Comments on "Investigation of Interface-Current Solution Techniques for Coupled Heterogeneous Cells"

I. INTRODUCTION

In the introduction to Ref. 1, Thomsen makes a statement about a technique that we contributed a few years ago.[2] Thomsen states that we could not conclude that the system matrix originating from the interface-current method can be symmetrized. Symmetrization is indeed possible, but Thomsen may have been misled by a few errors in some of our formulas. However, our paper is correct once these errors are corrected. Any reader interested in this interface-current symmetrization process may also refer to another presentation (with different notations but with the same results) at the Paris conference eight years ago.[3]

II. CORRIGENDUM FOR SEC. III

In Eq. (4a), we assumed that unknowns corresponding to zones with zero scattering cross sections and external faces with zero albedos (i.e., zero incoming currents) are eliminated. Because flux/current values for these unknowns can be reconstructed directly from the solution vectors $\boldsymbol{e}^K$, these are not independent unknowns of the interface-current system to be solved.

As for the second equation, which involves the boundary conditions, instead of producing multiple unrelated equations for each cell as in Eq. (4a), we will get a global coupling equation. The global feedback matrix $\mathbf{R}$ can be written as the product of a diagonal matrix $\mathbf{U}$ with a symmetric orthogonal matrix $\mathbf{P}$ used to couple the interface currents. The components of the diagonal matrix assigned to cell K are defined as

$$U^K_{i,j} = 4\pi V_i \Sigma^s_i \delta_{ij} \ ,$$

$$U^K_{L+\alpha,L+\beta} = \pi S_\alpha A_\alpha \delta_{\alpha\beta} \ ,$$

and

$$U^K_{L+\alpha,i} = U^K_{i,L+\alpha} = 0 \ ,$$

where A_α is the albedo if surface α is an external face and is equal to one if surface α is an interface.

We are now able to state the second set of interface-current equations for cell K as Eq. (4b) in Ref. 2. The problem of solving the transport equation inside domain D has therefore been reduced to the simultaneous resolution of the two sets of interface-current equations [Eqs. (4a) and (4b)], which we will now combine into a single symmetric linear equation. To do this, let us first invert the boundary condition matrix $\mathbf{R}$ as

$$(\mathbf{R}^{-1})^{KL} = \mathbf{T}^{KL} + \delta^{KL}(\mathbf{B}^K)^{-1} \ ,$$

where

$$\mathbf{T}^{KL} = (1 - \delta^{KL})\mathbf{P}^{KL}(\mathbf{U}^L)^{-1}$$

and

$$(\mathbf{B}^K)^{-1} = \mathbf{P}^{KK}(\mathbf{U}^K)^{-1} \ .$$

The global system may then be reduced to the form given by Eq. (5) in Ref. 2 where the global system matrix $\underline{\mathbf{M}} = \{\mathbf{M}^{KL}\}$ is defined as

$$\mathbf{M}^{KL} = \delta^{KL}\mathbf{D}^K + \mathbf{G}^K\mathbf{T}^{KL}(\mathbf{G}^L)^T$$

and the cell diagonal matrix is defined as

$$\mathbf{D}^K = \mathbf{G}^K(\mathbf{B}^K)^{-1}(\mathbf{G}^K)^T - \mathbf{Q}^K \ .$$

Note that the matrix $\underline{\mathbf{M}}$ is symmetric owing to the simple form of matrices $\mathbf{G}$ and $\mathbf{B}$.

The first error in our original paper comes from an inconsistent definition of the matrix $\mathbf{T}$, incorrectly declared as orthogonal because we forgot to include the geometric scaling factors. The second error is that the subtraction of the $\mathbf{Q}^K$ matrix was forgotten in the cell diagonal matrices $\mathbf{D}^K$.

III. A NUMERICAL EXAMPLE

A simple numerical example will now be presented to help in understanding the symmetrization process that is implicit in our solution algorithm. A two-cell assembly is constructed as indicated in Fig. 1, with the one-speed cross sections and fixed source indicated in Table I.

These data were first processed by the EURYDICE-2 option of DRAGON (Ref. 4) using the DP-0 option, and the following cellwise-dependent response matrices were obtained:

$$\mathbf{Q}^1 = \begin{bmatrix} 8.7400 & 2.1852 & 2.5425 & 2.5425 & 2.5425 & 2.5425 \\ 2.1852 & 1.8328 & 1.3588 & 1.3588 & 1.3588 & 1.3588 \\ 2.5425 & 1.3588 & 0.0 & 0.9034 & 0.8397 & 0.8397 \\ 2.5425 & 1.3588 & 0.9034 & 0.0 & 0.8397 & 0.8397 \\ 2.5425 & 1.3588 & 0.8397 & 0.8397 & 0.0 & 0.9034 \\ 2.5425 & 1.3588 & 0.8397 & 0.8397 & 0.9034 & 0.0 \end{bmatrix}$$

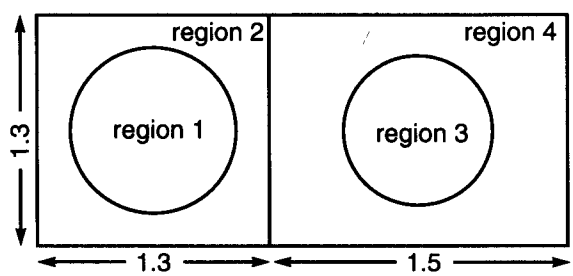

Fig. 1. Description of the two-cell assembly. The rod radii are equal to 0.6 and 0.5 cm in the square and rectangular cells, respectively. The neutrons are reflected isotropically around the assembly.

and

$$\mathbf{Q}^2 = \begin{bmatrix} 5.1067 & 3.0363 & 1.4290 & 1.4290 & 1.8013 & 1.8013 \\ 3.0363 & 6.3250 & 2.5231 & 2.5231 & 2.7639 & 2.7639 \\ 1.4290 & 2.5231 & 0.0 & 0.6807 & 0.8482 & 0.8482 \\ 1.4290 & 2.5231 & 0.6807 & 0.0 & 0.8482 & 0.8482 \\ 1.8013 & 2.7639 & 0.8482 & 0.8482 & 0.0 & 1.0518 \\ 1.8013 & 2.7639 & 0.8482 & 0.8482 & 1.0518 & 0.0 \end{bmatrix},$$

where the cell-dependent unknowns are the two fluxes followed by the X-oriented and Y-oriented interface currents, respectively.

The diagonal $\mathbf{G}^K$ and $(\mathbf{U}^K)^{-1}$ matrices are respectively given by

$$\mathbf{G}^1 = \text{diag}(14.2122\ 7.0249\ 4.0841\ 4.0841\ 4.0841\ 4.0841)$$

$$\mathbf{G}^2 = \text{diag}(9.8696\ 14.6348\ 4.0841\ 4.0841\ 4.7124\ 4.7124)$$

$$(\mathbf{U}^1)^{-1} = \text{diag}(0.2345\ 0.3559\ 0.2449\ 0.2449\ 0.2449\ 0.2449)$$

$$(\mathbf{U}^2)^{-1} = \text{diag}(0.3377\ 0.1708\ 0.2449\ 0.2449\ 0.2122\ 0.2122).$$

The global permutation matrix $\mathbf{P}$ corresponding to the volume and surface numbering is

$$\mathbf{P} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

The global system matrix $\underline{\mathbf{M}}$ is then obtained using Eq. (7):

$$\underline{\mathbf{M}} = \begin{bmatrix} 38.634 & -2.185 & -2.542 & -2.542 & -2.542 & -2.542 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -2.185 & 15.730 & -1.359 & -1.359 & -1.359 & -1.359 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -2.542 & -1.359 & 4.084 & -0.903 & -0.840 & -0.840 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -2.542 & -1.359 & -0.903 & 0.0 & -0.840 & -0.840 & 0.0 & 0.0 & 4.084 & 0.0 & 0.0 & 0.0 \\ -2.542 & -1.359 & -0.840 & -0.840 & 4.084 & -0.903 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ -2.542 & -1.359 & -0.840 & -0.840 & -0.903 & 4.084 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 27.792 & -3.036 & -1.429 & -1.429 & -1.801 & -1.801 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -3.036 & 30.262 & -2.523 & -2.523 & -2.764 & -2.764 \\ 0.0 & 0.0 & 0.0 & 4.084 & 0.0 & 0.0 & -1.429 & -2.523 & 0.0 & -0.681 & -0.848 & -0.848 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.429 & -2.523 & -0.681 & 4.084 & -0.848 & -0.848 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.801 & -2.764 & -0.848 & -0.848 & 4.712 & -1.052 \\ 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & 0.0 & -1.801 & -2.764 & -0.848 & -0.848 & -1.052 & 4.712 \end{bmatrix},$$

where we can observe the symmetry of this matrix.

TABLE I

Nuclear Data for the One-Speed Two-Cell Assembly

Region	Type of Material	Σ_t (cm^{-1})	Σ_t^s (cm^{-1})	Fixed Source ($s^{-1} \cdot cm^{-3}$)
1	Fuel	0.35	0.3	1.5
2	Water	0.45	0.4	0.0
3	Fuel	0.4	0.3	2.5
4	Water	0.45	0.4	0.0

The linear system is next solved using the following fixed source:

$$\tilde{\boldsymbol{e}} = \text{col}(1.5\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0\ \ 2.5\ \ 0\ \ 0\ \ 0\ \ 0\ \ 0).$$

And, the corresponding solution is obtained as $\boldsymbol{e} = (\underline{\mathbf{M}})^{-1}\mathbf{Q}\tilde{\boldsymbol{e}}$. The neutron fluxes are finally given by

$$\phi = \begin{bmatrix} e_1/\Sigma_1^s \\ e_2/\Sigma_2^s \\ e_7/\Sigma_3^s \\ e_8/\Sigma_4^s \end{bmatrix} = \begin{bmatrix} 5.072/0.3 \\ 6.633/0.4 \\ 4.964/0.3 \\ 6.462/0.4 \end{bmatrix} = \begin{bmatrix} 16.907 \\ 16.583 \\ 16.547 \\ 16.156 \end{bmatrix}.$$

As one can see, the interface-current symmetrization process is rather difficult to explain, and we apologize for these few errors that led Thomsen to conclude that symmetrization was impossible.

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Reply to "Comments on 'Investigation of Interface-Current Solution Techniques for Coupled Heterogeneous Cells' "

The corrigendum by Roy, Hébert, and Marleau[1] has been of great help in understanding their transformations of the multicell system equations. While retaining Eqs. (4) and (5) of the original paper,[2] Roy, Hébert, and Marleau replace all the associated, unnumbered equations (except the G terms) by the new ones. I shall not hesitate any further to recognize the symmetrization of the system matrix and the subsequent application of the alternate direction implicit (ADI) procedure, which seems to overcome the problem that the symmetric matrix is not positive definite.

Having grasped the basic idea, however, Roy, Hébert, and Marleau's formulation seems unnecessarily complicated. Furthermore, the same principles can be applied to the multiple-flight probability, interface-current equations in which the fluxes are eliminated. I do not share Roy, Hébert, and Marleau's concerns about this reduction (based on some "computational discrepancies" that they seem to have had earlier[2]). On the contrary, I found that the reduction works well, and in my view, it is preferable to iterate on the smaller system of currents only. Hence, it is interesting to discuss the symmetrization of the latter system in some detail.

Substituting the current densities $J_n^{\pm} = j_n^{\pm}/A_n$ into the cell equations [Eq. (9) of my paper[3]], we have

$$A_n J_n^{+} = c_n + \sum_l p_{nl} A_l J_l^{-},$$

where it may be recalled that c_n is the outgoing current due to sources [Eq. (22)] and that symmetry is ensured by the reciprocity relation for multiple-flight transmission probabilities $p_{nl}A_l = p_{ln}A_n$.

The corresponding system equation in matrix notation is expressed as

$$\mathbf{A}\mathbf{J}^{+} = \mathbf{C} + \mathbf{P}\mathbf{A}\mathbf{J}^{-} ,$$

where $\mathbf{A}$ is a diagonal matrix and $\mathbf{P}$ is a block-diagonal matrix, assuming cellwise organization of the current vectors.

The coupling equation is

$$\mathbf{J}^{+} = \mathbf{T}\mathbf{J}^{-} ,$$

where the nonzero entries of the symmetric connectivity matrix $\mathbf{T}$ are 1 for interfaces and α_b^{-1} for boundaries (diagonal or off-diagonal for reflective or cyclic boundary conditions, respectively).

Now, eliminating $\mathbf{J}^{+}$ and dropping the superscript on $\mathbf{J}^{-}$, we obtain after some reorganization

$$(\mathbf{T} - \mathbf{P})\mathbf{A}\mathbf{J} = \mathbf{C} .$$

Since any pair of symmetric entries in $\mathbf{T}$ corresponds to the two sides of an interface (or corresponding boundaries in the cyclic case) having the same area, the system matrix is seen to be symmetric. Based on the conservation equation [Eq. (15)], the column sums of the system can be seen to be nonnegative. However, the system matrix is not diagonally dominant, which is a prerequisite for using point successive overrelaxation.

Apparently, the lack of diagonal dominance is not important when using the ADI procedure, which gave good convergence as described by Roy, Hébert, and Marleau in Sec. IV of their paper.[2] Hence, it seems fair to assume that this also holds for the reduced system considered here.

Assume that we renumber the currents, starting with all the currents parallel to the X axis, taken cell by cell and line by line, followed in the same way by the currents along the other coordinate direction(s). Here, we further limit our discussion to the case with reflective boundary conditions. Then, the diagonal blocks containing all the nonzero entries of $\mathbf{T}$ will become tridiagonal. In the ADI iterations, all the off-diagonal blocks are moved to the right side of the equation, where we use the most recent currents. This matrix splitting allows a simple iteration calculation based on the forward elimination and backward substitution method.

The question is whether this special ADI method with overrelaxation (reminiscent of successive line overrelaxation) can be made more efficient than the point iterative method I described in my paper. Considering the increased number of operations per ADI iteration, this requires an improved convergence rate. The answer to this question is not obvious. For the time being, however, I am quite satisfied with the performance of my old method, so I shall leave the question open to other investigators.

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