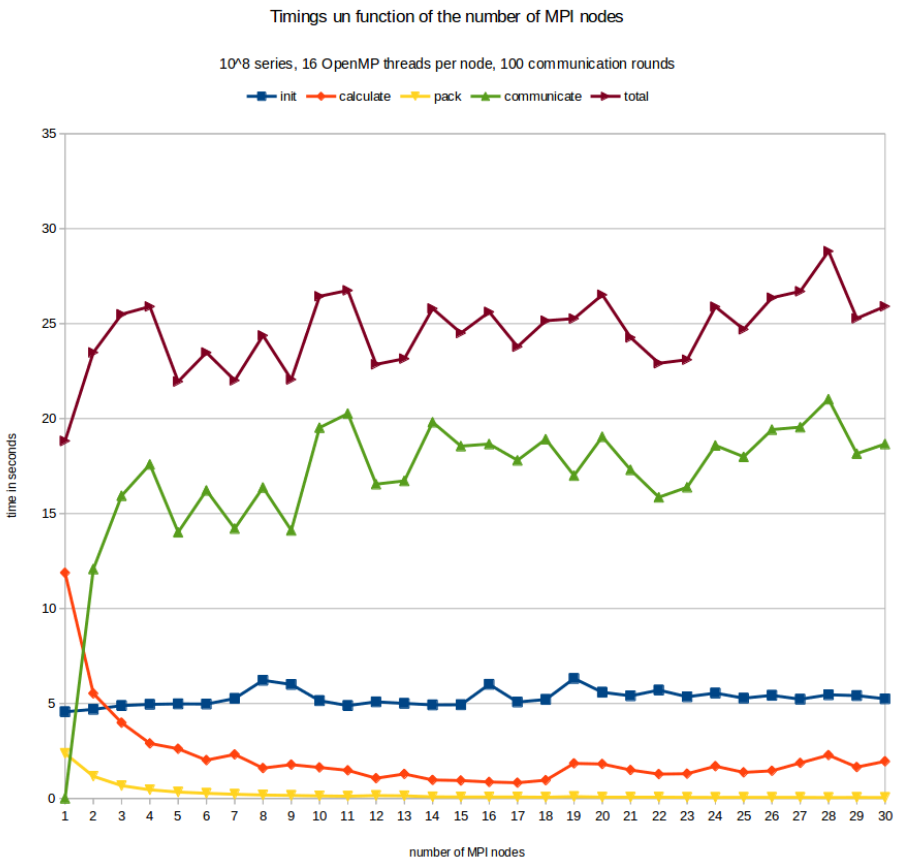

Figure 9: Time in function of the number of MPI nodes

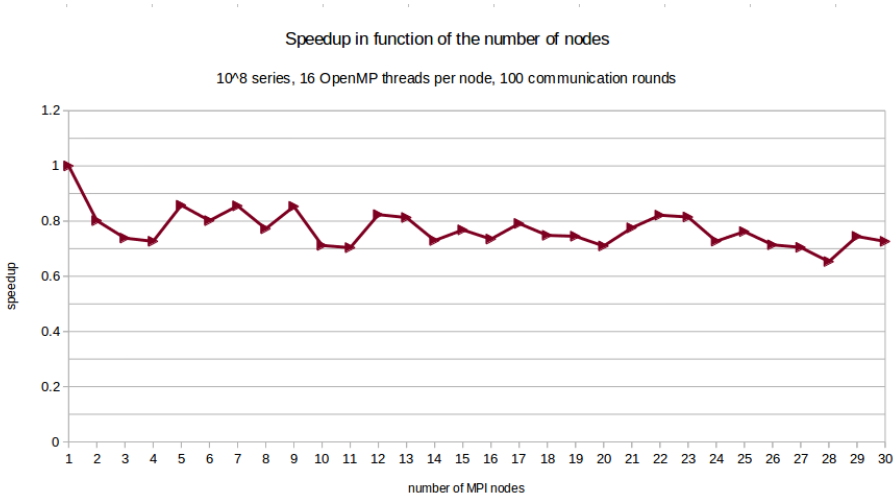

Figure 10: Speedup with 16 OpenMP thread per node

It make sense because here we multiplied to local computing power (that means we divided C_2) but did'nt change the newtork (represented by C_5)

Conclusion

In this project the theoretical analysis was pretty accurate. But this problem is not well suited for high performance computing because there are too many data dependencies.