

# Project 3 of "Metodi Del Calcolo Scientifico"

Academic Year 2019/2020

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# Contents

1	Introduction	3
2	Implementation	3
3	Validation study	10
4	Conclusion	21

# 1 Introduction

The main purpose of this project was to implement different solvers of systems of linear equations and organize them into a library. In particular, the following iterative solvers had to be implemented, limiting to the case of symmetric and positive definite matrices:

- The Jacobi method;
- The Gauß-Seidel method;
- the Gradient method;
- the Conjugate Gradient method.

This document consists of three sections: Section 2 describes how the library has been implemented; Section 3 describes the validation study that has been conducted with the developed library and, finally, Section 4 concludes this work.

## 2 Implementation

The required library has been implemented using the **Python** [1] programming language because it is open source, very powerful and it provides all the functionalities and libraries needed to achieve the goals of the project. In particular, the following libraries have been exploited:

- **NumPy** [2], which is the core library for scientific computing in Python [1], which mainly adds support for dense multidimensional arrays. In particular, it provides the *ones()* and the *zeros()* functions to generate a vector with all the entries equal to 1 or to 0, respectively;
- **SciPy** [3], which is a Python-based ecosystem of open-source software for mathematics, science and engineering, which also adds support for sparse matrices.

In order to improve the readability of the code and, thus, its maintainability, the software has been organized into the following modules and classes:

- **main.py**, which is the entry point of the program and which controls the execution flow of the program;
- **input\_parser.py**, which implements the logic for validating the user input in the *InputParser* class;

- **mtx\_file\_reader.py**, which contains the *MTXFileReader* class, whose purpose is to implement the logic for loading the matrix in input from an .mtx file and store it in memory;
- **iterative\_solver\_comparator.py**, containing the *IterativeSolverComparator* class, which is responsible for comparing the four aforementioned solvers in terms of their execution time, relative error and number of iterations.
- **abstract\_iterative\_solver.py**, which contains the *AbstractIterativeSolver* class, which is the template for all the iterative solvers of the library, i.e., it implements the logic of a general iterative solver;
- **jacobi\_solver.py**, containing the *JacobiSolver* class, which realizes the logic for updating the approximate solution based on the Jacobi updating strategy;
- **gauss\_seidel\_solver.py**, containing the *GaussSeidelSolver* class, which implements the logic for updating the approximate solution based on the Gauß-Seidel updating strategy;
- **gradient\_solver.py**, containing the *GradientSolver* class, which realizes the logic for updating the approximate solution based on the Gradient updating strategy;
- **conjugate\_gradient\_solver.py**, containing the *ConjugateGradientSolver* class, which realizes the logic for updating the approximate solution based on the Conjugate Gradient updating strategy;

From an architectural point of view, Figure 1 shows the structure of the project through a **UML** [4] diagram. It is a simple diagram showing both the dependencies between the software components and the attributes and methods of each class at a high level of abstraction. In fact, every software class is modelled as a rectangle: on top there is the name of the class, in the middle there are the attributes of the class (if any), each specified by a data type, and on the bottom there are the signatures of the methods. The links between the rectangles model the relationships between the software components: a class can use another class in its implementation or a class can extend another class. Note that the *main.py* module is just a simple script that implements the entry point of the program and that controls the execution flow of the program. This is why it has not been modelled as a class rectangle.

More in detail, as it is shown in the UML diagram and in Figure 2, the *main.py*

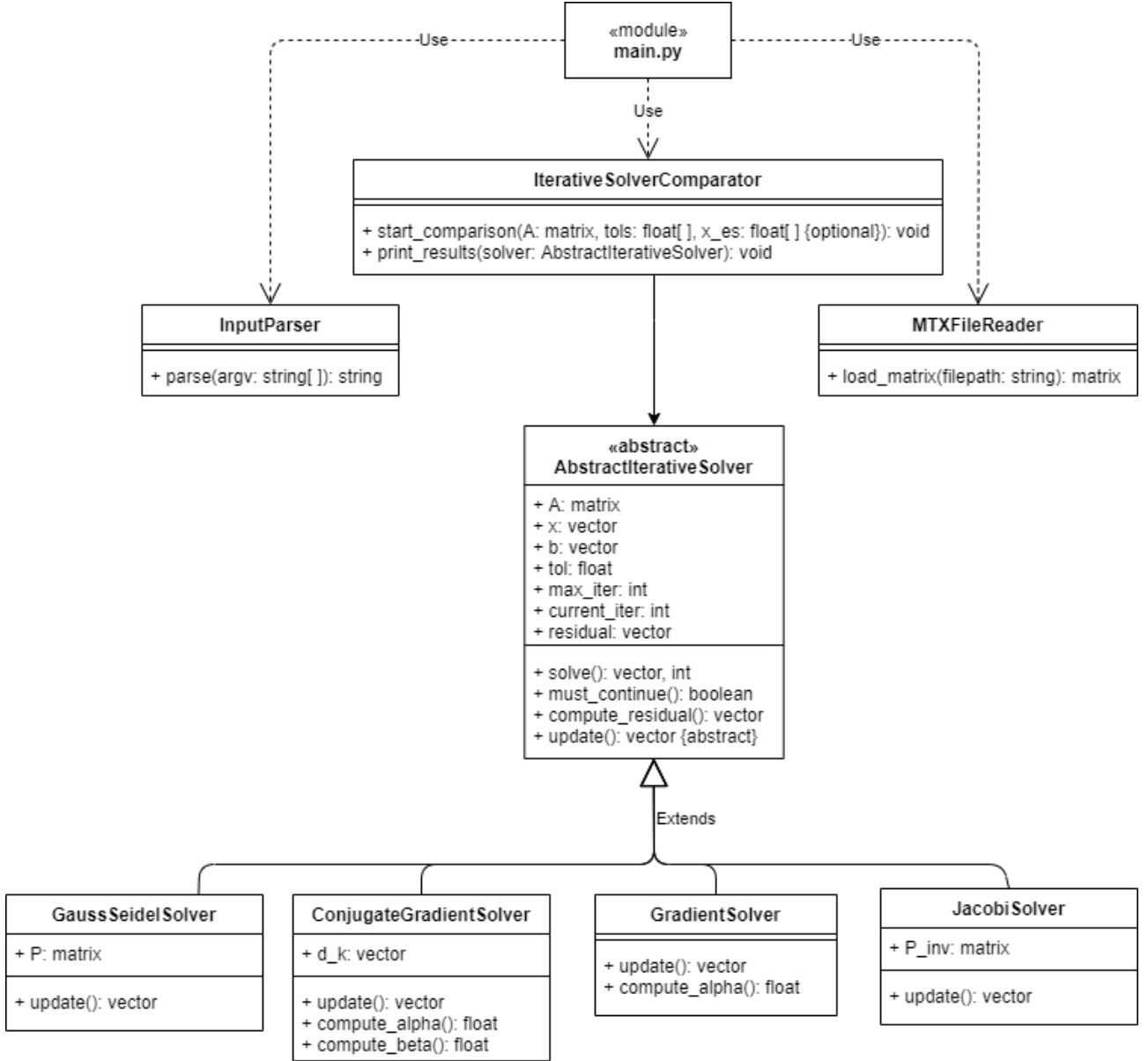


Figure 1: A UML [4] diagram that shows the structure of the software

module uses the *InputParser* class to parse and validate the user input, that is, it checks whether the .mtx file exists in the file system. Then, as soon as the user input has been validated, the *main.py* module uses the *MTXFileReader* class to load the matrix from the file system and store it in memory as sparse. Finally, the *main.py* module uses the *IterativeSolverComparator* class to start the comparison between the different solver implementations and to print the results obtained at the end of the comparison.

```

def main(argv):
    # input validation
    mtx_file = InputParser().parse(argv)

    # matrix extraction from the .mtx file
    A = MTXFileReader().load_matrix(mtx_file)

    # launch comparison
    tols = [1e-4, 1e-6, 1e-8, 1e-10]
    IterativeSolverComparator().start_comparison(A, tols)

```

Figure 2: Code inside the *main.py* module

```

class IterativeSolverComparator:

    # This is a helper method for the start_comparison() method:
    # it simply prints the results achieved by a solver to the console
    def print_results(self, solver, x_es):
        time_start = time()
        x_app, num_iter = solver.solve()
        time_end = time()
        exec_time = "{:.32e}".format(time_end - time_start)
        rel_error = "{:.32e}".format(norm(x_es - x_app) / norm(x_es))
        formatted_tol = "{:.0e}".format(solver.tol)
        solver_name = type(solver).__name__
        print("\n%s results with tolerance = %s:" % (solver_name,
                                                    formatted_tol))

        print("Relative error = %s" % rel_error)
        print("Number of iterations = %d" % num_iter)
        print("Execution time = %s\n" % exec_time)

    # This method simply solves the linear systems with the four different
    # solver to the varying of the tolerance and shows the achieved results
    # on the console
    def start_comparison(self, A, tols, x_es=None):
        if x_es is None:
            x_es = ones(A.shape[0])
        b = A.dot(x_es)
        for tol in tols:
            self.print_results(JacobiSolver(A, b, tol), x_es)
            self.print_results(GaussSeidelSolver(A, b, tol), x_es)
            self.print_results(GradientSolver(A, b, tol), x_es)
            self.print_results(ConjugateGradientSolver(A, b, tol), x_es)

```

Figure 3: Code inside the *IterativeSolverComparator* class

As shown in Figure 3, when the *start\_comparison()* method of the *IterativeSolverComparator* class is called, first the *x\_es* vector and the *b* vector are generated: the former has all its entries equal to 1 and it represents the exact solution of the system of equations, while the latter represents the right-hand side coefficients of the system and it is generated by using the *A* matrix in input

and the just created  $x_{es}$  vector. Note that it is still possible to use a different  $x_{es}$  vector, as also specified in the signature of the method. Soon afterwards, the *IterativeSolverComparator* class uses all the different solvers to solve the system of equations  $Ax = b$  to the varying of the tolerance, which is a value among  $[10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}]$ , and prints on the screen the relative error, the number of iterations and the execution time needed to generate a solution.

```
class AbstractIterativeSolver:

    # Constructor
    def __init__(self, A, b, tol):
        self.A = A
        self.b = b
        self.tol = tol
        self.x = zeros(A.shape[0]) # A.shape[0] gets the first dimension
        self.max_iter = 20000
        self.current_iter = 1
        self.residual = self.compute_residual()

    # Helper method that computes the residual
    def compute_residual(self):
        return self.b - self.A.dot(self.x)

    # Helper method that returns TRUE if the solver must continue to
    # iterate, FALSE otherwise.
    def must_continue(self):
        if self.current_iter > self.max_iter:
            print("[WARNING] max number of iterations reached: solver failed
                  to achieve convergence!")

            return False
        return norm(self.residual) / norm(self.b) >= self.tol

    # Template method for a general iterative method
    def solve(self):
        while self.must_continue():
            self.x = self.update()
            self.residual = self.compute_residual()
            self.current_iter += 1
        return self.x, self.current_iter

    # Method that must be overridden by the subclasses.
    def update(self):
        raise NotImplementedError("[ERROR] This method has not been
                                  implemented yet")
```

Figure 4: Implementation of the general iterative solver

All the solvers extend the *AbstractIterativeSolver* class, thus inheriting all its methods and attributes. The code of such class can be inspected in Figure 4 and, as it can be seen, the *solve()* method implements the main loop, which stops if either the maximum number of iterations is reached or the scaled residual is less than the fixed tolerance. At each iteration of the main loop, the *update()* method updates the approximate solution, but, since the update strategy strictly depends on the specific solving method (e.g., the Jacobi method), the *update()* method is abstract. More in detail, an abstract method is such that all the iterative solvers that extend the *AbstractIterativeSolver* class must override it, providing an implementation of such method (abstract methods are analogous to the concept of virtual methods in the *C++* [5] programming language). With this design pattern, implementing the solvers is a trivial task, since they only have to extend the *AbstractIterativeSolver* class and implement the *update()* method.

```
class JacobiSolver(AbstractIterativeSolver):

    # Constructor
    def __init__(self, A, b, tol):
        super().__init__(A, b, tol)
        self.P_inv = csr_matrix(identity(A.shape[0]) / A.diagonal())

    # This function implements the update strategy of the Jacobi method
    def update(self):
        return self.x + self.P_inv.dot(self.residual)
```

Figure 5: Implementation of the Jacobi method

For instance, Figure 5 shows the implementation of the Jacobi method, which consists of just the *update()* method. It's worthwhile to notice that the inverse of the P matrix is computed only once inside the constructor, where the P matrix is the diagonal matrix resulting from the factorization of the A matrix.

Figure 6 shows the implementation of the Gauß-Seidel method. Note that also in this case, for matters of efficiency, the P lower triangular matrix is computed just once using the *tril()* function provided by the SciPy [3] library. In addition, the *spsolve\_triangular()* method, also provided by the SciPy [3] library, has been used to efficiently solve the system of equations where P is the coefficient matrix and the residual vector is the right-hand side of the system.

Lastly, Figure 7 and Figure 8 show the code used to implement the Gradient solver and the Conjugate Gradient solver, respectively. In order to improve the maintainability of the code, the *compute\_alpha()* and the *compute\_beta()* helper methods have been implemented.



```

class GaussSeidelSolver(AbstractIterativeSolver):

    # Constructor
    def __init__(self, A, b, tol):
        super().__init__(A, b, tol)
        self.P = tril(self.A, format="csr")

    # This method simply computes the next vector solution x
    def update(self):
        return self.x + spsolve_triangular(self.P, self.residual)

```

Figure 6: Implementation of the Gauß-Seidel method

```

class ConjugateGradientSolver(AbstractIterativeSolver):

    # Constructor
    def __init__(self, A, b, tol):
        super().__init__(A, b, tol)
        self.d_k = self.residual

    # This method computes the next vector solution x based on the Conjugate
    # Gradient update strategy
    def update(self):
        y_k = self.A.dot(self.d_k)
        alpha = self.compute_alpha(y_k)
        self.x = self.x + alpha * self.d_k
        self.residual = self.compute_residual()
        beta = self.compute_beta(y_k)
        self.d_k = self.residual - beta * self.d_k
        return self.x

    # This is a helper function for the update() method and simply computes
    # the value of "alpha"
    def compute_alpha(self, y_k):
        alpha_numerator = self.d_k.dot(self.residual)
        alpha_denominator = self.d_k.dot(y_k)
        return alpha_numerator / alpha_denominator

    # This is a helper function for the update() method and simply computes
    # the value of "beta"
    def compute_beta(self, y_k):
        beta_numerator = self.d_k.dot(self.A.dot(self.residual))
        beta_denominator = self.d_k.dot(y_k)
        return beta_numerator / beta_denominator

```

Figure 7: Implementation of the Conjugate Gradient method

```

class GradientSolver(AbstractIterativeSolver):

    # This method computes the next x vector solution using the Gradient
    # update strategy
    def update(self):
        alpha = self.compute_alpha()
        return self.x + alpha * self.residual

    # This is a helper function for the update() method and simply computes
    # the value of "alpha"
    def compute_alpha(self):
        alpha_numerator = self.residual.dot(self.residual)
        alpha_denominator = self.residual.dot(self.A.dot(self.residual))
        return alpha_numerator / alpha_denominator

```

Figure 8: Implementation of the Gradient method

In conclusion, from a practical point of view, to launch this program it is sufficient to execute the following command on a command prompt window (e.g., Windows PowerShell or Linux Bash):

```
> python main.py <filepath>
```

For example, to launch it on the matrix saved in *my\_file.mtx*, it is sufficient to execute the following command:

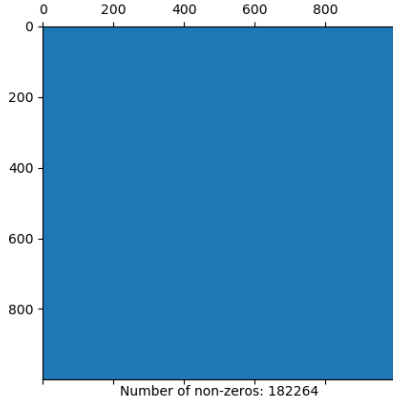
```
> python main.py my_file.mtx
```

For further details on the implementation of this library, all the code is available at:

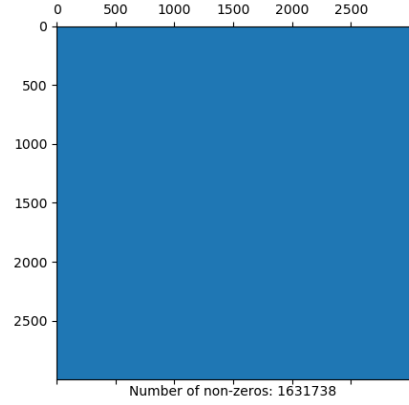
<https://bit.ly/3dvpX4y>.

### 3 Validation study

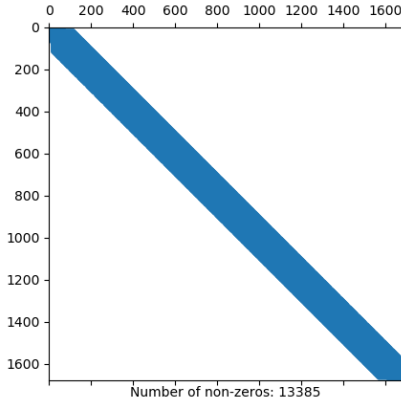
Once the library has been implemented, a validation study has been conducted with the aim of assessing the effectiveness and the efficiency of the different solvers of the library. The experiments have been conducted with the same machine equipped with an Intel Core i-7-4720HQ processor and 8 GB of RAM. In particular, the 4 sparse matrices (*spa1.mtx*, *spa2.mtx*, *vem1.mtx*, *vem2.mtx*) visualized in Figure 9 have been used. It's important to notice that *spa1.mtx* and *spa2.mtx* do not present a particular pattern, instead *vem1.mtx* and *vem2.mtx* have the non-zero coefficients concentrated on the main diagonal. In addition, Table 10 shows the condition numbers of the matrices.



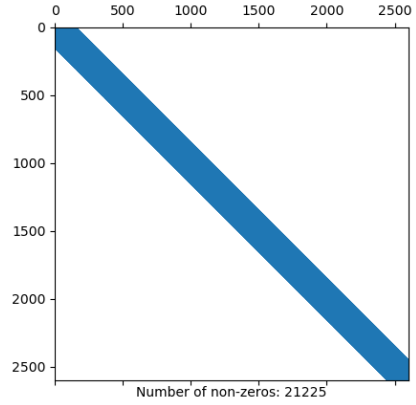
(a) spa1.mtx



(b) spa2.mtx



(c) vem1.mtx



(d) vem2.mtx

Figure 9: Spy plots of the matrices used during the experiments

Matrix	Condition number
spa1.mtx	2048.15
spa2.mtx	1411.97
vem1.mtx	324.64
vem2.mtx	507.02

Figure 10: Condition number of each matrix used for the experiments

Every solver of the library has been executed on the aforementioned 4 matrices using different values of the tolerance (i.e.,  $[10^{-4}, 10^{-6}, 10^{-8}, 10^{-10}]$ ). For each execution, the following quantities have been registered:

- Number of iterations;
- Relative error, computed as  $\frac{\|x_{app} - x_{es}\|}{\|x_{es}\|}$ , where  $x_{app}$  is the approximate solution returned by a solver and  $x_{es}$  is the exact solution;

- Execution time in seconds.

While the number of iterations and the relative error do not depend on the specific execution, because the methods are deterministic algorithms, the execution time strictly depends on the scheduler of the operating system, which decides how much CPU time to allocate to each process. For this reason, at each run of a method, a different execution time could be registered. To mitigate this problem, the experiment has been repeated 10 times and the execution time has finally been computed by averaging the values observed in such experiments. The results obtained are shown in the following tables (the results in the table have been rounded to the second decimal place):

<b>spa1.mtx with Tolerance: <math>10^{-4}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	115	$1.77 \times 10^{-3}$	$2.30 \times 10^{-2}$
Gauß-Seidel	9	$1.82 \times 10^{-2}$	$7.30 \times 10^{-2}$
Gradient	143	$3.46 \times 10^{-2}$	$5.20 \times 10^{-2}$
Conjugate Gradient	49	$2.08 \times 10^{-2}$	$3.50 \times 10^{-2}$

<b>spa1.mtx with Tolerance: <math>10^{-6}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	181	$1.80 \times 10^{-5}$	$3.50 \times 10^{-2}$
Gauß-Seidel	17	$1.3 \times 10^{-4}$	$1.20 \times 10^{-1}$
Gradient	3577	$9.68 \times 10^{-4}$	1.28
Conjugate Gradient	134	$2.55 \times 10^{-5}$	$9.40 \times 10^{-2}$

<b>spa1.mtx with Tolerance: <math>10^{-8}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	247	$1.82 \times 10^{-7}$	$5 \times 10^{-2}$
Gauß-Seidel	24	$1.71 \times 10^{-6}$	$1.71 \times 10^{-1}$
Gradient	8233	$9.82 \times 10^{-6}$	2.89
Conjugate Gradient	177	$1.32 \times 10^{-7}$	$1.30 \times 10^{-1}$

<b>spa1.mtx with Tolerance: <math>10^{-10}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	313	$1.85 \times 10^{-9}$	$6.30 \times 10^{-2}$
Gauß-Seidel	31	$2.25 \times 10^{-8}$	$2.20 \times 10^{-1}$
Gradient	12919	$9.82 \times 10^{-8}$	4.64
Conjugate Gradient	200	$1.20 \times 10^{-9}$	$1.39 \times 10^{-1}$

spa2.mtx with Tolerance: $10^{-4}$			
Method	Iterations	Rel. error	Time (in seconds)
Jacobi	36	$1.77 \times 10^{-3}$	$7.80 \times 10^{-2}$
Gauß-Seidel	5	$2.60 \times 10^{-3}$	$1.47 \times 10^{-1}$
Gradient	161	$1.81 \times 10^{-2}$	$5,78 \times 10^{-1}$
Conjugate Gradient	42	$9.82 \times 10^{-3}$	$3.23 \times 10^{-1}$

spa2.mtx with Tolerance: $10^{-6}$			
Method	Iterations	Rel. error	Time (in seconds)
Jacobi	57	$1.67 \times 10^{-5}$	$1.10 \times 10^{-1}$
Gauß-Seidel	8	$5.14 \times 10^{-5}$	$2.39 \times 10^{-1}$
Gradient	1949	$6.69 \times 10^{-4}$	7.27
Conjugate Gradient	122	$1.20 \times 10^{-4}$	$9.28 \times 10^{-1}$

spa2.mtx with Tolerance: $10^{-8}$			
Method	Iterations	Rel. error	Time (in seconds)
Jacobi	78	$1.57 \times 10^{-7}$	$1.49 \times 10^{-1}$
Gauß-Seidel	12	$2.79 \times 10^{-7}$	$3.59 \times 10^{-1}$
Gradient	5087	$6.87 \times 10^{-6}$	$1.87 \times 10^{+1}$
Conjugate Gradient	196	$5.59 \times 10^{-7}$	1.47

spa2.mtx with Tolerance: $10^{-10}$			
Method	Iterations	Rel. error	Time (in seconds)
Jacobi	99	$1.48 \times 10^{-9}$	$2.11 \times 10^{-1}$
Gauß-Seidel	15	$5.57 \times 10^{-9}$	$5.64 \times 10^{-1}$
Gradient	8285	$6.94 \times 10^{-8}$	$3.42 \times 10^{+1}$
Conjugate Gradient	240	$5.32 \times 10^{-9}$	2.00

vem1.mtx with Tolerance: $10^{-4}$			
Method	Iterations	Rel. error	Time (in seconds)
Jacobi	1314	$3.54 \times 10^{-3}$	$7.10 \times 10^{-2}$
Gauß-Seidel	659	$3.51 \times 10^{-3}$	6.67
Gradient	890	$2.70 \times 10^{-3}$	$6.70 \times 10^{-2}$
Conjugate Gradient	38	$4.08 \times 10^{-5}$	$5.01 \times 10^{-3}$

<b>vem1.mtx with Tolerance: <math>10^{-6}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	2433	$3.54 \times 10^{-5}$	$1.28 \times 10^{-1}$
Gauß-Seidel	1218	$3.53 \times 10^{-5}$	$1.23 \times 10^{+1}$
Gradient	1612	$2.71 \times 10^{-5}$	$1.23 \times 10^{-1}$
Conjugate Gradient	45	$3.73 \times 10^{-7}$	$7 \times 10^{-3}$

<b>vem1.mtx with Tolerance: <math>10^{-8}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	3552	$3.54 \times 10^{-7}$	$1.95 \times 10^{-1}$
Gauß-Seidel	1778	$3.52 \times 10^{-7}$	$2.05 \times 10^{+1}$
Gradient	2336	$2.70 \times 10^{-7}$	$2.25 \times 10^{-1}$
Conjugate Gradient	53	$2.83 \times 10^{-9}$	$9.01 \times 10^{-3}$

<b>vem1.mtx with Tolerance: <math>10^{-10}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	4671	$3.54 \times 10^{-9}$	$3.46 \times 10^{-1}$
Gauß-Seidel	2338	$3.51 \times 10^{-9}$	$2.81 \times 10^{+1}$
Gradient	3058	$2.71 \times 10^{-9}$	$2.90 \times 10^{-1}$
Conjugate Gradient	59	$2.19 \times 10^{-11}$	$9.99 \times 10^{-3}$

<b>vem2.mtx with Tolerance: <math>10^{-4}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	1927	$4.97 \times 10^{-3}$	$1.37 \times 10^{-1}$
Gauß-Seidel	965	$4.95 \times 10^{-3}$	$1.85 \times 10^{+1}$
Gradient	1308	$3.81 \times 10^{-3}$	$1.75 \times 10^{-1}$
Conjugate Gradient	47	$5.73 \times 10^{-5}$	$1.10 \times 10^{-2}$

<b>vem2.mtx with Tolerance: <math>10^{-6}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	3676	$4.97 \times 10^{-5}$	$3.35 \times 10^{-1}$
Gauß-Seidel	1840	$4.94 \times 10^{-5}$	$3.34 \times 10^{+1}$
Gradient	2438	$3.79 \times 10^{-5}$	$2.27 \times 10^{-1}$
Conjugate Gradient	56	$4.74 \times 10^{-7}$	$1.00 \times 10^{-2}$

<b>vem2.mtx with Tolerance: <math>10^{-8}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	5425	$4.97 \times 10^{-7}$	$3.66 \times 10^{-1}$
Gauß-Seidel	2714	$4.96 \times 10^{-7}$	$5.63 \times 10^{+1}$
Gradient	3566	$3.81 \times 10^{-7}$	$3.30 \times 10^{-1}$
Conjugate Gradient	66	$4.30 \times 10^{-9}$	$1.30 \times 10^{-2}$

<b>vem2.mtx with Tolerance: <math>10^{-10}</math></b>			
<b>Method</b>	<b>Iterations</b>	<b>Rel. error</b>	<b>Time (in seconds)</b>
Jacobi	7174	$4.96 \times 10^{-9}$	$4.88 \times 10^{-1}$
Gauß-Seidel	3589	$4.95 \times 10^{-9}$	$6.77 \times 10^{+1}$
Gradient	4696	$3.80 \times 10^{-9}$	$5.86 \times 10^{-1}$
Conjugate Gradient	74	$2.25 \times 10^{-11}$	$1.70 \times 10^{-2}$

The results in the tables above have been shown for completeness, but it is actually difficult to grasp the differences between the solvers with such tabular representations. For this reason, the results have been further analysed and different visualization techniques have been used to highlight the strengths and weaknesses of the four solvers.

Let's first discuss what happens when the solvers are given a sparse matrix that has not any pattern in its structure, that is, let's first consider the matrices in *spa1.mtx* and in *spa2.mtx*.

Concerning the convergence of the solvers in terms of the value of the scaled residual to the varying of the iterations, Figures 11 and 12 show the results obtained in *spa1.mtx* and in *spa2.mtx* using a tolerance value equals to  $10^{-10}$ . As it is shown, the Gradient method has difficulty converging to the solution: it requires a great number of iterations; instead, the Gauß-Seidel method takes very few iterations to reach the convergence. On the other hand, focusing the attention on the execution time, Figures 13 and 14 show that the Gauß-Seidel method is not the most efficient method, even if it takes less than 20 iterations to converge. This is due to the fact that a generic iteration in the Gauß-Seidel method is expensive in terms of time complexity, because at each iteration a system of linear equations must be solved. In addition, the last two figures confirm once again that the Gradient method is the slowest method.

Now, let's consider the other two matrices, which have the coefficients concentrated on their main diagonals, that is, let's consider the matrices in *vem1.mtx* and in *vem2.mtx*.

Also in this case, Figures 15 and 16 show the convergence of the solvers in terms

of the value of the scaled residual to the varying of the iterations. Contrary to what happened with the previous matrices *spa1.mtx* and *spa2.mtx*, it is possible to see that both the Gradient and the Conjugate Gradient methods take less iterations to converge, because the condition numbers of the considered matrices are smaller than the ones of the previous matrices, while the Gauß-Seidel method now is having difficulty converging. Furthermore, the Jacobi method requires a higher number of iterations to reach the convergence than the other methods. In addition, focusing on the time needed to achieve the convergence, Figures 17 and 18 show that the Gradient and the Conjugate Gradient methods are the fastest solvers, while the Gauß-Seidel method appears to be very slow. Interestingly, the Jacobi method is still fast, even if it takes a lot of iterations to converge and this can be explained by the fact that updating the current approximate solution is not so expensive in terms of time complexity.

It's worthwhile to notice that, considering the scaled residual curve to the varying of the iterations, the Gradient and Conjugate Gradient methods have a more irregular convergence, as also shown in Figure 19. The figure shows a zoomed view of both the Gradient graph and the Conjugate Gradient graph with respect to Figure 16. In particular, it is possible to see that both the methods do not present a monotonous decrease in the scaled residual and this can be explained by the fact that the Gradient and the Conjugate gradient methods are not based on splitting and, thus, Proposition 1 does not hold.

**Proposition 1.** *Suppose that  $A$  can be factored as  $A = P - N$ , where  $A$  and  $P$  are symmetric and definite positive matrices. If  $2P - A$  is also a definite positive matrix, then the iterative method defined as  $x^{(k+1)} = P^{-1}Nx^{(k)} + P^{-1}b$  converges for each initialization of  $x^{(0)}$  and*

$$|\lambda_{\max}| < 1,$$

where  $\lambda_{\max}$  is the maximum-modulus eigenvalue of the  $P^{-1}N$  matrix. In addition, the convergency is monotonous with respect to the norms  $\|\cdot\|_p$ .

However, the Conjugate Gradient method was introduced in the literature also to solve the "zig-zag" problem of the simple Gradient method and this is why it converges with less iterations and the curve of the residuals in Figure 19 is more regular.

In conclusion, it's important to underline that the Gradient and the Conjugate Gradient methods performed better with the *vem1.mtx* and the *vem2.mtx* matrices because they have lower condition numbers and, thus, the choice of the initial solution  $x^{(0)}$  has less influence on convergence. Instead, in the *spa1.mtx*



and the *spa2.mtx* matrices the initial solution  $x^{(0)}$  has a greater impact on the convergence.

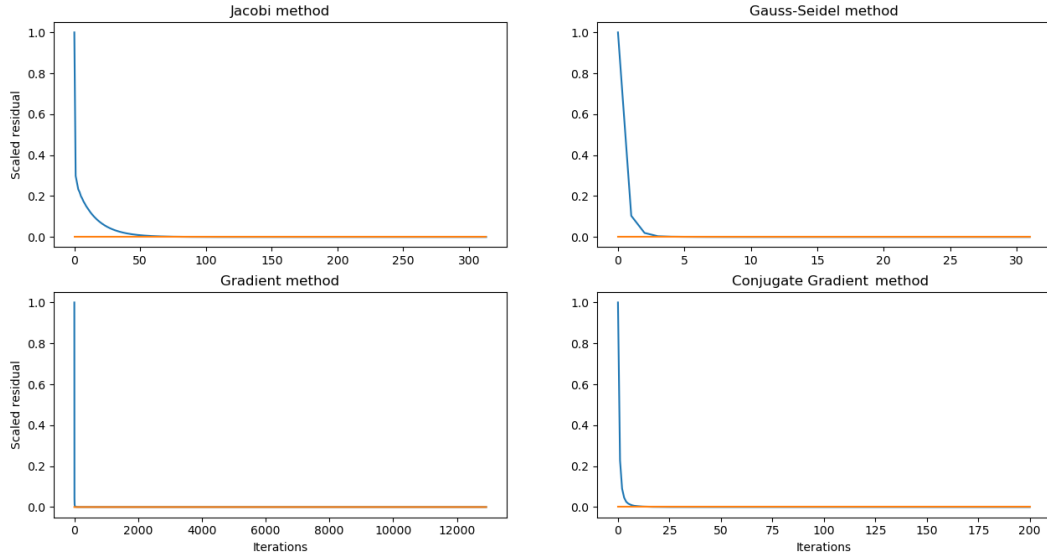


Figure 11: Comparison between the solvers in terms of the scaled residual and the number of iterations in *spa1.mtx* with tolerance equals to  $10^{-10}$

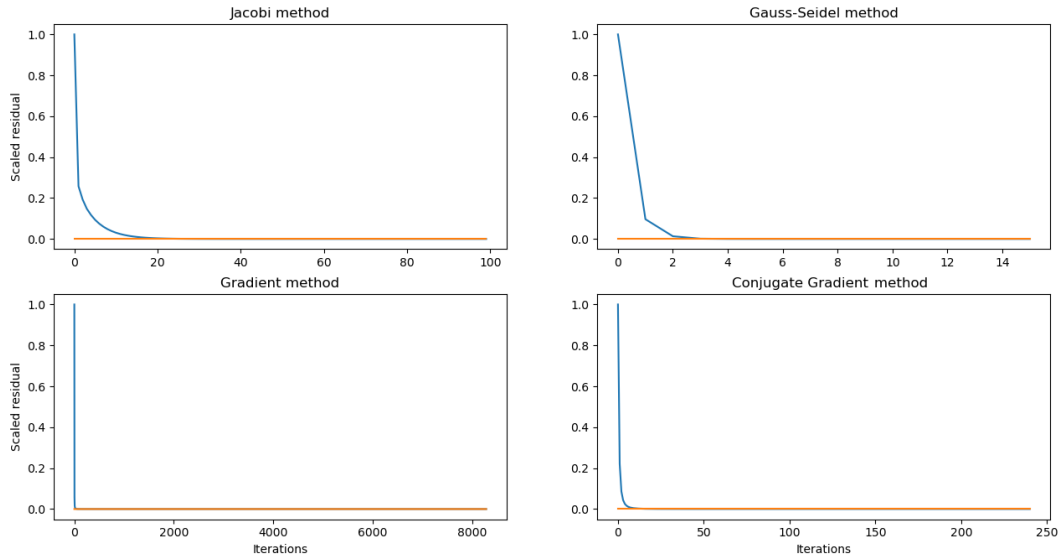


Figure 12: Comparison between the solvers in terms of the scaled residual and the number of iterations in *spa2.mtx* with tolerance equals to  $10^{-10}$

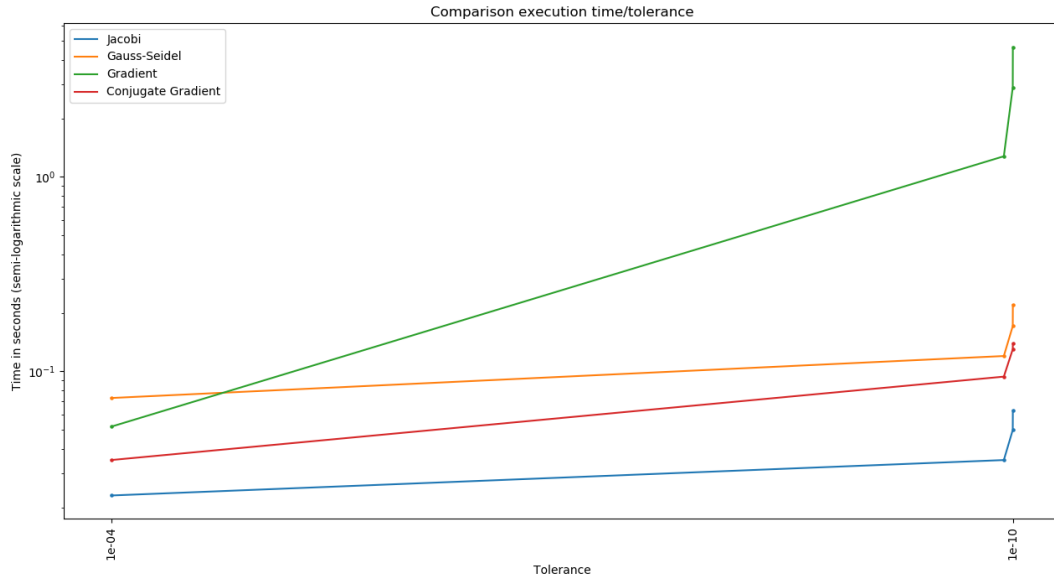


Figure 13: Semilog plot that compares the solvers in terms of time needed to achieve the convergence to the varying of the tolerance in *spa1.mtx*

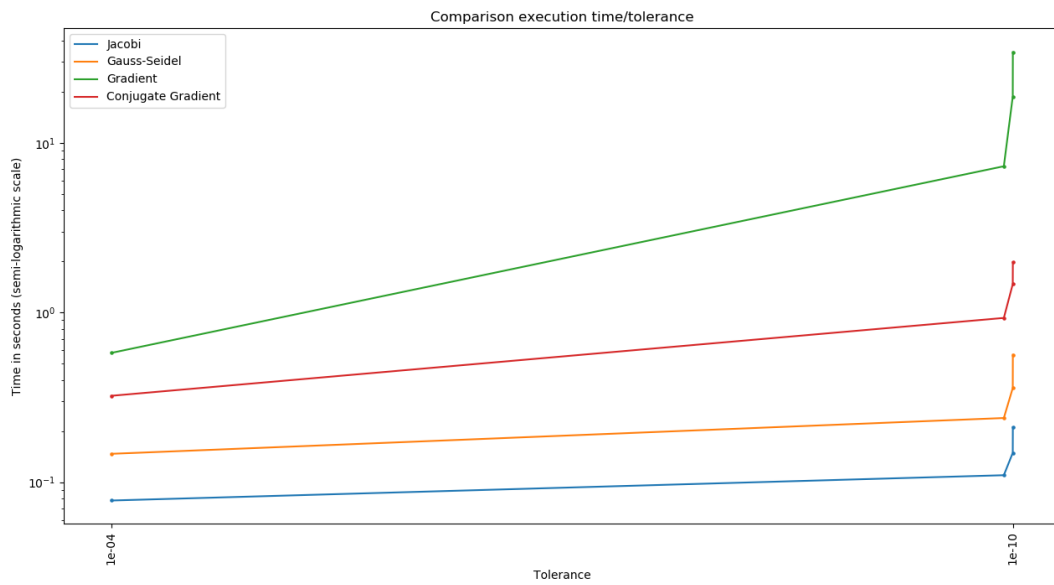


Figure 14: Semilog plot that compares the solvers in terms of time needed to achieve the convergence to the varying of the tolerance in *spa2.mtx*

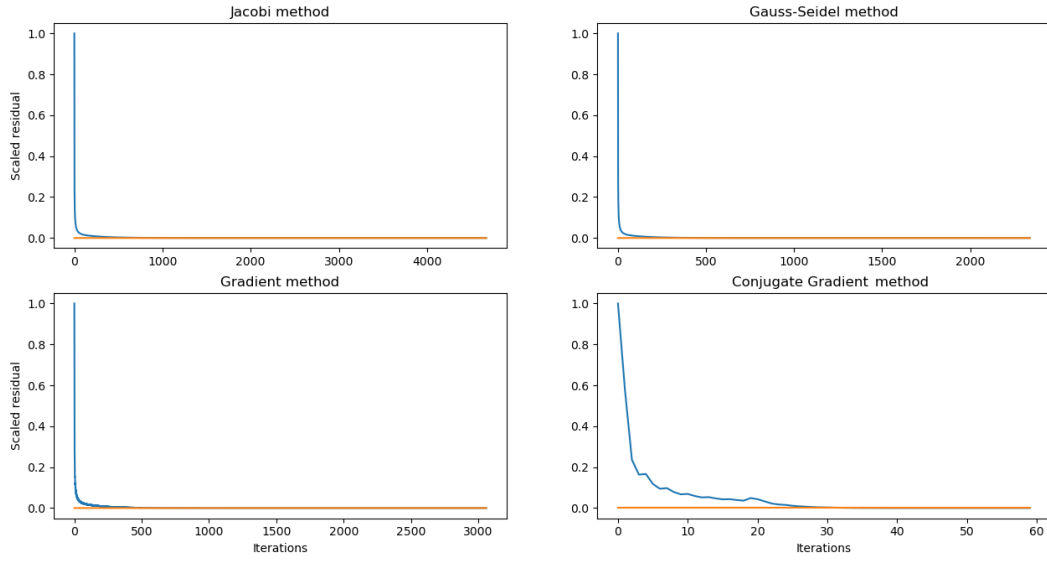


Figure 15: Comparison between the solvers in terms of the scaled residual and the number of iterations in *vem1.mtx* with tolerance equals to  $10^{-10}$

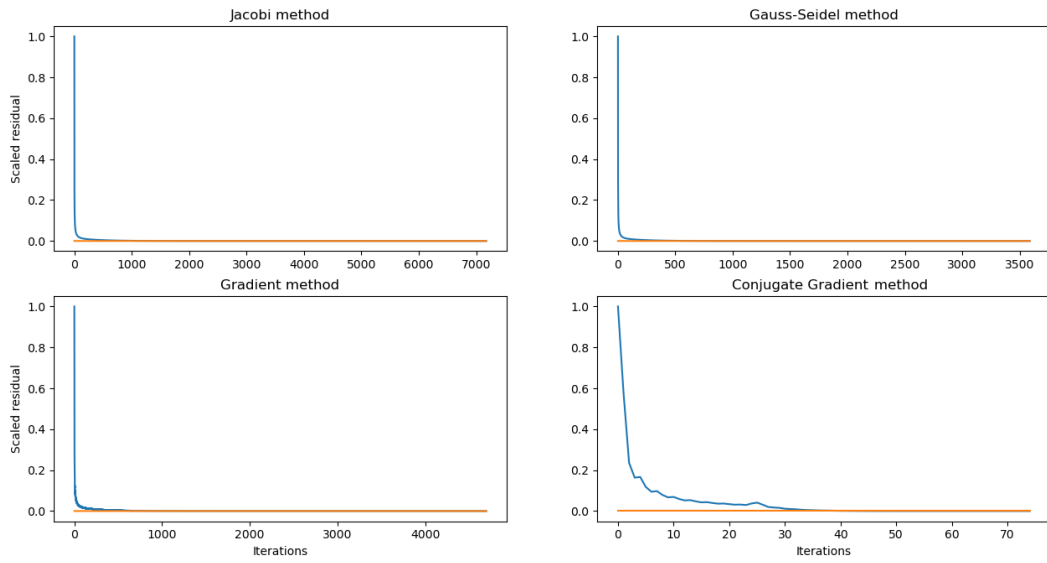


Figure 16: Comparison between the solvers in terms of the scaled residual and the number of iterations in *vem2.mtx* with tolerance equals to  $10^{-10}$

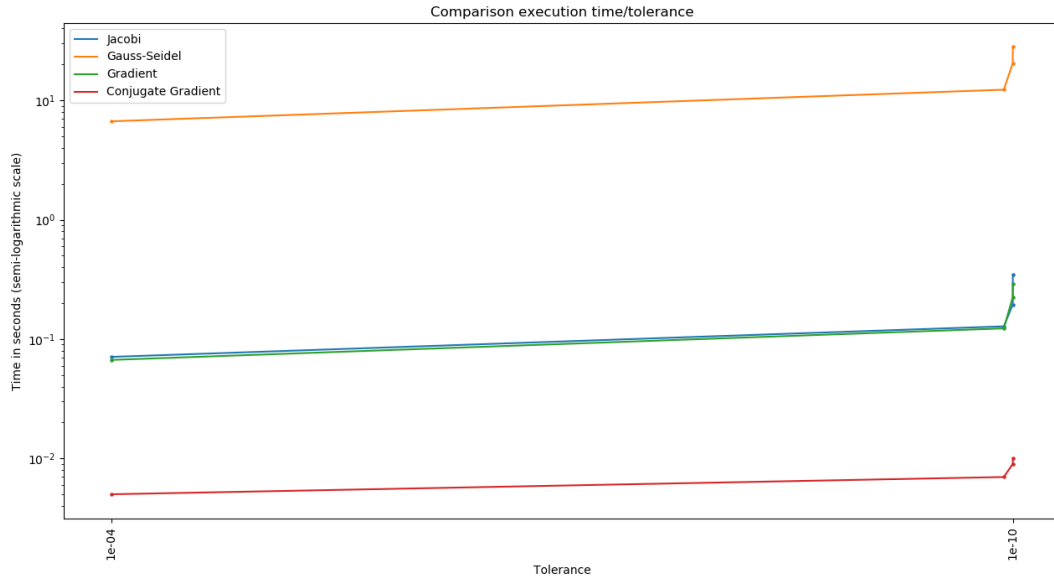


Figure 17: Semilog plot that compares the solvers in terms of time needed to achieve the convergence to the varying of the tolerance in *vem1.mtx*

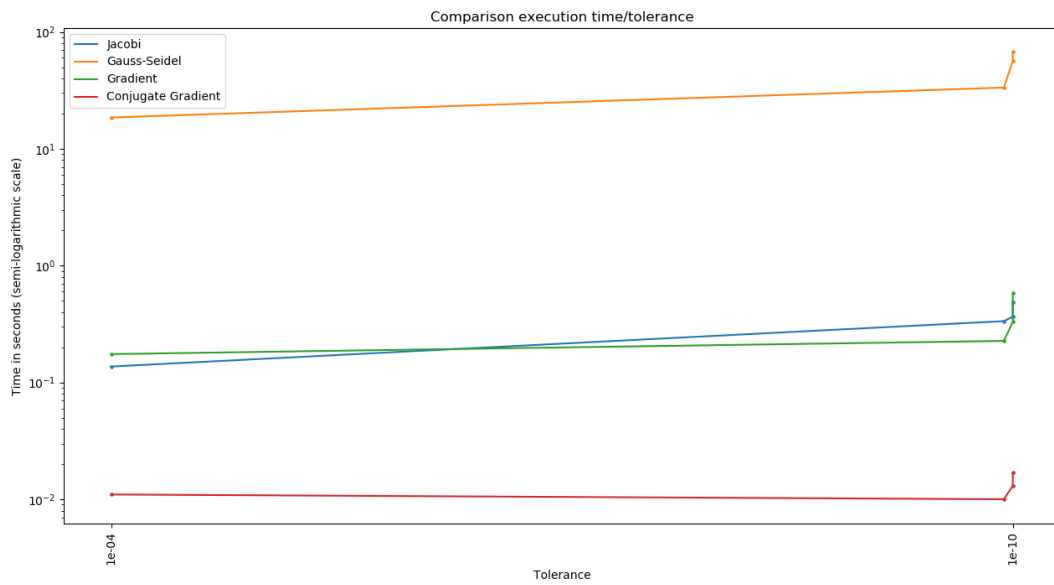


Figure 18: Semilog plot that compares the solvers in terms of time needed to achieve the convergence to the varying of the tolerance in *vem2.mtx*

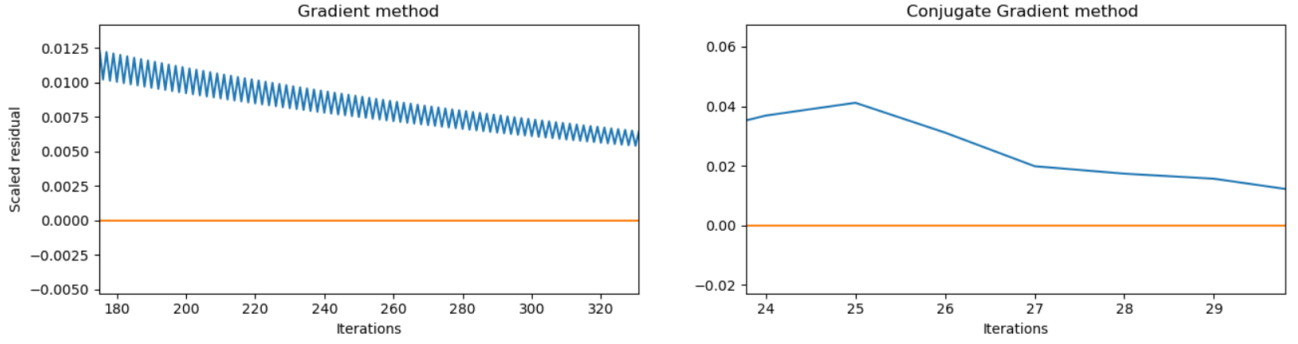


Figure 19: Zoomed view of the graphs in Figure 16 related to the Gradient and the Conjugate Gradient methods

## 4 Conclusion

This work has first presented in Section 2 the implementation of a library for solving systems of linear equations  $Ax = b$ , where  $A$  is a sparse matrix. In particular, the library contains the implementations of the following iterative methods: Jacobi method, Gauß-Seidel method, Gradient method and Conjugate Gradient method.

Then, this work has presented in Section 3 the validation study that has been conducted on the implemented library. This study revealed the strengths and weaknesses of the different methods and, in particular, this study has empirically demonstrated that there is no more efficient solver suitable for all possible systems of equations. In fact, from the results of the study, it has emerged that if the matrix does not have a particular pattern in its structure, the Jacobi and the Gauß-Seidel methods are faster in convergence than the Gradient and the Conjugate Gradient methods; instead, if the matrix presents the majority of the coefficients concentrated along its main diagonal, then the Gradient and the Conjugate Gradient methods perform well, while the Gauß-Seidel method is very inefficient. However, in both the cases, the Jacobi method does not seem to be inefficient.

## References

- [1] Guido Van Rossum and Fred L Drake Jr. *Python reference manual*. Centrum voor Wiskunde en Informatica Amsterdam, 1995.
- [2] Travis Oliphant. *Guide to NumPy*. 01 2006.
- [3] Pauli Virtanen, Ralf Gommers, Travis E. Oliphant, Matt Haberland, Tyler Reddy, David Cournapeau, Evgeni Burovski, Pearu Peterson, Warren Weckesser, Jonathan Bright, Stéfan J. van der Walt, Matthew Brett, Joshua Wilson, K. Jarrod Millman, Nikolay Mayorov, Andrew R. J. Nelson, Eric Jones, Robert Kern, Eric Larson, CJ Carey, İlhan Polat, Yu Feng, Eric W. Moore, Jake VanderPlas, Denis Laxalde, Josef Perktold, Robert Cimrman, Ian Henriksen, E. A. Quintero, Charles R Harris, Anne M. Archibald, Antônio H. Ribeiro, Fabian Pedregosa, Paul van Mulbregt, and SciPy 1.0 Contributors. SciPy 1.0: Fundamental Algorithms for Scientific Computing in Python. *Nature Methods*, 17:261–272, 2020.
- [4] Steve Cook, Conrad Bock, Pete Rivett, Tom Rutt, Ed Seidewitz, Bran Selic, and Doug Tolbert. Unified modeling language (UML) version 2.5.1. Standard, Object Management Group (OMG), December 2017.
- [5] Bjarne Stroustrup. *The C++ Programming Language*. Addison-Wesley Professional, 4th edition, 2013.