The Capacitance of Concentric Containers

A Chronicle in C++

Practical Numerical Simulations
Assignment 2

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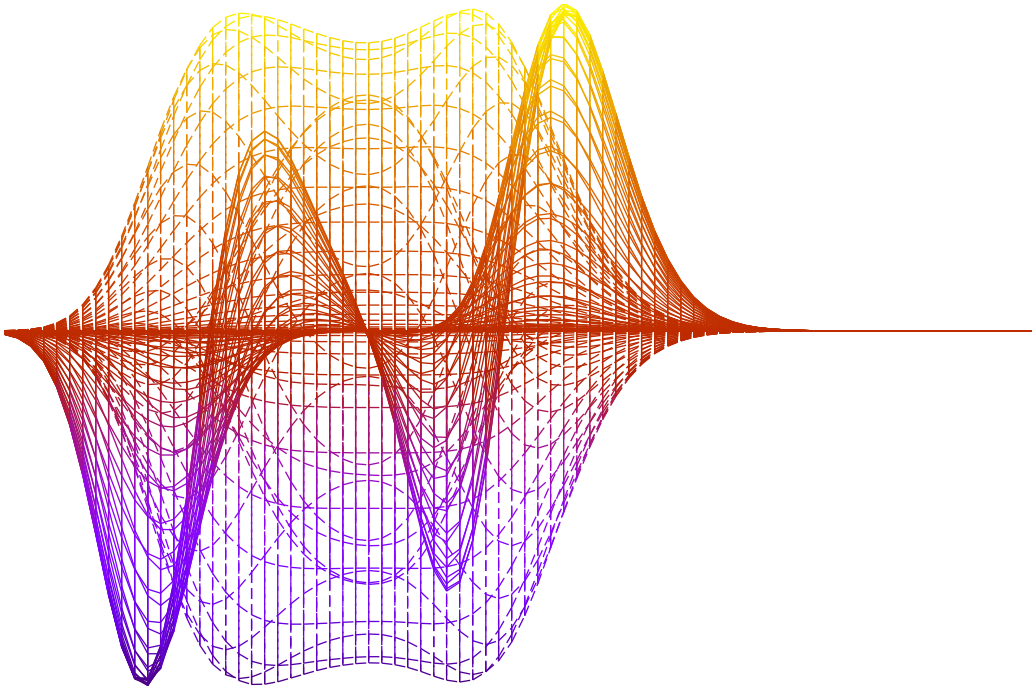

1 Introduction

In this code, the Gauss-Seidel algorithm was applied to solve the partial differential equations that describe electrostatic fields. The fields were evaluated throughout a bounded region R, whose boundary ∂R was held at a constant potential.

2 Tubes Within Tubes

The physical problem is concerned with a region R whose boundary is held at a fixed potential. Contained inside this region is a smaller region R', where the potential is constant on this smaller inner boundary just as before.

The outer boundary is held at a potential $u = 1$ and the inner boundary held at $u = 0$. For the electromagnetic field, this $u = u(x, y)$ is the voltage.

The sides of the outer boundary are of unit length. The inner boundary has sides of length 0.3, 0.2. Finally, we will define the lower right corner of the boundary to be at the point (a, b).

The dependence of u on x and y is governed by the Laplace equation

$$\nabla^2 u(x, y) = 0, \tag{1}$$

the vanishing case of the Poisson equation $\nabla^2 u = f$. Here $\nabla^2 = \triangle$ is the Laplacian operator in Euclidean space and u and f are real-valued functions mapping $\mathbb{R}^2 \mapsto \mathbb{R}$.

Equation 1 is an elliptic second-order partial differential equation. The solution to this equation, and its behaviour, will be the subject of the remainder of this report.

3 High-Sidelity

Now that we have abstracted our physical problem to that of solving a PDE, we must then think of a way to do this. We are looking for a harmonic function $u(x, y)$ which satisfies certain boundary conditions.

By representing the second-order derivative using a Taylor expansion, we may transform our problem into one of solving a set of coupled ODEs.

Equation 1 may be approximated by finite difference as

$$u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j} = 0.$$

Notice that this equation allows us to consider $u_{i,j}$ as the average of its nearest neighbours. In matrix form,

$$A\vec{u} = \vec{0},$$

where the matrix A is sparse. We are thus looking for the kernel, or null space, of A.

We can rewrite $A\vec{u} = \vec{0}$ as $P\vec{u} = -(A-P)\vec{u}$, which is suggestive of the iterative scheme

$$Pu_{k+1} = -(A-P)u_k.$$

Defining the difference as $u_k - u_{k+1} \equiv d_k$, we can write

$$d_{k+1} = \underbrace{(I - P^{-1}A)}_{\chi} d_k$$

provided P is invertible. This scheme converges if the eigenvalues λ of χ lie within the unit circle, $|\lambda| \leq 1$. That is, $u_{k+1} = u_k + \varepsilon$ for a sufficiently small ε.

The Gauss-Seidel algorithm is an iterative technique for solving such linear systems (both homogeneous and inhomogeneous). We must choose P such that it is close to A and easy to invert. Decomposing $A = L + D + U$, the Gauss-Seidel method chooses $P = D + L$. In this scheme, we may then describe our equation as

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

This shall be our iterative scheme for solving our physical problem.

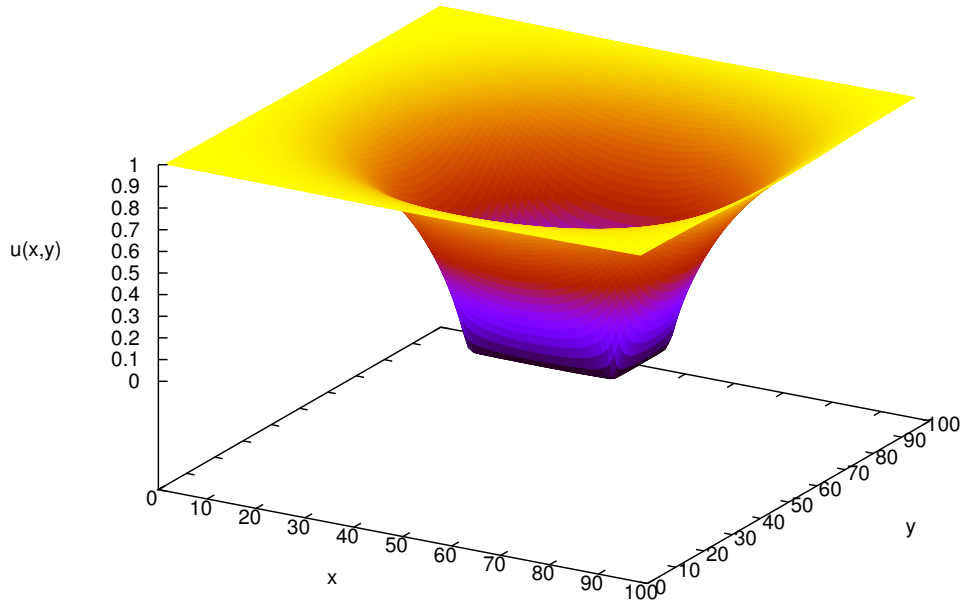

Figure 1: The potential $u(x,y)$ as it varies in space. Here, $x, y \in \mathbb{N} < 100$ are the discretised spatial variables and $(a,b) = (0.4, 0.4)$.

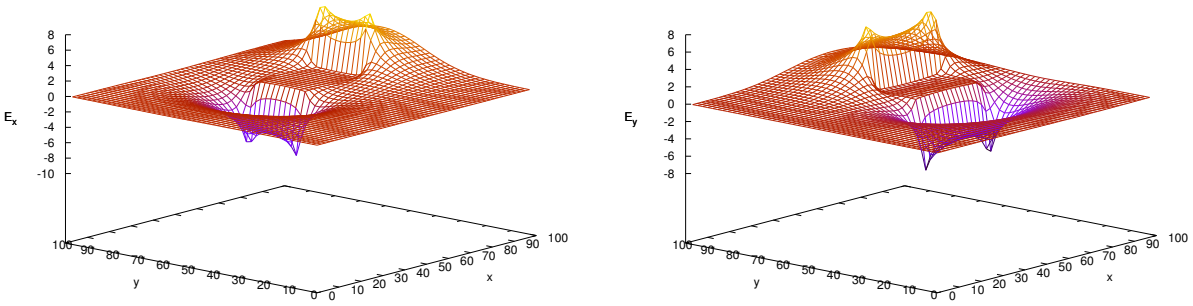

Figure 2: E_x, E_y varying over space.

4 The Electrostatic Potential u

Once the boundary conditions are initialised, the Gauss-Seidel algorithm computes the potential $u(x, y)$ as we have seen in §3. This is done by creating a `class Potential` which takes two arguments, `i` and `j`, like an array, and iterating over them.

The boundary of the inner region, $\partial R'$, is held at zero, which implies that $u(x, y) = 0$ for the entire inner region, i.e. $u(x, y) = 0$ for $(x, y) \in R'$. This means for $(x, y) \in R \setminus R'$ near $\partial R'$, the slope becomes large very quickly. This can be seen in fig. 1.

5 The Electric Field

The electric field is defined as

$$\vec{E} \equiv \vec{\nabla} u, \qquad (E_x, E_y) \equiv \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \right).$$

The uniqueness theorem for the Poisson equation states that the solution has a unique gradient. This ensures that if we find an electric field which satisfies our boundary conditions, it is the entire electric field.

This was evaluated everywhere in R by approximating the derivatives as three-point finite difference quotients, i.e.

$$\frac{\partial u}{\partial x} \approx \frac{u(x+h, y) - u(x-h, y)}{2h}, \qquad \frac{\partial u}{\partial y} \approx \frac{u(x, y+h) - u(x, y-h)}{2h}.$$

These expressions approach the true derivative in the limit $h \to 0$.

We can now visualise how the x- and y-components of the field change over space, as seen in fig. 2.

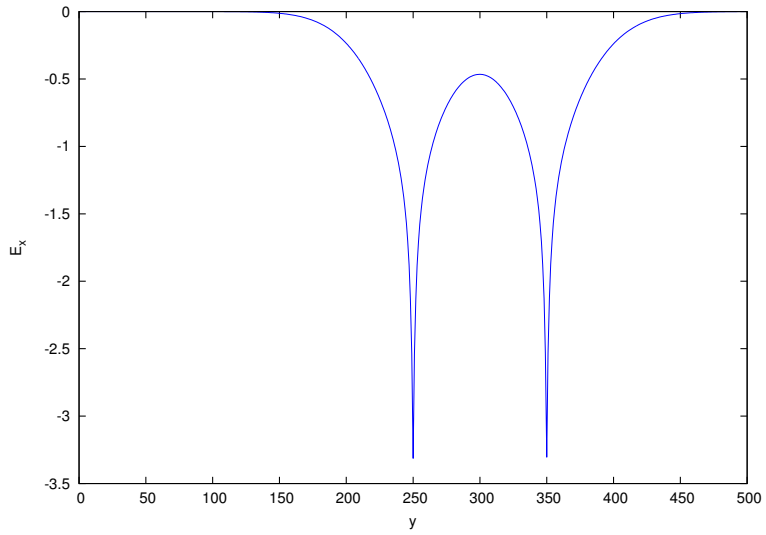

Figure 3: E_x versus y at $x = \frac{1}{2}$. Here, our mesh size is $n = 500$.

Choosing $x = \frac{1}{2}$ defines a vertical line in our region. It is useful to consider how E_x changes with y along this cross-section. This is visualised in fig. 3. As we expect, the field is close to vanishing inside the smaller region as there is no curvature in the potential here. As we move from the smaller region to the larger one, there is a discontinuity in the potential which is manifest in the gradient as a large spike, which falls off as we approach the outer boundary ∂R.

Gauss's law states that over a closed surface $\partial\Omega$,

$$\Phi_E \equiv \oint_{\partial\Omega} \vec{E} \cdot \mathrm{d}\vec{A} = \frac{Q}{\varepsilon_0}, \tag{3}$$

where Q is the total enclosed charge. By the divergence theorem, (3) can be rewritten in its differential form as

$$\vec{\nabla} \cdot \vec{E} = \frac{\rho}{\varepsilon_0}, \tag{4}$$

for ρ the charge density.

Fig. 4 illustrates the behaviour of the electric field E_x for increasing mesh size. As n increases, the curvature of the field in the inner and outer regions approaches 0. Hence, in the continuum limit, $\partial_x E_x \to 0$ and, by symmetry, $\partial_y E_y \to 0$. Thus,

$$\vec{\nabla} \cdot \vec{E} \xrightarrow{n\to\infty} 0.$$

By equation 4, this implies $\rho \to 0$. As we are considering cross-sections of an infinitely long tube, we must have a zero charge density. Thus, these results are compatible with Gauss's law.

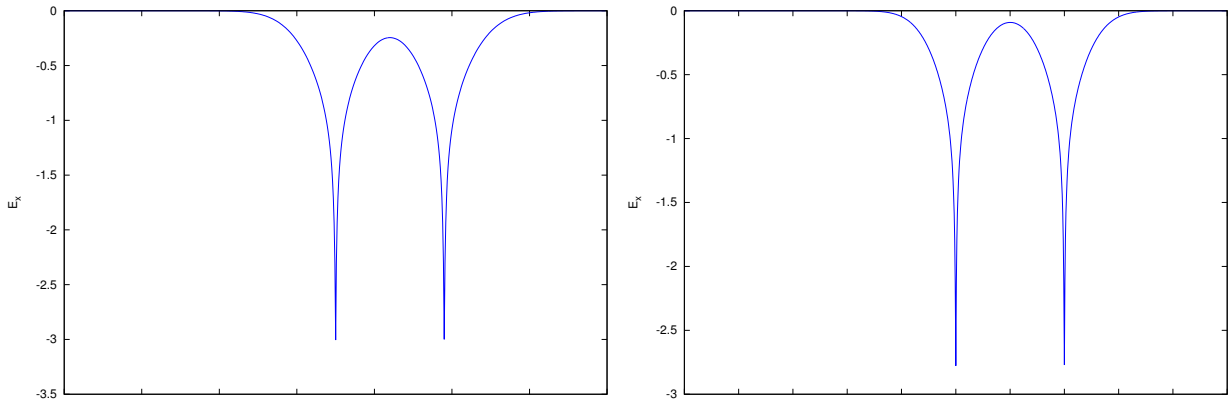

Figure 4: Fig. 3 replotted for mesh sizes of $n = 700, 1000$.

We are also free to evaluate the integral

$$\begin{aligned} L &= \iint_R \vec{E}^2 \, \mathrm{d}A \\ &= \int_0^1 \int_0^1 (E_x^2 + E_y^2) \, \mathrm{d}x \, \mathrm{d}y. \end{aligned}$$

This can be done by considering L as double Riemann or Darboux integrals and approximating them by their corresponding summation, so

$$L \approx \sum_i \sum_j \frac{1}{n^2} \vec{E} \cdot \vec{E},$$

where n is the size of our discretised space and (i, j) are the points.

For a fixed (a, b), L will obviously evaluate to a number. Indeed, for $(a, b) = (0.5, 0.5)$, the program outputs

```
The integral is L = 6.04447.
```

However, we may be more interested to see the behaviour of L as the inner region moves in space. Indeed, we will consider $L = L(b)$, for $a = 0.2$ and $b \in [0.05, 0.95]$. This is plotted in fig. 5.
There is a discontinuity here at $b \sim 80$, where the inner region hits the outer region. In this situation the area of the inner region decreases and the area of the outer region which the field can change in increases, so we are dealing with a different physical problem.

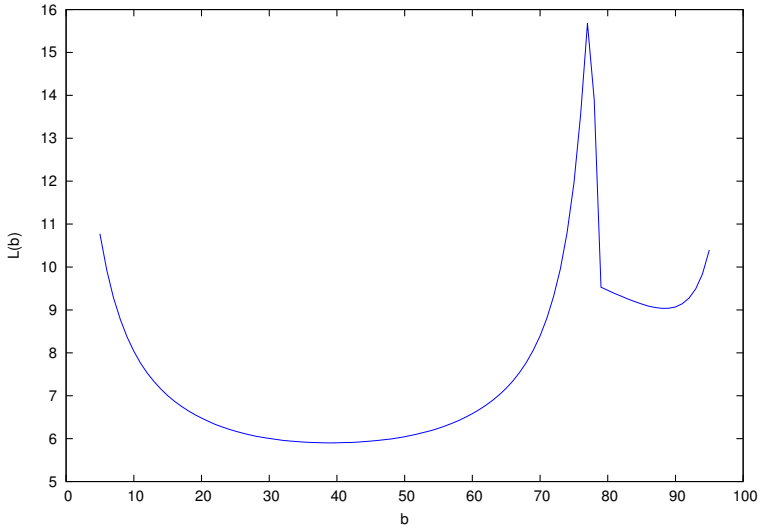

Figure 5: L as b varies in $[0.05, 0.95]$.

6 Successive Over-Relaxation

If we consider $u_{\text{GS}}^{k+1}(i,j)$ to be the $u_{i,j}^{k+1}$ element of the Gauss-Seidel sequence as in equation 2, the over-relaxed Gauss-Seidel method is given by

$$\begin{aligned} u^{k+1}(i,j) &= (1-\omega)u_{\text{GS}}^{k+1}(i,j) - \omega u^k(i,j) \\ &= (1-\omega)\frac{1}{4}\left(u_{i+1,j}^k + u_{i-1,j}^{k+1} + u_{i,j+1}^k + u_{i,j-1}^{k+1}\right) - \omega u^k(i,j) \end{aligned}$$

for some free parameter ω. As $\omega \to 0$, we recover our original scheme. For appropriate values of ω, this method will converge faster than the traditional Gauss-Seidel method.

Choosing $(a,b) = (0.5, 0.5)$, it was found that the best choice is $\omega = 0.92$. This can be seen in fig. 6.

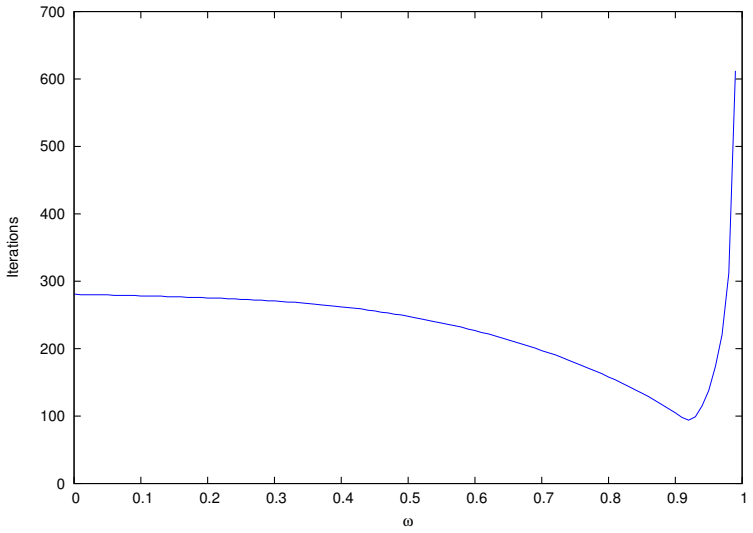

Figure 6: ω versus iteration time. We can see that $\omega = 0.92$ is the optimal value.

7 Tarball

The following is a list of files included in the tarball `Fionn_Fitzmaurice_Assignment2.tgz`.

1. `electric_field.cpp`. This file mostly concerns itself with the trials of part two, discussed in §5.
2. `relax.cpp`. This file concerns itself with over-relaxation, such as is discussed in §6.
3. `seidel.pdf`. "The Capacitance of Concentric Containers", i.e. this document.

The omission of a `C++` file for part 1, §§3-4, is not a serious one, as all of the code used to generate data in these sections is a subset of the two included `.cpp` files.