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 Zlâmal[15] in a quite recent work.

*J. P. Hennart**

Instituto Politécnico Nacional
Departamento de Ingeniería Nuclear
Apartado Postal 75-189
México 14, D. F., México

January 29, 1974

[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).

[12] C. A. FELIPPA and R. W. CLOUGH, in *Proc. Symp. Numerical Solution of Field Problems in Continuum Physics*, p. 210, G. BIRKHOFF and R. S. VARGA, Eds., American Mathematical Society, Providence, Rhode Island (1970).

[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).

*On leave of absence from the University of Brussels, Belgium.

[15] I. BABUŠKA and M. ZLÂMAL, *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).

By expanding $\hat{\phi}$ in terms of the v_{ig} we generate a system of equations of the form

$$B\hat{\boldsymbol{\phi}} = \boldsymbol{q} \quad ,$$

where the matrix B is given in detail in Ref. (2). By the assumptions of the problem, B is positive definite and therefore B inverse exists.

The truncation error in the approximation is given by

$$B\boldsymbol{\phi} - \boldsymbol{q} = \boldsymbol{\tau} \quad ,$$

with $\boldsymbol{\phi}$ a column vector of the analytic solution evaluated at the mesh points. Now consider the case of a homogeneous system; ϕ is then an analytic function and the truncation error $\boldsymbol{\tau}$ can be evaluated by Taylor series methods. By direct expansion it is easy to show, for our Hermite basis functions, that the truncation error is $0(\Delta r^{2m_r+1}) + 0(\Delta E^{2m_E+1})$, where we have assumed the energy spectrum to be sufficiently differentiable. The pointwise error in the function, $\boldsymbol{\phi} - \hat{\boldsymbol{\phi}}$, is given by

$$B(\boldsymbol{\phi} - \hat{\boldsymbol{\phi}}) = \boldsymbol{\tau} \quad ,$$

so that

$$||\boldsymbol{\phi} - \hat{\boldsymbol{\phi}}||_\infty \leq ||B^{-1}||_\infty ||\boldsymbol{\tau}||_\infty \quad .$$

The norm of B^{-1} is bounded by $0(1/h)$ as Hennart suggests. Further, our basis functions satisfy Descloux's[4] coerciveness conditions to problems in three spatial dimensions, and we limit ourselves to, at most, 3-D problems. Thus,

$$||\boldsymbol{\phi} - \hat{\boldsymbol{\phi}}||_\infty \leq 0(\Delta r^{2m_r}) + 0(\Delta E^{2m_E}) \quad ,$$

and not $2m_r$-1 as suggested by Hennart.

In the case of material discontinuities but no singular points, for example a two-region problem, we can still use Taylor series methods. However, the limits on the spatial portion of the truncation error become $0(\Delta r^2)$. In general the bound is $0(\Delta E^2)$ for the energy variable also.

The analytic solution is in class C^1 and, from the previous results we have

$$||\boldsymbol{\phi} - \boldsymbol{\phi}||_\infty \leq 0(\Delta r) + 0(\Delta E) \quad ,$$

which is consistent with our Theorem 7.

We now turn to the more realistic case of a problem with singular points. The method of proof is based on the triangle inequality as follows: From Eqs. (1) and (2) we have

$$a(\phi - \hat{\phi}, v_{ig}) = 0 \quad .$$

Let $\tilde{\phi}$ be the Hermite interpolate of ϕ, and write the above as

$$a(\hat{\phi} - \tilde{\phi}, v_{ig}) = a(\phi - \tilde{\phi}, v_{ig}) \quad . \tag{3}$$

The interpolation error is bounded as

$$||\phi - \phi||_\infty \leq K_1 \Delta r^{\mu_r} + K_2 \Delta E^{\mu_E} \quad , \tag{4}$$

with $\mu_r = \min(2m_r, t_r)$, $\mu_E = \min(2m_E, t_E)$. The interpolation theorem is valid for μ_r, $\mu_E > 0$. Establishing the theorem in the energy variable is trivial since there is no differentiation and the slowing down kernel is bounded. For the spatial domain the interpolation theorem is classic for $t \geq 1$. For $0 < t < 1$ the interpolation error bound is established by the following lemma:

For a function $f(x) \epsilon C^t[0,h]$, with $0 < t < 1$, and with $f(0) = f(h) = 0$, then

$$||f||_\infty \leq K_3 h^t \quad .$$

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

We note that the interpolation error, $\phi - \tilde{\phi}$, is indeed zero at $x = 0,h$. The fractional derivative of f is written,[5]

$$\frac{d^t f}{dx^t} = p^t f \quad .$$

The inverse operator p^{-t} is defined such that $p^{-t}p^t f = f$ and p^{-t} can be written

$$p^{-t}g(x) = K_4 \frac{d}{dx} \int_0^x dx' \, g(x') \, (x - x')^t \quad .$$

We then have

$$||\phi - \tilde{\phi}||_\infty = ||p^{-t}p^t(\phi - \tilde{\phi})||_\infty \leq ||p^{-t}||_\infty \, ||p^t(\phi - \tilde{\phi})||_\infty \quad ,$$

and, since ϕ, $\tilde{\phi} \epsilon C^t[0,h]$, we have

$$||p^t(\phi - \tilde{\phi})||_\infty \leq K_5 \quad .$$

Thus,

$$||\phi - \tilde{\phi}||_\infty \leq \frac{K_5}{K_6} ||p^{-t}K_6||_\infty = \frac{K_5}{K_6} K_4 \frac{d}{dx} \int_0^h dx' K_6 (x - x')^t \quad ,$$

or

$$||\phi - \tilde{\phi}||_\infty \leq K_4 K_5 h^t \quad \text{QED} \quad .$$

By direct integration by parts, it is easy to show that

$$\Big(\boldsymbol{\nabla}\big(\phi(E) - \tilde{\phi}(E)\big), \, \boldsymbol{\nabla} u_i(\boldsymbol{v})\Big)_\Omega \leq K(E) \Delta r^{\mu_r} \tag{5}$$

for our basis functions, which are called "uniform" by Strang and Fix.[6] Using Eqs. (4) and (5) it is easy to show that

$$a(\phi - \tilde{\phi}, v) \leq K_7 \Delta r^{\mu_r} + K_6 \Delta E^{\mu_E} \quad . \tag{6}$$

Now define the quantity $e(\boldsymbol{r},E)$ as $\hat{\phi} - \tilde{\phi}$. The $e(\boldsymbol{r},E)$ is thus a polynomial of degree $2m_r - 1$ in $\boldsymbol{r}$ and $2m_E - 1$ in E, and can be represented as

$$e(\boldsymbol{r},E) = \sum_{g=1}^{G} \sum_{i=1}^{G} e_{ig} u_g(E) \, u_i(\boldsymbol{r}) \quad .$$

Then Eq. (3) leads to

$$B\boldsymbol{e} = \boldsymbol{K}_9 \, \Delta r^{\mu_r} + \boldsymbol{K}_{10} \, \Delta E^{\mu_E} \quad ,$$

where the composition of B is given in Ref. 2. Then

$$\boldsymbol{e} = B^{-1}\boldsymbol{K}_9 \, \Delta r^{\mu_r} + B^{-1}\boldsymbol{K}_{10} \, \Delta E^{\mu_E} \quad .$$

The vectors $\boldsymbol{K}_9$ and $\boldsymbol{K}_{10}$ consist of a sum of two vectors. The first is composed of components with coefficients Δr^{2m_r} and ΔE^{2m_E} corresponding to the smooth solution. The second vector has coefficients Δr^{t_r} and ΔE^{t_E} and a finite number of nonzero terms since there are only a finite number of singular points. This last term dominates the solution since $t_r < 2m_r$, $t_E < 2m_E$. The ∞ - norm of $\boldsymbol{e}$ is bounded as

$$||\boldsymbol{e}||_\infty \leq ||B^{-1}\boldsymbol{K}_9||_\infty \, \Delta r^{t_r} + ||B^{-1}\boldsymbol{K}_{10}||_\infty \, \Delta E^{t_E} \quad .$$

The norms consist of a finite sum of finite terms and hence the errors behave as Δr^{t_r} and ΔE^{t_E} as stated in Theorem 7. This completes the proof.

Hennart questions the usefulness of a theorem which could not prove convergence in a finite element approximation. We too would question such a theorem, but since we believe our results to be correct there is no question of proposing a nonconvergent method. Finally, we used the L_∞ norm to obtain bounds because we thought the approach

[5] R. COURANT and D. HILBERT, *Methods of Mathematical Physics*, Vol. II, p. 518, Interscience Publishers (1962).

[6] G. STRANG and G. FIX, *An Analysis of the Finite Element Method*, p. 136, Prentice-Hall, Inc. (1973).

the simplest. Our results are intended for use in the nuclear audience where interest is in eigenvalues, reaction rates, and flux distributions, not the pointwise behavior of the function.

2. We cannot understand how our choice of Set A as an example of "the only simple way to satisfy the interface condition" can be interpreted as either implying that the true solution satisfies such a condition or advocating use of such a condition. A sizable portion of the text[2] (particularly pp. 468-469) was given to discussing singular points, and we were and are well aware that the solution has an infinite first derivative as such points. It is not *simple* to satisfy infinite conditions at interfaces with either Hermite or Lagrange element functions.

We proposed set A to demonstrate that poor convergence is obtained by using basis functions which satisfy improper continuity conditions. We thought the text and results made it clear that we used set A to demonstrate what *not* to do!

With regard to using Lagrange elements we neither agree nor disagree with Hennart's recommendations of using them. We feel that it is an open question as to which is best. One is interested in Hermite methods so that continuity conditions can be imposed to reduce the number of basis functions and number of unknowns. Conversely, Lagrange methods do not require any special treatment at interfaces and perhaps, with static condensation, the number of unknowns can be reduced to as few as with Hermite basis functions. We know of no definite study on the subject.

3. Hennart is correct in observing that piecewise flat element functions are nonconforming and probably should not be used in the weak form of the diffusion problem.

C. M. Kang
K. F. Hansen

Massachusetts Institute of Technology
Department of Nuclear Engineering
Cambridge, Massachusetts 02139

October 30, 1974