Investigation of partial differential equations through the use of relaxation methods

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Investigation of partial differential equations through the use of relaxation methods

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The aim of this code was to use the relaxation methods Jacobi and Gauss-Seidel to solve static partial differential equations. The associated standard deviation error of the Gauss-Seidel method was found to be in the order of 10^{-1} smaller than that of the Jacobi. Hence the Gauss-Seidel method was used to model of a capacitor. Through the used of the Backward Time Difference method, the heat diffusion equation was solved with both Von Neumann and Dirichlet boundary conditions.

RELAXATION ITERATIVE METHODS

The relaxation method is used to continuously update solutions of simultaneous equations to improved solutions. Within the relaxation method, it is possible to implement the differential equations with the corresponding finite difference equations [1]. These methods are of particular importance when solving linear systems of elliptic partial differential equations. The practical details will be explored in the solutions to Poisson's equations for a capacitor.

This paper will primarily focus on the Jacobi and Gauss-Seidel as means of solving the systems of linear equations. To obtain solutions using these iterative methods, the set up is initially the same for both methods. It requires multi-nodal spatial grid with well defined boundary conditions i.e. at fixed values. The non-boundary nodes were all set to an initial guess and the finite difference equations were bounded within a convergence criterion. To implement the Jacobi method, a new value for the entire grid is computed and then the full grid is updated. This method requires a new and old copy of the grid. Thus during the computations for the new grid, the known values of the nodes were updated from the previous iteration. This method is known as the simultaneous displacement method [2]. By contrast, the Gauss-Seidel method uses updated solutions as soon as they were computed and therefore only one grid is required and this is known as the successive displacement method.

SOLVING POISSON'S EQUATION

Consider Poisson's equation in 1D:

$$\nabla^2 V(x) = \frac{\partial^2 V(x)}{\partial x^2} = \frac{-\rho(x)}{\epsilon_0}, \tag{1}$$

where V(x) is the electric potential, $\rho(x)$ is the charge density, and ϵ_0 is the permittivity of free space.

This an example of a static equation that is solved using boundary conditions for a region of space with known behaviour at that boundary. The derivative operators were approximated for three points of the second derivative using the finite differences method:

$$\frac{\partial^2}{\partial^2} V(x_i) = \frac{V(x_{i-1}) + V(x_{i+1}) - 2V(x_i)}{h^2} \tag{2}$$

where h is the step size of the multi-nodal grid.

To calculate a generalized 2D Poisson equation, EQ. 2 may be plugged in to EQ. 1 and solved for $V(x_i, y_i)$:

$$V(x_i, y_i) = \frac{1}{4}(V(x_{i-1}, y_j) + V(x_{i+1}, y_j) + V(x_i, y_{j-1}) + V(x_i, y_{j+1})) + \frac{\rho(x_i, y_j)h^2}{4} \tag{3}$$

In this model ρ is taken to be 0 and ϵ_0 is taken to be 1. This equation demonstrates that every sample of voltage, $V(x_i, y_i)$ is dependent on the four closest neighbours. The computational molecule of this set up is depicted below:

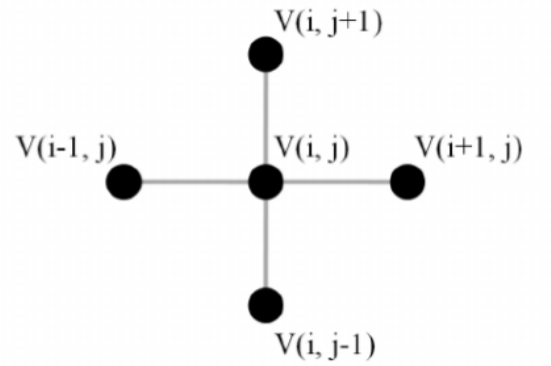

FIG. 1. Graphical representation of the five-point star computational molecule

The interior grid points for the new potential were calculated with boundary conditions set to zero. Both the Jacobi and the Gauss Seidel method were utilized and compared.

Method Comparison

A convergence condition was set until a minimum specified difference of node value between successive iterations

was obtained. When considering the sensitivity of both methods, it was found that the Jacobi method took double the number of iterations, and therefore time to converge compared to the Gauss method for a given convergence factor:

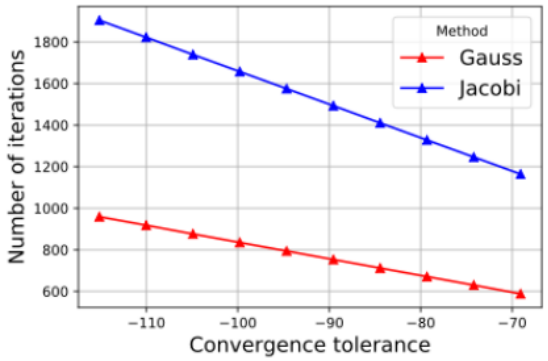

FIG. 2. Logarithmic graph of the number of iterations required for a specific convergence factor for the Gauss and Jacobi method

In FIG 2., the Gauss-Seidel method is shown to converge twice as fast as the Jacobi method. Therefore, a solution computed using both methods for the same number of iterations will produce a greater error in the solutions than those calculated using the Jacobi method. As a consequence of this finding, the Gauss Seidel method was selected as the method for the rest of this investigation.

The density of the grid spacing also has an effect on the number of iterations required until the convergence condition is satisfied. Due to the fact that the grid is dimensionless, changing the size of the grid has the same effect as changing the density of the grid.

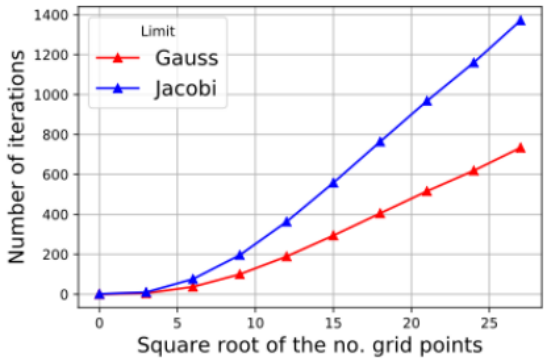

FIG. 3. Comparison the number of iterations for the Gauss and Jacobi methods as the number of grid points i.e. grid density

Error analysis was completed by taking the standard deviation of the solutions for the nodes of changing the density of the grid and changing the convergence factor. It was found that the standard deviation remained the same for both methods irrespective of grid size. However, it was noticeable that for the Gauss-Seidel method, the standard deviation was in the order of $\sigma = 10^{-5}$, whereas the Jacobi method was in the order of $\sigma = 10^{-4}$. This reiterates the premise that the Gauss Seidel method is a favourable method, for both speed and associated error. Tritsiklis [3] verifies that there are numerous algorithms that the Jacobi method fails to converge but the Gauss-Seidel method equivalent is able to and hence the preferential method.

For a box with boundary conditions set to zero, the interior grid points should eventually converge to zero. Therefore, taking the absolute error of the converged grid and the expected value to zero was a suitable test to ensure that the Poisson's equation returned the correct solutions.

PHYSICAL EXAMPLES

The Capacitor

Following evaluation of the Gauss-Seidel and Jacobi method, it was evident that the Gauss-Seidel was a better method. Hence, the Gauss-Seidel method was used to calculate the potential and electrical field within and around a a parallel plate capacitor with finite dimensions.

Using a contour plot, the voltage of the associated capacitor could be modelled:

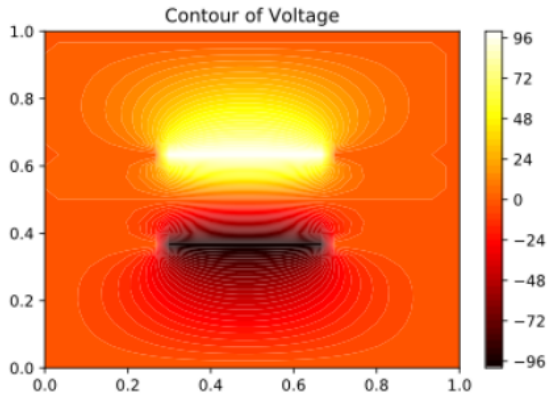

FIG. 4. Contour plot of the voltage of a capacitor with plate separation = 4 and plate length = 12

For a very large capacitor length, the capacitor can be approximated as an infinite plate capacitor. Here the field between the plates will follow the form $E = V/d$ and everywhere outside the plate will have an E field equal to zero. The edge effects were due to the imposed boundary conditions. An improvement would be to include computational molecules that mirror the missing fourth neighbour of the five point-star at the boundaries.

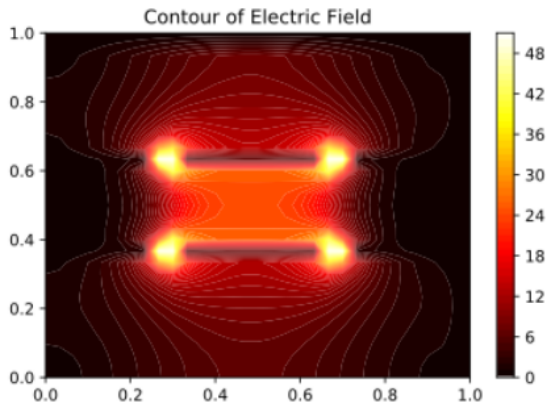

FIG. 5. Contour plot of the Electric field of a capacitor with plate separation = 4 and plate length = 12

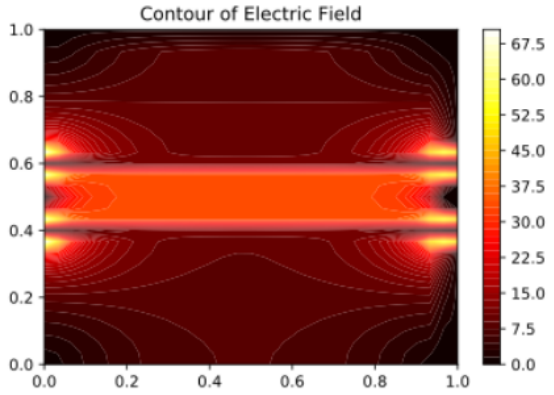

FIG. 6. Contour plot of the Electric field of a capacitor with plate separation = 4 and plate length = 1e6, used to approximate an infinite capacitor

Heat diffusion in a one-dimensional rod

The diffusion equation was investigated for an iron poker of length 50 cm with an initial temperature of 293 K. This rod is discretised into n nodes for a one dimensional grid. To solve the diffusion equation:

$$\alpha\nabla^2\phi = \alpha\frac{\partial^2\phi}{\partial^2 x} = \frac{\partial\phi}{\partial t} \tag{4}$$

the spatial derivative can be approximated using the second -order central difference operators at position x_i in conjunction with backward difference at time t_{n+1}.

The backward time difference method is favoured over the forward time difference method as for any Δt the solutions do not oscillate [4]. However, using the forward time difference method results in replacing the the true derivative with a discrete derivative. Therefore, from the first iteration, there is an error introduced.

$$\alpha\nabla^2\phi = \alpha\frac{\partial^2\phi}{\partial^2 x} = \frac{\partial\phi}{\partial t} \tag{5}$$

where α The computational molecule used in this case is known as the implicit method stencil

$$\frac{\phi\prime(x_i) - \phi(x_i)}{\delta t} = \frac{\alpha}{h^2}[\phi\prime(x_{i-1} + \phi\prime(x_{i+1} - 2\phi\prime(x_i] \tag{6}$$

where in this case, $\phi\prime$ is the temperature at the point x_i after the time step δT from ϕ, the initial temperature.

Rearranging for $\phi\prime$:

$$-\frac{\alpha\Delta t}{h^2}\phi\prime(x_{i-1}) + (1 + \frac{2\alpha\Delta t}{h^2}\phi\prime(x_i) - \frac{\alpha\Delta t}{h^2}\phi\prime(x_{i+1}) = \phi(x_i) \tag{7}$$

Using this equation, the temperature distribution of the one dimensional rod can be solved using a tridiagonal sparse matrix:

$$\begin{bmatrix} BC & BC & BC & BC & BC & BC \\ - & - & - & - & - & - \\ -a & 1+2a & -a & 0 & 0 & 0 \\ 0 & -a & 1+2a & -a & 0 & 0 \\ 0 & 0 & -a & 1+2a & -a & 0 \\ 0 & 0 & 0 & -a & 1+2a & -a \\ - & - & - & - & - & - \\ BC & BC & BC & BC & BC & BC \end{bmatrix} \begin{bmatrix} \phi\prime(x_0) \\ - \\ \phi\prime(x_1) \\ \phi\prime(x_2) \\ \vdots \\ \phi\prime(x_n) \\ - \\ \phi\prime(x_{n+1}) \end{bmatrix} = \begin{bmatrix} \phi(x_0) \\ - \\ \phi(x_1) \\ \phi(x_2) \\ \vdots \\ \phi(x_n) \\ - \\ \phi(x_{n+1}) \end{bmatrix} \tag{8}$$

where a is $\frac{\alpha\Delta t}{h^2}$ and BC are the boundary conditions imposed on the rod.

To solve this equation in the form $\boldsymbol{Ax} = \boldsymbol{b}$, the product of the inverse of the matrix of time dependent coefficients $\boldsymbol{A}$, and the ϕ vector, $\boldsymbol{b}$ is taken to find the values for $\phi\prime$, $\boldsymbol{x}$. After each iteration, $\boldsymbol{x}$ is set equal $\boldsymbol{b}$ and the product is taken again for a given time.

First, consider a poker with one end in a furnace at 1273 K and an ice bath at 273 K. In this case, both ends will remain at the fixed temperatures so the upper and lower boundary conditions come from the identity operator. This type of boundary condition is called the Dirichlet boundary conditions.

In the case where one end of the rod is held constant at 1293 K there is no heat loss from the far end of the poker, the heat diffusion gradient at the far end is constant, i.e $\frac{\partial\phi}{\partial x} = 0$. In this case, the $\phi_n = \phi_{n+1}$ so the lower boundary conditions take the form:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & -a & 1+a \end{pmatrix} \tag{9}$$

This type of boundary condition is known as the Von Neumann boundary conditions [5].

For case I, with both ends held at fixed temperature, after a given time the rod's temperature distribution becomes a linear distribution from temperature A to temperature B:

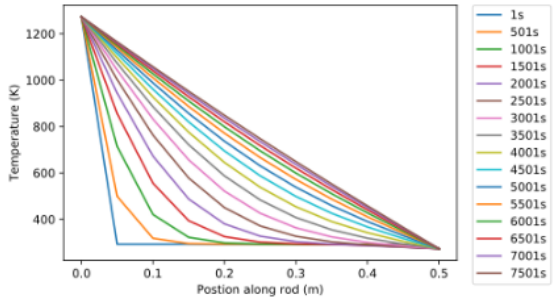

FIG. 7. Change in heat distribution over time for a rod with one end at T = 1273 K and T =273 K

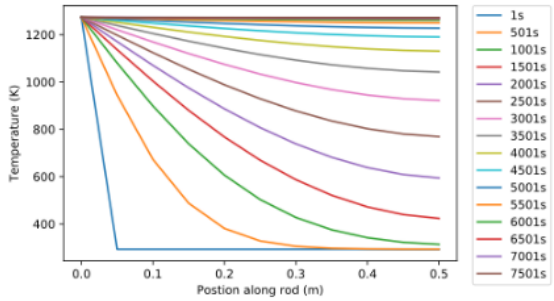

FIG. 8. Change in heat distribution over time for a rod with one end at T = 1273 K and no heat loss to the surroundings

CONCLUSION

In conclusion, the Gauss-Seidel method was found to be both faster and more accurate than the Jacobi method. The standard deviation associated with the Gauss-Seidel was σ = 5.4 x 10^{-5}, whereas the Jacobi method was σ = 1.5x 10^{-4}. Gauss-Seidel was also found use half the amount of iterations to get to the meet the convergence conditions as the Jacobi method.

The capacitor plate length was varied and the infinite plate capacitor was modelled. However, the boundary conditions of the grid did not allow an accurate simulation. An improvement would be to use a different computational molecule at the edges of the grid.

When investigating the heat diffusion equation, the backward time difference method was utilised due to its stability and reduction of error compared to the forward time difference. Von Neumann and Dirichlet boundary conditions were applied to a one dimensional rod for two different cases. The rods converged to the predicted temperature distribution after a certain time.

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GENERAL COMMENTS

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