Letters to the Editor

Comments on "Finite-Element Methods for Reactor Analysis"

Recently, Kang and Hansen[1] applied the finite-element technique to the numerical solution of the space-, energy-, and time-dependent neutron diffusion equations. Regarding that excellent paper, several comments seem to be in order:

1. In Part I, the authors present several theorems which bound the approximation error, and they choose to use the $L\infty$ norm for the distance function because "the $L\infty$ norm is equal to or larger than any other L_p norm" and thus their "error results certainly apply in the L_2 norm also." The final result of this choice is their Theorem 7, which is supposed to provide "a rigorous error bound for approximations of various orders." For two- and three-dimensional spatial approximations, I believe that this theorem is not correct in its present form, and I claim moreover that it has not been demonstrated at all.

The Sobolev imbedding theorem[2] from $W^1(\Omega)$ into $C^0(\Omega)$ is actually valid only in the one-dimensional case where all members of $W^1(\Omega)$ are also members of $C^0(\Omega)$ and where one has:

$$||u||_{L\infty} \leq C\ ||u||_{w1}\ ,\ \forall u \in W^1(\Omega) \quad . \tag{1}$$

In two and three dimensions, this is no longer the case and some members of $W^1(\Omega)$ are not continuous [for example, $\log \log (1/r)$ (Ref. 3)]. Since the Galerkin procedure takes place in $W_0^1(\Omega) \subseteq W^1(\Omega)$, error bounds are most naturally derived in the "energy" norm $a(u,u)^{1/2}$ or in the usually equivalent Sobolev norm $||u||_{w1}$. Since we always have

$$||u||_{L2} \leq C\ ||u||_{w1}\ ,\quad \forall u \in W^1(\Omega) \quad , \tag{2}$$

these error bounds directly induce approximation errors in the L_2 norm. The latter are not sharp because the square of a gradient appears in either the energy norm or in the Sobolev norm. They can be sharpened in the absence of singularities (i.e., the exponent of $\overline{\Delta r}$ increased by one) using, for instance, a technique originally developed by Nitsche.[4] Since Eq. (1) fails to apply in multidimensional geometries, one usually cannot obtain error bounds in the $L\infty$ norm, unless stronger smoothness assumptions are made for the flux. These assumptions would be quite unrealistic for the reactor case.

Although I do not have the details of the proof at hand, I believe that the results of Descloux[5] used to "demonstrate" Theorem 7 have been misinterpreted at least twice. In the space-dependent case, B, as defined on p. 471 of Ref. 1, becomes a generalized "stiffness" matrix whose terms are explicitly listed on p. 472. Theorem 3 of Ref. 5 actually bounds the inverse of such matrices in norm $L\infty$, but, first, a coerciveness relation should be satisfied. This is true in the 1-D case (using precisely the Sobolev imbedding theorem mentioned above) but not in the 2-D and 3-D cases. This was pointed out by Descloux[5] in his Remark 2. Even if this restriction could be relaxed, as conjectured by Descloux in a more recent work[6], and if his theorem could be applied here, the exponent of $\overline{\Delta r}$ in Theorem 7 should be defined as $\min(2m_r - 1, t_r)$ and not as $\min(2m_r, t_r)$; this comes from the fact that in Descloux's Theorem 3 the bound invoked by Kang and Hansen actually depends on $\overline{\Delta r}$ and in this case would be proportional to $\overline{\Delta r}^{-1}$. This is clearly shown in the example proposed in the third paragraph in Descloux's paper, with the same normalization for the basis functions as in Kang and Hansen's work.

Finally, even if the bounds claimed by Kang and Hansen in 2-D and 3-D cases could be proven, which I doubt, I cannot help questioning the usefulness of a theorem that in any realistic multidimensional calculation (i.e., one that involves more than one material zone) would not prove the convergence of the finite element approximation when the mesh is successively refined. Actually, t_r (and consequently μ_r) would always reduce to zero for such a calculation because the solution is only continuous and does not admit a piecewise continuous derivative in the presence of singularities.[7] Although it is true, as the authors remark on p. 469, that their "approximate solutions will converge to the exact solution, including the singular behavior," it cannot in any case be presented as a consequence of the "rigorous error bounds" that the authors claim to obtain for the finite element solution. Actually, the multigroup flux has square-summable first derivatives, and convergence can be proven in the energy, Sobolev, or L_2 norm. These derivatives should be the only ones used for 2-D and 3-D calculations such as those of Ref. 8 (and, in particular, in a similar theorem that I also stated erroneously two years ago in the $L\infty$ norm[9]). In one-dimensional cases, bounds can be derived in the $L\infty$ norm

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[1] C. M. KANG and K. F. HANSEN, *Nucl. Sci. Eng.*, **51**, 456 (1973).

[2] K. YOSIDA, *Functional Analysis*, Springer Verlag, Berlin (1968).

[3] G. STRANG, *Numer. Math.*, **19**, 81 (1972).

[4] J. NITSCHE, *Numer. Math.*, **11**, 346 (1968).

[5] J. DESCLOUX, *SIAM J. Numer. Anal.*, **9**, 260 (1972).

[6] J. DESCLOUX, *Proc. Equadiff III*, Brno (1972).

[7] I. BABUŠKA and R. B. KELLOGG, in *Numerical Reactor Calculations*, International Atomic Energy Agency, Vienna (1972).

[8] J. P. HENNART, in *Proc. Conf. Mathematical Models and Computational Techniques for Analysis of Nuclear Systems*, CONF-730414, Part II, Paper VII-67-93, U.S. Atomic Energy Commission (1974).

[9] J. P. HENNART, A. JAUCOT, and V. RENDA, in *Numerical Reactor Calculations*, International Atomic Energy Agency, Vienna (1972).

using Eq. (1) and sharpened, without the help of Descloux's work, but rather by techniques like those developed by Perrin et al.[10] and used, for instance, in Ref. 11.

Kang and Hansen claim, of course, that their results confirm their theoretical analysis, but I could find nowhere in Part II of their work a numerical example where the approximation error on the flux was analyzed in the L_∞ norm (not even for the safe 1-D cases). Most of the results presented are in terms of the fundamental eigenvalue, which is essentially an integral parameter and for which, in 2-D and 3-D, the error analysis should be performed, for the same reasons as above, entirely in the L_2 or W^1 norm, along the lines proposed at the end of Sec. III. B. 2. In this case, the authors would not have to conjecture, as they do, an extension of Theorem 7 to bound something that is practically always unbounded in the norm they have chosen, as pointed out in my next comment.

2. In Part II, several choices of bivariate cubic basis functions are considered. Set A, in particular, for which $\partial\phi/\partial x$ and $\partial\phi/\partial y$ are required to be zero at singular points, is presented as the "only simple way to satisfy the interface condition" at such points. This choice, which incidentally provides a poorly convergent approximation, is in complete contradiction to what should be well known from the works initiated by Babuška and Kellogg more than two years ago (see, for example, Ref. 7): Namely, that $\partial\phi/\partial x$ and $\partial\phi/\partial y$ are actually infinite (and not zero) at singular points and that the behavior of ϕ is in r^α around these points with α comprised between 0 and 1. This points out once more that the use of Hermite-type elements long favored by numerical analysts is not necessarily the best choice for reactor problems that, unlike the smooth test problems usually studied by the same numerical analysts, exhibit characteristically piecewise constant material properties. Actually, at the singularities, some of the parameters used in conjunction with Hermite elements completely lose their pointwise significance, and it could be more interesting for reactors with a fine structure, such as the pressurized water and boiling water reactors, to use Lagrange-type elements with static condensation techniques[12] to minimize the size of the algebraic systems to be solved.

3. In Table XV, the authors mention the possibility of using piecewise-constant elements for the spatial representation. Although I believe the authors never intended to use them, I would like to point out that these elements are "nonconforming," or, in other words, that the space they determine is not a subspace of $W_0^1(\Omega)$. Although nonconforming elements have been successfully used in several applications, convergence is usually subject either to the success of the so-called "patch test" devised by Bazeley et al.[13] and analyzed recently by Strang,[14] or to the use of a finite element method with penalty as proposed by Babuška and Zlámal[15] in a quite recent work.

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[10]F. M. PERRIN, H. S. PRICE, and R. S. VARGA, *Numer. Math.*, **13**, 180 (1969).

[11]J. P. HENNART, *Nucl. Sci. Eng.*, **50**, 185 (1973).

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[13]G. P. BAZELEY, Y. K. CHEUNG, B. M. IRONS, and O. C. ZIENKIEWICZ, in *Proc. Air Force Conf. Matrix Methods in Structural Mechanics*, Air Force Institute of Technology, Wright-Patterson, Ohio (1965).

[14]G. STRANG, in *The Mathematical Foundations of the Finite Element Method with Applications to Partial Differential Equations*, A. K. AZIZ, Ed., Academic Press, New York and London (1972).

[15]I. BABUŠKA and M. ZLÁMAL, *SIAM J. Numer. Anal.*, **10**, 863 (1973).

Response to "Comments on 'Finite Methods for Reactor Analysis'"

The following remarks reply to the recent Letter by Hennart.[1]

1. We believe our Theorem 7 of Ref. (2) is correct as stated, Hennart's comments notwithstanding. Hennart is correct in observing that the Sobolev imbedding theorem is valid only in one dimension, but since we make no use of the theorem, the comment is also irrelevant. Our theorem combines the errors in the spatial and energy variables for diffusion problems. The result concerning the L_∞ norm of the error in the spatial variable is not new; a similar result is given by Babuška and Kellogg.[3] Our approach is different, and we add the energy variable, but we make no claim to a new result in the L_∞ norm.

The fundamental problem seems to be one of notation. We assume the solution is in a space C_p^t, and $t > 0$. Indeed, solutions to multidimensional diffusion problems are in C_p^t. At singular points $0 < t < 1$, while at other points $t \geq 1$. Apparently Hennart has assumed we consider t to be only an integer, which is neither the case nor our intention.

To clarify the situation we reproduce the proof below with the following assumptions: We assume a region of configuration space, Ω, divided into a finite number of subregions, Ω_l, within which material properties are constant. Properties may differ from region to region. We also assume the conditions specified in the statement of Theorem 7. Finally we assume that all mesh spacings converge, i.e., $\Delta x = C_x h$, $\Delta y = C_y h$, $\Delta z = C_z h$, $\Delta E = C_E h$, with the C_i independent of x, y, z, or E. Throughout the development we will use K_i, $i = 1, 2, \ldots$ to mean a positive constant independent of h.

The original problem can be written on the weak form as

$$a(\phi,v) = (Q,v) \quad , \tag{1}$$

and we seek an approximate solution $\hat{\phi}$ from the relation

$$a(\hat{\phi},v_{ig}) = (Q,v_{ig}) \quad , \tag{2}$$

where

$$v_{ig} = u_i(\mathbf{r})u_g(E) \text{ for } i = 1, 2, \ldots, N;\ g = 1, 2, \ldots, G \quad .$$

[1]J. P. HENNART, *Nucl. Sci. Eng.*, **56**, 225 (1975).

[2]C. M. KANG and K. F. HANSEN, *Nucl. Sci. Eng.*, **51**, 456 (1973).

[3]I. BABUŠKA and R. B. KELLOGG, in *Proc. Conf. Mathematical Models in Computational Techniques for Analysis of Nuclear Systems*, CONF-730414, Part II, Paper VII-67-93, U.S. Atomic Energy Commission (1974).