Poisson Solver (2D)

Nikos Tryfonidis

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Abstract

The current report summarizes the structure, use and results of a two-dimensional Poisson solver, created for the purpose of being integrated into a 2D Particle-In-Cell (PIC) code. After a brief introduction regarding the numerical solution of the 2D Poisson PDE in chapter 1, the structure of the code will be described in chapter 2. Verification of the code will be given in chapter 3, through a number of test cases. Finally, the different iterative methods that have been implemented will be discussed in chapter 4, along with a review of their performance.

Contents

Chapter 1

2D Poisson Equation: Numerical Solution

The Poisson Equation and the associated boundary conditions form what is generally known as a *Poisson Problem*:

$$\nabla^2 u = u_{xx} + u_{yy} = f(x, y) \tag{1.1}$$

The Poisson Problem is one of the most well-known Elliptic Partial Differential Equations (PDE). A brief description of the numerical method followed in the code will be given here. Detailed analysis of the Poisson PDE and other methods can be found in most numerical analysis textbooks (for example [1]).

1.1 The Finite Difference Scheme

The 5-point stencil discretization scheme is followed. A uniform Cartesian grid is used, where each point x_i, y_j describes a point in 2D space, with $x_i = i\Delta x$ and $y_j = j\Delta y$. We assume that $0 \leq x \leq 1$ and $0 \leq y \leq 1$ for simplicity. Replacing the derivatives u_{xx} and u_{yy} in (1.1) with centered finite difference schemes, we end up with the following discretization scheme:

$$\frac{1}{(\Delta x)^2}(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}) + \frac{1}{(\Delta y)^2}(u_{i,j-1} - 2u_{i,j} + u_{i,j+1}) = f_{i,j} \tag{1.2}$$

Assuming that $\Delta x = \Delta y = h$, we get the simple finite difference scheme

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j} = h^2 f_{i,j} \tag{1.3}$$

For a grid of $N \times N$ points in total, this scheme gives a linear system of $(N-2)\times(N-2)$ equations for the $(N-2)\times(N-2)$ unknowns (the excluded values are the boundaries, which are considered known). As an example to illustrate the system of equations, suppose we have a 5×5 grid of points, including boundaries, that represent our 2D space.

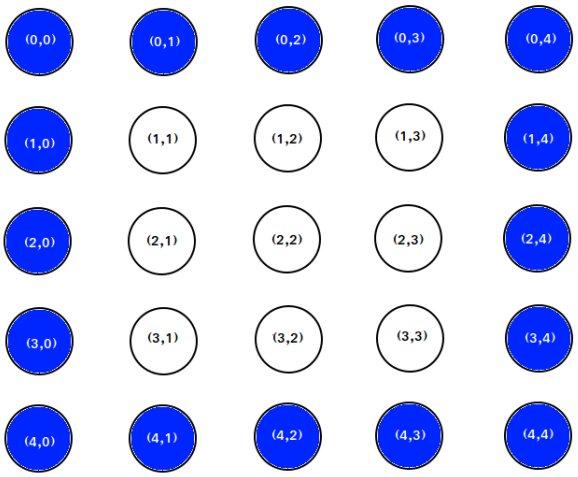


Figure 1.1: A 5×5 two-dimensional grid. Boundary points, for which the solution is known, are shown in blue.

Applying the finite difference scheme (1.3) to each inner grid point $u_{i,j}$ leads us to a system of $(5-2)\times(5-2) = 9$ equations:

$$\boldsymbol{u_{1,1}}: \quad u_{0,1} + u_{2,1} + u_{1,0} + u_{1,2} - 4u_{1,1} = h^2 f_{1,1} \tag{1.4a}$$
$$\boldsymbol{u_{1,2}}: \quad u_{0,2} + u_{2,2} + u_{1,1} + u_{1,3} - 4u_{1,2} = h^2 f_{1,2} \tag{1.4b}$$
$$\boldsymbol{u_{1,3}}: \quad u_{0,3} + u_{2,3} + u_{1,2} + u_{1,4} - 4u_{1,3} = h^2 f_{1,3} \tag{1.4c}$$
$$\boldsymbol{u_{2,1}}: \quad u_{1,1} + u_{3,1} + u_{2,0} + u_{2,2} - 4u_{2,1} = h^2 f_{2,1} \tag{1.4d}$$
$$\boldsymbol{u_{2,2}}: \quad u_{1,2} + u_{3,2} + u_{2,1} + u_{2,3} - 4u_{2,2} = h^2 f_{2,2} \tag{1.4e}$$
$$\boldsymbol{u_{2,3}}: \quad u_{1,3} + u_{3,3} + u_{2,2} + u_{2,4} - 4u_{2,3} = h^2 f_{2,3} \tag{1.4f}$$
$$\boldsymbol{u_{3,1}}: \quad u_{2,1} + u_{4,1} + u_{3,0} + u_{3,2} - 4u_{3,1} = h^2 f_{3,1} \tag{1.4g}$$
$$\boldsymbol{u_{3,2}}: \quad u_{2,2} + u_{4,2} + u_{3,1} + u_{3,3} - 4u_{3,2} = h^2 f_{3,2} \tag{1.4h}$$
$$\boldsymbol{u_{3,3}}: \quad u_{2,3} + u_{4,3} + u_{3,2} + u_{3,4} - 4u_{3,3} = h^2 f_{3,3} \tag{1.4i}$$

We have arranged the equations row-wise, grouping elements with the same row number (i index) together. We also see the boundary grid points in blue. These are considered to be known from the given boundary conditions.

We can now present the linear system of equations in matrix form,

$$\overleftrightarrow{\mathbf{A}} \cdot \overrightarrow{\mathbf{u}} = \overrightarrow{\mathbf{b}}, \tag{1.5}$$

where $\overleftrightarrow{\mathbf{A}}$ is the matrix equation, $\overrightarrow{\mathbf{u}}$ is the vector of unknowns and $\overrightarrow{\mathbf{b}}$ is the right-hand-side of the system of equations. Note that we will move the known boundary grid points to the right-hand-side of the matrix equation (again, shown in blue). The resulting matrix equation is

$$\begin{pmatrix}
\boldsymbol{u_{1,1}} & \boldsymbol{u_{1,2}} & \boldsymbol{u_{1,3}} & \boldsymbol{u_{2,1}} & \boldsymbol{u_{2,2}} & \boldsymbol{u_{2,3}} & \boldsymbol{u_{3,1}} & \boldsymbol{u_{3,2}} & \boldsymbol{u_{3,3}} \\
-4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4
\end{pmatrix} \cdot \begin{pmatrix} u_{1,1} \\ u_{1,2} \\ u_{1,3} \\ u_{2,1} \\ u_{2,2} \\ u_{2,3} \\ u_{3,1} \\ u_{3,2} \\ u_{3,3} \end{pmatrix} = \begin{pmatrix} h^2 f_{1,1} + u_{0,1} + u_{1,0} \\ h^2 f_{1,2} + u_{0,2} \\ h^2 f_{1,3} + u_{0,3} + u_{1,4} \\ h^2 f_{2,1} + u_{2,0} \\ h^2 f_{2,2} \\ h^2 f_{2,3} + u_{2,4} \\ h^2 f_{3,1} + u_{4,1} + u_{3,0} \\ h^2 f_{3,2} + u_{3,2} + u_{4,2} \\ h^2 f_{3,3} + u_{4,3} + u_{3,4} \end{pmatrix}$$

We see that the resulting $\overleftrightarrow{\mathbf{A}}$ matrix is block-tridiagonal:

$$\overleftrightarrow{\mathbf{A}} = \begin{pmatrix} \boldsymbol{T} & \boldsymbol{I} & \mathbf{0} \\ \boldsymbol{I} & \boldsymbol{T} & \boldsymbol{I} \\ \mathbf{0} & \boldsymbol{I} & \boldsymbol{T} \end{pmatrix} \tag{1.6}$$

$$\boldsymbol{T} = \begin{pmatrix} -4 & 1 & 0 \\ 1 & -4 & 0 \\ 0 & 1 & -4 \end{pmatrix}, \quad \boldsymbol{I} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{1.7}$$

This linear system of equations can be solved with a variety of methods (direct, iterative etc). Our focus will be on iterative methods.

1.2 Error and Stability

We will not go into the details of error and stability analysis in this report, since these are well-known and can be found in most relevant texts (e.g. [1]). We should simply keep in mind that the local truncation error of the 5-point stencil finite difference scheme we are using is $O(h^2)$ and that the method is stable, so the global error of the method is also $O(h^2)$. In case we do not assume $\Delta x = \Delta y = h$, this simply means that the error is $O\left((\Delta x)^2, (\Delta y)^2\right)$.

Chapter 2

The Code

In this chapter, the structure and use of the code will be described. The project has been arranged into separate directories. The source code is in "src", with corresponding header files in "headers", one for each .c source file (other than "main.c"). Object files (".o") are automatically placed into the "obj" directory by the makefile. Output files are also placed into the "output" directory. The python visualization script used for plotting the output is also in "output". Finally, "documentation" contains the current report.
In the following sections, we will briefly go through instructions on how to use the code, and we will review its structure.

2.1 Compilation and Execution

The code does not contain any external libraries and should compile without problems on any linux system with a C compiler. To compile, go to the central directory of the project, where the makefile is located, and type "make". This will create the executable file in the same directory, with object files in "obj". To delete the executable and the object files, type "make clean".
To run, simply run the executable from the command line, giving two arguments (number of grid points in dimensions X and Y, respectively). For example, the following will run the program with 101 grid points in X and Y:

```
./poisson2D 101 101
```

2.2 Code Structure

Here we will briefly go through the code structure, by explaining the work done by each of the source files.

main.c The main file simply wraps all pieces of the program together and can be seen as a program outline. First it reads the command line arguments and it allocates the required memory. Then, it sets up the problem, by setting the appropriate Boundary Conditions and right-hand-side function f(x,y) (see "setup.c").

io.c Contains functions that read command line arguments and write file output.

setup.c Contains functions that set boundary conditions and the right-hand-side function. This is where the user can specify the Poisson problem he/she wants to solve. *Boundary conditions* can be set for each one of the four boundaries separately, by the "$setBoundaries2D$" function. The RHS function is set by "$setRHS2D$".

memory.c Contains the "$array2D_contiguous$" function, that dynamically allocates a two-dimensional array of doubles, contiguous in memory. Also contains the "$free_array2D_contiguous$" function, that frees memory allocated by the previous function.

poisson2D.c The solver function. It iterates the solution for the appropriate number of iterations, until the desired accuracy is reached (or a maximum number of iterations is done). The iteration method of choice is passed into the function as an argument (function pointer). Error tolerance, maximum iterations, iterations per residual check are all set in this function. Also contains the residual calculation function.

iterative.c Contains the different iterative methods that may be used, and that are called by "$solvePoisson2D$". Currently, the Jacobi, Gauss-Seidel and Successive Overrelaxation methods have been implemented.

The space dimensions $(x_0, x_L), (y_0, y_L)$ are set in *definitions.h*, inside the *headers* directory.

2.3 Data Structures

The main data structure used is a two-dimensional array of doubles, that represents the discretized space grid. The dimensions of the grid are given

from the command line arguments the user provides. Memory for the 2D array is allocated by the "$array2D_contiguous$" function in *memory.c*.

Also, another two-dimensional array of the same dimensions is the right-hand-side function (RHS) of the Poisson Equation, $f(x, y)$. Memory for the RHS function is allocated in the same way as for the grid. The values of RHS for each grid point is set by the "$setRHS2D$" function in *setup.c*.

2.4 Solving a Poisson Problem

To solve a given Poisson problem, the user must perform the following actions:

1. Set Boundary Conditions in *setBoundaries2D* (setup.c).
2. Set the RHS function of the Poisson problem in *setRHS2D* (setup.c).
3. Choose the desired iterative method in main function (main.c).
4. Compile the program by typing "make" in the main directory (where the makefile is located).
5. Run the executable with the desired number of grid points in each of the two dimensions.

2.5 Output

Output is written in the "output" directory. Two output files are written:

output.txt Contains the 2D solution grid.

gridData.txt Contains grid data $((x_0, x_L), (y_0, y_L))$, step sizes (dx, dy) and number of grid points in each dimension (N_x, N_y). Data from this file is read by the visualization python script in the same folder, in order to create a plot of the results.

The solution is visualized by the python script *visualize.py*, in the output directory. The script requires *numpy* and *matplotlib*, two well-known packages for scientific computing in Python.
These can be easily installed in any Linux system, for example in Ubuntu:

```
sudo apt-get install python-numpy python-matplotlib
```

This python script reads grid meta-data from *gridData.txt* and the solution from *output.txt* and creates a 3D plot of the solution.
To create the plot, the user must simply run the script by typing:

```
python visualize.py
```

Chapter 3

Verification

In this chapter we will verify the correctness of the 2D Poisson solver, through three basic examples that have known analytic solutions. By comparing the numerical solution with the analytic one, we will show that the solver produces correct results.

Each example has detailed instructions on how to set up the Poisson problem studied, so the following sections can also be used as examples on how to use the code. The *Gauss-Seidel* iterative method was chosen for these examples, with a tolerance of Δx^2 for the residual check.

For the following examples, the domain was chosen to be $0 \leq x, y \leq 1$, which is set in *headers/definitions.h* as follows:

```
#define X0 0.0
#define XL 1.0
#define Y0 0.0
#define YL 1.0
```

We also used 101 grid points for each dimension, dividing each dimension into $(101 - 1)$ pieces, so that

$$\Delta x = \Delta y = (Length)/(101 - 1) = 1.0/100 = 0.01 \tag{3.1}$$

3.1 Zero RHS (Laplace Equation)

In this problem, we will solve a Poisson problem with no right-hand-side function. Let us assume that the (known) solution $u(x, y)$ is

$$u(x, y) = 3x + 4y \tag{3.2}$$

The corresponding Poisson problem is then

$$\nabla^2 u = u_{xx} + u_{yy} = 0 \tag{3.3a}$$

$$u(x, 0) = 3x \qquad u(x, y_L) = 3x + 4y_L \tag{3.3b}$$

$$u(0, y) = 4y \qquad u(x_L, y) = 3x_L + 4y \tag{3.3c}$$

Equation (3.2a), along with boundary conditions (3.2b) and (3.2c) are also known as a Laplace problem, a special case of the Poisson problem with a zero right-hand-side function. We will now solve this Poisson problem and compare the numerical solution with the analytic (3.1).

Setting Up The Problem

As explained in paragraph *2.4*, the functions that are used to set up the desired Poisson problem are in *setup.c*. Boundary conditions are given by the known solution *(3.1)*, while the RHS function is zero for this problem.

We set the Boundary Conditions:

```
double fBC(double x, double y)
{
    return 3.0*x + 4.0*y;
}
```

and the RHS function:

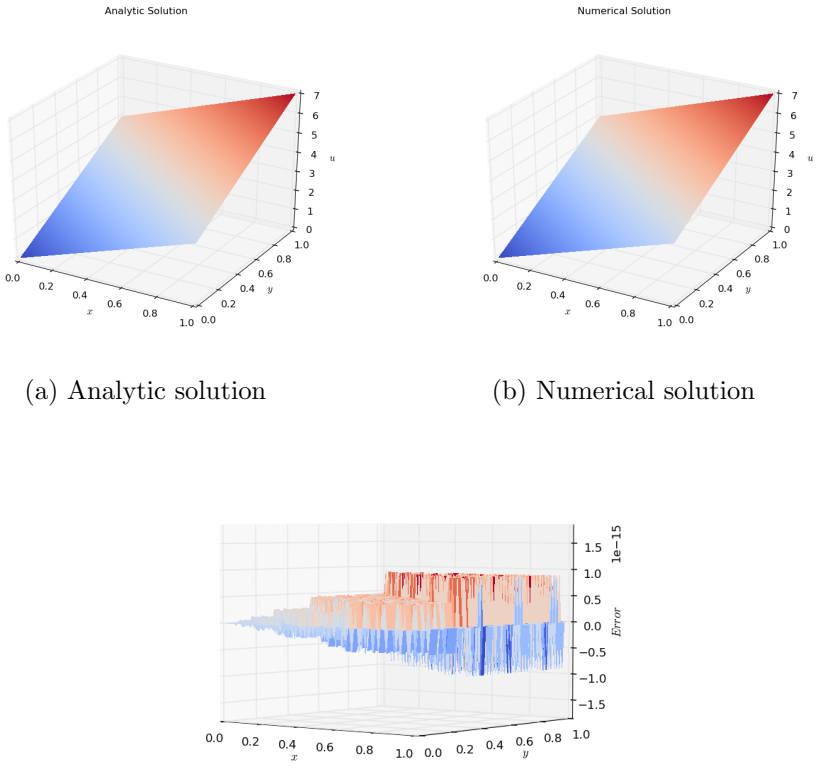
```
double f(double x, double y)
{
    return 0.0;
}
```

Running the Solver

After we set up the problem as shown, we compile the program and run. To specify 101 grid points for x and y, we run the executable as follows:

```
./poisson2D 101 101
```

Once the program has finished, output is ready in *output/output.txt*. We can plot the solution by running the python script *visualize.py*, which will create a 3D surface plot of our solution. In the next figure, the analytic and numerical solutions are shown side by side for comparison:



(a) Analytic solution

(b) Numerical solution

(c) Error

Figure 3.1: Analytic (a) and numerical (b) solution for the current Poisson problem, with a surface plot of the error in (c).

We see that the numerical solution is identical to the analytic one, and the error is shown to be of the order of 10^{-15} (machine precision, since with a constant right-hand-side we are effectively calculating averages).

3.2 Simple Linear RHS

Now, we will solve a Poisson problem with a simple linear right-hand-side function. Let us assume that the (known) solution $u(x, y)$ is

$$u(x, y) = x^2 + y^2 \tag{3.4}$$

The corresponding Poisson problem is now

$$\nabla^2 u = u_{xx} + u_{yy} = 2 + 2 = 4 \tag{3.5a}$$

$$u(x, 0) = x^2 \qquad u(x, y_L) = x^2 + (y_L)^2 \tag{3.5b}$$

$$u(0, y) = y^2 \qquad u(x_L, y) = (x_L)^2 + y^2 \tag{3.5c}$$

We will now solve this Poisson problem and compare the numerical solution with the analytic (3.4).

Setting Up The Problem

We set up the desired Poisson problem, as shown in the previous example, in *setup.c*. Boundary conditions are given by the known solution *(3.4)*, while the RHS function is equal to 4 for this problem.

We set the Boundary Conditions:

```
double fBC(double x, double y)
{
    return x*x + y*y;
}
```

and the RHS function:

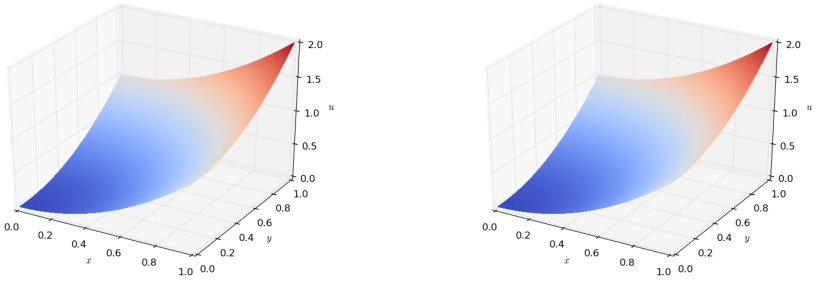
```
double f(double x, double y)
{
    return 4.0;
}
```

Running the Solver

We compile and run, once again, with 101 grid points in each dimension, as before:

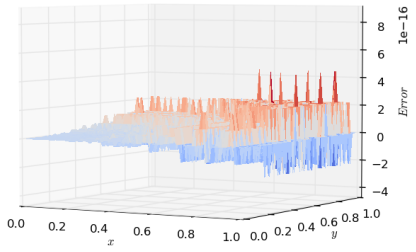
```
./poisson2D 101 101
```

We produce the surface plot of the results with *visualize.py*. In the next figure, the analytic and numerical solutions are shown side by side for comparison:



(a) Analytic solution

(b) Numerical solution



(c) Error

Figure 3.2: Analytic (a) and numerical (b) solution for the current Poisson problem, with a surface plot of the error in (c).

We see that the numerical solution is identical to the analytic one, and the error is shown to be of the order of 10^{-16} (machine precision again, since with a constant right-hand-side we are effectively calculating averages).

3.3 Sinusoidal RHS

Now, we will solve a Poisson problem with a slightly more complex right-hand-side function. Let us assume that the (known) solution $u(x, y)$ is

$$u(x, y) = sin\left[2\pi\left(x + y\right)\right] \tag{3.6}$$

The corresponding Poisson problem is now

$$\nabla^2 u = u_{xx} + u_{yy} = -8\pi^2 sin\left[2\pi\left(x + y\right)\right] \tag{3.7a}$$

$$u(x, 0) = sin\left[2\pi\left(x\right)\right] \qquad u(x, y_L) = sin\left[2\pi\left(x + y_L\right)\right] \tag{3.7b}$$

$$u(0, y) = sin\left[2\pi\left(y\right)\right] \qquad u(x_L, y) = sin\left[2\pi\left(x_L + y\right)\right] \tag{3.7c}$$

We will now solve this Poisson problem and compare the numerical solution with the analytic (3.6).

Setting Up The Problem

We set up the desired Poisson problem, as shown in the previous examples, in *setup.c*. Boundary conditions are given by the known solution *(3.6)*, while the RHS function is $f(x, y) = -8\pi^2 sin\left[2\pi\left(x + y\right)\right]$ for this problem.

We set the Boundary Conditions:

```
double fBC(double x, double y)
{
    return sin(2.0*M_PI*(x+y));
}
```

and the RHS function:

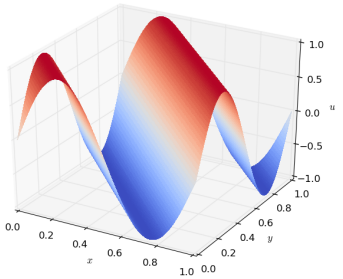
```
double f(double x, double y)
{
    return -8.0*M_PI*M_PI*sin(2.0*M_PI*(x+y));
}
```

Running the Solver

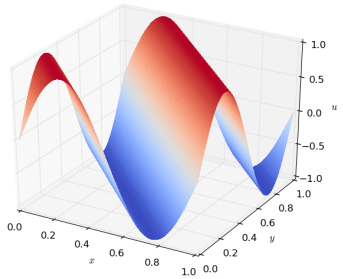
We compile the program and run with 101 grid points in each dimension, as before:

```
./poisson2D 101 101
```

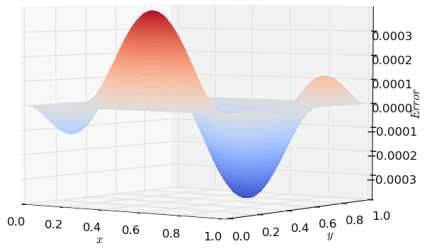
We produce the surface plot of the results with *visualize.py*. In the next figure, the analytic and numerical solutions are shown side by side for comparison. Also, the error surface plot is shown; this was created by plotting the difference of the analytic minus the numerical solution.



(a) Analytic solution



(b) Numerical solution



(c) Error

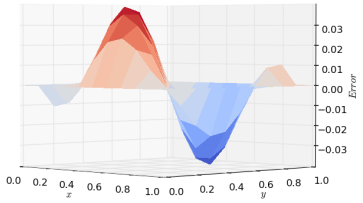
Figure 3.3: Analytic (a) and numerical (b) solution for the current Poisson problem, with a surface plot of the error in (c).

We see that the numerical solution is identical to the analytic one, and the error is shown to be, as expected, of the order of $O(h^2) = O(0.0001)$, where $h = \Delta x = \Delta y = 0.01$.

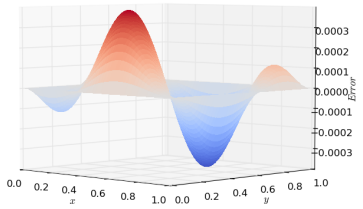
3.4 Minimizing the Error

As a last verification test, we will show that our solution becomes better (i.e. the error becomes smaller), as we refine our grid. We will use the previous section's Poisson problem to show this.

We will plot the error, using an increasing number of grid points. We expect the error to get smaller as dx, dy become smaller. The results are shown in the following two figures:



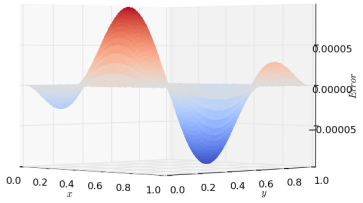
(a) $N = 10 \quad (h = 0.1)$



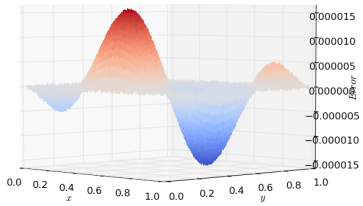
(b) $N = 100 \quad (h = 0.01)$

Figure 3.4: Error ($u_{analytic} - u_{numerical}$) for decreasing $h = dx = dy$. The error gets smaller as we go from 10 to 100 grid points (see Error axis range).

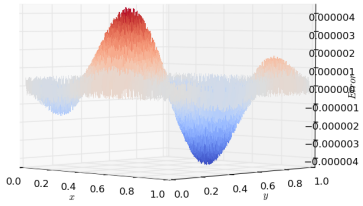
We notice that the error does get smaller as h decreases, and also it is of order $O(h^2)$, as expected. Even smaller h choices are shown in the next figure:



(a) $N = 200 \quad (h = 0.005)$



(b) $N = 500 \quad (h = 0.002)$



(c) $N = 1000 \quad (h = 0.001)$

Figure 3.5: Error ($u_{analytic} - u_{numerical}$) for decreasing $h = dx = dy$. The error gets smaller as we go from 200 to 1000 grid points (see Error axis range).

Chapter 4

Iterative Methods

In this chapter, we will briefly describe the different iterative methods that have been implemented for the solution of the linear system of equations of the Poisson problem. After that, a convergence review will be given for the methods. A detailed analysis of the iterative methods is outside the scope of this report, but can be found in most numerical PDE books (e.g. [1]).

The code for the iterative methods described in this chapter can be found in the *iterative.c* source file. The desired iterative method can be chosen in *main.c*, where it is passed as function pointer to the Poisson solver function.

4.1 Jacobi Method

The Jacobi method is the simplest iterative method that we will examine, and also the least efficient, as it has the slowest convergence. However, it is useful, not only as an example, but as a smoother in multigrid methods [1].

The Poisson problem we are solving can be written as follows, assuming that $dx = dy = h$, from equation (1.3):

$$u_{i,j} = \frac{1}{4}\left(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1}\right) - \frac{h^2}{4} f_{i,j} \tag{4.1}$$

The Jacobi method can be described by the following algorithm:

$$u_{i,j}^{k+1} = \frac{1}{4}\left(u_{i-1,j}^{k} + u_{i+1,j}^{k} + u_{i,j-1}^{k} + u_{i,j+1}^{k}\right) - \frac{h^2}{4} f_{i,j} \tag{4.2}$$

where u^k is the *current* state of the solution, while u^{k+1} is the new estimation. It is obvious that this method requires more memory, as the previous estimation of the solution has to be stored.

Alternatively, if we do not assume that $dx = dy$, as in equation (1.2), we write the Poisson problem as follows:

$$\begin{aligned} u_{i,j} &= \frac{1}{2(dx^2+dy^2)}\left((u_{i-1,j}+u_{i+1,j})dy^2+(u_{i,j-1}+u_{i,j+1})dx^2\right) \\ &\quad - \frac{dx^2dy^2}{2(dx^2+dy^2)}f_{i,j} \end{aligned} \tag{4.3}$$

and the Jacobi method is now

$$\begin{aligned} u_{i,j}^{k+1} &= \frac{1}{2(dx^2+dy^2)}\left((u_{i-1,j}^{k}+u_{i+1,j}^{k})dy^2+(u_{i,j-1}^{k}+u_{i,j+1}^{k})dx^2\right) \\ &\quad - \frac{dx^2dy^2}{2(dx^2+dy^2)}f_{i,j} \end{aligned} \tag{4.4}$$

4.2 Gauss - Seidel Method

The Gauss-Seidel method is a variation of the Jacobi method; it improves the solution by using the already calculated values for the new estimation. This simply translates to the following algorithm:

$$u_{i,j}^{k+1} = \frac{1}{4}\left(u_{i-1,j}^{k+1}+u_{i+1,j}^{k}+u_{i,j-1}^{k+1}+u_{i,j+1}^{k}\right) - \frac{h^2}{4}f_{i,j} \tag{4.5}$$

or, keeping $dx \neq dy$:

$$\begin{aligned} u_{i,j}^{k+1} &= \frac{1}{2(dx^2+dy^2)}\left((u_{i-1,j}^{k+1}+u_{i+1,j}^{k})dy^2+(u_{i,j-1}^{k+1}+u_{i,j+1}^{k})dx^2\right) \\ &\quad - \frac{dx^2dy^2}{2(dx^2+dy^2)}f_{i,j} \end{aligned} \tag{4.6}$$

The Gauss-Seidel method converges roughly twice as fast as the Jacobi method, and it does not require additional memory. However, it is less straightforward to parallelize (but can be parallelized using a red-black scheme [2]).

4.3 Successive Overrelaxation

Successive overrelaxation (SOR) is an improvement on the Gauss-Seidel method, using an additional scalar parameter ω, which is essentially moves the solution farther than Gauss-Seidel if $\omega > 1$ (and nearer if $\omega < 1$). SOR can be described by the following algorithm:

$$u_{i,j}^{k+1} = \frac{\omega}{2}\left(u_{i-1,j}^{k+1} + u_{i+1,j}^{k} + u_{i,j-1}^{k+1} + u_{i,j+1}^{k}\right) - \frac{h^2}{4} f_{i,j} \tag{4.7}$$

and, in case that $dx \neq dy$:

$$\begin{aligned} u_{i,j}^{k+1} \quad = \quad & \omega\left[\frac{1}{2(dx^2+dy^2)}\left((u_{i-1,j}^{k+1} + u_{i+1,j}^{k})dy^2 + (u_{i,j-1}^{k+1} + u_{i,j+1}^{k})dx^2\right)\right. \\ & \left. -\frac{dx^2dy^2}{2(dx^2+dy^2)} f_{i,j}\right] + (1-\omega)u_{i,j}^{k} \end{aligned} \tag{4.8}$$

It should be mentioned that SOR is unstable for $\omega > 2$, while for $\omega = 1$ it is equivalent to the Gauss-Seidel method. Regarding the optimal choice for ω, in general it depends on the problem (and may be hard to find). However, for the Poisson problem it can be shown that $\omega_{opt} \simeq 2 - 2\pi h$ ([1], par. 4.2.2).

4.4 Residual Checking

Before commenting on the convergence of the previous methods, it will be useful to show the method followed in order to validate our iterative solution. The method followed is the well-known *residual checking* method. This involves calculating the estimated solution between a fixed number of steps checking if the residual is smaller than a predetermined tolerance.

If $\boldsymbol{A}$ is the equation matrix and $\boldsymbol{u}$ is the estimated solution after a number of iterations, then

$$\boldsymbol{Au} = \boldsymbol{f}_{est} \tag{4.9}$$

But since we already know the right-hand values of our equations, we can quantify the correctness of our estimation by measuring how much our estimation differs from the actual right-hand side, by calculating the *residual*:

$$r = \boldsymbol{Au} - \boldsymbol{f}_{est} \tag{4.10}$$

and stopping when it becomes smaller than some value that we set:

$$\sqrt{\sum_{i,j} r_{i,j}^2} < tolerance \tag{4.11}$$

This procedure is carried out by the *residual* function in *src/poisson.c*.

4.5 Convergence Comparison

In this section we will show a brief comparison of the three iterative methods described in the revious sections. For this comparison, the Poisson problem shown in section (3.3) was solved, using 201×201 grid points.

To produce the following results, the program was altered slightly in order to output the residual in every iteration. Checking for the residual in every iteration is probably not worth the effort in general, but it is useful in order to evaluate the convergence of the three iterative methods.

We have set the maximum number of iterations to 1000 and the tolerance to zero; in this way, we can see the convergence of all three methods for 1000 iterations. Results are shown below using semi-log axes:

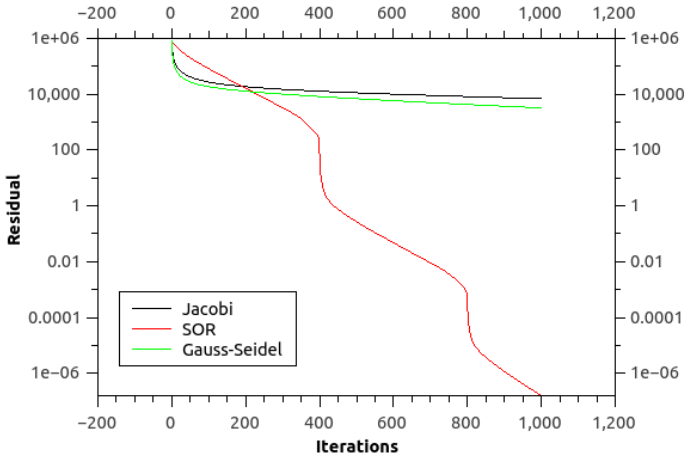


Figure 4.1: Residual versus number of iterations, for 3 different iterative methods (Jacobi, Gauss-Seidel, SOR). Problem size: 201×201

We see that SOR is by far the most effective method. However, we should keep in mind that we are using the optimal ω value for SOR, which is known for this problem. Gauss-Seidel converges roughly twice as fast compared to Jacobi, something that is well known in general. Further analysis regarding the convergence of the iterative methods is outside the scope of this report, but can be found in [1], [2].

Bibliography

[1] Randall J. LeVeque *Finite Difference Methods for Ordinary and Partial Differential Equations.* 2007.

[2] George Em. Karniadakis, Robert M. Kirby *Parallel Scientific Computing in C++ and MPI.* 2003