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Full Length Research Paper

Solving three-dimensional (3D) Laplace equations by successive over-relaxation method

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Motivated by the assertion that all physical systems exist in three space dimensions, and that representation in one or two space dimensions entails a large degree of approximations. The main objective of this paper is to extend the successive over-relaxation (SOR) method which is one of the widely used numerical methods in solving the Laplace equation, the most often encountered of the Elliptic partial differential equations (PDEs) in two dimensions to solving it in three dimensions. This is done by providing an easier procedure to obtain proper estimates to the SOR parameter and the stability criterion which are the two determinant elements used in facilitating convergence to the solution when solving PDEs by the SOR method. The hope is that, with the emergence of this finding, the representation of physical and environmental science problem will be closer to reality by representing them in three dimensions.

Key words: Stability criterion, over relaxation parameter, Laplace equation, finite differencing, successive over-relaxation.

INTRODUCTION

To describe changes in a most physical system, there is a need to study partial differential equations (PDEs). The general linear equations governing physical fields take the form:

$$A\frac{\partial^2 U}{\partial x^2} + 2B\frac{\partial^2 U}{\partial x\,\partial y} + C\frac{\partial^2 U}{\partial y^2} = D\frac{\partial U}{\partial x} + E\frac{\partial U}{\partial y} + FU + G \quad (1)$$

By letting the parameters A to G assume positive, negative or zero magnitude, the PDE could be classified as being hyperbolic, parabolic or elliptic. For instance, if $AC > B^2$, the equation is termed elliptic. The same situation will arise if B is 0, and A and C are positive. This classification of PDEs into these three categories is necessary because the basic analytical and numerical methods for treating field problems are different for the three types of equations (Vemuri and Karplus, 1981). It is also possible for an equation to be of more than one type, depending on the values of the coefficients. As an example, the equation $y\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial x\,\partial y} = 0$, is elliptic for $y > 0$, parabolic for $y = 0$, and hyperbolic for $y < 0$ (Kallin, 1971b).

In this research, interest is in the elliptic type of equation and specifically in the Poisson equation. The most often encountered of the elliptic PDE, and indeed of all PDEs in applied physical sciences and physics, is Laplace's equation as stated by Brandt and Diskin (1999). This is a special case of the Poisson equation and it arises when all the terms on the right hand side of the Poisson equation equal zero. The prototypical elliptic equation in three dimensions is the Poisson equation of the form:

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} = \rho(x, y, z), \quad (2)$$

where the source term ρ is given. Thus, if this source term is equal to zero, the equations become Laplace's equation. The cross product term is not included because there is no theoretical foundation to expect convergence in such a case as seen in Kallin (1971a).

The advantage of the Poisson equation as stated by Reynolds (1988) lies in its mode of solution. That is, the

Poisson equation also has the important benefit of behaving well numerically. Thus, when the equations are expanded by finite differencing into a set of linear algebraic equations, they can be solved iteratively to obtain a unique solution. This behaviour is especially convenient since the set of equations varies as the boundary points respond to changes.

SOLVING THE THREE-DIMENSIONAL (3D) LAPLACE EQUATION

In order to solve the Laplace equation which is also an example of a boundary value problem, it is necessary to:

1) Specify boundary values along the perimeter of the region of interest,
2) Set the forcing term ρ to the Laplacian; otherwise ρ is set to zero.

One of the methods of solving this equation is the finite difference method as stated by Kallin (1971a). The resulting set of simultaneous equation can be solved either by elimination or by iterative methods as shown in Dorn and McCracken (1972). It is worth noting that solving simultaneous equations by elimination is not a simple task, especially with a large system of algebraic equations. In fact, even for computers, the solution of a large system of algebraic equations by elimination may not be practicable because of storage requirements and accumulation of round-off errors. McCracken (1974) and Edgar (1992) provided some guidelines on how to build computer codes to solve systems of algebraic equations. Therefore, the best approach is to use an iterative method. This has the advantage over elimination in that it is self-correcting in the sense that the arithmetic error at any stage is eventually suppressed as described by Kallin (1971b).

Since the resulting matrix arising from this finite-differencing is sparse, it can be solved easily using the relaxation method. A somewhat more physical way of looking at the relaxation method, which also enhances convergence, is by making use of the diffusion equation. Therefore writing Equation 2 as a diffusion equation, with *t* as the time-step, the following equation is obtained.

$$\frac{\partial U}{\partial t} = \frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + \frac{\partial^2 U}{\partial z^2} - \rho(x,y,z), \tag{3}$$

As $t \rightarrow \infty$, the solution to this problem is a solution to the original elliptic Equation 2.
This can then be represented using finite differencing as:

$$U_{i,j,k}^{n+1} = U_{i,j,k}^{n} + \frac{\Delta t}{\Delta^2}(U_{i+1,j,k}^{n} + U_{i-1,j,k}^{n} + U_{ij+1,k}^{n} + U_{ij-1,k}^{n} + U_{i,j,k+1}^{n} + U_{i,j,k-1}^{n} - 6U_{i,j,k}^{n}) - \Delta t \rho_{i,j,k}$$

Where Δ represents the difference between two points in either the *i, j* or *k* directions and Δt represents the time-step from one iteration to another. The solution of the system of linear simultaneous equations, resulting from this expression when all the boundary conditions have been applied, can be obtained by the relaxation method.

The concern here shall be to establish the procedures for obtaining the stability criterion and the over-relaxation parameter which are the two determinant elements used in facilitating convergence to the solution when solving PDEs by the successive over-relaxation (SOR) method.

Obtaining the stability criterion for 3D finite differencing

The stability criterion for one-dimensional finite differencing of the diffusion equation is $\frac{\Delta t}{\Delta^2} \leq \frac{1}{2}$ and in the two-dimensional case, it is $\frac{\Delta t}{\Delta^2} \leq \frac{1}{4}$, where Δt represents the time-step from one iteration to another. Empirically, the criterion for higher-dimensions can be obtained as follows:

1) Let the number of dimensions (the number of spatial variables) be *k* and
2) Let *y* be the order of the partial derivative,
3) Then the stability criterion can be calculated as $\frac{\Delta t}{\Delta^2} \leq \frac{1}{ky}$.

Following this procedure, it is easy to see that the condition for stability for the 3D case when calculated will be $\frac{\Delta t}{\Delta^2} \leq \frac{1}{6}$. This matches with the suggestion of Roberts (2001) on the multi-grid solution of Poisson's equation using diagonally oriented grids.

Obtaining the over-relaxation parameter for 3D finite differencing

To the best of my knowledge, the only attempt to estimate the optimum SOR parameter for higher order Laplace's equation has been made by T.J. Randall, Department of Physics and Mathematics, John Dalton College of Technology, Manchester 1 Technical report, 400–401. This was for the case of 3D region with axial symmetry. The approach used here is from Frankel (1950) point of view. From his formula for obtaining the over-relaxation parameter in two dimensions, an

Table 1. The values obtained for the over-relaxation parameter in the 3D case, with varying dimensions.

m	n	l	α
10	10	10	1.528
15	20	10	1.621
40	35	20	1.796
200	100	50	1.920
230	65	46	1.907
1000	1000	1000	1.994
2000	2000	2000	1.997
10000	10000	10000	1.999

In all the cases, the value obtained lies between 1 and 2. This falls in line with the fact that the over-relaxation parameter should always lie between this ranges.

extension to obtain this parameter for the 3D case was approached intuitively as follows:

1) A close observation of the formula indicates that the calculation of the parameter does not depend on any other variable except the number of grid points and the number of spatial variables. This means that, if $k = 2$ is the number of spatial variables (that is, in the 2D case), and m and n are the number of grid points in the various directions (that is, the area is of dimension $m \times n$), then a general rule for obtaining the over-relaxation parameter could be given as: $\alpha = 2[1 + sincos^{-1}\frac{1}{k}\left(cos\frac{\pi}{m} + cos\frac{\pi}{n}\right)]^{-1}$.

To extend this to three dimensions, the following modifications can be made.

2) In the parentheses containing $\left(cos\frac{\pi}{m} + cos\frac{\pi}{n}\right)$, a third term was added containing the number of grid points in the third spatial variable, say l. This became $\left(cos\frac{\pi}{m} + cos\frac{\pi}{n} + cos\frac{\pi}{l}\right)$,

3) The multiplying factor of $\frac{1}{k}$, is $\frac{1}{2}$ when k = 2 in the 2D case, therefore, in three dimensions, k= 3 and thus the multiplier becomes $\frac{1}{3}$.

4) Thus, the formula for calculating the over-relaxation parameter in the 3D case can then be written as: $\alpha = 2[1 + sincos^{-1}\frac{1}{3}\left(cos\frac{\pi}{m} + cos\frac{\pi}{n} + cos\frac{\pi}{l}\right)]^{-1}$, or in the case where $m = n = l$, the shorter formula used was: $\alpha = \frac{2}{(1 + \sin\frac{\pi}{n})}$. This matches what is described in Thompson (1961).

NUMERICAL ILLUSTRATION

Table 1 shows the values of over-relaxation parameters obtained using the idea proposed in the work for solving 3D problems with some selected numbers of grid points. The numbers of grid points in each dimension are given as m, n and l and the relaxation parameter (α) is then calculated as previously described.

To test whether the over-relaxation parameters so obtained are optimum, the following example of 3D problem was solved using different numbers of equally sized grid points from 10 to 100. The convergence criterion was set to 1×10^{-6} and the maximum number of iterations allowed was 10000. The numbers of iterations at the point of convergence were recorded at different over-relaxation parameters and then compared to the numbers of iterations at convergence when the over-relaxation parameter calculated using the developed formula was used.

Example 1

Let $u = x^2z + 3z^3y^2 + y^3x^2z + 1$, found in Spiegel (1974), be considered in the interval [(0; 1); (0; 1); (0; 1)], with the x-axis divided into $i = 1,...,m$, the y-axis into $j = 1,...,n$ and the z-axis into $k=1,...,l$ grid points. The working surface is thus of dimension $m \times n \times l$. To solve this problem, it is necessary to start by looking for the derivatives with regards to all the spatial variables. That is,

$$\frac{\partial u}{\partial x} = 2xz + 2xy^3z; \qquad \frac{\partial^2 u}{\partial^2 x} = 2x(1 + y^3);$$

$$\frac{\partial u}{\partial y} = 6z^3y + 3x^2y^2z; \qquad \frac{\partial^2 u}{\partial^2 y} = 6z^3 + 6yx^2z);$$

$$\frac{\partial u}{\partial z} = x^2 + 9z^2y^2 + y^3x^2; \qquad \frac{\partial^2 u}{\partial^2 z} = 18z^2y^2;$$

The boundary conditions are:

$$f(x_0, y_0, z_0) = 1$$

$$f(x_1, y_1, z_1) = 6$$

Table 2. The comparison of the rate of convergence when using different fixed over-relaxation parameters and those calculated using the formula herein developed.

Relaxation coefficient	α							
	1.99	1.9	1.8	1.7	1.6	1.5	$2/\sin(\pi/n)$	
Grid points	Iteration	Iteration	Iteration	Iteration	Iteration	Iteration	α	iteration
10	1500	146	74	54	35	30	1.528	31
20	1504	172	79	70	110	148	1.728	65
30	1499	178	96	175	248	326	1.811	97
40	1534	162	192	309	430	561	1.854	129
50	1508	166	302	473	653	849	1.881	160
60	1494	192	431	666	916	1188	1.901	192
70	1519	261	577	886	1215	1575	1.914	223
80	1520	350	741	1132	1551	2007	1.924	254
90	1607	446	922	1404	1920	2483	1.932	285
100	1538	550	1119	1701	2323	3001	1.939	316

$$f(x_0, y_j, z_k) = 3z_k^3 y_j^2 + 1$$

$j = 2,\ldots,n-1;\ k = 2,\ldots,l-1$

$$f(x_1, y_j, z_k) = z_k + 3z_k^3 y_j^2 + y_j^3 z_k + 1$$

$j = 2,\ldots,n-1;\ k = 2,\ldots,l-1$

$$f(x_i, y_0, z_k) = x_i^2 z_k + 1;$$

$i = 2,\ldots,m-1;\ k = 2,\ldots,l-1$

$$f(x_i, y_1, z_k) = 2x_i^2 z_k + 3z_k^3 + 1;$$

$i = 2,\ldots,m-1;\ k = 2,\ldots,l-1$

$$f(x_i, y_j, z_0) = 1$$

$i = 2,\ldots,m-1;\ j = 2,\ldots,n-1$

$$f(x_i, y_j, z_1) = x_i^2 + 3y_j^2 + y_j^3 x_i^2 + 1$$

$I=2,\ldots,m-1; j=2,\ldots,n-1$

$$f(x_i, y_j, z_k) = 2z_k + 2y_j^3 z_k + 6z_k^3 + 6y_j x_i^2 z_k + 18y_j^2 z_k;$$

$i = 2,\ldots,m-1;\ j = 2,\ldots,n-1;\ k = 2,\ldots,l-1$

The calculated over-relaxation parameter was the same irrespective of whether the long form or the short form of the formula was used. The number of grid points was assumed equal in all the axes.

Table 2 shows the results obtained. From Table 2, it is clear that when using the over-relaxation parameter computed from the formula given, convergence is attained faster than when fixed values are used. Note the closeness in iteration numbers between relaxation parameters very close to those obtained using the formula. Thus, this formula gives an effective choice of the parameter and shall be used throughout the rest of this research when necessary. After having obtained the stability criterion and the over-relaxation parameter for the 3D case, the Gauss-Seidel scheme for solving the system of simultaneous equations resulting from this can be written in its extrapolated Liebmann form as follows:

$$U_{i,j,k}^{n+1} = U_{i,j,k}^{n} + \alpha\left(\frac{1}{6}\left(U_{i+1,j,k}^{n} + U_{i-1,j,k}^{n+1} + U_{i,j+1,k}^{n} + U_{i,j-1,k}^{n+1} + U_{i,j,k+1}^{n} + U_{i,j,k-1}^{n+1} - 6U_{i,j,k}^{n}\right) - \frac{\Delta^2}{6}\rho_{i,j,k}\right).$$

This can be written in short form as:

$$U_{i,j,k}^{n+1} = U_{i,j,k}^{n} + \alpha R_{i,j,k}^{n},$$

This matches with what is shown in Oort (1983) and Southwell (1946), where:

(1) $R_{i,j,k} = \nabla^2 U_{i,j,k} - \rho_{i,j,k}$ is the residual which must be less than a stated tolerance limit ε for convergence to be attained, and $\nabla^2 U_{i,j,k}$ is calculated from the recently obtained U as: $\nabla^2 U_{i,j,k} = (U_{i+1,j,k}^{n} + U_{i-1,j,k}^{n+1} + U_{i,j+1,k}^{n} + U_{i,j-1,k}^{n+1} + U_{i,j,k+1}^{n} + U_{i,j,k-1}^{n+1}$

2) The superscript n is the iteration number, while

3) α is the over-relaxation parameter.

The choice of the over-relaxation parameter determines the rapidity of convergence. If the parameter is equal

to 1, the method reduces to the Gauss-Seidel scheme as described by Ames (1972). If the parameter is less than 1, then there is under-correction as seen in Press et al. (1992). This scheme is then iterated until convergence is attained. The convergence set thus obtained is the solution field of the process.

Conclusion

We have been able to provide intuitively a procedure for obtaining the stability criterion and the over-relaxation parameter which are the two determinant elements used in facilitating convergence to the solution when solving PDEs by the SOR. These parameters were obtained for the 3D case by a natural extension of the one and 2D formulae developed by Frankel (1950).

Since the approach is intuitive, the main focus was to match this with reality. Thus, the detail derivation by Frankel (1950) has not been included. Instead, comparisons to the conditions of optimality posed by Frankel (1950) were tested on the obtained values. The performances of the parameters obtained from the procedure herein developed can be seen clearly in Table 2. The belief is that, with this development, many physical problems which were hitherto approximated by the use of 1D or 2D PDEs shall be explicitly expressed in three dimensions and be solved easily.

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