Computing Exercise 2: Solving partial differential equations to investigate voltage and temperature gradients

Saskia Jackson

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INTRODUCTION

Partial differential equations are a common occurrence in everyday physics, for example they appear in large amounts of the equations that describe heat, diffusion, sound, electrostatics, quantum mechanics, fluid dynamics and more.

Therefore it is very important to be able to solve these type of equations accurately and efficiently. There are many techniques to solve such equations, one of the more accurate being the finite difference method.

A commonly used example of a cyclic partial differential equation is Laplace's equation. [2]

$$\text{Laplace:} \quad \nabla^2 V = 0 \qquad\qquad \text{Poisson:} \quad \nabla^2 V = \frac{\rho}{\epsilon_0} \tag{1}$$

Relaxation method

This can be solved computationally using a relaxation method. This works by describing an area as a mesh grid of various points in space. The voltage (in the example of the Laplace equation) at any point on this grid (x_i, y_j) can be determined as a sum of the voltages of the four points around it.

Taking the Taylor expansion of the voltage at this point, as described by the points around it, gives an equation to describe $\nabla^2 V$ in terms of these points. [1]

$$\nabla^2 V \approx \frac{V(x_{i+1}, y_j) + V(x_{i-1}, y_j) + 2V(x_i, y_j)}{h^2} + \frac{V(x_i, y_{j+1}) + V(x_i, y_{j-1}) + 2V(x_i, y_j)}{h^2} \tag{2}$$

where h represents the spacing between grid points.

This can then be equated to 0 as shown in the Laplace equation and rearranged to give an equation for $V(x_i, y_j)$ in terms of the points around it.

In order for the relaxation method to work, initial conditions must be set for the points on the grid with fixed nodes on the boundaries of the grid and the remainder of the points at an initial guess. These boundary conditions can be used to set up various simulations, such as creating capacitor plates within the grid.

Gauss Seidel Method

The relaxation method works hand in hand with various iteration methods to produce an accurate representation of the changing voltage.

The most common iteration methods used are the Jacobi and Gauss Seidel methods. These are very similar methods of solving simultaneous equations that can be applied to the relaxation method in order to update each grid value in terms of the points around it.

The difference in methods is that in the Jacobi method, each point is determined from the grid from the previous iteration whereas in the Gauss Seidel method the points are determined from the points around it as they are updated.

In order for there to be an end to the iterations, there needs to be some sort of convergence conditions which determines when the result is accurate enough that no more iterations are needed. There a many different convergence conditions that can be used, for example finding the average value of the grid before and after each iteration and stopping iterations when the difference between these averages reaches a certain limit. It is much more efficient to compare a sum or maximum value of an array rather than comparing each point. [1]

The convergence condition method used in this exercise was to find the difference between the grid before and after each iteration and then find the percentage difference between the maximum value of this compared to the grid after iteration.

The diffusion equation

The diffusion equation is similar to the Poisson equation.

$$\alpha \nabla^2 \phi = \frac{\partial \phi}{\partial t} \tag{3}$$

where α is the collective diffusion coefficient and is calculated from the thermal conductivity (k), density (ρ) and specific heat (c) using the equation $\alpha = k/\rho c$.[3]

When α is a constant, the diffusion equation can be used to describe how temperature varies over time and space and is therefore referred to as the heat equation.[3]

It is possible to use the same method as in the relaxation method to find an equation to describe ϕ (earlier voltage) at a time $t + \Delta t$ calculated from the surrounding points at a time t. This forward time method is, however, not as stable as the backwards time method.

Therefore the backwards time method is used to form a set of simultaneous equations that can be described using a matrix equation.

$$\begin{pmatrix} 1+3x & -x & 0 & 0 \\ -x & 1+2x & -x & 0 \\ 0 & -x & 1+2x & -x \\ 0 & 0 & -x & 1+y \end{pmatrix} \cdot \begin{pmatrix} \phi'_{i-2} \\ \phi'_{i-1} \\ \phi'_{i} \\ \phi'_{i+1} \end{pmatrix} = \begin{pmatrix} \phi_{i-2} + 2xT_1 \\ \phi_{i-1} \\ \phi_i \\ \phi_{i+1} + z \end{pmatrix} \tag{4}$$

where $x = \alpha \cdot dt/h^2$, dt represents the time step size, h represents the space step size, ϕ represents the temperature with ϕ' representing this at a time $t + \Delta t$, T_1 represents the temperature at the first set boundary condition. When there is only one set boundary condition, $y = x$ and $z = 0$. When there are boundary conditions at both ends of the rod represented by the ϕ matrix, $y = 3x$ and $z = 2xT_2$ where T_2 represents the temperature at the second set boundary condition.

This matrix can then be solved to find the temperature matrix (consisting of ϕ') at multiple iterations to investigate how the temperature changes over time of a one dimensional object.

PART ONE: USING LAPLACE's EQUATION TO FIND A VOLTAGE GRADIENT

This section of the exercise was focused around using the relaxation method and Laplace's equation to show the voltage at some varying boundary conditions. Firstly a known case was investigated, in this case the known case was an initial conditions grid with a voltage of 100 along one edge, zeros along the remaining edges and an initial guess of 1 elsewhere. This returned a grid with a voltage gradient from the edge with voltage 100 as shown in the left hand side graph in figure 1.

The number of iterations can be plotted for increasing grid sizes to investigate how the number of points on the grid affects the convergence condition. This is shown in the right hand side graph in figure 1.

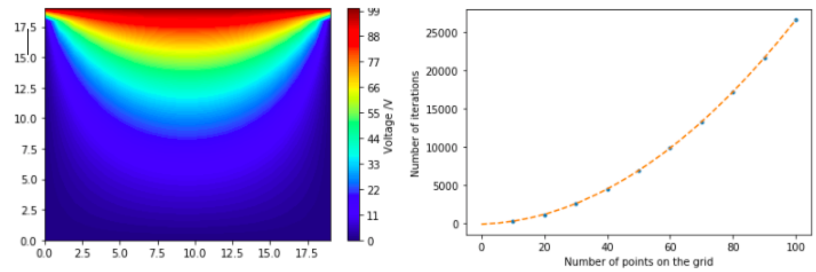

Figure 1: Left: A contour plot of the voltage across the grid for an initial grid with a voltage of 100V along the top edge. Right: A plot showing how the number of iterations varies as the size of the grid increases. The blue circles show the data plots and the orange curve demonstrates the polynomial fit.

The next part of the exercise involved investigating the voltage around two oppositely charged parallel plate capacitors.

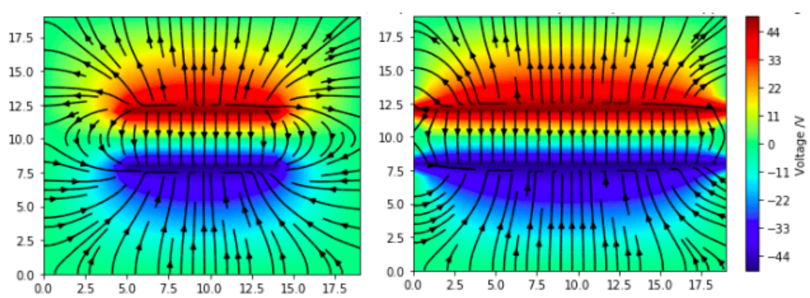

Figure 2: Left: A contour plot showing the voltage surrounding parallel capacitors with a length of half the grid and a width of 20% of the grid. Right: A similar contour plot to show how the voltage acts when A/d is large.

PART TWO: USING THE DIFFUSION EQUATION TO FIND THE TEMPERATURE GRADIENT OF A ROD

This section of the exercise is to investigate how the temperature of a one dimensional rod with one side in a furnace at $1000^{o}C$ varies over time.

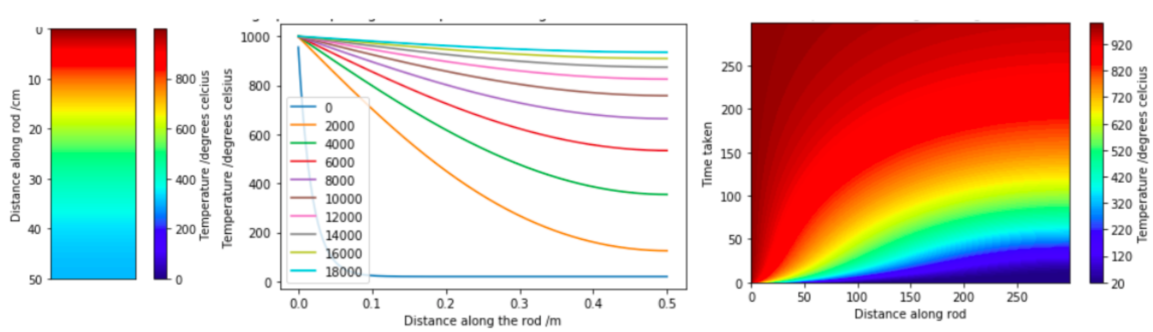

Figure 3: All plots are for when there is no heat loss from the other end of the rod. Left: A snapshot of the temperature gradient at 3600s. Middle: A plot of the temperature against the distance along the rod for various times. Right: A gradient comparison of the middle graph.

There were two sections to this part; one in which there was no heat lost from the other end of the rod and one in which the other end of the rod was immersed in ice at 0^oC. When the rod is immersed in ice, there are two boundary conditions and thus the appropriate matrix equation must be used, as described in equation 4.

The right hand plot in figures 3 and 4 are a gradient plot of how the temperature gradient along the rod (on the x axis) changes with time (plotted on the y axis). In these figures, it can clearly be seen that as time increases, the temperature along the rod also increases. It can also be seen that for the simulation where one side of the rod is kept at 0^oC, after a certain time the temperature gradient stays relatively the same, most likely as thermal equilibrium has been reached.

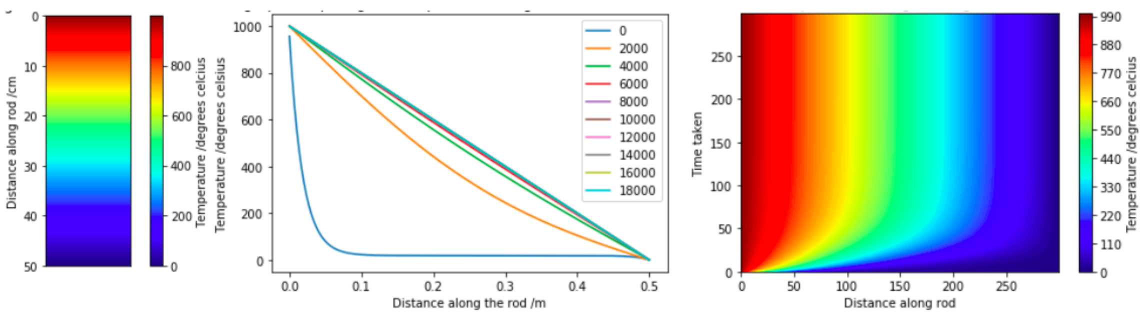

Figure 4: All plots are for when one end of the rod is immersed in ice at 0^oC. Left: A snapshot of the temperature gradient at 3600s. Middle: A plot of the temperature against the distance along the rod for various times. Right: A gradient comparison of the middle graph.

DISCUSSION

The Gauss Seidel method will converge much faster than the Jacobi method, due to the new points being used in the equation much earlier in the iteration thus less iterations are needed to meet the convergence condition. This therefore makes the Gauss Seidel method the more accurate and additionally the more efficient method to use to solve partial differential equations.

The speed of the code to determine the voltage gradients can be improve upon by changing the convergence conditions to a condition such that additional arrays do not need to be created as this increases the time it takes for the code to run thus reducing the efficiency.

An additional improvement would be to test the code by investigating more known cases to ensure its working and ensure it is accurate. A point charge is not a reasonable known case to investigate in order to check the code because, while this is a known case in 3 dimensions, it is more difficult to interpret in 2 dimensions.

The accuracy of the method used to determine the temperature of the rod in time increases if you decrease the time difference. The increase in accuracy comes at the price of speed of the code unfortunately, as the time taken for the code to run depends on the number of iterations there must be.

1 References

[1] David G. Robertson *Relaxation Methods for Partial Differential Equations: Applications to Electrostatics* Department of Physics and Astronomy Otterbein University, Westerville, OH 43081 (2010)

[2] Nicole Nikas *Using the Relaxation Method to solve Poisson's Equation* (2015)

[3] Matthew J. Hancock *The 1-D Heat Equation 18.303 Linear Partial Differential Equations* (2006)