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ASYMPTOTIC SOLUTION OF THE TRANSVERSE INTEGRATED DIFFUSION EQUATION IN A NEAR-CRITICAL NODE

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ABSTRACT

When the Analytic Nodal Method (ANM) is applied to problems that contain near-critical nodes, numerical instabilities are possible. This problem of numerical instability becomes even more pronounced when Legendre moments of the transverse-integrated one-dimensional flux are calculated. To overcome the numerical difficulties associated with the evaluation of nodal coupling coefficients and flux Legendre moments the asymptotic solution to the transverse-integrated diffusion equation is developed. This solution limits to the true solution of the one-dimensional inhomogeneous diffusion equation for the case of zero fundamental mode eigenvalue and it further provides recurrent relations for the calculation of the higher order terms in the Taylor series expansion of the transverse-integrated one-dimensional flux.

Key Words: Asymptotic Solution, Near-Critical Nodes, Legendre Moments

1 INTRODUCTION

Transverse-integration nodal diffusion methods [1] are in widespread use in production codes for global reactor analysis. The Analytic Nodal Method (ANM) [2] is one such method and its most attractive feature is that it is more accurate than the widely used polynomial methods. On the other hand, the ANM can, dependent on how the nodal current-to-flux coupling coefficients are computed, exhibit numerical instabilities when a reactor core contains near-critical nodes [3]. The same problem occurs when the analytic solution to the one-dimensional transverse-integrated equation or the Legendre moments of this solution have to be evaluated numerically. The Legendre moments may be needed in various parts of the nodal solution algorithm, such as in the calculation of the intra-nodal cross-section source contribution (as in [4]), in the construction of transverse-leakage moments or in the determination of intra-nodal homogeneous flux distributions. One way of overcoming the numerical problems associated with the evaluation of nodal coupling coefficients and flux Legendre moments is to use Taylor series expansions. Unfortunately, such an approach becomes cumbersome when the inhomogeneous source in the transverse-integrated diffusion equation is represented by a variable order polynomial. In this paper, an alternative solution to these numerical problems is sought by employing the asymptotic solution to the transverse-integrated diffusion equation. The layout of the paper is as follows.

First, the analytic solution (both for non-zero and zero fundamental mode eigenvalue) to the one-dimensional transverse-integrated diffusion equation is presented in terms of its complementary and particular solutions and recurrence relations for the Legendre moments of this solution are derived. Next, the local asymptotic solution of the transverse-integrated flux is derived for the case of a near-critical node. Numerical comparison between the analytic and asymptotic calculation of the flux Legendre moments in the case of a near-zero eigenvalue is made to demonstrate the utility of the asymptotic method.

2 ANALYTIC SOLUTION OF THE TRANSVERSE-INTEGRATED DIFFUSION EQUATION

We consider the transverse-integrated one-dimensional diffusion equation in G energy groups:

$$\frac{\mathrm{d}^2 \underline{\Phi}(u)}{du^2} + \widehat{b}^2 \underline{\Phi}(u) = \underline{S}(u), \qquad -1 \leq u \leq +1 \qquad , \tag{1}$$

where $\underline{\Phi}(u)$ is the $G \times 1$ column vector of group fluxes, $\widehat{b}^2$ is the $G \times G$ dimensionless buckling matrix, and $\underline{S}(u)$ is the $G \times 1$ vector of intra-nodal group sources (due to transverse leakage and intra-nodal cross-section shape contribution). We assume that the $G \times G$ matrix $\widehat{b}^2$ has G distinct eigenvalues and we denote the largest one, the fundamental mode eigenvalue, by α^2. The matrix $\widehat{b}^2$ can be diagonalized through the similarity transformation $\widehat{U}^{-1}\widehat{b}^2\widehat{U}$ where $\widehat{U}$ is the modal matrix of $\widehat{b}^2$. The same transformation will also diagonalize the system of equations (1). We single out the fundamental mode equation:

$$\frac{\mathrm{d}^2 f(u)}{du^2} + \alpha^2 f(u) = Q(u), \qquad -1 \leq u \leq +1 \tag{2}$$

with boundary conditions $f(\pm 1) = f^{\pm}$. We assume for the moment that $\alpha^2 \neq 0$. The analytic solution of this boundary value problem can be written as follows:

$$f(u) = f_c(u) + f_p(u) \qquad . \tag{3}$$

Here $f_c(u)$ is the solution of the complementary problem that satisfies the original boundary conditions at $u = \pm 1$:

$$\frac{\mathrm{d}^2 f_c(u)}{du^2} + \alpha^2 f_c(u) = 0, \qquad -1 \leq u \leq +1 \qquad , \tag{4}$$

$$f_c(\pm 1) = f^{\pm} \qquad . \tag{5}$$

This solution can be written as follows:

$$f_c(u) = f^{+} \left[\frac{\sin(\alpha(1+u))}{\sin 2\alpha} \right] + f^{-} \left[\frac{\sin(\alpha(1-u))}{\sin 2\alpha} \right] \qquad . \tag{6}$$

$f_p(u)$ is the solution of the following problem:

$$\frac{\mathrm{d}^2 f_p(u)}{du^2} + \alpha^2 f_p(u) = Q(u), \qquad -1 \le u \le +1 \qquad , \tag{7}$$

$$f_p(\pm 1) = 0 \qquad , \tag{8}$$

i.e. $f_p(u)$ is the contribution of the particular part of the solution of problem (2) due to the source $Q(u)$ that satisfies zero boundary conditions at $u = \pm 1$. This solution can be written as follows:

$$f_p(u) = Z(u) - Z^+ \left[\frac{\sin(\alpha(1+u))}{\sin 2\alpha}\right] - Z^- \left[\frac{\sin(\alpha(1-u))}{\sin 2\alpha}\right] \qquad , \tag{9}$$

where $Z(u)$ is the particular solution due to the source $Q(u)$:

$$Z(u) = \frac{1}{\alpha}\int^u sin(\alpha(u-t))Q(t)dt \tag{10}$$

and $Z^{\pm} = Z(\pm 1)$. If the source $Q(u)$ is given as a Legendre polynomial series (up to some arbitrary order L)

$$Q(u) = \sum_{l=0}^{L} d_l P_l(u) \tag{11}$$

then the particular solution is also given as Legendre polynomial series:

$$Z(u) = \sum_{l=0}^{L} b_l P_l(u) \qquad . \tag{12}$$

The coefficients of the Legendre polynomial series of the particular solution (Legendre moments of the particular solution) are obtained by inserting Eqs. (11) and (12) into Eq. (7). Multiplying this equation by $P_n(u)$ and integrating over the interval $[-1, +1]$, the following upper-triangular system of equations for coefficients b_l is obtained:

$$\sum_{m=l+2}^{L} a_{lm} b_m + \alpha^2 b_l = d_l, \qquad l = 0, 1, \ldots, L \qquad , \tag{13}$$

where

$$a_{lm} = \frac{2l+1}{4}\left[1 + (-1)^{l+m}\right][m(m+1) - l(l+1)] \qquad . \tag{14}$$

The system of equations (13) can be easily solved via backward substitution:

$$b_L = \frac{1}{\alpha^2} d_L,$$

$$b_{L-1} = \frac{1}{\alpha^2} d_{L-1}, \tag{15}$$

$$b_l = \frac{1}{\alpha^2}\left[d_l - \sum_{m=l+2}^{L} a_{lm} b_m\right], \qquad l = L-2, \ldots 1, 0 \qquad .$$

Thus, a recursive relation has been obtained for the moments of the particular solution.

Hence, in the case of a polynomial source, Eq. (9) can be written as follows:

$$f_p(u) = \sum_{l=0}^{L} b_l P_l(u) - \left(\sum_{l=0}^{L} b_l\right)\left[\frac{\sin(\alpha(1+u))}{\sin 2\alpha}\right] - \left(\sum_{l=0}^{L} (-1)^l\, b_l\right)\left[\frac{\sin(\alpha(1-u))}{\sin 2\alpha}\right] \qquad . \qquad (16)$$

Substituting Eqs. (6) and (16) into Eq. (3), we can write the analytic solution in the case of a polynomial source as follows:

$$f(u) = f^+\left[\frac{\sin(\alpha(1+u))}{\sin 2\alpha}\right] + f^-\left[\frac{\sin(\alpha(1-u))}{\sin 2\alpha}\right]$$

$$-\left(\sum_{l=0}^{L} b_l\right)\left[\frac{\sin(\alpha(1+u))}{\sin 2\alpha}\right] - \left(\sum_{l=0}^{L} (-1)^l\, b_l\right)\left[\frac{\sin(\alpha(1-u))}{\sin 2\alpha}\right] + \sum_{l=0}^{L} b_l P_l(u) \qquad . \qquad (17)$$

2.1 Analytic Solution for Zero Eigenvalue

When the fundamental mode eigenvalue α^2 is equal to zero, the fundamental mode equation (2) reduces to the following equation:

$$\frac{\mathrm{d}^2 g(u)}{du^2} = Q(u), \qquad -1 \le u \le +1 \qquad . \qquad (18)$$

The boundary conditions remain unchanged: $g(\pm 1) = f^{\pm}$. The analytic solution of this boundary value problem can still be written as the sum of the complementary part of the solution and the contribution of the particular part of the solution:

$$g(u) = g_c(u) + g_p(u) \qquad . \qquad (19)$$

Here $g_c(u)$ is the solution of the complementary problem that satisfies the original boundary conditions at $u = \pm 1$:

$$\frac{\mathrm{d}^2 g_c(u)}{du^2} = 0, \qquad -1 \le u \le +1 \qquad , \qquad (20)$$

$$g_c(\pm 1) = f^{\pm} \qquad . \qquad (21)$$

This solution can be written as follows:

$$g_c(u) = f^+ \left[\frac{1}{2}(1+u)\right] + f^- \left[\frac{1}{2}(1-u)\right] \quad . \tag{22}$$

We note that we could have obtained this solution from Eq. (6) (complementary part of the solution for non-zero eigenvalue) by taking the limit as $\alpha \to 0$. This means that the function $g_c(u)$ is the zero order term in the Taylor series expansion (in α) of the function $f_c(u)$ (function $f_c(u)$ is given by Eq. (6)). $g_p(u)$ is the solution of Eq. (18) with homogeneous (zero) boundary conditions:

$$\frac{\mathrm{d}^2 g_p(u)}{du^2} = Q(u), \qquad -1 \le u \le +1 \quad , \tag{23}$$

$$g_p(\pm 1) = 0 \quad . \tag{24}$$

This solution can be written as follows:

$$g_p(u) = R(u) - R^+ \left[\frac{1}{2}(1+u)\right] - R^- \left[\frac{1}{2}(1-u)\right] \quad , \tag{25}$$

where $R(u)$ is the particular solution due to the source $Q(u)$:

$$R(u) = \int^u (u-t)Q(t)dt \tag{26}$$

and $R^\pm = R(\pm 1)$. We again note that we could have obtained Eqs. (25) and (26) from Eqs. (9) and (10) respectively, by taking the limit as $\alpha \to 0$. This means that the function $g_p(u)$ is the zero order term in the Taylor series expansion (in α) of the function $f_p(u)$ (function $f_p(u)$ is given by Eq. (9)). If the source $Q(u)$ is given as a Legendre polynomial series (Eq. (11)), then the function $g_p(u)$ will also be given as a Legendre polynomial series:

$$g_p(u) = \sum_{l=0}^{L+2} p_l P_l(u) \quad . \tag{27}$$

This follows directly from Eq. (23). In order to obtain the polynomial coefficients p_l, we first integrate Legendre polynomials explicitly in Eq. (26) to obtain the particular solution $R(u)$. Next, we calculate the values of the particular solution $R(u)$ at $u = \pm 1$, $R^\pm$. We proceed by inserting $R(u)$ and $R^\pm$ into Eq. (25) and collecting all terms of equal Legendre polynomial index. This gives us the coefficients p_l explicitly. Using vector notation we can write:

$$\underline{p} = \widehat{M}^{(L+1)} \underline{d} \quad , \tag{28}$$

where $\underline{p}$ is the $(L+3) \times 1$ column vector of coefficients p_l, $\underline{d}$ is the $(L+1) \times 1$ column vector of coefficients d_l and $\widehat{M}^{(L+1)}$ is the $(L+3) \times (L+1)$ rectangular matrix. This matrix has the following special forms for $L = 0$ and $L = 1$:

$$\widehat{M}^{(1)} = \begin{bmatrix} -\frac{1}{3} \\ 0 \\ \frac{1}{3} \end{bmatrix} \qquad , \widehat{M}^{(2)} = \begin{bmatrix} -\frac{1}{3} & 0 \\ 0 & -\frac{1}{15} \\ \frac{1}{3} & 0 \\ 0 & \frac{1}{15} \end{bmatrix} \tag{29}$$

and the following general form when $L \geq 2$:

$$\begin{bmatrix} -\frac{1}{3} & 0 & \frac{1}{15} & 0 & 0 & & \cdots & & 0 \\ 0 & -\frac{1}{15} & 0 & \frac{1}{35} & 0 & \ddots & \cdots & & 0 \\ \frac{1}{3} & 0 & -\frac{2}{21} & 0 & \frac{1}{63} & \ddots & \ddots & & 0 \\ 0 & \frac{1}{15} & 0 & -\frac{2}{45} & 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & \frac{1}{35} & 0 & -\frac{2}{77} & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & & & & & \ddots & -\frac{2}{(2L-5)(2L-1)} & 0 & \frac{1}{(2L-1)(2L+1)} \\ 0 & & & & & \ddots & 0 & -\frac{2}{(2L-3)(2L+1)} & 0 \\ 0 & & & & & \ddots & \frac{1}{(2L-3)(2L-1)} & 0 & -\frac{2}{(2L-1)(2L+3)} \\ 0 & & & & & \ddots & 0 & \frac{1}{(2L-1)(2L+1)} & 0 \\ 0 & 0 & 0 & 0 & 0 & \ddots & 0 & 0 & \frac{1}{(2L+1)(2L+3)} \end{bmatrix} . \tag{30}$$

Substituting Eqs. (22) and (27) into Eq. (19) we obtain the analytic solution for zero eigenvalue:

$$g(u) = f^+ \left[\frac{1}{2}(1+u)\right] + f^- \left[\frac{1}{2}(1-u)\right] + \sum_{l=0}^{L+2} p_l P_l(u) \qquad . \tag{31}$$

3 LEGENDRE MOMENTS OF THE TRANSVERSE-INTEGRATED FLUX

The Legendre moments of the one-dimensional flux are defined as

$$f_n = c_n \int_{-1}^{+1} f(u) P_n(u) du \qquad , \tag{32}$$

where $c_n = \frac{2n+1}{2}$. Substituting Eqs. (3),(6) and (9), we have

$$f_n = (f^+ I_n^+ + f^- I_n^-) - (Z^+ I_n^+ + Z^- I_n^- - Z_n) \qquad , \tag{33}$$

where I_n^+ and I_n^- are the Legendre polynomial moments of the trigonometric functions $\sin(\alpha(1+u))/\sin 2\alpha$ and $\sin(\alpha(1-u))/\sin 2\alpha$, respectively, and Z_n are the Legendre moments of the particular solution $Z(u)$. They are defined as follows:

$$I_n^+ = I_n = c_n \frac{1}{\sin 2\alpha} \int_{-1}^{+1} \sin(\alpha(1+u)) P_n(u) du \qquad , \tag{34}$$

$$I_n^- = c_n \frac{1}{\sin 2\alpha} \int_{-1}^{+1} \sin(\alpha(1-u)) P_n(u) du = (-1)^n I_n \qquad , \tag{35}$$

$$Z_n = c_n \int_{-1}^{+1} Z(u) P_n(u) du \qquad . \tag{36}$$

The calculation of the Legendre moments of the trigonometric function $\sin(\alpha(1+u))/\sin 2\alpha$ denoted by I_n is described here. As a first step, the zero-order auxiliary functions Ω_0 and Θ_0 and the first-order auxiliary functions Γ_1 and H_1 are defined:

$$\Omega_0 = \frac{1}{\sin 2\alpha} \int_{-1}^{+1} \sin(\alpha(1+u)) P_0(u) du = \frac{\tan\alpha}{\alpha} \qquad , \tag{37}$$

$$\Theta_0 = \frac{1}{2\alpha \sin\alpha} \int_{-1}^{+1} \cos(\alpha u) P_0(u) du = \frac{1}{\alpha^2} \qquad , \tag{38}$$

$$\Gamma_1 = \frac{1}{\sin 2\alpha} \int_{-1}^{+1} \sin(\alpha(1+u)) P_1(u) du = \frac{1}{\alpha^2}\left(1 - \frac{\alpha}{\tan\alpha}\right) \qquad , \tag{39}$$

$$H_1 = \frac{1}{2\alpha \cos\alpha} \int_{-1}^{+1} \sin(\alpha u) P_1(u) du = \frac{1}{\alpha^2}\left(\frac{\tan\alpha}{\alpha} - 1\right) \qquad . \tag{40}$$

After twice integrating by parts in Eq. (34), the following recurrence relations are obtained for even n $(n = 2, 4, \ldots)$:

$$\Omega_n = \Omega_{n-2} - 2c_{n-1} H_{n-1} \qquad , \tag{41}$$

$$H_{n+1} = \frac{2c_n}{\alpha^2}\Omega_n + H_{n-1} \qquad , \tag{42}$$

$$\Theta_n = \Theta_{n-2} - \frac{2c_{n-1}}{\alpha^2}\Gamma_{n-1} \qquad , \tag{43}$$

$$\Gamma_{n+1} = 2c_n \Theta_n + \Gamma_{n-1} \qquad . \tag{44}$$

The Legendre moments of the trigonometric function $\sin(\alpha(1+u))/\sin 2\alpha$ can then be calculated as

$$I_n = \begin{cases} c_n \Omega_n, & \text{for even } n \\ c_n \Gamma_n, & \text{for odd } n \end{cases} \qquad . \tag{45}$$

If the source is given as a Legendre polynomial series (up to some arbitrary order L), then the particular solution is also given as a Legendre polynomial series and we can rewrite Eq. (33) for the Legendre moments of the one-dimensional flux as follows:

$$f_n = \left(f^+ + (-1)^n f^-\right) I_n - \left(\left(\sum_{l=0}^{L}\left(1+(-1)^{l+n}\right) b_l\right) I_n - b_n\right) \qquad . \tag{46}$$

This expression is valid for $\alpha^2 \neq 0$. When $\alpha^2 = 0$ we use the special form of the analytic solution (Eq. (31)) to obtain:

$$f_0 = \left[\frac{1}{2}\left(f^+ + f^-\right)\right] + p_0 \qquad ,$$

$$f_1 = \left[\frac{1}{2}\left(f^+ - f^-\right)\right] + p_1 \qquad , \tag{47}$$

$$f_n = p_n \qquad , n = 2, 3, \ldots, L+2 \qquad .$$

4 ASYMPTOTIC SOLUTION FOR SMALL EIGENVALUES

From Eqs. (15) we can conclude that the coefficient d_L will be divided $(L/2+1)$ times by α^2 in the expression for the b_0 coefficient. When the fundamental mode eigenvalue α^2 approaches zero a very large round-off error in the analytic expression for the one-dimensional flux, (Eq. (17)) and in expression (46) for the calculation of the flux moments can occur. When α^2 is equal to zero both expressions are undefined (because of division by α^2 in the recursive relations (15) for the calculation of the b_l coefficients). This problem was circumvented by developing a special form of the analytic solution when the eigenvalue α^2 is equal to zero (Eq. (31)) so that the calculation of the flux Legendre moments is facilitated through Eqs. (47).

The work in progress will require higher order terms in the Taylor series expansion (in α) of the analytic expression for the one-dimensional flux (Eq. (17)) for arbitrary order L of the polynomial source. The direct approach requires the Legendre polynomial coefficients of the particular solution (the b_l coefficients) to be expressed in terms of the Legendre polynomial coefficients of the source (the d_l coefficients). This requires the direct inversion of the upper-triangular matrix of the system of equations (15). Unfortunately, this direct inversion cannot be done recursively and the consequence is that the functional form of the Taylor series coefficients depends on the polynomial order L of the source.

The more elegant approach is to bridge the analytic solutions for non-zero and zero eigenvalues by developing a special form of solution for small eigenvalues. We derive that solution by applying an asymptotic expansion to Eq. (2) for the fundamental mode. (The source $Q(u)$ is given as a Legendre polynomial series (up to some arbitrary order L).) We again write the solution in the form given by Eq. (3).

Assuming that α^2 is small, we write the complementary part of the solution, and the contribution of the particular part of the solution, as the power series in α^2:

$$f_c(u) = f_c^{(0)}(u) + \alpha^2 f_c^{(1)}(u) + \alpha^4 f_c^{(2)}(u) + \ldots \quad , \tag{48}$$

$$f_p(u) = f_p^{(0)}(u) + \alpha^2 f_p^{(1)}(u) + \alpha^4 f_p^{(2)}(u) + \ldots \quad . \tag{49}$$

4.1 Asymptotic Solution of the Complementary Problem

After inserting Eq. (48) into Eq. (4) and equating terms with equal powers of α^2 we obtain the following system of equations:

$$\frac{\mathrm{d}^2 f_c^{(0)}(u)}{du^2} = 0, \qquad -1 \le u \le +1$$

$$\frac{\mathrm{d}^2 f_c^{(i)}(u)}{du^2} + f_c^{(i-1)}(u) = 0, \qquad -1 \le u \le +1, \qquad i = 1, 2, \ldots \quad , \tag{50}$$

with the following boundary conditions:

$$f_c^{(0)}(\pm 1) = f^{\pm},$$

$$f_c^{(i)}(\pm 1) = 0, \qquad i = 1, 2, \ldots \quad . \tag{51}$$

The problem satisfied by the function $f_c^{(0)}(u)$ is identical to the complementary problem for zero eigenvalue (given by Eqs. (20) and (21) in Subsection 2.1). Hence, the function $f_c^{(0)}(u)$ is actually the solution of the complementary problem for zero eigenvalue and it is given by Eq. (22).

We now recognize that the boundary value problem satisfied by the function $f_c^{(i)}(u)$ $(i = 1, 2, \ldots)$ is identical in its form to the problem given by Eqs. (23) and (24). Hence, we can follow the same solution procedure as in calculating the analytic form of the function $g_p(u)$ to obtain the function $f_c^{(i)}(u)$ as follows:

$$f_c^{(i)} = \frac{1}{2} f^+ \left[\sum_{n=0}^{2i+1} q_n^{(i)+} P_n(u) \right] + \frac{1}{2} f^- \left[\sum_{n=0}^{2i+1} q_n^{(i)-} P_n(u) \right], \qquad i = 1, 2, \ldots \tag{52}$$

where the coefficients $\underline{q}^{(i)\pm}$ are given by the following recurrence relation:

$$\underline{q}^{(i)\pm} = -\widehat{M}^{(2i)} \underline{q}^{(i-1)\pm}, \qquad , i = 1, 2, \ldots \quad . \tag{53}$$

Here $\underline{q}^{(i)\pm}$ are $(2i+2) \times 1$ column vectors of coefficients $q_n^{(i)\pm}$ and $\widehat{M}^{(2i)}$ is $(2i+2) \times (2i)$ rectangular matrix given by Eq. (30). Also,

$$\underline{q}^{(0)\pm} = col \left[\begin{array}{cc} 1 & \pm 1 \end{array} \right] \quad . \tag{54}$$

For example, we can write Eq. (52) for $i = 1$ explicitly as follows:

$$f_c^{(1)} = \frac{1}{2} f^+ \left[\frac{1}{3} P_0(u) + \frac{1}{15} P_1(u) - \frac{1}{3} P_2(u) - \frac{1}{15} P_3(u) \right]$$

$$+ \frac{1}{2} f^- \left[\frac{1}{3} P_0(u) - \frac{1}{15} P_1(u) - \frac{1}{3} P_2(u) + \frac{1}{15} P_3(u) \right] \quad . \tag{55}$$

We have noted earlier (in Subsection 2.1) that the function $g_c(u)$ (i.e. $f_c^{(0)}(u)$) is the zero-order term in the Taylor series expansion (in α) of the function $f_c(u)$ (function $f_c(u)$ is given by Eq. (6)). It is easy to show that the function $f_c^{(1)}(u)$ given by Eq. (55) is the next order term ($O(\alpha^2)$) in the same Taylor series expansion and, in general, that the function $f_c^{(i)}(u)$ given by Eq. (52) is $O(\alpha^{2i})$ term. It is also easy to show that

$$q_n^{(i)-} = (-1)^n q_n^{(i)+} \quad . \tag{56}$$

So, we can rewrite Eq. (52) as follows:

$$f_c^{(i)} = \sum_{n=0}^{2i+1} \left[f^+ + (-1)^n f^- \right] \frac{q_n^{(i)+}}{2} P_n(u) \quad . \tag{57}$$

We now insert Eq. (57) into Eq. (48) and truncate the asymptotic expansion after $M + 1$ terms to obtain:

$$f_{c,as}^{(M)}(u) = \sum_{i=0}^{M} \alpha^{2i} \sum_{n=0}^{2i+1} \left[f^+ + (-1)^n f^- \right] \frac{q_n^{(i)+}}{2} P_n(u) \quad . \tag{58}$$

After exchanging the summation order, we have:

$$f_{c,as}^{(M)}(u) = \sum_{n=0}^{2M+1} \left[f^+ + (-1)^n f^- \right] \left[\sum_{i=[n/2]}^{M} \frac{q_n^{(i)+}}{2} \alpha^{2i} \right] P_n(u) \quad . \tag{59}$$

Here [ ] denotes the largest integer part. The term in the second bracket we can identify as the power series approximation (in α^2) of the Legendre moments of the trigonometric function $\sin(\alpha(1+u))/\sin 2\alpha$:

$$I_{as,n}^{(M)}(\alpha) = \sum_{i=[n/2]}^{M} \frac{q_n^{(i)+}}{2} \alpha^{2i} \quad . \tag{60}$$

4.2 Asymptotic Approximation of the Contribution of the Particular Part

After inserting Eq. (49) into Eq. (7) and equating terms with equal powers of α^2 we obtain the following system of equations:

$$\frac{\mathrm{d}^2 f_p^{(0)}(u)}{du^2} = Q(u), \qquad -1 \leq u \leq +1$$

$$\frac{\mathrm{d}^2 f_p^{(i)}(u)}{du^2} + f_p^{(i-1)}(u) = 0, \qquad -1 \leq u \leq +1, \qquad i = 1, 2, \ldots \tag{61}$$

with the following boundary conditions:

$$f_p^{(0)}(\pm 1) = 0,$$

$$f_p^{(i)}(\pm 1) = 0, \qquad i = 1, 2, \ldots \qquad . \tag{62}$$

The problem satisfied by the function $f_p^{(0)}(u)$ is identical to the problem given by Eqs. (23) and (24) in Subsection 2.1. Hence, the function $f_p^{(0)}(u)$ is actually the solution of the contribution of the particular part of the solution for zero eigenvalue and it is given by Eq. (25) (or by Eq. (27) for polynomial source). We now recognize that the boundary value problem satisfied by any of the higher order functions $f_p^{(i)}(u)$ is identical in its form to the problem given by Eqs. (23) and (24). Hence, we can follow the same solution procedure as in obtaining the analytic form of the function $g_p(u)$ to obtain the functions $f_p^{(i)}(u)$ as follows:

$$f_p^{(i)}(u) = \sum_{n=0}^{L+2+2i} p_n^{(i)} P_n(u), \qquad i = 1, 2, \ldots \qquad , \tag{63}$$

where the coefficients $p_n^{(i)}$ are given by the following recurrence relation:

$$\underline{p}^{(i)} = -\widehat{M}^{(L+2i+1)} \underline{p}^{(i-1)}, \qquad i = 1, 2, \ldots \qquad . \tag{64}$$

Here $\underline{p}^{(i)}$ is the $(L + 2i + 3) \times 1$ column vector of coefficients $p_n^{(i)}$ and $\widehat{M}^{(L+2i+1)}$ is the $(L + 2i + 3) \times (L + 2i + 1)$ rectangular matrix given by Eq. (30). Also,

$$\underline{p}^{(0)} = \underline{p} = \widehat{M}^{(L+1)} \underline{d} \qquad . \tag{65}$$

It is possible (but not trivial!) to show that the function $f_p^{(i)}(u)$ given by Eq. (63) is the $O(\alpha^{2i})$ term in the Taylor series expansion (in α) of the function $f_p(u)$ given by Eq. (16). As we explained at the beginning of the Section 4, the difficulty in performing the Taylor series expansion of the Eq. (16) is that we have to express the Legendre polynomial coefficients of the particular solution (b_l coefficients) in terms of the Legendre polynomial coefficients of the source (d_l coefficients) explicitly. The consequence is that the functional form of the Taylor series coefficients will depend on the polynomial order of the source L. This is undesirable from a coding point of view. On the other hand, our recursive formula (64) generates the Taylor series coefficients explicitly.

We now insert Eq. (63) into Eq. (49) and truncate the asymptotic expansion after $M+1$ terms to obtain:

$$f_{p,as}^{(M)}(u) = \sum_{i=0}^{M} \alpha^{2i} \sum_{n=0}^{L+2+2i} p_n^{(i)} P_n(u) \qquad . \tag{66}$$

After exchanging the summation order, we have:

$$f_{p,as}^{(M)}(u) = \sum_{n=0}^{L+2(M+1)} \left[\sum_{i=i_{min}}^{M} p_n^{(i)} \alpha^{2i} \right] P_n(u) \qquad , \tag{67}$$

where

$$i_{min} = \begin{cases} 0, & n \le L+2 \\ \lceil (n-L-1)/2) \rceil, & L+3 \le n \le L+2M+2 \end{cases} \qquad . \tag{68}$$

The term in the bracket in Eq. (67) we can identify as the power series approximation (in α^2) of the Legendre moments of the contribution of the particular solution (given by Eq. (16)):

$$p_{as,n}^{(M)}(\alpha) = \sum_{i=i_{min}}^{M} p_n^{(i)} \alpha^{2i} \qquad . \tag{69}$$

We now can insert Eqs. (59) and (67) into Eq. (3) to obtain the asymptotic solution as follows:

$$f_{as}^{(M)}(u) = \sum_{n=0}^{2M+1} \left[f^+ + (-1)^n f^- \right] I_{as,n}^{(M)}(\alpha) P_n(u) + \sum_{n=0}^{L+2(M+1)} p_{as,n}^{(M)}(\alpha) P_n(u) \tag{70}$$

The Legendre moments of the asymptotic one-dimensional flux will be:

$$f_{as,n}^{(M)} = \left[f^+ + (-1)^n f^- \right] I_{as,n}^{(M)}(\alpha) + p_{as,n}^{(M)}(\alpha) \qquad . \tag{71}$$

The asymptotic solution given by Eq. (70) correctly limits to the solution for zero eigenvalue given by Eq. (31). We also note that only the first $L+2$ coefficients in the contribution of the particular part of the solution (p_n coefficients) are $O(0)$ quantities. It is obvious that it is not correct to use the solution for zero eigenvalue, (Eq. (31)) when the eigenvalue is small but not zero, since we are neglecting the higher-order asymptotic terms.

5 NUMERICAL EXAMPLES

In standard transverse integrated nodal diffusion codes the transverse leakage and the intra-nodal cross-section shape source are usually approximated by a quadratic polynomial.

In Table I we compare the analytic calculation of the Legendre moments of the one-dimensional solution (given by Eq. (46)) and the asymptotic one with $M = 2$ (given by Eq. (71)) and for two values of the fundamental mode eigenvalue: $\alpha^2 = 10^{-8}$ and $\alpha^2 = 0.01$. The Legendre coefficients of the source expansion are $d_0 = d_1 = d_2 = 1$ and the boundary conditions are $f^{\pm} = 1$.

The analytic calculation suffers from the round-off error (mostly due to analytic calculation of the Legendre moments of the trigonometric function $\sin(\alpha(1+u))/\sin 2\alpha$). This error is not removed even in a double precision calculation when $\alpha^2 = 10^{-8}$. Also, the round-off error is larger for higher order Legendre moments (the analytic formula in double precision calculation for $\alpha^2 = 10^{-2}$ gives only 3 significant digits for f_4). On the other hand, the asymptotic calculation has a truncation error of $O(\alpha^6)$ and this error can be reduced, if needed, by simply increasing the order of the asymptotic expansion M in Eq. (71).

Table I. Comparison of Analytic and Asymptotic Calculations of the Legendre Moments of the One-Dimensional Flux for $\alpha^2 = 0.01$ and $\alpha^2 = 10^{-8}$

	Double Precision			
	$\alpha^2 = 0.01$		$\alpha^2 = 10^{-8}$	
	Analytic	Asymptotic	Analytic	Asymptotic
f_0	0.735628	0.735628	1.945313	0.733333
f_1	-0.0667302	-0.0667302	1.717970	-0.0666667
f_2	0.235863	0.235863	-1.81905E+09	0.238095
f_3	0.0667408	0.0667408	-6.24629E+09	0.0666667
f_4	0.0285229	0.0285114	1.14600E+19	0.0285714

	Single Precision			
	$\alpha^2 = 0.01$		$\alpha^2 = 10^{-8}$	
	Analytic	Asymptotic	Analytic	Asymptotic
f_0	0.738011	0.735628	1.00000	0.733333
f_1	-0.0678539	-0.0667302	1.00000E+08	-0.0666667
f_2	-3.32609	0.235863	1.50000E+17	0.238095
f_3	4.00491	0.0667408	-3.50000E+17	0.0666667
f_4	2.24189E+04	0.0285114	-9.45000E+26	0.0285714

In the second example we consider the modified OECD-L-336 C5 Benchmark Problem [5]. Material data for this problem are given in Table II. Following [6], we changed the thermal fission cross in material 4 to produce a near-critical fundamental mode eigenvalue $\alpha^2 = 8.589616 \times 10^{-9}$. Results are summarized in Figure 1. Reference results are generated by the higher-order nodal diffusion code CASTOR [7] using one node per assembly mesh size and 6th order spatial approximation. (Higher-order calculation does not suffer from the round-off error since it utilizes the analytic solution of the within-group diffusion equation and the group removal cross-sections in this example are fairly large.) The ANM results are generated by the MGRAC code [8] also using one node per assembly mesh size. The MGRAC code utilizes the Taylor series expansions for the expressions for the nodal current-to-flux coupling coefficients, so there was no difficulty in obtaining results that are very close to the reference ones.

Table II. Material Parameters for Modified OECD-L-336 Benchmark Problem

Material	Group	D [cm]	Σ_a [cm^{-1}]	$\Sigma_s^{h\to g}$ [cm^{-1}]	$\nu\Sigma_f$ [cm^{-1}]
M1(UX)	1	1.20	0.009226	0.02043	0.00457
	2	0.40	0.092656	-	0.113525
M2(PuX)	1	1.20	0.0137912	0.0158634	0.00685243
	2	0.40	0.231602	-	0.344439
M3(Refl)	1	1.20	0.001	0.05	-
	2	0.40	0.04	-	-
M4(PuX)	1	1.20	0.0137912	0.0158634	0.00685234
	2	0.40	0.231602	-	0.29773208

Figure 1. Results for Modified OECD-L-336 Benchmark Problem

M1 1.460 1.460	M4 0.823 0.821
M2 1.241 1.243	M1 0.477 0.475

x.xxx: Ref. CASTOR Assembly Powers
x.xxx: MGRAC Assembly Powers

CASTOR k_{eff}=0.91855957
MGRAC k_{eff}=0.91875657

In the same MGRAC calculation we obtained the Legendre moments of the transverse-integrated one-dimensional fluxes. In Table III we give the Legendre moments of the one-dimensional fluxes in x-direction in node M4 calculated using the MGRAC code (analytic and asymptotic expressions) and the CASTOR code (reference results). The first harmonic mode solution is handled using analytical formula (the first harmonic eigenvalue is large and negative, $\alpha_1^2 = -68.536$). So, we compare the results when the fundamental mode solution is handled analytically (using Eq. (46)) and using the asymptotic formula (71) with $M = 2$. Although we used quadruple precision in the analytic calculation of the Legendre moments of the trigonometric function $\sin(\alpha(1+u))/\sin 2\alpha$, the analytic results still suffer from round-off error.

We note that the MGRAC Legendre moments of the transverse-integrated one-dimensional fluxes compare well to reference moments calculated via the higher-order calculation. This is encouraging for our future work that includes the calculation of the intra-nodal cross-section shape contribution, the construction of transverse-leakage moments, and the determination of intra-nodal homogeneous flux distributions.

6 CONCLUSIONS

We developed the local asymptotic solution of the one-dimensional transverse-integrated diffusion equation. When applied to calculation of the Legendre moments of the transverse-integrated flux, this solution gives round-off error free expressions in case of a near-critical node.The conditions under which a critical node may be encountered are rare in practice. However, errors in the analytic calculation of the Legendre moments can occur in nodes with relatively large eigenvalues (see first example).

We are currently developing models that require arbitrary order of the polynomial source expansion. The asymptotic solution developed in this paper provides for this requirement. Furthermore, the model is easily implemented in a computer code, since the same matrix (Eq. (30)) is used for any expansion order.

Table III. Legendre Moments of the One-Dimensional Flux in x-direction in Node M4

	Fast Flux			Thermal Flux		
	Analytic	Asymptotic	Reference	Analytic	Asymptotic	Reference
f_0	2.37500	2.71348	2.72062	0.164062	0.220875	0.221141
f_1	-1.65916	-1.66686	-1.66510	-0.120061	-0.120095	-0.126497
f_2	0.340948	0.00868399	0.00757123	0.127607	0.0903912	0.0912479
f_3	-0.000149735	-0.000426483	-0.00127049	-0.0133987	-0.0128055	-0.0104434
f_4	-0.0367151	-0.0313071	-0.0307598	0.0771101	0.0677983	0.0667826

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