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Letters to the Editor

Comments on the "Weinberg" Issue

It is quite fitting that *Nuclear Science and Engineering* (NS&E) pay tribute to Alvin Weinberg, and I am pleased that the editors and authors have done so in the August 1985 issue. It is particularly appropriate because of his warm support to the journal over the years.

Dr. Weinberg was a member of the Board of Directors of the American Nuclear Society and of its Publications Committee at the inception of NS&E in early 1956, and he surely contributed, together with other officials, to the likely intense discussions that established a project so important to a then young organization. For a decade during the 1960s, when the editorial office was at the Oak Ridge National Laboratory (ORNL), he was a dedicated member of the Editorial Advisory Committee providing encouragement and guidance to fledglings in that office. I am sure my predecessor would join me in these thanks for that counsel.

In a more specific vein, I also take this opportunity to add an historical footnote to Art Snell's recounting¹ of his many contributions to the Manhattan Project. He accurately and adequately tells of the early efforts at the Clinton Laboratories to provide guidance in nuclear criticality safety at the Oak Ridge Gaseous Diffusion Plant (K-25). To the credit of the segment of the Union Carbide organization then operating K-25, a predecessor of its Nuclear Division, and of its management under the late Clark Center, I add the following.

I am confident that the potential for undesired nuclear reactions within the gaseous diffusion cascade was recognized early in its design and that, within the limits of available knowledge, provision was made for their avoidance. The degree of ²³⁵U enrichment was, of course, an important consideration. In 1945, there was established at K-25 a criticality safety study that included a series of experiments in early 1946 at the Los Alamos National Laboratory under the personal guidance of Louis Slotin. Those initial measurements utilized a mixture containing uranium of >90% ²³⁵U, and they were repeated in Oak Ridge with 30% ²³⁵U. In both cases the nuclear properties of the test material closely resembled those of UF₆. During the following several years, an extensive parametric study was made of the nuclear critical dimensions of solutions containing highly ²³⁵U-enriched uranium.

Subsequently, with Union Carbide, the contractor for the three major operations in Oak Ridge, all research of this kind was consolidated within the ORNL organization. The back-

ground and experience gleaned at K-25 were a basis for an invitation to me by Dr. Weinberg in 1950 to assume the responsibilities noted by Dr. Snell on p. 363. For that invitation, I shall always be grateful.

I thank the editors for this opportunity to make a small personal contribution to the encomium.

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August 30, 1985

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An Additional Comment on the "Weinberg" Issue

In the recollections of early years at Oak Ridge National Laboratory (ORNL) as described in the August 1985 issue of this journal, I regret an oversight in my description of the 1945 criticality tests of UF₆ at the 24% level of enrichment of ²³⁵U. Actually, these measurements at ORNL were supplemented by probably more pertinent tests at enrichment levels of well over 90% by a collaboration between a group at the Gaseous Diffusion Plant itself and Louis Slotin at Los Alamos National Laboratory. Clifford K. Beck, A. Dixon Callihan, and Raymond L. Murray describe the first of a series of such studies in their ORGDP Special Hazards Report No. A-4716 entitled "Critical Mass Studies" and issued June 10, 1947. Thus, my implication that the ORNL work was solely responsible for the safety at the diffusion plant was an overstatement. My conjecture at present would be that knowledge of the transfer of the UF₆ criticality work to a capable group at the diffusion plant was received with relief by me; I could then forget about further work on UF₆, as I apparently did. In any event, all concerned can feel satisfaction in the absence of criticality accidents

at the diffusion plant as it brings to a close its history of 40 years of productive operation.

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Comments on the Richardson Extrapolation

In a recent letter to the editor,¹ Makai pointed out the efficiency of the Richardson extrapolation method² in obtaining finite difference (FD) solutions of higher accuracy from two FD solutions of lower accuracy. We confirm the efficiency and accuracy of this method, as shown by a number of calculations we have made³ for various fast reactor configurations using two- and three-dimensional multigroup FD neutron diffusion computer codes in r - z , x - y , and x - y - z geometries. Good results have been reported by others, as well (for example, see Refs. 4 and 5).

The purpose of this letter to the editor is to bring out some other points concerning the application of this method in reactor calculations:

1. Not only is the computer time reduced by the use of this extrapolation procedure but, perhaps more importantly, the memory storage requirements are greatly reduced. It should be recalled that for a three-dimensional FD problem the computer memory requirements increase as the cube of the number of meshes. We made particular use of the Richardson extrapolation method in problems where the fine mesh case just did not fit into the computer.

2. The method could fail when the higher order terms of the discretization error series are not negligibly small. Hence, the applicability of the procedure to each class of problems must be separately established before routine use. This can most easily be checked by making a series of calculations with gradually finer meshes. A straightforward Richardson extrapolation of two coarse-mesh solutions should not be made if the successive approximations do not approach the true value monotonically, since in this case the higher terms of the error series cannot be neglected.

3. By having solutions with three different mesh sizes, it is possible to have an estimate of the order j of the first term of the discretization error series. For example, with three solutions u_1 , u_2 , and u_3 corresponding to mesh sizes h , $2h$, and $4h$, we have

$$j \approx \frac{\ln \left(\frac{u_2 - u_3}{u_1 - u_2} \right)}{\ln 2}$$

4. For the conventional FD neutron diffusion equation, the truncation error is of $O(h^2)$ if there is a single homogeneous region and uniform mesh width. However, at boundaries between different regions in a reactor, the truncation error becomes of $O(h)$. Hence, if there are a large number of different regions or nonuniform mesh widths in the considered problem, an h^2 extrapolation of two coarse-mesh solutions may not be valid.

5. There is a slight discrepancy in Ref. 1. In Eqs. (3) and (6), the first term of the discretization error series has been indicated as $j = 1$. However, the weighting factors $\nu_1 = -\frac{1}{3}$ and $\nu_2 = \frac{1}{3}$ that have been used in the case study correspond to a single term error series starting with $j = 2$.

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Reply to "Comments on Richardson Extrapolation"

The advantages of applying Richardson extrapolation can be summarized as follows:

1. A solution of given accuracy is cheaper due to the larger mesh size, which leads to a faster algorithm, reduced memory requirement, and larger numerical stability.
2. The method is flexible; applications to r - z , x - y , x - y - z (see Refs. 1 and 2) and hexagonal geometry^{3,4} have been reported.
3. The method is applicable to a large number of problems, including finite difference²⁻⁴ (FD), finite element,⁵ coarse-mesh, and diverse transport theory methods. Application to the S_N method has been reported in Ref. 6.

Let us return to the FD method and pay attention to the problem of extrapolating k_{eff} . By definition,

$$k_{eff} = \frac{\text{production}}{\text{absorption} + \text{leakage}}, \quad (1)$$

where both production and absorption are integrals over the core, while leakage is an integral over the surface of the core. Some difficulty is caused by the FD method's having different truncation errors at material boundaries and in homogeneous regions, excluding the legitimacy of extrapolating the nominator and denominator of Eq. (1) in the same way.² That approximation, though not correct, is often useful. It is even more convenient to assume k_{eff} to behave as any reaction rate³ in a homogeneous region and to express the truncation error as

$$k_{eff} = K_{eff} + a \cdot h^2, \quad (2)$$

TABLE I
WVER-1000 Benchmark ($h = 14$ cm) Results
by HEXAGA-III

i	h_i^a	Points/ Hexagon	k_{eff}	Time (s, CYBER 73)
1	1	3	1.11715	6
2	2	12	1.11375	14
3	3	27	1.11279	34
4	4	48	1.11240	60
5	6	108	1.11211	237

^aThe value h_i is mesh size in relative units.

where h is the mesh size. We would recommend here a useful method proposed by Koch.⁷ The problem considered below is a WVER-1000 benchmark⁸ and the results were obtained by the HEXAGA program.⁹

Table I shows the eigenvalues k_{eff} obtained at five mesh sizes. The extrapolation procedure is given in Table II. The proposed value is

$$K_{eff} = 1.11187 \pm 0.00002,$$

which is just k_{15} and the error is $(k_{15} - k_{14})$.

All in all, the reader is encouraged to use the Richardson extrapolation.

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TABLE II
Extrapolation of k_{eff} by Koch's Method

h_i	k_i			
1	1.11715			
2	1.11375 ^a	$k_{12} = p_1 k_2 + p_2 k_1 = 1.11262$	$k_{13} = v_1 k_{23} + v_2 k_{12} = 1.11195$	$k_{14} = u_1 k_{24} + u_2 k_{13} = 1.11185$
3	1.11279	$k_{23} = p_3 k_3 + p_4 k_2 = 1.11202$	$k_{24} = v_3 k_{34} + v_4 k_{23} = 1.11186$	$k_{25} = u_3 k_{35} + u_4 k_{24} = 1.11187$
4	1.11240	$k_{34} = p_5 k_4 + p_6 k_3 = 1.11190$	$k_{35} = v_5 k_{45} + v_6 k_{34} = 1.11187$	
5	1.11211	$k_{45} = p_7 k_5 + p_8 k_4 = 1.11188$		

$$\begin{aligned}
 &^a p_1 = \frac{1}{3}; p_2 = -\frac{1}{3}; p_3 = \frac{2}{3}; p_4 = -\frac{1}{3}; p_5 = \frac{16}{7}; p_6 = -\frac{2}{7}; p_7 = \frac{2}{3}; p_8 = -\frac{1}{3} \\
 &v_1 = \frac{2}{8}; v_2 = -\frac{1}{8}; v_3 = \frac{1}{3}; v_4 = -\frac{1}{3}; v_5 = \frac{2}{3}; v_6 = -\frac{1}{3} \\
 &u_1 = \frac{16}{15}; u_2 = -\frac{1}{15}; u_3 = \frac{2}{8}; u_4 = -\frac{1}{8} \\
 &w_1 = \frac{36}{35}; w_2 = -\frac{1}{35}
 \end{aligned}$$