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INVARIANT IMBEDDING IN TWO DIMENSIONS

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INTRODUCTION

J. Corones [1] has noted that the doubling and addition formulas of invariant imbedding can be extended conceptually to very general situations. All that is needed is a black box "process" with n "ports." The ith port has vector input I_i and vector output J_i. (In Fig. 1, such a process is represented as an n-gon, but this is only a visual device.)

Addition formulas result when two or more of these processes are joined together to form a new process in some regular way. For example, four congruent squares can be juxtaposed to form a larger square. (This program is carried out in some detail in Sec. 2.) At each join, the output of one process becomes the input of the other and vice versa. (We always suppose the join to occur at one or more ports.) Addition formulas result from the combination of these shared quantities. Corones has thus pointed out that invariant imbedding is not, as is sometimes asserted, an inherently one-dimensional (1-D) method, but works conceptually in any number of dimensions; some previous work that is conceptually along these lines, with references to other such works, can be found in Refs. 2-4. The details can, of course, become very complicated. We shall show that the method is computationally feasible for certain two-dimensional (2-D) problems. To conform to the thrust of these proceedings, we shall usually phrase our discussions in terms of transport theory rather than speaking of more abstract processes.

* This work was performed under the auspices of the U.S. Department of Energy

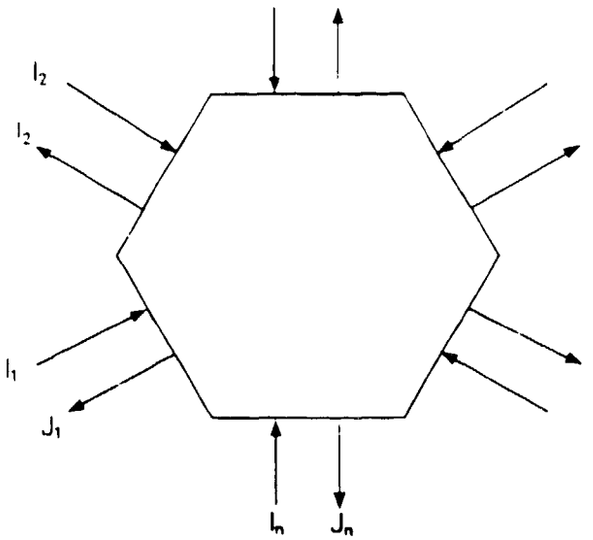


Figure 1. N - port process.

1 INVARIANT IMBEDDING IN 1-D

1.1 The Addition Formulas

Consider an infinite slab of material of thickness z. Linear transport of particles occurs in the slab in a manner independent of the x and y coordinates. We suppose no internal particle sources. The left face of the slab may be considered a "port," as may the right side. The input of particles at the left face is described by a vector I_1, which may have as components energies, directions, etc. These are assumed to be discrete quantities. The vector I_1 will not be allowed to depend on the x and y coordinates. (We are considering the entire left face to be a port). For instance, I_1 might be the vector whose components give the number of particles per unit area entering the left face at six different angles. Similarly, I_2, J_1, and J_2 are input and output vectors as shown in Fig. 2. (Note that the indexing does not agree with Fig. 1.)

The components of the input and output vectors are sometimes referred to as states (see [5]). Although energies and directions are often the physically interesting states, such descriptors as color, size, and generation number are quite admissible.* Observe that the symbol I is used in Fig. 2 for "input," with J for "output." Also, we do not mention anything about the particles inside the slab, save to emphasize that all processes are linear.

We associate with this process a transition matrix

$$A = A(z) , \tag{1.1}$$

which has the property that its entries (α,β) give the probability that an input particle in state α will lead to an output particle in state β. Thus

* The number of states can become very large easily. Suppose input particles can move in any of eight directions at any of 12 energies. There are then 96 possible states, and the input (and output) vectors will have 96 components.

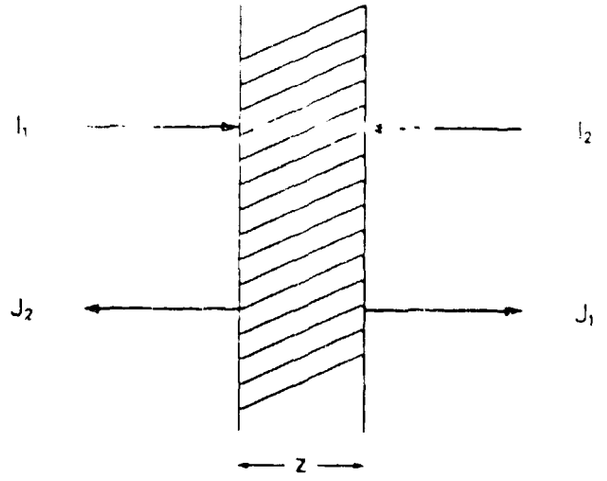


Figure 2. Slab of width z.

$$\begin{bmatrix} J_1 \\ J_2 \end{bmatrix} = A \begin{bmatrix} I_1 \\ I_2 \end{bmatrix} . \tag{1.2}$$

Because I and J are vectors, A is not a simple two-by-two matrix. It is customarily written in block form:

$$A = \begin{bmatrix} T_+ & R_+ \\ R_- & T_- \end{bmatrix} . \tag{1.3}$$

To understand the meaning of the T and R matrices, observe that (1.2) gives

$$J_1 = T_+ I_1 + R_+ I_2 . \tag{1.4}$$

If $I_2 = 0$ this yields

$$J_1 = T_+ I_1 . \tag{1.5a}$$

Thus T_+ provides the information about particles transmitted through the slab to the right when the only input is at the left face.

Again, suppose $I_1 = 0$. Then

$$J_1 = R_+ I_2 . \tag{1.5b}$$

Hence R_+ provides information about particles reflected from the slab to the right when the only input is at the right face; T_- and R_- may similarly be understood.

In many cases of interest the material is isotropic* it does not know its right from its left.* Then

$$R = R_+ = R_- , \quad T = T_+ = T_- . \tag{1.6}$$

*Note that the word isotropic here applies to the material's "sense of direction." It has nothing to do with the details of scattering processes.

In some of what follows we assume (1.6) holds. Suppose we now have two slabs of thicknesses z_1 and z_2. Assume that we know the transition matrices $A(z_1)$ and $A(z_2)$. Let us juxtapose the two slabs forming one of thickness $z_1 + z_2$. Can we find the resulting transition matrices, which we denote by $A(z_1 + z_2)$?

This problem was first addressed by R. Redheffer (see [6]) and the bibliography therein) but in a somewhat different context. We shall sketch the fundamental derivation.

Refer to Fig. 3. Obviously we wish, for example, to consider the output vector J_1 from the slab of thickness z_1 as an input vector K_1 for the slab of thickness z_2. This requires a certain compatability amongst the input and output vectors. The details are best left to the reader. Also, we must require that when we form the slabs, J_1 does indeed become K_1, etc. No particles are created or absorbed. This is a fundamental continuity assumption physically appropriate to transport phenomena (and many other processes).

For notational convenience, write

$$A(z_i) = \begin{bmatrix} T_+(i) & R_+(i) \\ R_-(i) & T_-(i) \end{bmatrix}, \quad i = 1,2 . \tag{1.7}$$

We seek the matrix

$$A(z_1 + z_2) = C = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \tag{1.8}$$

such that

$$\begin{bmatrix} J_2 \\ L_1 \end{bmatrix} = C \begin{bmatrix} I_1 \\ K_2 \end{bmatrix} . \tag{1.9}$$

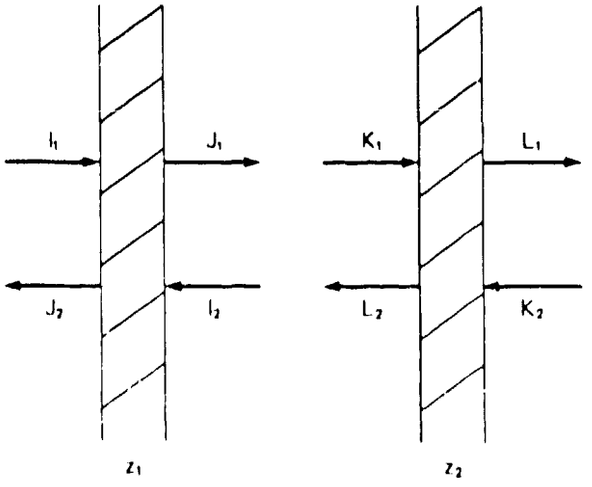


Figure 3. Two slabs to be "joined."

From Fig. 3 we have (see (1.2) and (1.3))

$$\begin{aligned} J_1 &= T_+(1)I_1 + R_+(1)I_2 \\ J_2 &= R_-(1)I_1 + T_-(1)I_2 \\ L_1 &= T_+(2)K_1 + R_+(2)K_2 \\ L_2 &= R_-(2)K_1 + T_-(2)K_2 \ . \end{aligned} \tag{1.10}$$

The continuity requirement implies

$$J_1 = K_1 \ , \quad I_2 = L_2 \ . \tag{1.11}$$

Eliminating J_1, I_2, K_1, L_2 from (1.10) and (1.11) finally gives (observe that the unsubscripted I denotes the identity)

$$\begin{aligned} J_2 &= T_-(1)\,[R_-(2)(I - R_+(1)R_-(2))^{-1}R_+(1)T_-(2)]\,K_2 \\ &\quad + [T_-(1)R_-(2)(I - R_+(1)R_-(2))^{-1}T_+(1) + R_-(1)]\,I_1 \\ L_1 &= [T_+(2)(I - R_+(1)R_-(2))^{-1}R_+(1)T_-(2) \\ &\quad + R_+(2)]\,K_2 + [T_+(2)(I - R_+(1)R_-(2))^{-1}T_+(1)]\,I_1 \ . \end{aligned} \tag{1.12}$$

We now easily identify the elements of C (Eq. (1.8)), which we write as $R_\pm(z_1 + z_2)$ and $T_\pm(z_1 + z_2)$. Reverting to the R and T notation yields

$$\begin{aligned} C_{11} &= T_+(z_1 + z_2) = T_+(z_2)(I - R_-(z_1)R_+(z_2))^{-1}T_+(z_1) \\ C_{12} &= R_+(z_1 + z_2) = T_+(z_2)(I - R_-(z_1)R_+(z_2))^{-1}R_-(z_1)T_-(z_2) + R_-(z_2) \\ C_{21} &= R_-(z_1 + z_2) = T_-(z_1)R_+(z_2)(I - R_-(z_1)R_+(z_2))^{-1}T_+(z_1) + R_+(z_1) \\ C_{22} &= T_-(z_1 + z_2) = T_-(z_1)[R_+(z_2)(I - R_-(z_1)R_+(z_2))^{-1}R_-(z_1)T_-(z_2) + T_-(z_2)] \ . \end{aligned} \tag{1.13}$$

Equation (1.13) is often written in the form

$$A(z_1 + z_2) = A(z_1) * A(z_2) \ , \tag{1.14}$$

where the "*product" is obtained by forming the elements of $A(z_1 + z_2)$ by use of (1.13). Clearly, the inverse of the particular matrix $(I - R_-(z_1)R_+(z_2))$ must exist. In the transport theory of neutrons, the existence or non-existence of this inverse is closely connected with the problem of physical criticality of the system.

1.2 The Doubling Formulas

Finally, if the medium is isotropic (see Eq. (1.6)) and if $z_1 = z_2 = z$, we find

$$\begin{aligned} T(2z) &= T(z)(I - R^2(z))^{-1}T(z) \\ R(2z) &= T(z)(I - R^2(z))^{-1}R(z)T(z) + R(z) \ . \end{aligned} \tag{1.15}$$

These so-called "doubling" formulas obviously make it possible to calculate the R and T functions for "thick" slabs starting only with knowledge of a single "thin" slab. Equations (1.15) were apparently first noted by the astrophysicist van der Hulst [7].

These formulas were very effectively used by G. Hughes et al. [5] who made extensive calculations involving direction dependent neutron transport. The continuous angle dependence was first discretized by careful "binning," a process conceptually easy but nontrivial in practice. As many as 256 bins were considered. The initial slab was taken sufficiently thin to make it possible to employ the single scattering transport approximation. Excellent results were obtained.

1.3 The *-Product

The properties of the *-product invite investigation, and a considerable amount of work has been done. The operation is associative and has the identity

$$Iden = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix} . \tag{1.16}$$

Under certain conditions there is an inverse. To pursue the properties of the *-product in detail would take us far afield.

2 INVARIANT IMBEDDING IN TWO DIMENSIONS

2.1 Discussion of the Problem

We have implied that invariant imbedding in more than 1-D is conceptually possible, but gives promise of being quite complicated. In this section we shall face some of those complications. Transport in 2-D appears to be a somewhat unrealistic process. To see that it is actually meaningful we simply consider an infinitely long cylinder and confine our investigations to a cross section of the cylinder. (This is the analogue of what was done with the infinite slab in Sec. 1). To keep matters as simple as possible, we consider that cross section to be a square, or, at worst, a rectangle. Later, we shall note that more complicated regions, which can be approximated by unions of squares, can be handled.

Continuing our emphasis on particle transport, we intuitively see at once that particle direction is going to be the most difficult matter to handle. Energy, particle size or kind, or other types of states usually offer much less complication. We shall therefore consider particle directions as the only states.

Consider the case of a square. A particle impinging on one side of the square can result in outputs on the adjacent sides as well as on the opposite side. Clearly, more than the simple R and T functions are needed. As another complication, we note that location of the point of entry on the square side is probably going to play a role, a difficulty avoided in the slab geometry by our assumption that there was no (x,y) dependence.

From the 1-D analysis, we see that it is probably reasonable to start with a very small fundamental square in the hope of getting, in some way, results for this "element." The

addition and doubling formulas (Eqs. (1.13), (1.15)) suggest that we may then be able to "add" (juxtapose) these elements to obtain "thin" rectangles and then "add" these rectangles to eventually "double" the original element. This is the essence of the program we shall describe.

2.2 Notation and Operators

We shall not at this point describe how to obtain results for the fundamental square element Σ. That matter will be taken up in Sec. 3. We suppose all that information is available. For convenience we assume the square Σ is isotropic. It does not distinguish its top from its sides or bottom. More accurately, it is insensitive to 90° rotations.

Figure 4 schematically shows Σ with input vectors denoted by u and outputs by v. When four Σ elements are joined–hence a doubling–the picture looks like Fig. 5. Here the heavy arrows labeled V denote overall outputs resulting from the inputs u to each of the four fundamental squares Σ_i. Figure 6 indicates the situation after five doublings. In none of these diagrams is any quantitative relationship among the u's and V's implied.

Let us now introduce the necessary reflection and transmission operators. Figure 7 indicates an input vector u on the left side of the square Σ. This results in four output vectors.

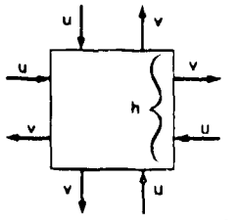


Figure 4. Fundamental square of width h.

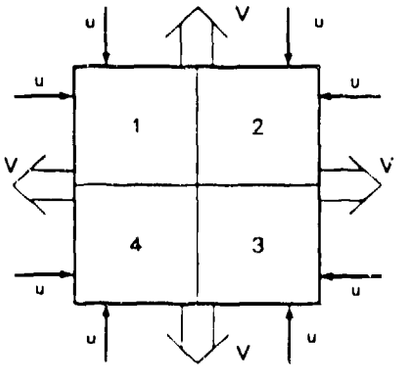


Figure 5. Four fundamental squares "joined" together resulting in a 2hx2h square with known flux values.

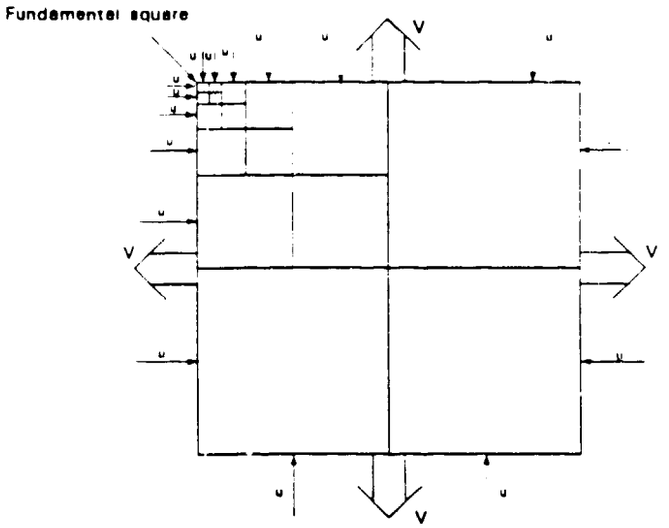


Figure 6. Result after five doublings (32hx32h, 2^5hx2^5h).

one from the left face, one from the right, and one from each of the two sides. The last are new. There are no analogues in 1-D. We denote the required operators by $R, T, S, \tilde{S}$. If we call the output vectors V_E, V_W, V_S, V_N, as shown in Fig. 8 (note that the indexing corresponds to the customary way of labeling wind direction), and similarly write $u = u_W$, we have (assuming momentarily that $U_S = U_E = U_N = 0$)

$$\begin{aligned} V_S &= SU_W \\ V_W &= TU_W \\ W_N &= \tilde{S}U_W \\ V_E &= RU_W \quad . \end{aligned} \tag{2.1}$$

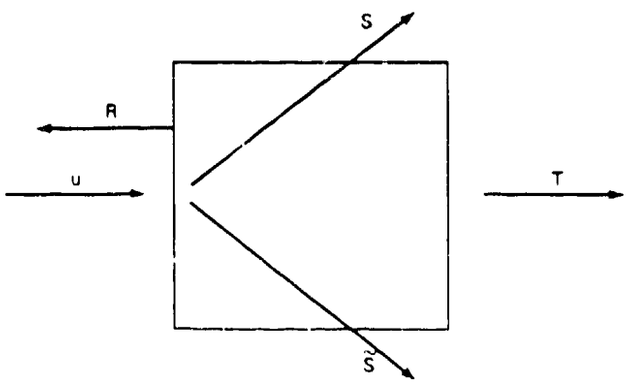


Figure 7. Possible exit vector operators R, S, $\widetilde{S}$, and T associated with an incident vector u.

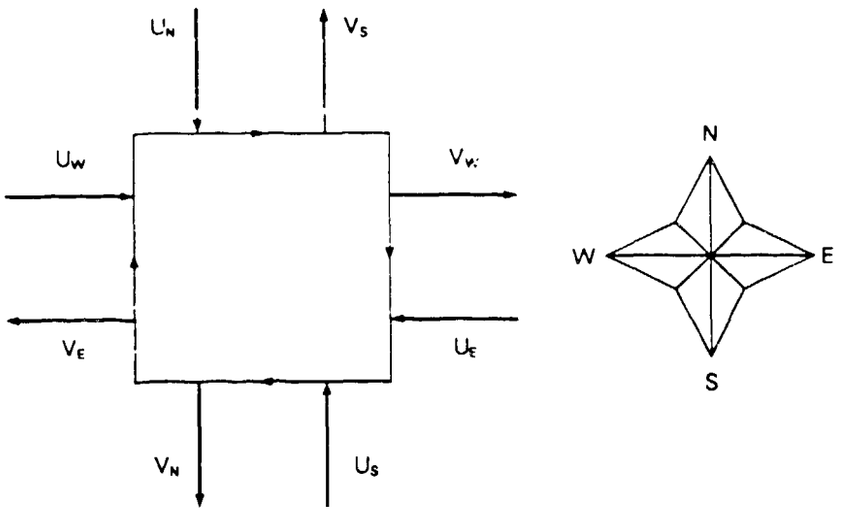


Figure 8. Incident and exit vectors U_N, U_E, U_S, U_W and V_N, V_E, V_S, V_W, respectively.

Now recall the fact that Σ is isotropic. We see at once that

$$\tilde{S} = S^* \quad , \tag{2.2}$$

where * indicates adjoint (transpose in this real case). Also we see that if the input is only from the south, the same operators (permuted) apply. Thus, finally,

$$\begin{pmatrix} V_N \\ V_E \\ V_S \\ V_W \end{pmatrix} = \begin{pmatrix} T & S & R & S^* \\ S^* & T & S & R \\ R & S^* & T & S \\ S & R & S^* & T \end{pmatrix} \begin{pmatrix} U_N \\ U_E \\ U_S \\ U_W \end{pmatrix} . \tag{2.3}$$

The four-by-four matrix operator (recall the elements themselves are matrices) is the precise analogue of the transition matrix A of Sec. 1.1.

2.3 Addition

We now wish to adjoin two of the fundamental squares Σ. We do so as shown in Fig. 9. Using the continuity assumption introduced in Sec. 1.1 we see

$$\begin{aligned} V_{W1} &= U_{W2} \\ U_{E1} &= V_{E2} \end{aligned} \tag{2.4}$$

The R, T, S, S^* are the same for the individual squares Σ_1 and Σ_2. We now need to find the transition matrix $A_{\mathcal{R}}$ relating the input vector

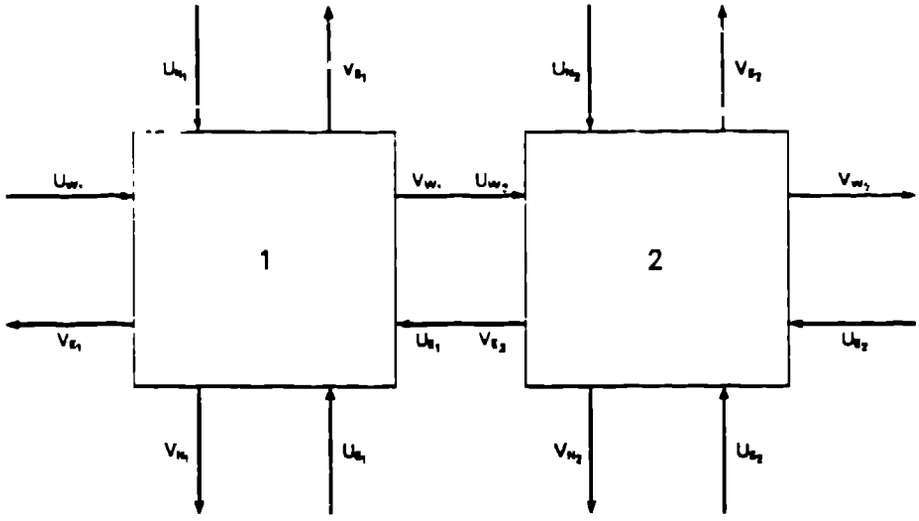


Figure 9. "Joining" two squares.

$$U = \begin{bmatrix} U_{N1} \\ U_{N2} \\ U_{E2} \\ U_{S2} \\ U_{S1} \\ U_{W1} \end{bmatrix} \tag{2.5}$$

to the output vector

$$V = \begin{bmatrix} V_{N1} \\ V_{N2} \\ V_{E2} \\ V_{S2} \\ V_{S1} \\ V_{W1} \end{bmatrix} . \tag{2.6}$$

Obviously, Eq. (2.3) yields four equations for each square, a total of eight. Two of these may be eliminated by use of (2.4). After a very considerable amount of algebra we find

$$V = A_{\mathcal{R}} U \ . \tag{2.7}$$

where

$$A_R = \left(\begin{array}{cc:cc:cc}
T + S(I - R^2)^{-1}RS & S(I - R^2)^{-1}S^* & S(I - R^2)^{-1}T & S(I - R^2)^{-1}S & R + S(I - R^2)^{-1}RS^* & S^* + S(I - R^2)^{-1}RT \\
S^*(I - R^2)^{-1}S & I + S^*(I - R^2)^{-1}RS^* & S + S^*(I - R^2)^{-1}RT & R + S^*(I - R^2)^{-1}RS & S^*(I - R^2)^{-1}S^* & S^*(I - R^2)^{-1}T \\
\hdashline
S^* + T(I - R^2)^{-1}RS & T(I - R^2)^{-1}S^* & T(I - R^2)^{-1}T & T(I - R^2)^{-1}S & S + T(I - R^2)^{-1}RS^* & R + T(I - R^2)^{-1}RT \\
\hdashline
S(I - R^2)^{-1}S & R + S(I - R^2)^{-1}RS^* & S^* + S(I - R^2)^{-1}RT & T + S(I - R^2)^{-1}RS & S(I - R^2)^{-1}S^* & S(I - R^2)^{-1}T \\
R + S^*(I - R^2)^{-1}RS & S^*(I - R^2)^{-1}S^* & S^*(I - R^2)^{-1}T & S^*(I - R^2)^{-1}S & T + S^*(I - R^2)^{-1}RS^* & S + S^*(I - R^2)^{-1}RT \\
\hdashline
T(I - R^2)^{-1}S & S + T(I - R^2)^{-1}RS^* & R + T(I - R^2)^{-1}RT & S^* + T(I - R^2)^{-1}RS & T(I - R^2)^{-1}S^* & T(I - R^2)^{-1}T
\end{array}\right) \tag{2.8}$$

Clearly, $A_{\mathcal{R}}$ is an analogue of $A(z_1 + z_2)$. Rewrite (2.8)

$$A_{\mathcal{R}} = \begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix} , \tag{2.9}$$

where the A_{ij} are the block matrices indicated by the dotted lines in (2.8). Also set

$$\begin{aligned} \vec{U}_N &= \begin{bmatrix} U_{N1} \\ U_{N2} \end{bmatrix} , \ \vec{U}_E = (U_{E2}) , \ \vec{U}_S = \begin{bmatrix} U_{S2} \\ U_{S1} \end{bmatrix} , \ \vec{U}_W = (U_{W1}) \\ \vec{V}_N &= \begin{bmatrix} V_{N1} \\ V_{N2} \end{bmatrix} , \ \vec{V}_E = (V_{E1}) , \ \vec{V}_S = \begin{bmatrix} V_{S2} \\ V_{S1} \end{bmatrix} , \ \vec{V}_W = (V_{W2}) . \end{aligned} \tag{2.10}$$

Equation (2.7) can be rewritten

$$A_{\mathcal{R}} \vec{U} = \vec{V} . \tag{2.11}$$

For example,

$$\vec{V}_N = A_{11}\vec{U}_N + A_{12}\vec{U}_E + A_{13}\vec{U}_S + A_{14}\vec{U}_W . \tag{2.12}$$

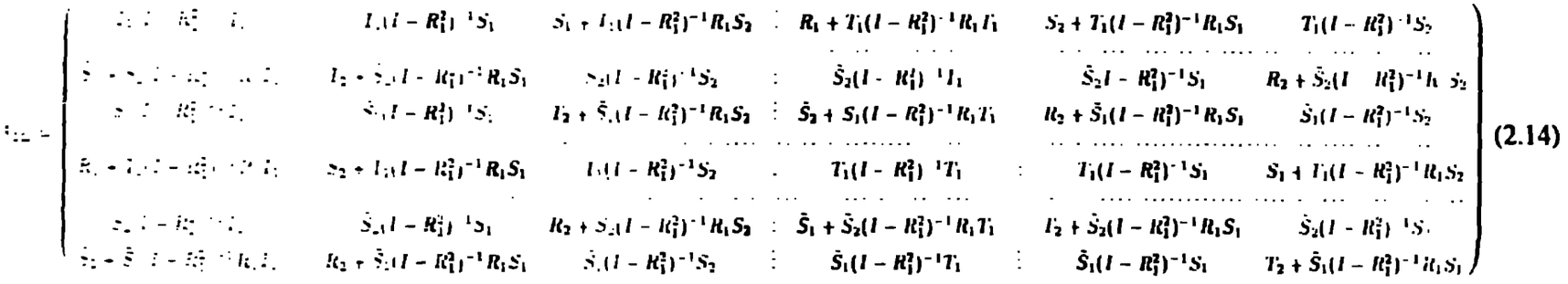
From this equation we see that A_{11} is a T-like matrix, A_{12} is S-like, A_{13} is R-like, and A_{14} is again S-like. Making this identification for the other A_{ij} and noting that some certain blocks in $A_{\mathcal{R}}$ occur more than once, we get

$$A_{\mathcal{R}} = \begin{bmatrix} T_1 & S_1 & R_1 & S_2 \\ \hat{S}_1 & T_2 & \hat{S}_2 & R_2 \\ R_1 & S_2 & T_1 & S_1 \\ \hat{S}_2 & R_2 & \hat{S}_1 & T_2 \end{bmatrix} . \tag{2.13}$$

We now have results for a rectangle $\mathcal{R}$. The operator can be repeated to obtain $A_{2\mathcal{R}}$, the transition matrix for a rectangle twice as long, but of the same width. Instead we wish to "build" a square 2Σ, the double of Σ.

2.4 Doubling

We double the original square element by juxtaposing two rectangles, as indicated in Fig. 10. The reasoning is straightforward but the algebra is messy. We simply write the final result.



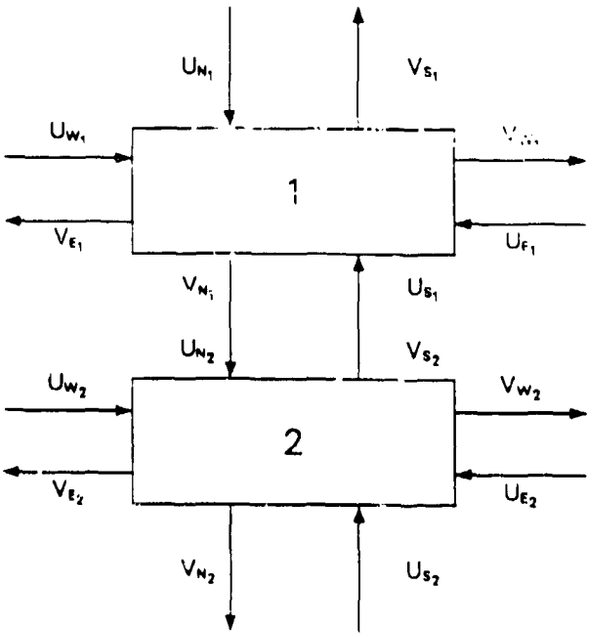


Figure 10. Joining two rectangles.

In Eq. (2.14)

$$A_{2\Sigma}\begin{bmatrix} U_{N1} \\ U_{E1} \\ U_{E2} \\ U_{S2} \\ U_{W1} \\ U_{W1} \end{bmatrix} = \begin{bmatrix} V_{W2} \\ V_{E1} \\ V_{E2} \\ V_{S1} \\ V_{W2} \\ V_{W1} \end{bmatrix}, \tag{2.15}$$

or again in block notation

$$A_{2\Sigma}\begin{bmatrix} \tilde{U}_N \\ \tilde{U}_E \\ \tilde{U}_S \\ \tilde{U}_W \end{bmatrix} = \begin{bmatrix} \tilde{V}_W \\ \tilde{V}_E \\ \tilde{V}_S \\ \tilde{V}_W \end{bmatrix}, \tag{2.16}$$

where the U's and V's with tildes take their meanings from (2.15) and are not the same as vectors defined by (2.10). The operator $A_{2\Sigma}$ may be written

$$A_{2\Sigma} = \begin{bmatrix} T_1 & S_1 & R_1 & S_2 \\ \hat{S}_1 & T_2 & \hat{S}_2 & R_2 \\ R_1 & S_2 & T_1 & S_1 \\ \hat{S}_2 & R_2 & \hat{S}_1 & T_2 \end{bmatrix} \tag{2.17}$$

The elements of $A_{2\Sigma}$ take their meanings from (2.14) and are not to be confused with those in (2.13).

We may now treat 2Σ as the fundamental square, and, by iterating, find $A_{2^n\Sigma}$. Clearly, the matrices (and the input and output vectors) increase in order at each step. We shall say more about this and its consequences shortly.

3 MORE ABOUT THE FUNDAMENTAL ELEMENT S

3.1 General Comments

In Sec. 2, we have observed that to start the doubling process, it is necessary to begin with a fundamental square Σ for which the transition matrix is completely known. It was implied that Σ would probably be "small." This is not really necessary if, by one device or another, we have all of the needed R, T, and S information. However, in Sec. 1, we observed that for the calculations made in [5], a thin slab initiated the process, and for it the single scattering approximation sufficed. This suggests the probable usefulness of a small Σ, but the approximation is much less obvious on simple physical grounds. In Sec. 3.2, we shall outline one way of getting started. It is by no means the only way.

3.2 Details for a "Small" Σ Calculation

We begin with a specific transport problem in mind. This will provide enough information so that generalizations are fairly obvious, albeit perhaps unpleasant. The fundamental square Σ, of side h, is oriented with respect to x and y axes as shown in Fig. 11. Scattering is supposed isotropic so that the classical transport equation is, assuming macroscopic cross section unity,

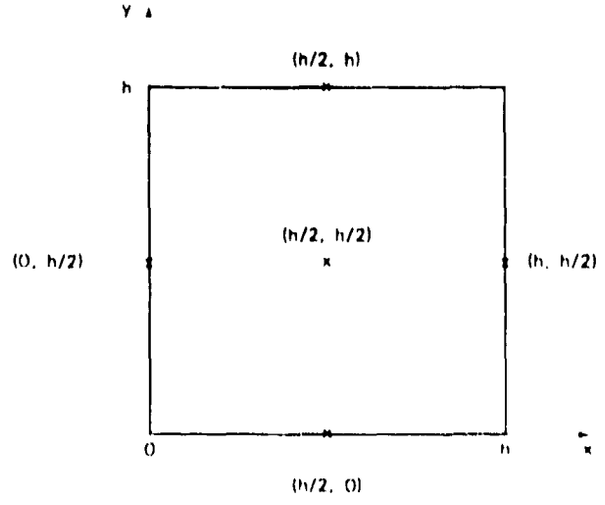


Figure 11 Stencil for difference scheme applied

$$\mu \frac{\partial \psi}{\partial x}(x,y,\mu,\eta) + \eta \frac{\partial \psi}{\partial y} + \psi(x,y,\mu,\eta) - \frac{c}{2}\int_{-1}^{1} \psi(x,y,\mu',\eta')d\mu' \ , \quad c = constant \ . \tag{3.1}$$

Here

$$\mu = \cos\theta \ , \quad \eta = \sin\theta \ , \tag{3.2}$$

where θ is the angle the particle direction makes with respect to the x-axis. In this example we discretize θ so that

$$\theta_j = (2(j-1)+1)\frac{\pi}{4} \ , \quad j = 1,2,3,4 \ .$$

(In the terminology of nuclear engineering, this is an S_2 approximation. See [8].)

Now we consider Σ as the fundamental cell in a finite difference scheme using a five-point stencil as indicated in Fig. 11. The discretized version of (3.1) becomes

$$\begin{aligned} \mu_j(\psi^j(h,\tfrac{h}{2}) - \psi^j(0,\tfrac{h}{2}) + \eta_j\psi^j(\tfrac{h}{2},h) \\ - \psi^j(\tfrac{h}{2},0)) + \psi^j(\tfrac{h}{2},\tfrac{h}{2}) \\ = \frac{c}{2}\sum_{k=1}^{4}\psi^k(\tfrac{h}{2},\tfrac{h}{2}) \ , \quad j = 1,2,3,4 \ ; \end{aligned} \tag{3.3}$$

the simplest quadrature formula approximates the integral in (3.1).

To determine the known quantities and the unknowns in (3.3), we examine Fig. 12. Clearly some of the ψ's are inputs (known) and some are outputs (unknowns). The function values $\psi^j(\frac{h}{2},\frac{h}{2})$ appear to be uncalculable. To overcome this we use a kind of central difference scheme often referred to by nuclear experts as the "diamond difference." Numerical analysts refer to it as the Crank-Nicholson method. We set

$$\psi^j(\tfrac{h}{2},\tfrac{h}{2}) = \frac{1}{2}(\psi^j(0,\tfrac{h}{2}) + \psi^j(h,\tfrac{h}{2})) \tag{3.4a}$$

and

$$\psi^j(\tfrac{h}{2},\tfrac{h}{2}) = \frac{1}{2}(\psi^j(\tfrac{h}{2},0) + \psi^j(\tfrac{h}{2},h)) \ . \tag{3.4b}$$

In the solution of the transport equation, this approximation is known to be of accuracy $O(h^2)$.

We may now write (3.3) in a somewhat different form. For specificity we select $\theta = \theta_1$. After some algebra we find, using the equations (3.4),

$$\frac{\sqrt{2}}{h}\left(\psi^1(h,\frac{h}{2})-\psi^1(0,\frac{h}{2})\right)$$

$$+\frac{1}{2}\left(\psi^1(\frac{h}{2},h)+\psi^1(0,\frac{h}{2})\right) \tag{3.5a}$$

$$=\frac{c}{4}\sum_{k=1}^{4}\left(\psi^K(0,\frac{h}{2})+\psi^k(\frac{h}{2},\frac{h}{2})\right)$$

and also

$$\frac{\sqrt{2}}{h}\left(\psi^1(h,\frac{h}{2})-\psi^1(\frac{h}{2},0)\right.$$

$$+\frac{1}{2}\left(\psi^1(h,\frac{h}{2})+\psi^1(0,\frac{h}{2})\right) \tag{3.5b}$$

$$=\frac{c}{4}\sum_{k=1}^{4}\left(\psi^k(0,\frac{h}{2})+\psi^k(h,\frac{h}{2})\right)\ .$$

Clearly, six further equations can be obtained by choosing $\theta = \theta_2,\theta_3,\theta_4$.

We have eight equations and sixteen ψ's. However, a glance at Figs. 12a and b reveal that eight of the ψ's are known inputs. It is convenient to write (3.5) and its analogues in the form

$$MS = NS\ , \tag{3.6}$$

where M and N are eight-by-eight matrices, and the u and v are input and output vectors, respectively. Specifically, we have

$$V = \begin{pmatrix} \psi^2(h,\frac{h}{2}) \\ \psi^1(\frac{h}{2},h) \\ \psi^1(h,\frac{h}{2}) \\ \psi^4(h,\frac{h}{2}) \\ \psi^4(\frac{h}{2},0) \\ \psi^3(\frac{h}{2},0) \\ \psi^3(0,\frac{h}{2}) \\ \psi^2(0,\frac{h}{2}) \end{pmatrix} \tag{3.7a}$$

$$U = \begin{pmatrix} \psi^2(\frac{h}{2},0) \\ \psi^1(\frac{h}{2},0) \\ \psi^1(0,\frac{h}{2}) \\ \psi^4(0,\frac{h}{2}) \\ \psi^4(\frac{h}{2},h) \\ \psi^3(\frac{h}{2},h) \\ \psi^3(h,\frac{h}{2}) \\ \psi^2(h,\frac{h}{2}) \end{pmatrix} . \tag{3.7b}$$

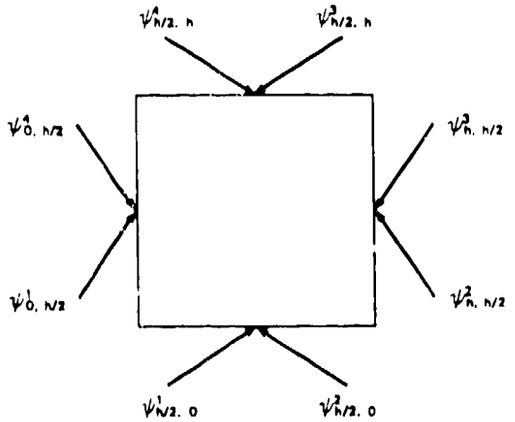


Figure 12a. Incident flux.

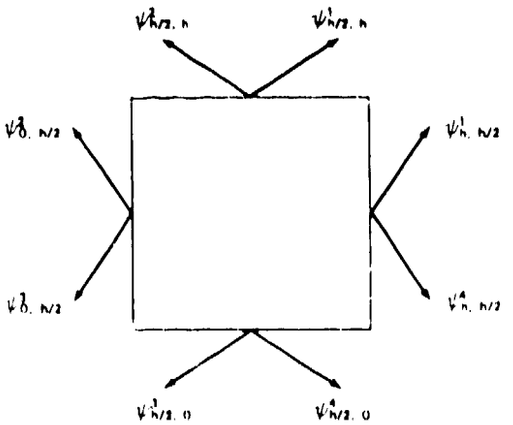


Figure 12b. Exit flux.

Also,

$$M = \frac{1}{h}\begin{bmatrix} \sqrt{2}\hat{I} & 0 & 0 & 0 \\ 0 & \sqrt{2}\hat{I} & 0 & 0 \\ 0 & 0 & \sqrt{2}\hat{I} & 0 \\ 0 & 0 & 0 & \sqrt{2}\hat{I} \end{bmatrix} + \begin{bmatrix} \beta & 0 & \gamma & 0 \\ 0 & \beta & 0 & \gamma \\ \gamma & 0 & \beta & 0 \\ 0 & \gamma & 0 & \beta \end{bmatrix}, \tag{3.8}$$

where the entries are two-by-two block matrices:

$$\hat{I} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{3.9a}$$

$$\beta = \frac{1}{2}\hat{I} + \gamma \tag{3.9b}$$

$$\gamma = -\frac{c}{4}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}. \tag{3.9c}$$

(The somewhat strange choice of the components of V has been made so that M is diagonally dominant for small h). Also

$$N = \begin{bmatrix} -\beta & \frac{\delta}{h} & -\gamma & \frac{\delta^*}{h} \\ \frac{\delta^*}{h} & -\beta & \delta & -\gamma \\ -\gamma & \frac{\delta^*}{h} & -\beta & \frac{\delta}{h} \\ \frac{\delta}{h} & -\gamma & \frac{\delta^*}{h} & -\beta \end{bmatrix}, \tag{3.10}$$

where

$$\delta = \begin{bmatrix} 0 & 0 \\ \sqrt{2} & 0 \end{bmatrix}. \tag{3.11}$$

To find V we must determine $M^{-1}N$. Write using (3.8)

$$hM = \sqrt{2}\,I + hP. \tag{3.12}$$

Thus

$$\frac{M^{-1}}{h} = \frac{1}{\sqrt{2}}\left(I + \frac{h}{\sqrt{2}}P\right)^{-1} = \frac{1}{\sqrt{2}}\left[I - \frac{h}{\sqrt{2}}P\right] + O(h^2). \tag{3.13}$$

(It suffices to retain only the term in h because the whole difference approximation is valid only to this order.) Now write (3.10) as

$$Nh = \begin{bmatrix} 0 & \delta & 0 & \delta^* \\ \delta^* & 0 & \delta & 0 \\ 0 & \delta^* & 0 & \delta \\ \delta & 0 & \delta^* & 0 \end{bmatrix} \tag{3.14}$$

$$+ hQ = \Delta + hQ \quad .$$

Thus

$$\begin{aligned} M^{-1}N &= \frac{1}{\sqrt{2}} \left(I - \frac{h}{\sqrt{2}} P\right) (\Delta + hQ) + 0(h^2) \\ &= \frac{\Delta}{\sqrt{2}} + h\left[\frac{Q}{\sqrt{2}} - \frac{P\Delta}{2}\right] + 0(h^2) \quad . \end{aligned} \tag{3.15}$$

The matrix $M^{-1}N$ is just the transition matrix A_Σ (see Sec. 2.2), and the entries are the blocks T, S, R, etc., properly arranged. Observe that if h is neglected, we get simply

$$M^{-1}N \simeq \frac{\Delta}{\sqrt{2}} \quad . \tag{3.16}$$

and the block in the (1,1) position is thus zero. A glance at Fig. 12 shows that indeed there can be no transmission to an opposite side without a collision, and (first) collisions are accounted for by the terms in h. Thus $M^{-1}N$ as given by (3.15) is the first collision approximation to the inverse of the transport operator (3.1).

Thus we have the analogue of what was done in [5]. Observe also that the (1,2) block is just δ and that it is an S block. Here no collision is needed for output.

Explicit expressions for the elements of $A_\Sigma = M^{-1}N$ can clearly be calculated. It does not seem worth while to list them here.

3.3 Some Computational Experiences

The approaches outlined in this section have been carried out in detail for the example described in the previous section as well as one for which particles were allowed to move in only the compass directions, N, E, S, W. Most of our discussion will be for the first case.

Most striking is the fact that even the initial square Σ involves vectors of length 8 and matrices containing 64 elements. On each doubling, the length of the former increases by a factor of 2, and of the size of the latter increases by a factor of 4. Computer memory restrictions are a clear threat. However, seven doublings were carried out on the CRAY-1 with no strain using only internal memory. The total time required was about 10 seconds. Interestingly enough, at each stage, most of the computer time was required for the last doubling. Hence, the sixth stage took about one second and the seventh took about nine seconds. The fundamental square Σ was chosen with $h = 10^{-2}$. (Recall the unit is a mean free path.) Thus the doublings brought the square to a bit over one and a quarter mean free

paths on a side. Direct comparison with other methods proved difficult, but results appeared reasonable.

An additional doubling was carried out in the N, E, S, W case in about the same amount of time. Observe that the first doubling in this case produces a system as large as that with which we start in the previous example.

In all instances standard matrix routines were employed. No efforts were made to optimize programs, and only the readily available machine memory was utilized.

4 REMARKS, SUMMARY, AND CONCLUSIONS–THE FUTURE

We have described in some detail how the conceptual program of Corones can be carried out in a particular 2-D geometry and have described some calculations to demonstrate that the approach is feasible. It may be argued, of course, that a square only one or two mean free paths on a side is not likely to be of great interest.

However, highly efficient programming, plus the use of auxiliary memory, could doubtless have allowed several more doublings without excessive expenditure of time. More important, the advent of the parallel processor probably changes the time and memory considerations greatly. The structure of the equations developed makes parallel processing seem ideal for invariant imbedding.

Assuming all this comes about, of what use might the method be? First, quite irregular regions can be approximated by unions of squares, even if the lengths of their sides are related by multiples of two. Once the basic transition matrices have been calculated and recorded, the joining problems are fairly straightforward.

At a simple level, consider three rectangles of different materials forming a sandwich. Suppose the middle rectangle can be made of any of several materials with the aim of constructing the most effective shield. This problem, even now, is virtually within grasp. Instead of computing each shield separately, one would only have to call up the appropriate A matrices and "join."

A geometry that is extremely difficult (or impossible) to handle with all standard computational transport methods except Monte Carlo is illustrated in Fig. 13. Obviously, the imbedding method could be employed quite easily.

What about 3-D? That, at present, does not look too promising. Simple operation counts suggest that invariant imbedding may not be competitive with classical numerical approaches. But that pessimistic view is based on devices similar to the one we have outlined (not on future computing machines). Further research is strongly suggested.

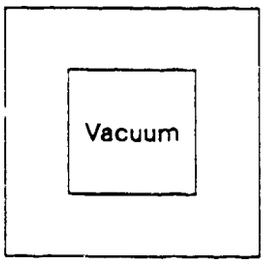


Figure 13. Medium with imbedded vacuum region.

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