Letters to the Editor

Comments on Variation Flux Synthesis Methods for Multigroup Diffusion Theory

Stacey[1] has made some erroneous remarks concerning my work on Lagrange multiplier functionals. The remark that the Lagrange multiplier functional does not remove the overdetermination difficulty is false, as I shall show. Moreover, he states that the second order Lagrange multiplier functional is equivalent to the functional which he calls $F_{12} = F_1 + F_2$. The two principles are *not* equivalent from the viewpoint of generating variational approximations to the neutron diffusion equation.

For the convenience of the reader, I shall review briefly some of the work given in the report[2] on the application of the Lagrange multiplier principles to axial synthesis. There is a summary of this work in Ref. 3. Moreover, the Lagrange multiplier functionals are discussed in Ref. 4, and applied there to the problem of interface conditions for few group equations with flux-adjoint weighted constants. The functionals discussed in Ref. 4 are for the continuous energy $P-1$ equations instead of the few-group diffusion equations but the differences are minor. Both first and second order Lagrange multiplier functionals are presented in Ref. 4.

Consider the functional

$$F(u,u^*,\alpha,\beta) = F_v(u,u^*) + F_s(u,u^*,\alpha,\beta) \quad , \tag{1}$$

where

$$F_v(u,u^*) = \sum_k \int_{R_k} \{\nabla u^{*T} \cdot D\,\nabla u + u^{*T}(A - \lambda^{-1}M)u\}\, d\boldsymbol{r} \tag{2}$$

and

$$F_s = \int_S \{\alpha^T(\boldsymbol{r})[u(+)-u(-)] + [u^*(+)-u^*(-)]^T \beta(\boldsymbol{r})\}\, dS \quad . \tag{3}$$

Here D, A, and M are $G \times G$ matrices and u, u^*, α, and β are $G \times 1$ column matrices. (Note that Stacey incorrectly wrote the Lagrange multipliers α and β as vectors in x, y, and z space). Here u and u^* are continuous within every R_k and vanish on the outer boundary of the reactor; S represents the totality of all interfaces across which u or u^* is discontinuous. When F is made stationary with respect to independent variation of *all* its argument functions u, u^*, α, and β, one obtains as Euler equations

$$-\nabla \cdot D\,\nabla u + (A - \lambda^{-1}M)\,u = 0 \text{ in every } R_k \quad , \tag{4}$$

and on S

$$u(+) - u(-) = 0 \tag{5}$$

$$D\,\nabla u(-) \cdot \boldsymbol{N} - \beta = 0 \quad , \qquad D\,\nabla u(+) \cdot \boldsymbol{N} - \beta = 0 \tag{6}$$

as well as analogous conditions on u^* and α which may be obtained from Eqs. (4), (5), and (6) by replacing D, A, and M by their adjoints D^*, A^*, M^*, and by replacing u and β by u^* and α. [Strictly speaking, Eq. (4) holds only within every subregion of R_k in which ∇u, ∇u^*, and D are continuous, and the usual current continuity conditions hold across any interface internal to R_k, since u and u^* are continuous within each R_k].

To use the functional F to obtain an approximate solution to the neutron diffusion equation for, say, the problem of axial synthesis, a family of trial functions is assumed for all the argument functions of the functional, including the Lagrange multipliers. As in Ref. 2, let us consider a reactor with k_0 axial zones, with the k'th axial zone lying between z_{k-1} and z_k. In the k'th axial zone choose trial functions for u and u^* as

$$u = \sum_{i=1}^{n(k)} f_i(z)\, g_i(x,y;k) \quad \text{and} \quad u^* = \sum_{i=1}^{n(k)} f_i^*(z)\, g_i^*(x,y;k) \quad . \tag{7}$$

On the interface $z = z_k$, choose trial functions for α and β given by

$$\alpha(x,y;z_k) = \sum_{i=1}^{m(k)} a_i(z_k)\, h_i^*(x,y;z_k)$$

$$\beta(x,y;z_k) = \sum_{i=1}^{m(k)} b_i(z_k)\, h_i(x,y;z_k) \quad . \tag{8}$$

Here k ranges over all interfaces, $k = 1, 2, \ldots k_0 - 1$. The g_i, g_i^*, h_i^*, and h_i are known column matrices and the functions $f_i(z)$, $f_i^*(z)$, and the constants $a_i(z_k)$, $b_i(z_k)$ are to be found by the variational method. The notation in which the trial functions for u and u^* is expressed is somewhat different from that of Stacey's. The expansion modes g_i and g_i^* are column vectors, and the functions $f_i(z)$ and $f_i^*(z)$ are scalars. The expansion modes Stacey uses are $G \times G$ diagonal matrices, and the coefficients of the expansion modes are column vectors. However, every trial function of Stacey's form can be written in the form of Eq. (7) by choosing for the g_i and g_i^* column vectors with only one nonzero element, the position of the nonzero element being in the g'th place, if g_i and g_i^* correspond to trial functions for the g'th group. In addition, Eqs. (7) can be used for group collapsed synthesis by appropriate choice of g_i and g_i^*.

Note that the trial functions of Eqs. (7) do *not* assume the same number of modes in each axial zone, although Stacey does not mention that this extension was made in Ref. 2. As is discussed in Ref. 2, the number of modes $m(k)$ in which the Lagrange multipliers for the surface $z = z_k$ are expanded must bear a certain relationship to the number of modes $n(k)$ and $n(k+1)$ in which the fluxes are expanded on either side of the interface, if the results are

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[1] WESTON M. STACEY, Jr., *Nucl. Sci. Eng.*, **47**, 449 (1972).

[2] A. J. BUSLIK, "A Variational Principle for the Neutron Diffusion Equation using Discontinuous Trial Functions," WAPD-TM-610, Bettis Atomic Power Laboratory (1966).

[3] A. J. BUSLIK, *Trans. Am. Nucl. Soc.*, **9**, 199 (1966).

[4] A. J. BUSLIK, *Nucl. Sci. Eng.*, **32**, 233 (1968).

to be physically reasonable. However, as will be seen, no overdetermination problems arise. The number of modes $m(k)$ which seem most reasonable is somewhere about midway between $n(k)$ and $n(k+1)$.

When the trial functions Eqs. (7) and (8) are substituted into the functional and the resulting reduced functional made stationary with respect to independent and arbitrary variations of $f_i(z)$, $f_i^*(z)$, $a_i(z_k)$, and $b_i(z_k)$, then the following Euler equations for the reduced functional are obtained. We have, in the k'th axial zone,

$$\int g_j^{*T}(x,y;k)\left[-\nabla\cdot\nabla D+(A-\lambda^{-1}M)\right]u\,dxdy=0\ ,\qquad j=1,2,\dots n(k)\ . \tag{9}$$

On the interface $z=z_k$ we have

$$\int h_i^{*T}(x,y;z_k)\left[u(z_k+\epsilon)-u(z_k-\epsilon)\right]dxdy=0\qquad i=1,2,\dots m(k)\ , \tag{10}$$

as well as

$$\int g_j^{*T}(x,y;k+1)\left[D(x,y,z_k+\epsilon)\left(\frac{\partial u}{\partial z}\right)_{z_k+\epsilon}-\beta\right]dxdy=0\qquad j=1,2,\dots n(k+1) \tag{11}$$

and

$$\int g_j^{*T}(x,y;k)\left[D(x,y,z_k-\epsilon)\left(\frac{\partial u}{\partial z}\right)_{z_k-\epsilon}-\beta\right]dxdy=0\ ,\qquad j=1,2,\dots n(k)\ . \tag{12}$$

In these equations, u and β are to be interpreted as the trial function expansions given by Eqs. (7) and (8). The analogous Euler equations determining the adjoint flux u^* and α will not be written. In addition, we have that the $n(1)$ functions $f_i(0)$ vanish at the bottom of the core $z=0$, and that the $n(k_0)$ functions $f_i(h)$ vanish at the top of the core $z=h$, since the admissible trial functions must vanish on the outer boundary of the reactor.

Stacey states that in synthesis applications of the Lagrange multiplier principle the interface overdetermination problem is avoided by choosing one of Eqs. (6) (of this letter) to guide the selection of trial functions for β. This is quite simply false. Regardless of whether or not the $h_i(x,y;z_k)$ are chosen so that one of Eqs. (6) is satisfied, one does not have an overdetermination problem. Associated with each interface there are $m(k)+n(k+1)+n(k)$ conditions, and in addition one has $n(1)$ conditions at the bottom of the core and $n(k_0)$ conditions at the top of the core resulting from the requirement that u vanish at $z=0$ and $z=h$. Thus we have

$$\sum_{k=1}^{k_0-1}\left[m(k)+n(k+1)+n(k)\right]+n(1)+n(k_0)$$

conditions. The number of arbitrary constants in the general solution of the differential equations in the k'th axial zone is $2n(k)$, and the unknown parameters $b_i(z_k)$ in the trial function for β are $m(k)$ in number at the k'th interface. Thus the number of unknown constants is equal to

$$\sum_{k=1}^{k_0}2n(k)+\sum_{k=1}^{k_0-1}m(k)\ ,$$

and this is just equal to the number of conditions on the unknown constants. Thus there is no overdetermination problem, contrary to what Stacey says.

Stacey states, in the construction of his table of extended variational principles, that he has reduced the Lagrange multiplier functional to an equivalent one by introducing the "requirements on the Lagrange multipliers" into the functional. It is *important* to realize that the so-called equivalent functional and the original Lagrange multiplier functional are not equivalent from the viewpoint of generating approximations. The reason for this is that the so-called "requirements" on the Lagrange multipliers, which requirements are Eqs. (6) of this letter (and the analogous equation relating α to u^*), are not restrictions on the class of admissible functions but are relationships satisfied by u, β, u^*, and α at the stationary point of the functional. This means that in selecting trial functions for α and β we need not satisfy Eqs. (6) (and their counterpart for α), but that by use of the variational method these equations will be approximately satisfied in just the same way as the neutron diffusion equation; Eq. (4), which is another Euler equation of the functional, will be satisfied approximately. In fact, we see that Eqs. (6) are not satisfied exactly by our solution but only approximately, in the weighted residual sense, as is shown by Eqs. (11) and (12). It is precisely this freedom to choose trial functions for β which do not satisfy Eqs. (6) exactly which permits the generation of new approximations by the Lagrange multiplier functional. These approximations cannot be derived from the functional which is obtained from the Lagrange multiplier functional by elimination of the Lagrange multipliers. An analogous situation occurs with the first order (Selengut-Wachspress) functionals. (These are the J-type functionals of Stacey's article as opposed to the second order F-type functionals.) If trial functions for a first order F-type functional are chosen so that the Euler equations $\boldsymbol{j}=-D\nabla\phi$ and $\boldsymbol{j}^*=-D^*\nabla\phi^*$ are satisfied exactly, then the results are entirely equivalent to the use of a second order type functional. Under these circumstances, the use of the same class of trial functions for ϕ in both functionals will yield the same reduced functional. In those cases where the F-type functional yields approximations not obtainable from the J-type functional the equations $\boldsymbol{j}=-D\nabla\phi$ and $\boldsymbol{j}^*=-D^*\nabla\phi^*$ are not satisfied exactly by the trial functions. An example of this is the "staggered interface" method of avoiding the overdetermination problem.

Later on in the article Stacey states that the Lagrange multiplier principle is equivalent to the principle $F_{12}=F_1+F_2$ because β is equal to a linear combination of $D\nabla\phi(+)\cdot\boldsymbol{N}$ and $D\nabla\phi(-)\cdot\boldsymbol{N}$. From what has been said earlier it should be clear why this relationship does not prove equivalence. The relationship Stacey writes is satisfied only at the stationary point of the functional and not at an arbitrary point within the domain of admissible functions. The relationship need not be satisfied exactly by trial functions for β and u.

I have therefore shown that there is no overdetermination problem with the Lagrange multiplier functional in the problem of axial synthesis, and have also shown that the Lagrange multiplier functional can yield results different from the functional F_{12} of Stacey, so that it is not equivalent to F_{12} from the viewpoint of generating approximations.

Another point which I should like to mention is that Stacey stated that I introduced a second order functional that admitted discontinuous trial functions and "Lambropolous and Luco subsequently provided mathematical proof that second-order variational principles could be constructed which admit spatially discontinuous trial functions." I had already proved that the Lagrange multiplier functional which I constructed admitted spatially discontinuous trial functions. I had shown that the functional I presented had the correct stationary point, and that the flux continuity condition was one of its Euler equations. I did this both in Ref. 2 and Ref. 4. As related to my work, the

Lambropolous and Luco contribution was merely to show that the volume term of the functional, which I wrote as a sum of integrals over disjoint regions R_k, could be written as an integral over the volume of the reactor if the integral is interpreted as a Riemann integral. For then the discontinuities do not contribute to the integral.

Let me now pass on to consider briefly the alternative method of removing the overdetermination problem suggested by Stacey. This involves the use of arbitrary diagonal matrices $\omega_{n'}(x,y)$ as weight functions on the $\delta\rho^*_{n+} = \delta\rho^*_{n-}$ condition (discussed on p. 456 ff of Stacey's article). In the case where the same number of flux and current expansion modes are used in each axial zone this method seems workable enough. However, it suffers from the defect that one does not have any guidelines on how to best choose these weight functions $\omega_{n'}(x,y)$. In the Lagrange multiplier method one knows that one should choose the modes in which β and α are expanded in such a way that they approximate the component normal to the interface of the current and adjoint current. If one is interested in obtaining accurate values of the functional, or in an eigenvalue problem an accurate value of the eigenvalue, this seems to be an important consideration. The remarks Kaplan[5] makes seem pertinent here.

There is, I believe, a more serious objection to Stacey's method when different number of flux and current expansion functions are used in adjacent axial regions. He then states that the same number N^* of adjoint flux and current expansion functions must be used in both regions, and that this number must equal the number of direct expansion functions in one of the regions. If, for concreteness, we assume $N^* = N_+$, then $N^* \neq N_-$. But the number of first order differential equations in each zone is, in a one group problem, just given by $4N^*$. These equations are Eqs. (11) through (14) of Stacey's article. [Actually, Eqs. (11) and (14) are differential equations; Eqs. (12) and (13) are algebraic equations.] The index n' in these equations runs over the adjoint functions, and hence it is easy to verify that there are $4N^*$ of these equations. The unknown flux and current variables in these equations are $4N$ in number. This means that one has $4N^*$ equations in the $4N$ flux and current variables in the zone on the minus side of the interface. If $N^* < N_-$, then one has more unknown functions in this zone than one has equations, and the solution of the problem is underdetermined. If $N^* > N_-$, an overdetermination problem occurs with more equations than unknown functions of z, and there is no solution possible.

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[5]S. KAPLAN, *Trans. Am. Nucl. Soc.*, **6**, 3 (1963).

Reply to "Comments on Variation Flux Synthesis Methods for Multigroup Diffusion Theory"

Buslik's comments[1] reflect more a difference in viewpoint than any difference in substance, and to some extent indicate a misinterpretation of my paper.[2] My basic position is that the Lagrange multipliers can equally well be written as currents evaluated at the interface [i.e., Eqs. (5a) or (5b) and (6a) or (6b) of my paper], in which case the Lagrange multiplier functional is identical to the more transparent functional represented by F_2, providing $\gamma, \Omega = 0, 1$ in the latter, in that either functional contains some one scalar function weighting the difference in flux at the interface. Just as the Lagrange multiplier function α may be expanded in trial functions which are independent of the flux trial functions in the volumes, so may the terms $D_+\nabla\phi^*_+$ be expanded (i.e., there is no constraint that the expansion functions for interface terms be related to expansion functions for volume terms in the synthesis application). His remarks indicate that Buslik has incorrectly read such a constraint into my paper.

Using the Lagrange multipliers, one comes upon the overdetermination problem in a different guise. There is no formal overdetermination in the derivation. However, when one looks to the Euler equations for guidance in selecting expansion functions, one is confronted with both Eq. (5a) and (5b) of my paper, and one must choose either one, some combination of the two, or neither. Using the functional F_2 one comes formally upon the overdetermination problem if the functional is required to be stationary for arbitrary independent variations of, for example, $D_+\nabla\phi_+$ and $D_-\nabla\phi_-$. Setting $\gamma = 0, 1$ formally eliminates the overdetermination, but leaves one with the choice $\gamma = 0$ or $\gamma = 1$. This choice influences the guidance in selecting expansion functions. Thus, one is faced with basically the same problem in both cases, and the same range of options is open for its resolution in each instance.

While I believe that most of Buslik's comments follow from the incorrect constraint assumption mentioned above, there are three points which I should like to respond to directly.

His Lagrange multipliers are scalars in his surface integrals [Eq. (3) of his letter], and he subsequently shows in his Eq. (6) that these scalars are identifiable with the normal components of the current at the surface. He commented that I incorrectly wrote the Lagrange multipliers as vectors. I wrote the Lagrange multipliers as the scalar product of the unit vector normal to the surface $\hat{n}$ and vector quantities $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$. This scalar product is used in my Eq. (14), which is identical to his Eq. (3); i.e., his α is my $\hat{n} \cdot \boldsymbol{\alpha}$, etc. Thus, his comment, appearing just after Eq. (3) in his letter, is incorrect.

Buslik also objects to the alternative method of removing the interface overdetermination which I suggested. He raises two points. First, he states that my method suffers from the fact that the weight functions $\omega_n(x,y)$ are arbitrary, which they are. At this point he argues, "In the Lagrange multiplier method one knows that one should choose the modes in which β and α are expanded in such a way that they approximate the component normal to the interface of the current and adjoint current. If one is interested in obtaining accurate values of the functional, or in an eigenvalue problem an accurate value of the eigenvalue, this seems to be an important consideration." Earlier in his letter, in striving to make another point, he seems to argue the opposite: "Stacey states that in synthesis applications of the Lagrange multiplier principle the interface overdetermination problem is avoided by choosing one of Eqs. (6) (of his Letter) to guide the selection of trial functions for β. This is quite simply false." He cannot have it both ways. Relative to his comment on the arbitrariness of my ω_n, I would like to point out that all weighting and expansion functions are arbitrary, in all synthesis

[1]A. BUSLIK, *Nucl. Sci. Eng.*, **49**, 112 (1972).
[2]W. M. STACEY, Jr., *Nucl. Sci. Eng.*, **47**, 449 (1972).