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THE CP METHOD IN THREE DIMENSIONS: CRITICALITY OF A CUBE

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ABSTRACT

A recently developed numerical method for computing collision probabilities in three dimensions is applied to the solution of the one-group critical problem for a cube. The method is based on a subdivision of the spatial zones, where the flat-flux approximation is used, into parts called *elements* and an assumption that the contribution from a source element to a sink element occurs along the path that joins their centers of mass. The calculation is repeated with the number of elements increased successively and Richardson extrapolation to infinite number of elements applied to the sequence of results, until convergence to the desired degree of accuracy in the collision probabilities is reached. The use of cube symmetries to reduce the required number of collision probability evaluations and the order of the resulting eigensystem that has to be solved for the dominant eigenvalue and the corresponding eigenvector is discussed. Numerical results are given for three test cases and compared with results from the MCNP and THREEDANT computer codes. It is concluded that the CP method can give fairly accurate results with low computational cost for this problem.

Key Words: CP method, criticality, collision probabilities, Richardson extrapolation

1. INTRODUCTION

In a recent work [1], we reported a new method for computing first-flight collision, escape and transmission probabilities in three dimensions. The method is based on a subdivision of the spatial domain into parts called *elements* and an assumption that neutrons are emitted only at the centers of mass of such elements, and can reach another element only if they travel along the path that joins the centers of mass of the source and the sink elements. The calculation is repeated as many times as necessary, increasing the number of elements successively and performing repeated Richardson extrapolation to infinite number of elements in the sequence of results, until convergence to a desired accuracy is obtained. Results for some test problems solved in Ref. 1 indicate that four (sometimes five) sequential steps of Richardson extrapolation are required to generate probabilities with an accuracy comparable to that of existing codes (typically $\sim 1\%$ of relative error). Furthermore, as discussed in Ref. 1, results from an optimized algorithm developed for cubic geometry [2] suggest that we may be able to obtain even more accurate results for the most common 3D geometries (rectangular, cylindrical and a combination of both) with reasonable computational effort, hopefully to the point where normalization schemes [3] commonly used to improve the accuracy of calculated collision, escape, and transmission probabilities in existing codes will not be needed in our method.

In this work, we apply the CP method with collision probabilities computed as in Refs. 1 and 2 to the solution of what we believe to be the simplest transport problem that can be formulated in three dimensions, namely the one-group criticality problem for a homogeneous cube with isotropic scattering. Our main objective in solving this problem is to have an initial appraisal of our method vis-à-vis existing 3D methods of solving the transport equation, both from the points of view of accuracy and computational efficiency.

2. THE CP METHOD

The CP method is an important tool in reactor design, and has been extensively applied to cell calculations since the 1960's. Because several good descriptions of the CP method are available (see, for example, Refs. 4–6), our presentation here is brief.

We consider a spatial domain of total volume V and surface S. Assuming one energy group, isotropic scattering, no extraneous sources in V, and zero incoming current on S, we can write the integral transport equation for the scalar flux $\phi(\mathbf{r})$, $\mathbf{r} \in V$, as

$$\phi(\mathbf{r}) = \frac{1}{4\pi} \int_V \mathrm{d}^3\mathbf{r}' \, \frac{\mathrm{e}^{-\tau(\mathbf{r},\mathbf{r}')}}{|\mathbf{r}-\mathbf{r}'|^2} \left[\Sigma_s(\mathbf{r}') + \frac{1}{k} \nu(\mathbf{r}') \Sigma_f(\mathbf{r}') \right] \phi(\mathbf{r}'), \tag{1}$$

where $\Sigma_s(\mathbf{r}')$ and $\Sigma_f(\mathbf{r}')$ are, respectively, the scattering and fission cross sections, $\nu(\mathbf{r}')$ is the mean number of neutrons produced per fission event, k is a factor to be determined so that Eq. (1) has a physically meaningful solution, and $\tau(\mathbf{r},\mathbf{r}')$ denotes the distance from $\mathbf{r}'$ to $\mathbf{r}$, measured in mean free paths. In general, $\tau(\mathbf{r},\mathbf{r}')$ is given by [4]

$$\tau(\mathbf{r},\mathbf{r}') = \int_0^{|\mathbf{r}-\mathbf{r}'|} \mathrm{d}s \, \Sigma(\mathbf{r}' + s\boldsymbol{\Omega}), \tag{2}$$

where $\Sigma(\mathbf{r})$ denotes the total cross section at position $\mathbf{r}$ and $\boldsymbol{\Omega}$ is the unit vector in the direction of $\mathbf{r}-\mathbf{r}'$. If the domain is homogeneous, $\tau(\mathbf{r},\mathbf{r}')$ reduces simply to $\Sigma|\mathbf{r}-\mathbf{r}'|$.

Now, if we subdivide the domain into N zones of volumes V_i, $i = 1, 2, \ldots, N$, use the flat-flux approximation [5]

$$\phi(\mathbf{r}) = \phi_i, \quad \mathbf{r} \in V_i, \tag{3}$$

and assume that the zones are piecewise homogeneous, we can integrate Eq. (1) over V_i to obtain

$$\Sigma_i V_i \phi_i = \sum_{j=1}^{N} \left(c_{s,j} + \frac{1}{k} c_{f,j} \right) P_{ij} \Sigma_j V_j \phi_j, \tag{4}$$

for $i = 1, 2, \ldots, N$, where $c_{s,j} = \Sigma_{s,j}/\Sigma_j$ and $c_{f,j} = \nu_j \Sigma_{f,j}/\Sigma_j$ are, respectively, the mean number of scattered and fission secondaries emitted per collision in zone j, and

$$P_{ij} = \frac{\Sigma_i}{4\pi V_j} \int_{V_i} \mathrm{d}^3\mathbf{r} \int_{V_j} \mathrm{d}^3\mathbf{r}' \, \frac{\mathrm{e}^{-\tau(\mathbf{r},\mathbf{r}')}}{|\mathbf{r}-\mathbf{r}'|^2} \tag{5}$$

is the probability that a neutron born uniformly and isotropically in zone j has its first collision in zone i. Once P_{ij} is calculated for $i, j = 1, 2, \ldots, N$, we can see that the system of equations defined by Eq. (4) for $i = 1, 2, \ldots, N$ is an eigenvalue problem of order N for the dominant k-eigenvalue, which we denote as k_{eff}, and the corresponding eigenvector, which has $\phi_i(k_{\mathrm{eff}})$, $i = 1, 2, \ldots, N$, as components.

3. COMPUTATION OF THE COLLISION PROBABILITIES

In this section, we summarize our method [1] of computing the collision probabilities P_{ij} for $i, j = 1, 2, \ldots, N$, in general 3D geometry.

The fact that the denominator $|\mathbf{r} - \mathbf{r}'|$ can be zero when $i = j$ in Eq. (5), making the kernel of the double integral in this equation singular, has motivated researchers to apply a variable transformation [7] to Eq. (5) in order to overcome this problem. Our method of computing collision probabilities that is described in Ref. 1 does not require transformations and deals directly with Eq. (5). It is based on subdividing the spatial zones into parts called *elements* and assuming, as an approximation, that the interaction between a source element and a sink element takes place only along the path that joins their centers of mass.

Using K elements per zone (the number of elements could be different for each zone if desired, but here we consider it to be the same for all zones) and denoting the locations of the centers of mass of these elements as $\mathbf{r}_{i,n}$, for $i = 1, 2, \ldots, N$ and $n = 1, 2, \ldots, K$, we can approximate Eq. (5) for $i \neq j$ by [1]

$$P_{ij} = \frac{\Sigma_i}{4\pi V_j} \sum_{n=1}^{K} \Delta V_{i,n} \sum_{m=1}^{K} \Delta V_{j,m} \frac{\mathrm{e}^{-\tau(\mathbf{r}_{i,n}, \mathbf{r}_{j,m})}}{|\mathbf{r}_{i,n} - \mathbf{r}_{j,m}|^2}, \tag{6}$$

where $\Delta V_{i,n}$ denotes the volume of element n in zone i.

When $i = j$, we can still use Eq. (6) provided all contributions for which the source and sink elements are the same are neglected in this expression. Our justification for doing so is physical: source neutrons that do not move from the point where they were born cannot contribute to the collision probability calculation. Thus, Eq. (6) is written, for $i = j$ and $K > 1$, as [1]

$$P_{ii} = \frac{\Sigma_i}{4\pi V_i} \sum_{n=1}^{K} \Delta V_{i,n} \sum_{\substack{m=1 \\ m \neq n}}^{K} \Delta V_{i,m} \frac{\mathrm{e}^{-\tau(\mathbf{r}_{i,n}, \mathbf{r}_{i,m})}}{|\mathbf{r}_{i,n} - \mathbf{r}_{i,m}|^2}. \tag{7}$$

Our numerical procedure for computing the collision probabilities can be summarized as follows. We start the calculation using a small value of K in Eq. (6) [or Eq. (7)] to find a first approximation for P_{ij} (or P_{ii}), and then we repeat the calculation, as many times as necessary, increasing the value of K and applying repeated Richardson extrapolation [8] to infinite number of elements, until the relative difference between two consecutive values of P_{ij} (or P_{ii}) in the sequence of calculations gets smaller than a prescribed tolerance ϵ.

To conclude this section, we note that the symmetry relation

$$\Sigma_j V_j P_{ij} = \Sigma_i V_i P_{ji}, \tag{8}$$

allows us to reduce the number of collision probability evaluations from N^2 to $N(N+1)/2$. The remaining $N(N-1)/2$ probabilities can then be obtained from Eq. (8).

4. THE CASE OF A HOMOGENEOUS CUBE

First of all, we note that Eq. (4) becomes, for the case of a homogeneous domain subdivided into equal-volume zones,

$$\phi_i = \left(c_s + \frac{1}{k} c_f \right) \sum_{j=1}^{N} P_{ij} \phi_j, \tag{9}$$

where the parameters c_s and c_f are now zone-independent. Defining the $N \times N$ matrix $\mathbf{P}$ that has the collision probabilities $\{P_{ij}\}$ as elements and the N-vector $\mathbf{\Phi}$ with the scalar fluxes $\{\phi_i\}$ as components, we can write Eq. (9) for $i = 1, 2, \ldots, N$ as

$$\mathbf{P}\mathbf{\Phi} = \lambda\mathbf{\Phi}, \tag{10}$$

where

$$\lambda = \frac{k}{kc_s + c_f}. \tag{11}$$

It is easy to see that λ increases monotonically with k, and therefore the largest eigenvalue $\lambda_{\max}$ of $\mathbf{P}$ is associated with (an approximation to) the effective multiplication factor k_{eff} that we seek. Thus, once $\lambda_{\max}$ is found, use of Eq. (11) yields

$$k_{\text{eff}} = \frac{c_f\lambda_{\max}}{1 - c_s\lambda_{\max}}, \tag{12}$$

and an approximate scalar flux distribution in the domain is provided by the corresponding eigenvector $\mathbf{\Phi}(\lambda_{\max})$.

Our implementation of the CP method for the case of a homogeneous cube makes use of equal-volume cubic zones, each of which can be identified in two different ways: (i) a positive integer in a sequence, as in Eq. (9), or (ii) a triplet of positive integers (α, β, γ) that gives the zone position in the cube with respect to the x,y,z coordinates. Thus, when we subdivide the edges of a cube into n equal-sized segments to obtain a total of $N = n^3$ equal-volume zones, we can refer to these zones either as

$$i, \quad \text{for } i = 1, 2, \ldots, N, \tag{13}$$

or

$$(\alpha, \beta, \gamma), \quad \text{for } \alpha, \beta, \gamma = 1, 2, \ldots, n, \tag{14}$$

and we can take the correspondence between these two kinds of identification to be

$$i = \alpha + (\beta - 1)n + (\gamma - 1)n^2. \tag{15}$$

The main advantage of the (α, β, γ) identification system is that it makes easier to visualize how to deal with the cube symmetries in the process of reducing the number of independent collision probability evaluations to a minimum. In fact, noting that the collision probability P_{ij} can also be denoted as $P_{(\alpha,\beta,\gamma)\leftarrow(\alpha',\beta',\gamma')}$, we can easily see that it is sufficient to consider the situations where $\alpha' - \alpha = 0, 1, \ldots, n-1$, along with $\beta' - \beta = 0, 1, \ldots, \alpha' - \alpha$ for each allowed value of $\alpha' - \alpha$, and $\gamma' - \gamma = 0, 1, \ldots, \beta' - \beta$ for each allowed value of $\beta' - \beta$, to define the independent collision probabilities in the cube. A simple calculation then shows that the required number of independent CP evaluations for n^3 equal-volume zones in a homogeneous cube is $n(n+1)(n+2)/6$. We recall from Section 3 that this number would be $n^3(n^3+1)/2$ (a factor of almost $3n^3$ higher) if the cube symmetries were not taken into account.

Next, each zone of the cube is subdivided into equal-volume cubic elements for computing the independent elements of collision probability matrix. The calculation is based on optimized versions of Eqs. (6) and (7) that were developed by grouping and counting the number of similar binary relations that describe the interaction between all elements in the source and sink zones [2]. The gain in computational efficiency when the optimized procedure is applied is substantial: while the CPU time for a direct implementation of Eqs. (6) and (7) increases quadratically with K (the number of elements per zone), the CPU time for the optimized implementation increases about linearly with K [1].

In addition to the simplification in the setting of the collision probability matrix just discussed, we can make use of flux symmetries to reduce the order of the eigensystem expressed by Eq. (10). By adopting the (α, β, γ) zone identification system, we can easily see that $\phi_{(\alpha,\beta,\gamma)}$ must be invariant by a change in the order of the indices α, β and γ. Moreover, as our computational implementation of the CP method always considers an even number of edge subdivisions, the cube symmetries in this case are such that when any of the indices α, β or γ is $> n/2$ it can be replaced by $n+1-\alpha$, $n+1-\beta$ or $n+1-\gamma$, respectively. Thus, we conclude that the number of independent flux components in a cube with n edge subdivisions is given by the number of distinct combinations of α, β and γ for $\alpha, \beta, \gamma = 1, 2, \ldots, n/2$ and $\alpha \geq \beta \geq \gamma$. This amounts to $n(n+2)(n+4)/48$ and represents a substantial reduction over the order of the original eigensystem, as can be seen in Table I.

Table I. Comparison of Eigensystem Orders

Number of Edge Subdivisions	Original Eigensystem	Reduced Eigensystem
2	8	1
4	64	4
8	512	20
16	4096	120
32	32768	816
64	262144	5984

5. NUMERICAL RESULTS

We have applied the CP formulation discussed in the previous sections to three test cases based on U-235 one-group isotropic cross sections extracted from a Los Alamos report [9].

To compute the effective multiplication factor k_{eff}, we have applied the power method with eigenvalue estimation given by the Rayleigh quotient [10] to find the largest eigenvalue $\lambda_{\max}$ of the reduced collision probability matrix obtained from $\mathbf{P}$ after using the cube symmetries, as discussed in Section 4. The iterative process of the power method was stopped when an estimate of $\lambda_{\max}$ did not differ from the previous one by more than 10^{-6}, in relative terms, three times consecutively. We then used Eq. (12) to find k_{eff}.

The fluxes came out as the components of the eigenvector associated with $\lambda_{\max}$, and were normalized by imposing that the integral of the flux distribution over the cube in the flat-flux approximation be equal to the total volume of the cube, i.e.

$$\int_0^a \mathrm{d}x \int_0^a \mathrm{d}y \int_0^a \mathrm{d}z\, \phi(x,y,z) \simeq (a/n)^3 \sum_{i=1}^{N} \phi_i = a^3, \tag{16}$$

where a denotes the length of the cube edge.

The cross-section set used in this work is given by $\Sigma = 0.32640$ cm^{-1}, $\Sigma_s = 0.248064$ cm^{-1}, $\Sigma_f = 0.065280$ cm^{-1}, and $\nu = 2.70$, and the three test cases differ only in the selected value of a. Case 1 has $a = 3$ cm, Case 2 has $a = 12$ cm, and Case 3 has $a = 50$ cm.

Table II shows our results for the effective multiplication factor k_{eff}, for various numbers of cube edge subdivisions. The results labeled as "accelerated" were obtained from the application of repeated Richardson extrapolation [8] with parameters $p_k = k$ and $q = 2$ to the "standard" results. Two different values of the tolerance ϵ (see Sec. 3) were used for the CP calculation: 10^{-3} for 2, 4, 8 and 16 edge subdivisions and 10^{-4} for 32 and 64 edge subdivisions. We have applied a larger tolerance to the CP calculations with 2, 4, 8 and 16 edge subdivisions in order to save some computer time. Since the inherent errors for these levels of discretization are relatively large, this has not caused any significant loss of accuracy in our calculation. Also shown in Table II are the MCNP and THREEDANT results generated for comparison purposes by Parsons [11]. The MCNP results were obtained with 2×10^8 histories for Case 1, 2.5×10^8 histories for Case 2, and 4×10^8 histories for Case 3, and the THREEDANT results with a Chebyshev-Legendre quadrature of order 24 and a 50×50×50 mesh for Case 1, a 60×60×60 mesh for Case 2, and a 80×80×80 mesh for Case 3, on 1/8 of the cube. We can see that our best results (64 edge subdivisions accelerated with 5 steps of repeated Richardson extrapolation) show relative deviations of $<0.01\%$ in magnitude with respect to the MCNP results, which we consider a pretty good agreement.

Table II. The Effective Multiplication Factor[a]

No. of Edge Subdivisions	Case 1		Case 2		Case 3	
	Standard	Accelerated	Standard	Accelerated	Standard	Accelerated
2	0.23395 (–9.2)	—	0.78990 (–18.3)	—	1.60870 (–19.3)	—
4	0.24731 (–4.0)	0.26067 (+1.2)	0.87473 (–9.5)	0.95956 (–0.70)	1.72619 (–13.4)	1.84368 (–7.6)
8	0.25431 (–1.2)	0.26154 (+1.6)	0.93431 (–3.3)	1.00533 (+4.0)	1.86828 (–6.3)	2.06593 (+3.6)
16	0.25665 (–0.34)	0.25773 (+0.08)	0.95710 (–0.96)	0.97092 (+0.47)	1.95117 (–2.2)	2.03854 (+2.2)
32	0.25730 (–0.09)	0.25751 (–0.003)	0.96389 (–0.26)	0.96622 (–0.02)	1.98185 (–0.62)	1.99757 (+0.16)
64	0.25748 (–0.02)	0.25754 (+0.009)	0.96572 (–0.07)	0.96634 (–0.003)	1.99099 (–0.17)	1.99419 (–0.006)
MCNP[b]	0.25752±0.00001		0.96637±0.00004		1.99431±0.00004	
THREEDANT[b]	0.25749		0.96626		1.99422	

[a]The figures in parentheses are the percent relative deviations with respect to the MCNP results.
[b]Results generated by Parsons [11].

Concerning computational requirements, we report in Table III the CPU times in seconds spent by our single-precision FORTRAN program on a 850-MHz Pentium III PC. The CPU-time distribution among the different tasks that have to be performed by the program is given in Table IV for Case 2. All of these CPU times are for standard calculations; CPU times for the accelerated calculations can be obtained by adding up the relevant times for standard calculations. For example, to find the CPU time for the accelerated calculation with 16 edge subdivisions we must add the CPU times for the standard calculations with 2, 4, 8 and 16 edge subdivisions. By comparison, the CPU times (in minutes) for the MCNP and THREEDANT runs carried out by Parsons [11] on a Sun Ultra 10 workstation (300-MHz clock) are given in Table V.

Table III. CPU Times for the CP Method[a]

No. of Edge Subdivisions	Case 1	Case 2	Case 3
2	0.2	0.9	6.4
4	0.3	0.3	3.5
8	0.6	1.1	9.0
16	0.7	5.5	8.0
32	20.7	67.6	74.1
64	437.0	544.4	1109.6

[a] In seconds, on a 850-MHz Pentium III PC.

Table IV. The CPU-Time Distribution for Case 2[a]

Program Section	Number of Edge Subdivisions					
	2	4	8	16	32	64
Calculation of the collision probabilities	0.9	0.3	1.1	5.4	60.1	78.4
Setting of the reduced $\mathbf{P}$ matrix	<0.1	<0.1	<0.1	0.1	6.6	363.1
Calculation of k_{eff} and $\{\phi_i\}$	<0.1	<0.1	<0.1	<0.1	0.9	102.9
Total	0.9	0.3	1.1	5.5	67.6	544.4

[a] CPU times in seconds.

In regard to storage space, our program requires approximately $(n^6 + 12n^5)/48^2$ floating-point words and $55n^3/48$ integer words of RAM, where, as before, n denotes the number of cube edge subdivisions.

Table V. CPU Times[a] for MCNP and THREEDANT

Case	MCNP	THREEDANT
1	253	184
2	582	567
3	1644	524

[a] In minutes, on a Sun Ultra 10 workstation [11].

Finally, to illustrate our flux results, we show in Fig. 1 the scalar flux distribution along the diagonal of the cube, from the vertex $x = y = z = 0$ to the center point $x = y = z = a/2$, for 4, 16 and 64 edge subdivisions applied to Case 2. The flux shown in this figure is normalized according to Eq. (16).

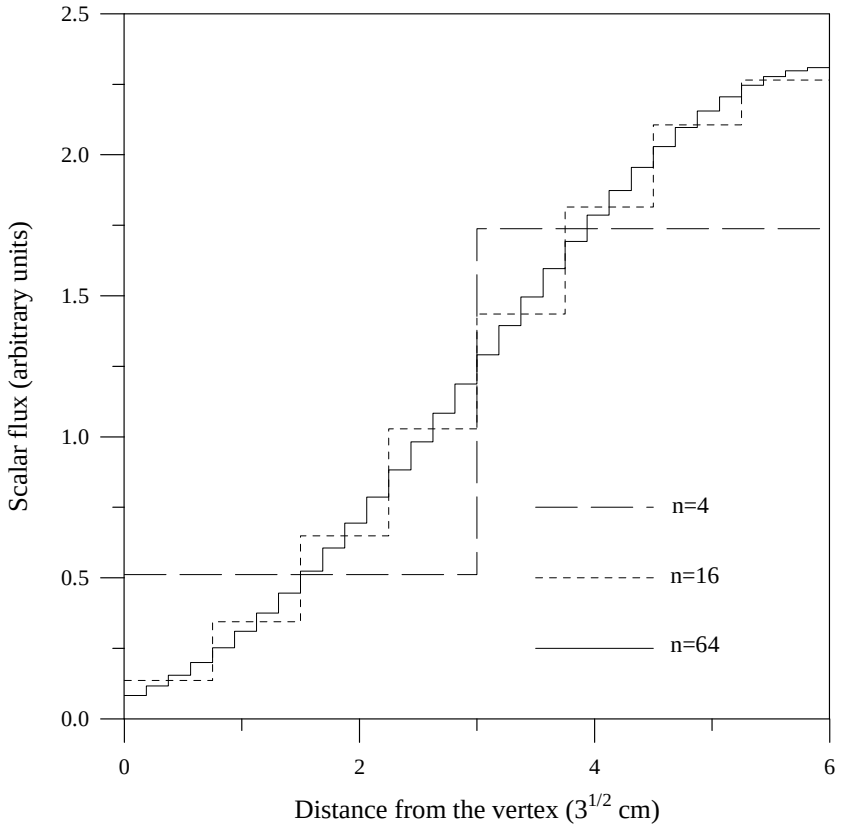

Figure 1. The Scalar Flux along the Cube Diagonal for Case 2

6. CONCLUSIONS

In this work, we have developed an optimized version of the CP method to solve the one-group critical problem for a cube. We conclude from the numerical results and comparisons with other methods that are

reported in Section 5 that our implementation of the CP method yields good results with modest computational effort for this problem. As is apparent from Tables II and III, using up to 32 edge subdivisions and four steps of Richardson extrapolation, we were able to obtain k_{eff} results with relative deviations of $<0.2\%$ in magnitude for all three cases, in CPU times that varied between 20 and 100 seconds per case on a 850-MHz Pentium III PC. Nevertheless, we should point out that discretization at the 64 edge-subdivision level sets a practical limit for the use of our current implementation, as both the CPU time and memory usage would be prohibitively high at the 128 edge-subdivision level.

To close this section, we would like to mention that we plan next to develop a similar kind of optimization for the case of a finite cylinder, in our continuing work on the CP method.

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REFERENCES

[1] R. D. M. Garcia, “A Numerical Method for Computing Collision, Escape and Transmission Probabilities in Three Dimensions,” *Nucl. Sci. Eng.* (accepted for publication).

[2] R. D. M. Garcia, “Optimized Algorithm for CP Calculations in Cubic Geometry” (to be submitted).

[3] G. J. Wu and R. Roy, “A New Characteristics Algorithm for 3D Transport Calculations,” *Ann. Nucl. Energy*, **30**, 1–16 (2003).

[4] R. Sanchez and N. J. McCormick, “A Review of Neutron Transport Approximations,” *Nucl. Sci. Eng.*, **80**, 481–535 (1982).

[5] R. J. J. Stamm’ler and M. J. Abbate, *Methods of Steady-State Reactor Physics in Nuclear Design*, Academic Press, London (1983).

[6] E. E. Lewis and W. F. Miller, Jr., *Computational Methods of Neutron Transport*, American Nuclear Society, La Grange Park, IL (1993).

[7] R. Roy, A. Hébert, and G. Marleau, “A Transport Method for Treating Three-Dimensional Lattices of Heterogeneous Cells,” *Nucl. Sci. Eng.*, **101**, 217–225 (1989).

[8] G. Dahlquist and Å. Björk, *Numerical Methods*, Prentice-Hall, Englewood Cliffs, NJ (1974).

[9] A. Sood, R. A. Forster, and D. K. Parsons, *Analytical Benchmark Test Set for Criticality Code Verification*, Report LA-13511, Los Alamos National Laboratory, Los Alamos, N. Mex. (1999).

[10] A. Jennings, *Matrix Computation for Engineers and Scientists*, Wiley, New York (1977).

[11] D. K. Parsons, Private communication (2002).