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NEW TRANSPORT METHODS AND CODES*

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ABSTRACT

New developments in deterministic numerical solution of the Boltzmann transport equation are reviewed. Applications of the finite element method in the FENT and TRIPLET codes to achieve flexible geometric representations are described. The role of the finite element method in mitigating ray effects is examined, and criteria for a next-generation transport code are suggested. The use of the finite element method to solve the integral transport equation is described.

A refinement of an already powerful method to accelerate convergence of transport iterative processes is discussed, and directions of future research in this area are outlined. The use of code restructuring and data management to improve the efficiency of large transport codes is discussed, and the implementation of such techniques in the DOT-IV code is described. Comments on the "economy" of computing are made.

1. INTRODUCTION

In the deterministic numerical solution of the Boltzmann transport equation, we see as important new developments the application of the finite element method, the development of new convergence acceleration techniques, and code restructuring coupled with improved data management. Use of the finite element method is important because it permits the systematic derivation of new approximate equations and has already made possible flexible geometric representations and mitigation of the ray effect. We discuss the finite element method and its application in specific codes in the next section.

Convergence acceleration methods offer the hope of reducing the total computational effort. A recent new concept in convergence acceleration has stimulated research which is described in Section 3. Similarly, code restructuring and improved data management can also make a computation less time consuming. In Section 4, we discuss this subject in general terms and as it occurs in the creation of specific codes. We conclude with remarks on the "economy" of computing.

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2. FINITE ELEMENT METHODS AND CODES

In the finite element method a functional form of the solution is assumed for each subdomain (element) of the space being considered. The functional form, often taken to be a polynomial, contains parameters which are determined systematically. For example, equations which the parameters must satisfy may be found by rendering stationary the second-order variational principle for the transport equation. Or, such equations may be found by substituting the functional form in the transport equation and then weighting the result (the residual) over the selected element with enough independent weights to determine all the parameters. Here, the procedure is much less well defined because of the wide choice of weights and domains possible. In either the variational or the weight-and-integrate process, the trial functions may be continuous or discontinuous. If discontinuous functions are used, care must be taken to treat the derivatives of the functions correctly.

In the transport equation, assuming the energy variable is treated by the multigroup approximation, there are six remaining independent variables which may be treated in whole or in part. For example, in the TRIPLET code (1,2) only the spatial variables are treated by the finite element method to derive a numerical approximation to the transport equation for a triangular grid. The angular variables are represented in a standard discrete ordinates approximation. In the FENT code (3), triangular elements, curved elements and a piecewise bilinear angular representation are combined to give not only a very general geometric capability, but also to give a more accurate (on a per unknown basis) approximation which has the important feature of greatly reducing ray effects. Ray effects are flux distortions caused by the discrete ordinates approximation which in effect restrains particles to stream only in directions corresponding to the discrete directions used in the calculation. If sources are isolated, then many locations in a system are not intersected by the discrete streaming paths from the source. When the system is absorbing, the flux at such locations is underestimated. The coupling introduced by the finite element method as used in FENT greatly reduces such distortions.

However, the angular coupling or the spatial coupling for finite element approaches which use continuous trial functions (as does FENT) has a disadvantage compared to standard discrete ordinates methods. The coefficient matrices are much less sparse and in particular are not lower triangular even in purely absorbing systems. This means that either a direct inversion of the coefficient matrix must be performed (which FENT does) or an iterative technique must be used. The direct inversion process, while eliminating the scattering source iteration used in discrete ordinates codes, has the drawback that both the storage requirements and solution times increase faster than linearly with problem size, while very little experience is available for iterative solution of finite element equations.

The TRIPLET code avoids the problem of spatial coupling by using discontinuous trial functions, and consequently, because it is combined with the discrete ordinates approximation, it uses standard iterative solution methods. Hence TRIPLET can solve large production problems without excessive storage requirements and with reasonable computing speed. On the other hand, TRIPLET does nothing to mitigate the ray effect.

Thus, neither FENT nor TRIPLET is completely satisfactory as a next-generation two-dimensional transport code. Research is in progress at Northwestern to develop iterative strategies for FENT and at Los Alamos to formulate a finite element method for both planar and finite cylindrical geometries while simultaneously reducing ray effects. Because a next-generation computer program should not be substantially slower than present programs, the latter is an ambitious undertaking. Because part of the extra computational effort of TRIPLET is devoted to testing for the orientation of triangles to ensure the stability of the different scheme, a first research effort at Los Alamos was to examine rectangular cells split by a single line of arbitrary orientation. By using a single finite element trial function over the whole rectangle, the testing of TRIPLET could be avoided while by allowing different material compositions on either side of the dividing line the flexibility of geometric representation could be retained. Furthermore, standard rectangular elements could be used when no material discontinuity is present. A number of different schemes were tested (4) and found unsatisfactory in comparison to the explicit representation possible in TRIPLET. Evaluation of these results has suggested two means for improvement of such schemes. TRIPLET apparently does well because it allows an explicit discontinuity at the material interface and because it preserves particle balance over each material zone separately. We are now considering a discontinuous linear trial function with a step function discontinuity along the line splitting the rectangular cell.

It seems clear from several years of research that ray effects cannot be mitigated without some form of coupling between angular domains. Consequently, the task is to devise schemes which reduce the ray effect as much as possible with a minimum amount of coupling. Because the discrete ordinates approximation is adequate in a large number of situations, it seems particularly desirable to have a formulation that reduces in a simple manner to the discrete ordinates equations. Indeed, it may be feasible to make this type of reduction selectively by space point. In methods which convert the discrete ordinates equations to spherical harmonic-like equations by adding a source, this source can be introduced selectively, and this might be done by multiplying it by a coefficient which is near unity in absorbing regions and small wherever the effective secondaries ratio is high. Similarly, coupling in a finite element method may be introduced by using a weight function which spans a variable angular region. Then, the parameters which define this region can be left free and used to locally alter the nature of the approximation. The effectiveness of such ideas remains to be explored.

An interesting variation of the finite element method is illustrated in the FEINT code (5). Designed to treat systems where isotropic scattering and sources are adequate, i.e., systems where collision probability methods are often applied, the FEINT code uses a finite element to discretize the spatial variables and then converts the resulting system of equations into integral equations for the scalar flux. The advantages of such an approach are several. First, if polynomial spatial representations are used, the method should be more accurate than collision probability methods which usually assume piecewise constant spatial variation. Second, by using curved and triangular elements, a wide variety of geometries can be represented precisely. Third, reflecting boundary conditions can be treated correctly. Work is continuing at Northwestern on refining the numerical techniques in the FEINT code so that it may be used for production-type problems.

3. CONVERGENCE ACCELERATION

Reed has shown (6) that both the rebalance and the synthetic convergence acceleration methods can be cast in a form with an iteration matrix given by

$$M' = (I - W_2 W^{-1})M \quad (1)$$

where M is the iteration matrix of the unaccelerated process, W is the exact solution operator matrix, and W_2 is a low-order solution operator matrix which is much cheaper to invert than W . In the synthetic acceleration method described by Gelbard (7), W_2 is related to the matrix of the diffusion operator and the solution proceeds by sweeping the mesh once with the transport operator and then solving the diffusion equations to improve the solution before repeating the process. In the rebalance method, W_2 is determined by enforcing particle balance. In contrast to the conventional synthetic method where W_2 remains constant, the W_2 of the rebalance process changes with each iterative cycle. The rebalance process is also nonlinear because W_2 depends on the unknowns being determined. In either case, the objective is to have the spectral radius of M' much smaller than that of M . From Eq. (1) it seems plausible that this will be true if W_2 is "close" to W , i.e., if $W_2 W^{-1}$ is nearly I so that the norm of M' is decreased.

Thus, if W_2 can be made "closer" to W without increasing the difficulty of its inversion, the effectiveness of the acceleration process should be increased. Although he was not addressing the problem in the context outlined here, Alcouffe (8) considered alternating between diffusion and transport solutions and, crucially, using the information generated by the transport solution to improve the quality of the diffusion solution. In particular, he generated anisotropic diffusion coefficients from the transport solution information. Painter, Rydin and Metcalf (9) systematized this approach and used the transport solution to provide improved diffusion coefficients and extrapolation distances after each transport solution. Hence, they modified W_2 at each iteration to make it closer to W . In a comparison on several standard one-dimensional test problems, this modified synthetic method was much more effective than a specially modified rebalance acceleration (9).

However, certain problems arise in the estimation of diffusion coefficients from the relation

$$\underline{J} = -\underline{D}\nabla\phi \quad (2)$$

where $\underline{J}$ and ϕ are assumed known from the transport solution and $\underline{D}$ is taken to be a diagonal tensor. In practice this definition may lead to negative or infinite values for the components of $\underline{D}$. To avoid this, Reed (10) suggested satisfying

$$\nabla \cdot \underline{J} = -\nabla \cdot \underline{D}\nabla\phi \quad (3)$$

instead. In one-dimensional finite difference form this leads to

$$\phi_i D_i = (J_{i+\frac{1}{2}} - J_{i-\frac{1}{2}})\Delta x + D_{i+\frac{1}{2}}\phi_{i+\frac{1}{2}} + D_{i-\frac{1}{2}}\phi_{i-\frac{1}{2}} \quad (4)$$

and Reed picked (again ϕ and J are known) D_1 from this equation after assuming $D_{i+\frac{1}{2}} = D_{i-\frac{1}{2}} = 1/3\sigma_{tr}$.

Much analytic work and numerical experimentation remains to be done in this area. The return is potentially great. In the test problems considered, marked reductions in the total number of iterations have been achieved, up to a factor of three in computing time, for both optically thick and optically thin media, and these comparisons are made against an improved re-balance method which has not been implemented in production codes. Derivation and testing of such methods should be performed for two-space dimensions and for coarse meshes, to minimize storage requirements.

To further improve the low-order operator it seems natural, when anisotropic scattering is present, to use the consistent P1 equations instead of diffusion theory as a low-order operator. Perhaps still more fruitful would be the use of the variable Eddington factor equations (11). The diffusion approximation is formed by assuming certain higher-order angular moments of the angular flux vanish. The Eddington factor approach assumes that these moments are proportional, with space-dependent factors, to the scalar flux and results in second-order equations no more complicated than the diffusion equations. By itself, the approach suffers from the difficulty of choosing the factors, but in an iterative acceleration context the transport solution is available for direct evaluation of the factors. Further, there are no numerical problems associated with evaluating these factors which are ratios of angular flux moments.

We feel that continued research in convergence acceleration measures is urgently needed. There is no reason that such methods cannot be applied to finite element or other approximations as well as to discrete ordinate techniques. Improved acceleration methods will ultimately make more feasible deterministic three-dimensional solutions.

4. CODE STRUCTURING AND DATA MANAGEMENT

Transport codes have grown in size to the point that overlay structures are common, and the size of problems solved with transport codes has increased to the extent that all available storage types are frequently used. Consequently, the structure of a code and the manipulation of the data within a code have come to play an increasingly important role in its efficiency. This, coupled with the desire to make codes operational on different machines within different operating systems has motivated research.

In present production codes the data handling is oriented toward a group-at-a-time solution process and it is tacitly assumed that the code is executed within about 500,000 words of fast memory, available either entirely as fast core on an IBM machine or within SCM and LCM on a CDC machine. This has precluded some installations from making effective use of the codes, and has required very large problems to be run in overlapping pieces. Currently, the two-dimensional DOT-IV program (12) is being developed to supplant DOT-III and is being organized around a line-at-a-time approach. This organization, in which a one-dimensional slice of the system is the working unit, is used partially in the TRANZIT (13) code and in the TWOTIME code now

under development at Los Alamos. Both TRANZIT and TWOTIME are time-dependent, two-dimensional transport codes where the entire angular flux is stored for use at the next time step.

The line-at-a-time organization has a satisfying simplicity and generality. It can apply to one, two or three space dimensional codes equally and makes possible the treatment of a large problem on a variety of machines. The Bettis Atomic Power Laboratory transport code (14) uses such an organization and performs an iteration on the line separately. That is, rather than sweeping the entire spatial mesh before updating scattering sources and accelerating convergence, more than one sweep on each line is made and this process, which is two-cyclic Chebyshev, is accelerated. This algorithm is used to reduce the amount of data transfer required for solution.

A line organization also facilitates two important innovations which are being made in DOT-IV. At specified planes, DOT-IV will permit the radial mesh to be changed. This will require either the interpolation or extrapolation of data, but makes possible the reduction of the number of mesh cells required in many problems. Similarly, at specified planes, DOT-IV will allow the N_Ω order to be changed, again allowing reduction of the total number of unknowns. Both of these options are conveniently executed after a line computation is complete.

In conjunction with a line organization, DOT-IV is to include a data management strategy to optimize storage and transmission between a three-level hierarchy of storage devices. Although the line is to be the basic unit, depending on problem size, blocks of line data may be the transmission unit. In any case, location of data in storage will be arranged according to problem size and local availability at execution time, with an attempt being made to optimize the positioning of the data. Similarly, simultaneous read, write, and compute algorithms will be used to minimize computing expense. DOT-IV is expected to be executing in its first version by 1 January 1975 and will include diffusion theory and consistent P1 theory options.

5. THE COMPUTING ECONOMY

It is interesting to note that workable deterministic numerical methods for solving the three-dimensional, time-dependent transport equations have been available for over ten years (15). However, ten years ago, it was thought to be an economic impossibility to implement these methods for three-dimensional problems. In the intervening years development has concentrated on methods to shorten execution times, and computers have become markedly faster, yet today three-dimensional methods seem to be as remote as they did ten years ago. This is in part because research has steadily increased the capability of the methods, with consequent increase of computational complexity. For example, anisotropic scattering has been added, methods to control negative fluxes have been implemented, acceleration techniques (which in two dimensions may themselves require an iterative solution) are used, more geometries are treated, and so on. This coupled with rising expectations on the part of the user to be able to solve problems with greater spatial and angular resolution has maintained the economic cost of two-dimensional computations approximately constant. Indeed, this state of affairs is probably a

corollary of Parkinson's law about work expanding to fill the time available. We feel, however, that this situation should be recognized in preparing for the development of three-dimensional codes. Part of the expansion has surely been a luxury, and certain features can be omitted from what should, at least at first, be a spartan undertaking. We do feel then, that by extracting the best from current development, three-dimensional finite difference solution of the transport equation will become a reality.

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