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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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June 13, 1995

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