# Parallel Solution of Laplace's Equation

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## Contents



**Abstract**

The main goal of this work is to develop a parallel way to solve numerically Laplace's Equation by using OpenMPI and to analyze how this process accelerates the computation compare to the serial way to do, and how exact are the results compared to the analytical solution. The using method in this project must have been Jacobi with red-black ordering. However there is no interest in doing red-black ordering with Jacobi as the old matrix has to be kept in memory, that's why I've decided to use Gauss Seidel method associated with red-black ordering.

The complete source code of this project may be found on Github: https://github.com/Soulou/HPC_Assignment It includes the analytical, the serial and the parallel methods, the scripts which have

been used to define the errors between results, how the benchmarks have been done, a link to the actual data resulting from the Astral computation and additionaly the LaTeX source code of this report.

# 1 The analytical solution

## 1.1 Solving the equation by using Fourier series

Finding the analytical solution basically consists in solving the following equation: 2

$$\frac{\partial^2\phi}{\partial y^2} + \frac{\partial^2\phi}{\partial x^2} = 0 \qquad x \in [0,1], y \in [0,1]$$

The homogeneous boundary conditions are:

$$\phi(x,0) = 0 \qquad \phi(x,1) = 0 \qquad \phi(1,y) = 0$$

The inhomogeneous boundary condition is:

$$\phi(0,y) = sin^2(\pi y)$$

After separating the variables: $\phi(x,y) = X(x)Y(y)$, so Laplace's equation becomes:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} + \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = 0$$

Let:

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = -k^2 \Leftrightarrow Y(y) = A_1\cos(ky) + B_1\sin(ky)$$

So:

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = k^2 \Leftrightarrow X(x) = A_2\cosh(kx) + B_2\sinh(kx)$$
$$Or: X(x) = A_2\cosh(k(x-1)) + B_2\sinh(k(x-1))$$

This second expression works better with $X(0) = 0$ as boundary condition. The result is:

$$\phi(x,y) = [A_1\cos(ky) + B_1\sin(ky)][A_2\cosh(k(x-1)) + B_2\sinh(k(x-1))]$$

Thanks to our boundary conditions, it can be deduced that

$$Y(0) = 0 \Rightarrow A_1 = 0 \qquad Y(1) = 0 \Rightarrow k = n\pi \qquad X(1) = 0 \Rightarrow A_2 = 0$$

Finally:

$$\phi_n(x,y) = B_n\sin(n\pi y)\sinh(n\pi(x-1)) \qquad for\ n \in \mathbb{N}^{+*}$$
$$\phi_n(x,y) = \sum_{n=1}^{\infty} B_n\sin(n\pi y)\sinh(n\pi(x-1)) \qquad (by\ superposition)$$

Thanks to the inhomogeneous boundary condition:

$$\phi(0, y) = \sum_{n=1}^{\infty} B_n sin(n\pi y) \sinh(-n\pi)$$

The Fourier coefficient is now $B_n \sinh(-n\pi)$:

$$B_n \sinh(-n\pi) = \int_0^1 \sin^2(\pi y) \sin(n\pi y) dy$$
$$B_n = \frac{2(\cos(\pi n) - 1)}{\pi(n^3 - 4n) \sinh(-n\pi)}$$

## 1.2 Implementation of the solution

The implementation has been done with the C programming language. The only constraint of using this language is that the resulting formula contains $\sinh(-n\pi)$. When $n$ gets bigger, a primitive variable type (double, long double) is not able anymore to have enough precision to compute correct results. This is why I've used the library GNU MPFR which is used to manipulate with high precision floating point numbers.

## 1.3 Illustration of the analytical solution

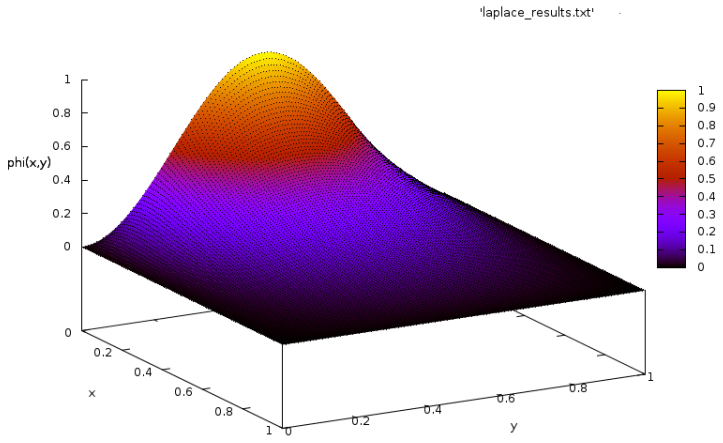



Figure 1: Representation of $\phi(x, y)$ for a stepsize of 1/120

# 2 The numerical solution - serial computation

## 2.1 Implementation

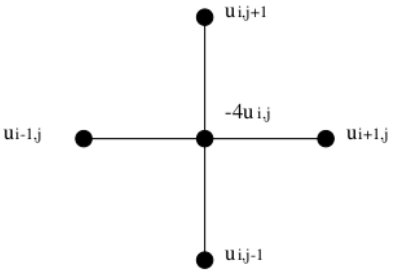



Figure 2: Finite difference stencil

The implementation of Gauss-Seidel method consists in a successive number of iterations of the following formula:

$$\phi_{i,j}^{k+1} = \frac{1}{4}(\phi_{i+1,j}^{k} + \phi_{i-1,j}^{k+1} + \phi_{i,j+1}^{k} + \phi_{i,j-1}^{k+1})$$

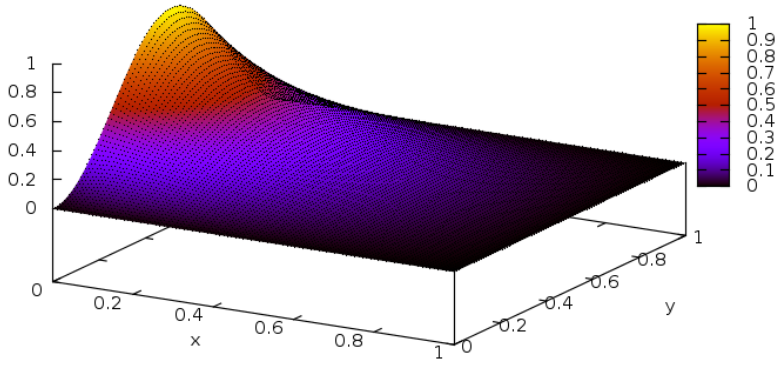
$$i \in [2; k-1], j \in [2; k-1]$$

As shown on the figure 2, the current value is calculated from the four values which circle it. This is really convenient to implement, because by iterating by line as in the following schema, when the point $o22$ is calculated, $\phi_{i-1,j}^{k+1}$ and $\phi_{i,j-1}^{k+1}$ have already been defined because they have been computed previously. Consequently, keeping a copy of the old matrix in memory is not mandatory, it is possible to iterate on in directly.

```
 ----------------------------
|                            |
| f   0   0   0   ...   0   0 |
| f  n11 n12 n13  ...  n1k  0 |
| f  n21 o22 o23  ...  o2k  0 |
|                            |
|                            |
|           .........        |
|                            |
|                            |
|                            |
|                            |
|____________________________|
```

Another important point, is the stopping condition. The following choice has been done: after each iteration the norm of the difference between the newly computed matrix and the previous one is compared to a certain tolerance the user has to give as argument to the software. When this norm is close to 0, it means that the newly generated matrix is not different anymore from the previous one. The algorithms stops iterating at that precise point.

$$||\phi^{k+1} - \phi^{k}|| < \epsilon$$




## 2.2 Aspect of the results

The results look similar as those obtained in the analytical computation:

## 2.3 Validation of the implementation

To know if the results are accurate, they are compared to the analytical solution. In order to achieve that, The small script: `diff_results.rb` compares two result files by calculating the difference of each $\phi(x, y)$ and finally printing the average difference in percents. The following table shows the difference between the analytical implementation and the Gauss-Seidel serial version, for different sizes of domain and different error tolerances [1].

- N: Number of steps/size of the result matrix
- $\bar{e}$: Average error
- t: convergence tolerance

| N | $\bar{e}$ ,t $= 10^{-2}$ | $\bar{e}$, t $= 10^{-3}$ | $\bar{e}$, t $= 10^{-4}$ | $\bar{e}$, t $= 10^{-5}$ |
|---|---|---|---|---|
| 20 | 0.1822 | 0.1325 | 0.1234 | 0.1227 |
| 40 | 0.2170 | 0.1086 | 0.0737 | 0.0708 |
| 60 | 0.2626 | 0.1091 | 0.0554 | 0.0500 |
| 80 | 0.3004 | 0.1171 | 0.0465 | 0.0388 |
| 100 | 0.3206 | 0.1228 | 0.0421 | 0.0320 |

Table 1: Difference between analytical and serial solutions

There are different things observable in this table. First, whatever is the size of the domain, the precision of the results is better when the tolerance is decreasing. Then, the results look accurate when the convergence tolerance is small enough. Actually when $t = 10^{-5}$ and $N \geq 60$, the numerical results

[1] Data generated by: analytical_serial_diff.sh

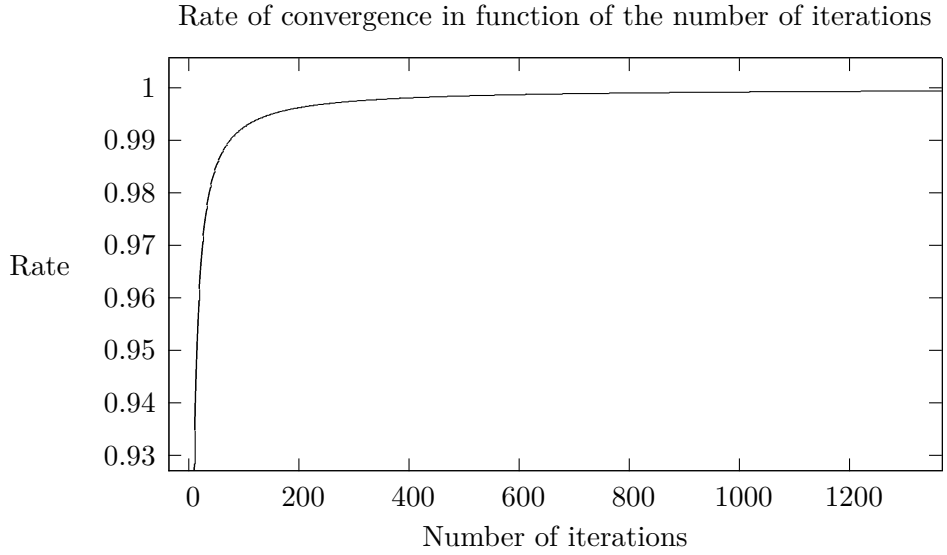
are less than 5% different from the analytical one. Finally, the bigger the domain, the smaller the required tolerance has to be to obtain good results. So, this way can be validated in order to measure the error and to detect the convergence.

## 2.4 Investigation of the rate of convergence

This rate is expressed like that:

$$\frac{||\phi^{k+1} - \phi^k||}{||\phi^k - \phi^{k-1}||}$$

It compares the previous error to the current one. In this case, it looks like the following graph:



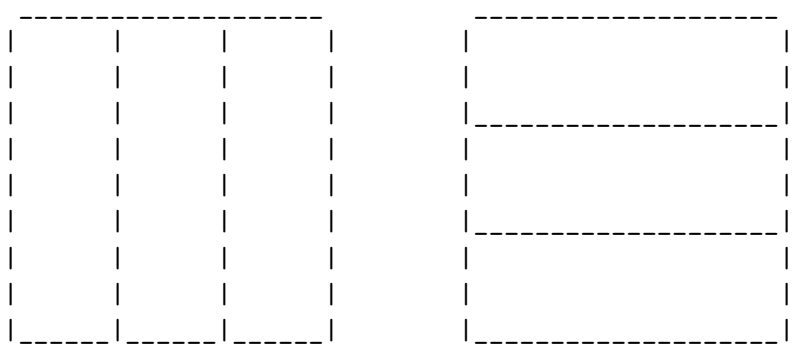

At the beginning, the value is really low, because the error is decreasing fast, after a couple hundreds iterations, the content of the result matrix begins to be more stable and more precise. This is why the rate of convegence is approaching 1. The bigger the asked precision, the closer to 1 will be the rate of convergence.

# 3 OpenMPI - parallel computation

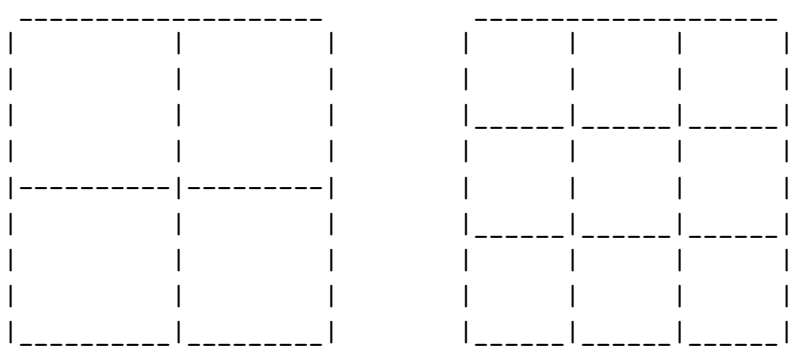
## 3.1 Computational domain decomposition

To divide a matrix, there are two main solutions:

- Panels:



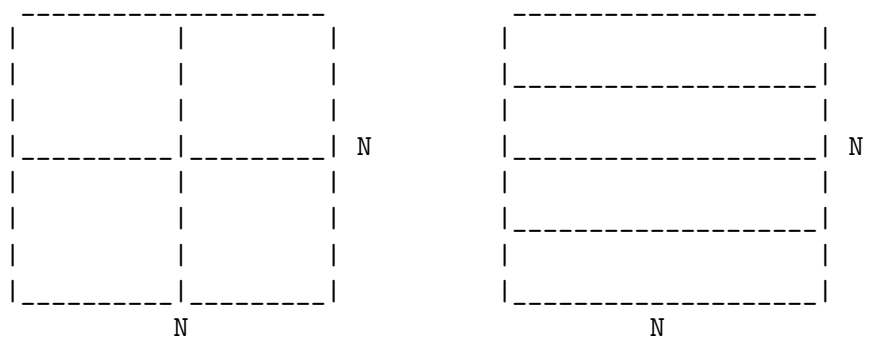
- Squares:



As shown above, the panels decomposition may be horizontal or vertical. Fondamentaly there is no difference between their characteristics, their are as many values to calculate and to exchange. However their is one difference which is linked to how caching is managed on the computing nodes. In our case the cache is storing lines, that's why it is much better to use horizontal panels than vertical.

## 3.2 Data exchange and halo nodes

The main advantage of the panels compare to the squares is that each process only needs to communicate with a maximum of 2 other instances (the one above and the one underneath). Even if by dividing the domain in squares, some processes would need to communicate with 4 other nodes, the amount of data which has to be exchanged by each process is smaller:




In both case the domain is divided in 4 equal parts, but with the square division there is only $2N$ of internal border. It means $4N$ of halo nodes to exchange during each iteration. Whereas, the strips division contains $3N$ of internal borders to exchange, it means $6N$ values. This difference is getting bigger and bigger.

### 3.3 Red Black Ordering

The main difference between red-black ordering is that the computation is divided two steps. The domain (or subdomain) has to be considered as a checkers board. According the index i and j, when $i + j$ is even, the values are in red, and otherwise if $i + j$ is odd, the values are in the other color: black.

```
 ---------------------
| R B R B R B R B R B |
| B R B R B R B R B R |
| R     .....       B |
| B                 R |
| R                 B |
| B                 R |
| R                 B |
|_____________________|
```

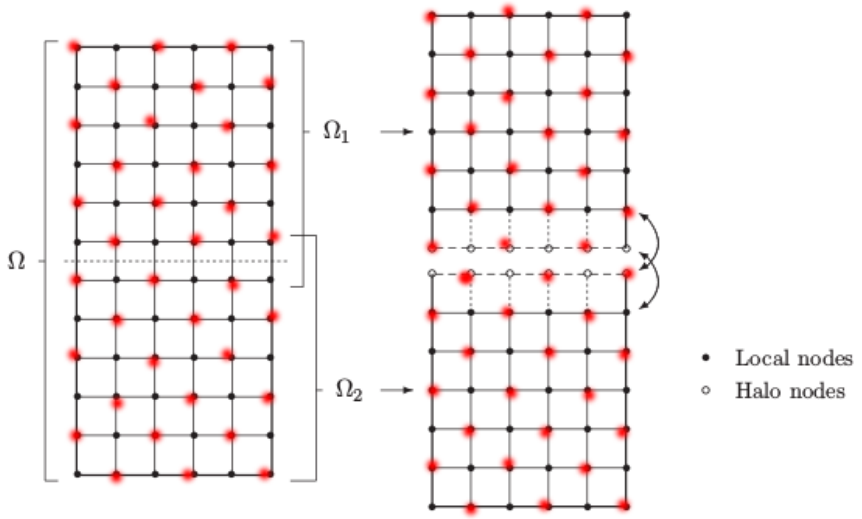
The algorithm is:

```
reapeat
  compute red values
  exchange red values from halo
  compute black values from new red values
  exchange black values from halo
  Every 30 iterations
    define new error
until the error is smaller than a given tolerance
```

> You can notice that in the case of parallel computing the error is not checked after each iteration. The reason is that to check the error, some additional calculations and data exchanges are required, so to optimize the speed, the algorithm avoids checking it every single time.

A direct consequence is that red values are only dependant of black values and vice versa. After calculating the new red values, The new black values can be obtained thanks to these recent figures. It avoids doing an iteration from the old data set. (difference between Jacobi and Gauss-Seidel)

Comparing to a standard division, the halo exchange is done in two different steps as it is shown in the pseudo-code algorithm above.




The best speedup which is expectable from this parallel computation is

$$S_p = N_p$$

With

- $S_p$: Speedup
- $N_p$: Number of processors

However, this result is really difficult to reach because the nodes have to communicate with each other. The following performance model can be defined:

$$S_p = \frac{T_{cr} + T_{cb} + T_{exr} + T_{exb}}{N_p}$$

- $T_{cr}$: Red value computation

- $T_{exr}$: Red value halo exchange
- $T_{cb}$: Black value computation
- $T_{exb}$: Black value halo exchange

When $N_p = 1 \qquad T_{exr} + T_{exb} \to 0$

### 3.4 Parallel execution on Astral

The main goal of high performance computing is to parallelize an algorithm to obtain results as fast as possible. A parallel algorithm may be slower that the original algorithm if only one processor is used, however this one is designed to able to reach high performance when it is running on multiple computational nodes. The speedup is probably the value the most interesting. It represents what is the acceleration between 1-node computation and $N$-node computation.

Two experiences have been done on Astral, the same algorithm has been executed twice with a different precision tolerance, the first one has been done with a low precision: $10^{-4}$ and the second with a high precision: $10^{-6}$. Both of them have been run with 1, 2, 4, 8, 16 and 32 processors. The algorithm used is Red-Black ordering Gauss-Seidel with a domain splitted in horizontal strips.

#### 3.4.1 Parallel execution with a low precision

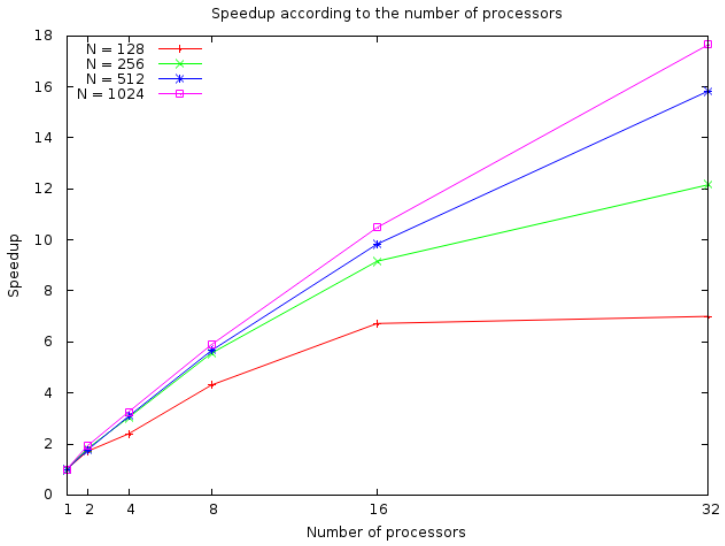



Figure 3: Speedup when the mesh size and the number of CPUs are varying (low precision)

Instead of the perfect result, the speedups are lower, when $N_p = 32$, the speedup is only 17. This difference can be easily explained. When there are more nodes, there are more data exchanges. These are expensive and cost a lot of time (processors cycles and networking latency). However, when the mesh is larger, each node has more calculations to do and there is a important speedup improvement.

The underneath table gives more details for the case $N_p = 32$.

| Number of processors | 1 | 2 | 4 | 8 | 16 | 32 |
|---|---|---|---|---|---|---|
| Execution time in seconds | 3506 | 2001 | 1019 | 602 | 356 | 201 |
| Number of iterations | 149,760 | 170,700 | 190530 | 216,360 | 249,360 | 289,980 |
| Speedup | 1 | 1.75 | 3.44 | 5.82 | 9.85 | 17.44 |
| Speedup evolution | - | $\times$1.75 | $\times$1.96 | $\times$1.69 | $\times$1.69 | $\times$1.77 |
| Difference with Optimal speedup | 0% | 12.5% | 14.0% | 27.3% | 38.4% | 45.5% |
| Average error with analytical | 10.5% | 8.3% | 6.6% | 5.1% | 3.8% | 3.4% |

Table 2: Data analysis of the obtained speedups with a $10^{-4}$ precision

The speedup evolution shows that its evolution is quite stable, not as fast as expected, but stable: $\approx 1.75$. However, as this value is not two, the results are going further and further from the optimal as it is illustrated by the difference with the linear speedup.
It is something to have a good speedup, but it's necessary to check if the results are good enough. All the previous figures have been done with a mesh of $1024 \times 1024$. With this precision, the average error is really high. Having results which are 10% different from the analytical one is not acceptable. However, the more the number of processors, the lower the error to the analytical solution. It can be explained by the way the stopping condition is implemented. The error is the sum the of all the local errors (of each subdomain), so more the domain is divided, the slower it will reach the acceptance step. This is why there are much more iterations when the number of CPUs is getting bigger.

### 3.4.2 Parallel execution with a high precision

The only difference in these results is the tolerance parameter, nothing else has changed.
The lines of this graph have exactly the same shape as the previous experience but the speedus are really much more higher. Whatever is the size of the mesh it is higher as there are much more iterations.

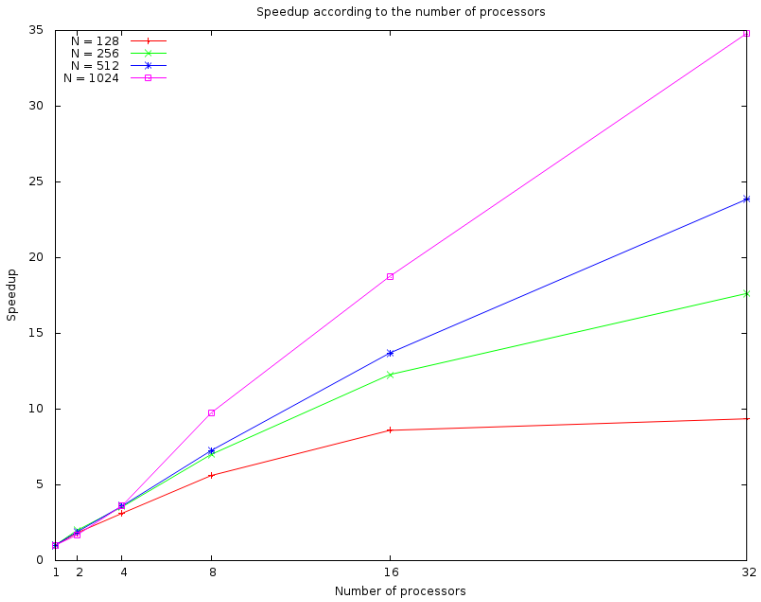



Figure 4: Speedup when the mesh size and the number of CPUs are varying (high precision)

| Number of processors | 1 | 2 | 4 | 8 | 16 | 32 |
|---|---|---|---|---|---|---|
| Execution time in seconds | 18771 | 11101 | 5212 | 1923 | 1000 | 539 |
| Number of iterations | 591,330 | 629,250 | 660,510 | 696,150 | 735,450 | 779,010 |
| Speedup | 1 | 1.69 | 3.60 | 9.76 | 18.77 | 34.3 |
| Speedup evolution | - | $\times$1.69 | $\times$2.13 | $\times$2.71 | $\times$1.92 | $\times$1.83 |
| Difference with Optimal speedup | 0% | -15.5% | -10.0% | +22.3% | +17.3% | +7.2% |
| Average error with analytical | 0.22% | 0.24% | 0.44% | 0.65% | 1.55% | 3.21% |

Table 3: Data analysis of the obtained speedups with a $10^{-6}$ precision

In this case the results are particularly good, a super-linear speedup has been reached. For 2 and 4 processors, the results are identical as the previous experience, the speedup is strongly increasing afterwards. ($> \times 2$).

These calculations have been done with a higher precision, the logical consequence is that the whole computation is longer, the number of iterations more important and mainly the average error compare to the analytical solution is closer to 0, it is what was expecting. The aspect is still the expecting result too:

How to explain such a high speedup: as horizontal strips are used, the domain is decomposed in large horizontal subdomains. With 32 processors it means, that each process is working on a $32 \times 1024$ matrix. The *double* is 8 bytes long, so each line is weighting 8KB, and the matrix itself 256KB.

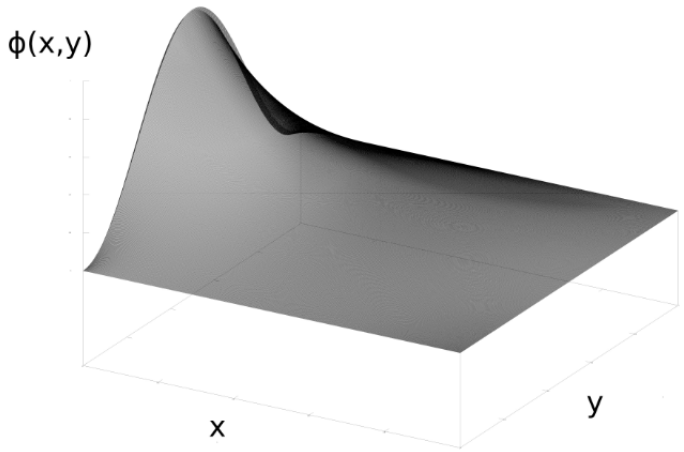



Figure 5: 3D drawing of a 1024 mesh

The Astral HPC uses processors with 32KB of L1 cache and 4MB of L2 cache, it means that the whole matrix can be stored in them. There are no need to use the RAM. When the algorithm is running on 1 CPU, the whole matrix can't fit in this cache and data exchanges from the RAM are necessary. Those slow down the global operation.

# 4 Methodology

All my source code have been regularly commited using GIT pushed on Github to a save in case of my laptop encounters any problem. I also use GIT to transfer everything from it to Astral to execute the different experiences. To debug the code and analyse partial results, I've developed some functions able to print and to do some operations on the matrices to be sure the data are valid and that the data exchange are correct too. All my results come from Astral even the results with a few processors. The reason is that I wanted an uniform envrionment of execution. There is no interest to run computation from different kinds of processor. The caches, the frequence must be identical to have a good comparaison of the results. To draw the differents graphs (2D and 3D) i've used gnuplot with its pm3d mod which enable isotherm drawing on 3D graphs. (The files which are used to generate those are in the "results" folder. I've used **ruby** to write the utility used to compare the results. Not because this language is great to manipulate numbers, but because I'm used to it.

## Conclusion

To conclude, we've seen that it's possible to reach a good speedup without sacrifying the precision of the results. But there are still a lot of possible improvements for a further study. The more logical is to investigate why does the speedup increase so much when the amount of computation is getting bigger. We can suppose things but that's nothing really precise and absolute. Aside, it may be great to continue increasing the number of CPUs and analyse the parallelism limits. Finally, it must be a great to compare these results with another domain division method. To know if there is really a big difference between strips and squares about cache usage or halo data exchange.
As we have to fill the module evaluation questionnaire before working on this assignment, I would like to give point of view over this work. According to me, it was great to introduce the power of OpenMPI and the use of a supercomputer like Astral. That something most of us haven't done before and it is really interesting to do. That's also a good opportunity to see how a parallel code can be difficult to debug if it was not well thought from the beginning and if the mathematical model hasn't been set up correctly.