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A REVIEW OF CHARACTERISTIC METHODS USED TO SOLVE THE LINEAR TRANSPORT EQUATION*

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We review a selection of characteristic methods used to solve the linear transport equation. Characteristic methods are based upon the solution of the transport equation written in the form

$$\psi(s) = \psi(s_0)\, e^{-\sigma_T(s - s_0)} + \int_{s_0}^{s} Q(t')\, e^{-\sigma_T(s - t')}\, dt'$$

where s is arc length along the characteristic.

The methods of solution distinguish themselves in how the characteristics used for computation are selected and how the source term is approximated. We conclude by recommending criteria upon which a production method should be based.

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A REVIEW OF CHARACTERISTIC METHODS USED TO SOLVE THE LINEAR TRANSPORT EQUATION

1. INTRODUCTION

During the past two decades several methods have been proposed (and many fewer implemented in production codes) to solve the multidimensional neutral particle linear transport equation. In this review we discuss two classes of such methods and concentrate on one class, called "characteristic" methods. In the following we shall describe these two classes and set up a framework from which we define and compare the various characteristic methods found in the literature.

To begin, we assume that the transport equation has been cast in a multigroup, discrete-ordinates approximation which is to be solved by source iteration. This procedure is the most practical one for multidimensional problems, and is widely used in production computer codes. Thus, with no loss of generality we may consider the one-group transport equation in a region R with a non-reentrant boundary ∂R:

$$\Omega\cdot\nabla\psi(\underline{r},\Omega) + \sigma_T(r)\,\psi(r,\Omega) = Q(\underline{r},\Omega) \quad , \tag{1}$$

$$Q(\underline{r},\Omega) = \int\sigma(\underline{r},\Omega\cdot\Omega')\,\psi(\underline{r},\Omega')\,d\Omega' + S(r,\Omega) \quad ,$$

where

$r\in R$,
Ω is the direction of particle travel,
σ_T is the total cross section,
$\sigma(\underline{r},\Omega\cdot\Omega')$ is the scattering cross section assuming an isotropic medium,
$S(\underline{r},\Omega)$ is an arbitrary (nonnegative) source.

The boundary condition is

$$\psi(\underline{r},\Omega) = b(\underline{r},\Omega) \qquad , \qquad r\in\partial R, \quad \Omega\cdot n < 0 \quad ,$$

where n is the outer normal at r.

We note two features of Eq. (1) which greatly impact the accuracy of the methods discussed below. First, the scattering integral couples all angles at the local space point r. The local-ness of this coupling contrasts with the second feature. The "streaming" term can be written in the form

$$\Omega\cdot\nabla\psi(r,\Omega) = \frac{d\psi}{ds}$$

where s is arc length along the straight line through $\underline{r}$ in the direction $\underline{\Omega}$. Thus, the equation

$$\frac{d\psi}{ds} = Q$$

implies

$$\psi(\underline{r},\underline{\Omega}) = \psi(\underline{r} + s\underline{\Omega},\underline{\Omega}) \quad ,$$

which states that the value of the flux at point r in the direction Ω depends upon the value of the flux at any other point on the line through $\underline{r}$ in the direction $\underline{\Omega}$. We view this as a "non-local" contribution to the flux. These properties of local and non-local contributions to the flux at point $\underline{r}$ distinguish our two classes of methods of solution to the transport equation.

The first class of methods is actually based upon the local property of the scattering integral; the non-local nature of the transport term is accounted for in an approximate way. In this class a (generally orthogonal) spatial coordinate system appropriate for the system at hand is used to express the operator $\Omega\cdot\nabla$, a grid of points defining mesh cells in the phase space (r,Ω) is selected, and a balance equation (obtained by integrating Eq. (1) over a cell) is used to simulate the differential equation. (This assures particle conservation and leads to straightforward iteration acceleration methods which are essential in scattering-dominated or eigenvalue problems.) In such methods the scattering integral is readily evaluated by a quadrature rule; this invariably serves as an excellent approximation. However, the streaming term in Eq. (1) generates a surface integral in the balance equation, and this is approximated by a finite difference or finite element method. The accuracy of this approximation is severely limited by the size of the mesh in multidimensional problems[1]. As a rule this class of methods (which includes the diamond difference and linear discontinuous methods) performs well for problems in which the scattering terms are important (this includes most reactor systems). It performs the worst in streaming problems (with regions of vacuum or very low cross section) and in deep penetration (shielding) problems where computing resources normally require the size of the mesh to be large in mean free paths.

The second class of methods we call "characteristic" methods. Since these methods are the main thrust of this article, we shall describe them in more detail. To display the general philosophy behind these methods, we invert the "streaming plus collision" operator on the left side of Eq. (1) and get

$$\psi(r,\Omega) = \psi(r_0,\Omega)\, e^{-\sigma_T s} + \int_0^s e^{-\sigma_T t}\, Q(r - t\Omega,\Omega)\, dt \quad , \tag{2}$$

where

$$\underline{r} = \underline{r}_0 + s\underline{\Omega} \quad ,$$

and where, for simplicity, we have assumed σ_T = constant.

Thus, along each characteristic we have handled the non-local transport term exactly; the problem now is to evaluate the integral term in Eq. (2). An associated problem is that we frequently want the solution to the problem at every mesh point in the medium. This can be formally done by passing characteristics through every point in the system for every direction Ω, but the practicality of numerical solutions requires that as few a number of characteristics be taken as possible for an "adequate" solution. This can place constraints on how the mesh points are chosen. Thus, most of the effort in devising an accurate characteristic method lies in choosing the mesh points and in representing Q.

Generally, this second class of methods is most useful and accurate when the scattering integral is not as important as the streaming term. This occurs in streaming and deep penetration problems, where meshes are large and scattering is small. Also, we note that if $Q(s) \geq 0$ in Eq. (2), then $\psi(r,\Omega) \geq 0$. Thus methods based on Eq. (2) will be positive provided the boundary and internal sources are positive.

In the next section we derive characteristic methods, using Eq. (2) as a starting point, and we show how various authors have tackled the problem of the selection of mesh points and evaluation of the scattering integral. Included are two methods which seek to combine features of both classes of methods discussed above. In Sec. III we offer some recommendations for further research in this area.

II. CHARACTERISTIC METHODS FOR MULTIDIMENSIONAL PROBLEMS

To give a uniform presentation of the various characteristic methods found in the literature, we shall take some liberties in interpreting each author's development of his method. Specifically, we consider one group of a multigroup problem, we assume that the solution is obtained by iteration on the scattering source, and we restrict ourselves to (x,y)-geometry. (The characteristics in (x,y)-coordinates are straight lines, which facilitates display of the methods.) The characteristic methods make use of a spatial coordinate system and a grid of points in r and Ω, just as in the first class of methods. However, each characteristic method differs in the selection of the grid and in how this grid fits into the operational aspects of the method.

II.A The Method of Takeuchi

This method has been developed in (r,z) geometry by K. Takeuchi[2-4] and is also outlined by Campbell[5]. (Takeuchi has used the method exclusively for shielding problems.) We refer to Figure 1 in which one mesh cell in (x,y)-geometry is displayed. In Takeuchi's method the fluxes at the mesh vertex points are the principle unknowns. The directions Ω of the characteristics are chosen independently of the

spatial mesh and can in fact be any of the quadrature sets presently incorporated in S_N codes[6]. Figure 1 displays a representative characteristic ray which passes through the vertex point D in the direction $\underline{\Omega}$ and intersects the boundary at point E. In the direction shown, the flux is known at points A,B, and C, the source is known at points A, B, C, and D, and we wish to determine the flux at point D. Eq. (2) implies

$$\psi(D,\underline{\Omega}) = \psi(E,\underline{\Omega})e^{-\sigma_T \ell} + \int_0^{\ell} e^{-\sigma_T t}\, Q(t)\, dt \quad , \tag{3}$$

where ℓ is the length of the line segement $\overline{DE}$. The value of the flux at E is obtained by linear interpolation, i.e.

$$\psi(E,\underline{\Omega}) = \rho\psi(A,\underline{\Omega}) + (1 - \rho)\, \psi(B,\underline{\Omega}) \quad ,$$

where

$$\rho = \frac{k\mu}{h\eta} \quad ,$$

and where μ and η are the direction cosines of $\underline{\Omega}$ in the x and y directions and h and k are the cell dimensions in the x and y directions. (The location of the point E in Fig. 1 implies $0 < \rho < 1$.) To evaluate the integral term in Eq. (3), the source Q(s) is assumed linear in s along the characteristics, i.e.

$$Q(s) = \frac{s}{\ell}\, Q(D) + (1 - \frac{s}{\ell})\, Q(E) \quad .$$

Again, the source at E is interpolated from those at A and B to obtain

$$Q(E) = \rho Q(A) + (1 - \rho)\, Q(B) \quad .$$

This method thus consists of a vertex-to-vertex evaluation. Since the angles of the characteristics are arbitrary, the method is very flexible and is readily extendable to any geometry and mesh arrangement. Also, since the approximations in the method are due only to linear interpolations, the method is inherently positive.

Some basic questions concerning this method are posed below.

(i) How should the spatial mesh be selected?

(ii) How many characteristics are sufficient? (In other words, how should the angular quadrature set be chosen?)

(iii) Is linear interpolation sufficient?

(iv) Is a linear representation of the source along a characteristic a good one?

We give the following comments to these questions in reverse order:

(iv) Our experience in one-dimensional slabs[7] has shown that a linear (versus a constant) representation of the source is essential for accuracy in characteristic methods. We note that Sasamoto and Takeuchi have considered exponential (rather than linear) variations in the source and have reported excellent results[4].

(iii) Since the values of the fluxes and sources are known at the vertices, a higher-order interpolation such as splines or other polynomials incorporating points from adjoining cells could be used to check the adequacy of linear interpolation. However, the solution of the discrete-ordinates equations has a discontinuous first derivative across "singular characteristics" which emanate from every corner of every material region in every discrete-ordinate direction in multi-dimensional geometries, and higher-order interpolation schemes requiring greater smoothness than actually exists in the transport equation solution may be inappropriate.

(ii) The question of an adequate number of characteristics (i.e., directions in the quadrature set) can probably only be answered by experiment.

(i) It is essential to pick large meshes in regions where the scattering source is zero or very small so that the linear boundary interpolations do not overly degrade the solution. The remaining meshes should be on the order of a mean free path.

In general, precise answers to the above questions can be obtained only by a careful and experimental test program. Takeuchi did undertake such a program in Ref. 4, but most of his results are stated for one-dimensional slabs. In our opinion these results are not necessarily indicative of those in multidimensions because of the special smoothness of the solutions in slab geometry.

It is now appropriate to make another comment. Takeuchi's method does not seem to satisfy a balance equation, and hence neutron conservation is not strictly enforced independently of mesh size. For example, the angle-integrated balance equation for a mesh in (x,y)-geometry (referring again to Fig. 1) is written

$$J_x^{BD} - J_x^{AC} + J_y^{CD} - J_y^{AB} + \sigma_T \phi_0 = Q_0 \qquad (4)$$

where

$$\phi_0 = \iint_{cell} \psi(x,y,\underline{\Omega})\, dx\, dy\, d\underline{\Omega} \quad ,$$

$$Q_0 = \iint_{cell} Q(x,y,\underline{\Omega})\, dx\, dy\, d\underline{\Omega} \quad , \tag{5}$$

$$J_x^{BD} = \iint_{B}^{D} \mu\psi(h,y,\underline{\Omega})\, dy\, d\underline{\Omega} \quad , \qquad \text{etc.}$$

In analogy to Eq. (4), one could imagine a relationship from the solution of Takeuchi's method such as

$$\frac{1}{2}(J_x^B + J_x^D) - \frac{1}{2}(J_x^A + J_x^C) + \frac{1}{2}(J_y^C + J_y^D) - \frac{1}{2}(J_y^A + J_y^B)$$

$$+ \frac{1}{4}\sigma_T(\phi^A + \phi^B + \phi^C + \phi^D) = \frac{1}{4}(Q^A + Q^B + Q^C + Q^D) \quad ,$$

where the quantities here are analogous to those defined in Eq. (5), but evaluated at the vertex points. However, there is no guarantee that this (or a related) equation is ever satisfied.

By contrast, it has historically been considered crucial for purposes of iteration acceleration methods and accuracy that numerical methods in the first class discussed in Sec. I (such as diamond difference and linear discontinuous) satisfy a cell balance equation. In fact, we have pointed out in Sec. I that the cell balance equation is the basic ingredient in these methods. In Takeuchi's method, however, this equation is completely absent.

II.B The Method of Wagner - Sorgis - Cohen

This method is described in Ref. 8 and extended somewhat in Ref. 9; it was developed to solve general (x,y,z)-geometry problems having a uniform spatial grid. We describe this method in (x,y)-geometry by means of Fig. 3. Again in order to resolve the source and calculate a local flux, this method resorts to a grid of points. The spatial grid is required to form a uniform mesh of rectangles such that the height k and width h are the same for each mesh cell. As we show in Fig. 3, only certain directions through the mesh are chosen as characteristic rays; these are the ones that pass through the vertices of the rectangles along the diagonals and through the center of the edges in the horizontal and vertical directions. This restriction on the characteristics along with the use of a uniform mesh allows the computation of the flux without interpolations and with a minimum of computational effort since the same exponential factors are used in every cell in each material region for attenuation along the characteristics. In Ref. 9 a scheme is mentioned which relaxes the requirement of a uniform mesh by a spatial interpolation, but details are not given so we shall not discuss this modification here.

The essential feature of this method which distinguishes it from Takeuchi's is that the source is taken to be constant throughout each mesh cell; the source integral is then readily evaluated for each characteristic. In the source iteration procedure, a method to compute the source is described which uses a balance equation similar to Eq. 4. This balance equation defines the cell-average scalar flux from which the constant source is computed.

In summary, this method is positive, simple, and presumably computationally fast. It appears to be most useful for deep penetration problems that can be described by a uniform rectangular mesh where the source contribution is small. The accuracy is limited because of the assumption of a constant source in each mesh and the restrictions on the characteristic directions used. The constant source assumption implies that very small mesh cells are required when scattering is an important contribution to the source and the restriction on the characteristic directions implies that general streaming in the void regions cannot be accurately calculated. However, this method's value lies in rapidity of calculation and the method should serve as a benchmark for assessing the impact of relaxing the restrictions upon the class of problems it was designed to solve.

At first glance it appears that another restriction on methods which proceed from vertex to vertex is that the characteristics be straight lines in the problem coordinate system. However, Askew has developed a method which for cylinders and spheres works on the same principles discussed above.

II.C The Method of Askew

This method, originally formulated by Askew[10], has been expanded to handle general problems for a variety of one- and two-dimensional geometrical situations[11-13]. Askew's method, although developed independently, takes ingredients from the methods described above. In Fig. 3 we display some of the aspects of the method for a rectangular mesh cell. We show three equally spaced characteristic rays passing through the cell in an arbitrary direction Ω. The characteristics need not be equally spaced, but for practical reasons[12] this restriction has been imposed on the method. The initial values of the flux in direction Ω are given at the points at which the characteristic rays enter the cell; the flux at the points at which the rays exit the cell is evaluated from the characteristic solution (Eq. 2). The source is assumed constant in the mesh cell as in the previous method. In order to compute the flux $\psi(r,\Omega)$ from which the source is evaluated, the following procedure is used. Each ray passes through the "center" of a volume as it sweeps through the cell and in the example this volume is

$$\delta A_m \ell_{im}$$

where δA_m is the spacing for angle m and ℓ_{im} is the length of the (i-th) ray passing through the cell. In general, the total volume swept by rays passing through the cell is not equal to the physical volume of the cell, and so each track length through the cell is modified as

$$\ell'_{im} = \ell_{im} \frac{V_{cell}}{\sum_m w_m \sum_{j\varepsilon\ cell} \delta A_m \ell_{jm}} \quad ,$$

where w_m is the angular weight.

Thus these modified "track lengths" will yield the correct cell volume when weighted and summed over all the characteristics passing through the cell. The motivation for doing this is to ensure neutron balance for the cell (and consequently the system). This balance is ensured by using the balance equation (Eq. 4) to compute the cell-average scalar flux which is then used to compute the source. This procedure is much the same as described for Wagner's method. A similar procedure is implemented for preserving balance in curvilinear geometries and is described in detail in the references.[10-13] Also detailed there are criteria for choosing the characteristics (i.e., their spacing and the angles), the impact of reflecting and periodic boundary conditions, considerations of non-constant σ in the cells (i.e., cells which contain non-rectangular subregions), and iteration acceleration procedures to converge the scattering source and to solve eigenvalue problems.

This method of characteristics has been implemented in impressive generality[12], and yet there are some attendant difficulties with it. Because the source is assumed constant it is necessary to take small mesh cells, on the order of a scattering mean free path, when the scattering contribution is large. In curvilinear geometries the manner of choosing the characteristics leads to many evaluations of the flux in the outer regions of the system, which is quite inefficient. This is clearly explained by Campbell[5], who presents a remedy for this. (Campbell's "long characteristic" method is similar to Askew's method). Another method which is similar is displayed next.

II.D The Streaming Ray Method of Filippone

Filippone's general-purpose (x,y)-geometry streaming ray method[14,15] is an attempt to develop a hybrid method: one which takes attributes of the class of characteristic methods and attributes of the local mesh methods and combines them into a single method. To describe this method we again refer to Fig. 3. As in Askew's method, equally spaced characteristics in a given direction $\underline{\Omega}$ are drawn which intersect the rectangular region. However, the problem is split into two parts; one part solves along the characteristics with the source assumed to be zero, and the other part solves the source problem in the rectangular region via a diamond differenced approximation with zero incoming boundary conditions. Mathematically we describe this as follows: Assume

$$\psi(\underline{r},\underline{\Omega}) = \psi^0(\underline{r},\underline{\Omega}) + \psi^c(\underline{r},\underline{\Omega})$$

where

$$\underline{\Omega}\cdot\nabla\psi^c + \sigma_t\psi^c = S(\underline{r},\underline{\Omega}) \qquad (6)$$

$$\psi^c = 0 \text{ on the incident faces} \ ,$$

Now solve Equation (6) via diamond differencing on the rectangular mesh to obtain

$$\psi_R^c \ , \ \psi_T^c \quad \text{and} \ \psi_{av}^c \quad .$$

Also solve the equation for ψ^0 along the characteristics to obtain

$$\psi^0_{out,i} = \psi^0_{in,i} \ e^{-\sigma_T \ell_i}$$

where i denotes a characteristic and $\psi_{in,i}$, $\psi_{out,i}$ are the fluxes evaluated at the intersection of the ray with the rectangular mesh at the incoming and outgoing boundary, respectively.

The average characteristic flux for the cell, ψ^0_{av}, is obtained by volume-averaging of the average fluxes along each streaming ray. Thus the total solution is

$$\psi_{av} = \psi^c_{av} + \psi^0_{av}$$

$$\psi_{out,i} = \psi^0_{out,i} + \psi^c_B$$

where ψ^c_B is the appropriate outward boundary flux from the diamond solution.

As implemented, this method assumes a uniform spatial mesh and special quadrature sets to minimize the number of exponential calculations. It also assumes a constant source, whose drawbark we have already commented on, but this source is used in a diamond sense and may not be as severe a restriction as in the other methods. Of a potentially more serious nature, the method does not explicitly satisfy a balance condition. On the other hand, the method is strictly positive because of the zero boundary conditions for the diamond solution. Also, the angular discretization for the diamond solution can usually be chosen to be much less than that for the characteristic solution. The reason for this is that in a source region the flux will generally be nearly isotropic and the angular corrections due to the boundary condition will presumably be picked up by the characteristic solution on the finer angular discretization. This consideration is important because streaming in void regions can be handled quite nicely and efficiently in an accurate way (note that the diamond solution will be zero in voids). Further details on this method and its calculational results are presented in the third paper of this session.

II.E The Linear Characteristic Method of Larsen

The general-purpose, (x,y)-geometry linear characteristic method[16,17] again is an attempt to more consistently utilize the advantageous properties of the two classes of methods. We use Figure 1 to illustrate the essential points. First, the characteristic equation (2) is solved explicitly for all points in the cell for the angle $\underline{\Omega}$, assuming linearly varying boundary conditions along the bottom and left edges of the cell and a source linear everywhere in the cell. The outgoing cell boundary fluxes required for the boundary conditions of the adjoining cells are evaluated from the analytic solution. The cell-averaged fluxes, required for constructing the source for the next iterate, are evaluated from neutron balance considerations. The details on this method are given in Ref. 18.

Thus the source term is handled much the same as a mesh-oriented code would and the transport from cell to cell is approximated by boundary averaged terms rather than point values. From the perspective of methods denoted C and D above, this method "fills" the cell with characteristics at angle $\underline{\Omega}$ but smears out the cell to cell communication by using boundary averages.

The advantages of the method lies in its simplicity, which is reflected in computational efficiency[16]. Also, it is mathematically clear in what sense the method is approximating the original differential equation, and neutron balance is rigorously assured. The algebraic simplicity of the method takes advantage of the fact that the characteristics are straight lines in (x,y)-geometry. In curvilinear geometry the analytic solution in the curvilinear coordinates is not simply expressed, and hence computational efficiency would require the storage of a large amount of data for solution.

III. RECOMMENDATIONS

It is apparent that many researchers have found the method of characteristics useful for solving certain classes of transport problems. In our view these are the problems in which the streaming term dominates the source contribution, such as in voids or deep penetration problems. The CACTUS code[12] does have the capability of solving a wide variety of problems, including eigenvalue problems, and its geometric flexibility is closer to that of Monte Carlo codes than any other code that has come to our attention. However, we view CACTUS as a special-purpose code because it appears to be much less efficient in terms of computer resources than other general purpose transport codes which solve eigenvalue and shielding problems[9,10]. We do believe that an efficient characteristic method can be developed for a general-purpose transport code. To do this will, however, involve additional research which we have divided into the following three areas.

III.A Balance Equation

Our experience in developing methods to solve and accelerate the solution of the transport equation indicates that having a balance equation appropriate to the method leads to an increase in accuracy and in the effectiveness of iteration acceleration schemes. The methods of Wagner and of Askew and the linear characteristic method do satisfy a balance equation. Such an equation for more general methods should be formulated and incorporated.

III.B Representation of the Source

All of the methods discussed in Section II make use of a mesh in the problem coordinate system to form the source. It is our experience that at least a linear representation for the source is necessary for an accurate characteristic method, especially for large meshes[17,18]. This at-least-linear representation also seems to be needed to satisfy the diffusion limit for scattering-dominated problems. Whether this representation is best done in the problem coordinates or strictly along the characteristics (as in Takeuchi's method) is an open question.

III.C Geometric Flexibility

A final distinguishing aspect of the methods displayed in Section II is the flexibility allowed in the placement of the calculational characteristic rays to solve the transport problem. In Wagner's method there is a minimum of flexibility since the spatial mesh determines the allowed directions for the characteristics. Askew and Filippone relax this restriction somewhat, although they prefer a regular placement of the characteristics (e.g. equal spacing, a fixed number per cell, etc.) Takeuchi's method places no restrictions; any direction can be chosen and the necessary cell boundary data are supplied by interpolation. The merit in the methods which depend on a uniform mesh is that a minimum amount of data needs to be computed and stored to allow the method to be vectorized. The implication here is that a vectorizable calculational method will ultimately be most efficient. In a vectorized mode one must have no cell-by-cell decisions made during calculation; this rules out methods based upon interpolation. On the other hand, interpolation can lead to a more accurate method with a given number of mesh points. Thus some compromise or melding of the two approaches could be optimum - perhaps along the lines implicit in Filippone's method.

In conclusion, the method of characteristics has the promise of leading to (but has not yet produced) a general-purpose method which alleviates many of the difficulties encountered by methods incorporated in existing general-purpose production codes.

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Fig. 1 X-Y cell used to Describe Takeuchi's Method

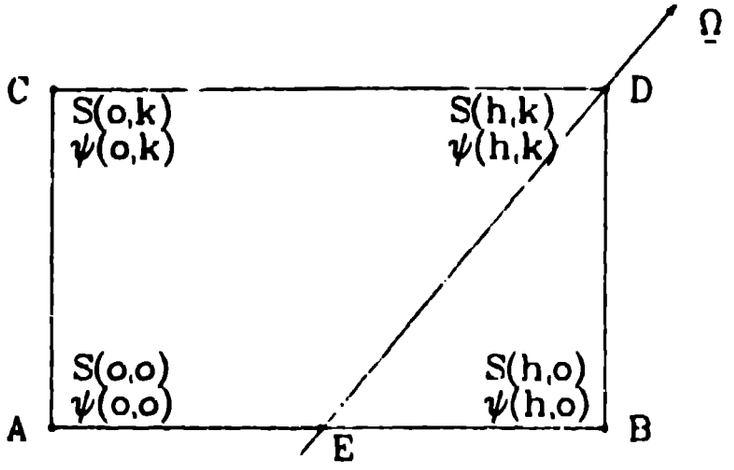

Fig. 2 X-Y cell used to Describe Wagner's Method

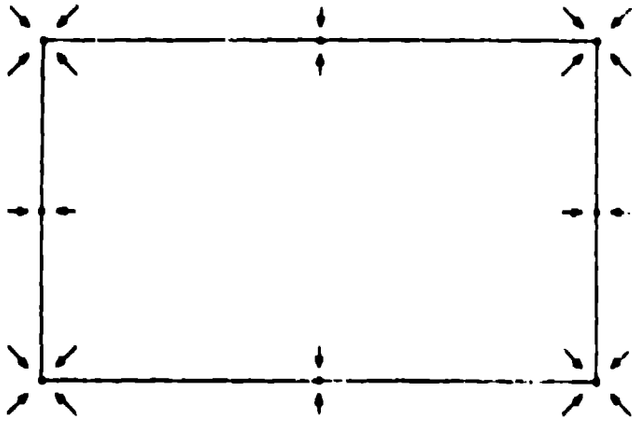

Fig. 3 X-Y cell used to Describe Askew's and Filippone's Method