Finite-Difference Methods for the Diffusion Equation

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Thesis submitted for the degree of
Doctor of Philosophy

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March 1988

Contents

Summary

The development of accurate finite-difference methods for solving the linear diffusion equation with constant coefficients, in either one or two spatial dimensions, is useful in the study of several physical phenomena, such as underground water flow and diffusion of heat through a solid body. As well as accuracy, however, the amount of computer time taken to generate a solution must be taken into account, since this may be an important practical constraint.

The approach taken has been to thoroughly examine the one-dimensional case and then, having found some good methods to solve this problem, use the knowledge gained to develop methods for solving the more complicated two-dimensional problem. This work can then be extended to solve the variable coefficient diffusion equation, or even the non-linear equation, by considering that over the size of the computational stencil used, the linearised constant coefficient equation is a good approximation to the equation being solved.

In order to determine the accuracy of a given finite-difference equation, the *modified equivalent equation,* developed by Warming and Hyett (1974) for their heuristic stability analysis, has been adapted and used. This approach allows the simple determination of the theoretical order of accuracy of any finite-difference equation, thus allowing methods to be compared with one another. Also, from the truncation error of the modified equivalent equation, it is possible to eliminate the dominant error terms associated with finite-difference equations that contain free parameters (weights), thus leading to more accurate methods.

Several different finite-difference methods for the one-dimensional diffusion equation are developed, and their theoretical and actual truncation errors, as well as the CPU time required for solution, are compared to determine the most practical methods. To determine the actual order of accuracy of the method, graphs of $\log\{(Gridspacing)\}$ against $\log\{|(Error)|\}$ are plotted for decreasing values of the grid spacing and the results are examined. These graphs should be straight lines, and the slopes of the lines give the actual order of accuracy of the method. In most cases, this order matches the theoretical prediction, and in those cases where this is not so, the reasons for the difference are investigated.

Where the normal derivative at one boundary (or even both boundaries) is specified rather than the boundary value, the approximations at grid points on the boundary must be calculated. It is shown that it is still possible to produce relatively accurate solutions although the results are not as accurate as when the boundary value is known. Also in this case the techniques for handling the problems that arise near the boundary from some of the finite-difference equations having spatially wide computational stencils must be revised.

The same techniques as were used for the one-dimensional case are then applied to developing accurate finite-difference equations for the two-dimensional diffusion equation. In this case the computational stencils contain more grid points, and therefore allow more weights to be included. However, the larger number of low-order error terms in the modified equivalent equation, arising from the added cross-derivative error terms, means that some of the extra weights must be used to maintain the same accuracy as was achieved for the one-dimensional problem. Again, many different stencils and their corresponding finite-difference equations are examined, in order to find the best methods which can be practically applied. The method for determining the actual order of accuracy of the method is the same as that used for the one-dimensional case.

The so-called "locally one-dimensional" methods are examined, where the very accurate methods developed for the one-dimensional case can be applied directly to the two-dimensional problem. The best of the one-dimensional methods used in this manner are then compared with the best of the fully two-dimensional methods, to deter-

mine the preferred solution method. Note that to implement these methods correctly it is necessary to split the two-dimensional diffusion equation into two one-dimensional equations, each of which is solved alternately. Doing this requires special consideration of values on the boundary in the cases where only diffusion in one direction has been modelled. If this is not done then the results are downgraded to second-order accurate, regardless of the order of the finite-difference equation used.

The other class of techniques in common use for solving the two-dimensional diffusion equation is the alternating direction implicit methods, which combine the advantages of implicit methods, particularly large stability ranges, with fast execution speed on a computer, which is the major problem with fully implicit equations for the two-dimensional problem. Two different kinds of equations are considered, those based on the "classical" ADI methods, and those based on a "marching" equation, which must be applied "left-to-right" and then "right-to-left" in each spatial direction, as well as alternating the spatial direction. The potential for generating accurate solutions is examined for each type of equation, since these methods prove to be the only way of obtained generally fourth-order accurate results without using spatially wide computational stencils.

Another important practical problem that arises when solving the two-dimensional problem is an irregular boundary, which results in the specified boundary values not coinciding with the grid points of a uniform grid. This problem can be overcome by developing special finite-difference equations which allow for a non-uniform grid spacing at such a boundary. The effect of using these equations, which have a theoretical accuracy one order lower than their uniform grid analogues, is examined.

In order to make this work feasible, computer programs were developed to perform the time consuming and mechanical tasks involved with developing the finite-difference equations by hand. Using these programs it is possible to start with a desired method of differencing the diffusion equation, and have the computer determine the finite-difference equation corresponding to that differencing, as well as its modified equivalent equation. Weights specified in the original differencing can then be used to eliminate the dominant error terms, which then leads to the optimal form of the finite-difference

equation. This optimal equation can then be checked for such things as time-stepping (von Neumann) stability, solvability and/or marching stability, as appropriate. In some cases it is possible to use some of the weights to enhance the stability region of the equation rather than to increase the accuracy.