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RATIONAL FUNCTION APPROXIMATION METHOD FOR DISCRETE ORDINATES PROBLEMS IN SLAB GEOMETRY

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ABSTRACT

In this work we use rational function approaches to obtain the transfer functions that appear in the spectral Green's function (SGF) auxiliary equations for one-speed isotropic scattering S_N equations in one-dimensional Cartesian geometry. For this task we use the computation of the Padé approximants to compare the results with the standard SGF method's applied to deep penetration problems in homogeneous domains. This work is a preliminary investigation of a new proposal for handling leakage terms that appear in the two transverse-integrated one-dimensional S_N equations in the exponential SGF method (SGF-ExpN). Numerical results are presented to illustrate the rational function approximation accuracy.

1. INTRODUCTION

Nodal methods (Badruzzaman, 1990) form a very accurate class of coarse-mesh methods for Cartesian geometry discrete ordinates (S_N) transport problems, where N is the angular quadrature set order. Larsen introduced the Extended Diamond (ED) method (Larsen, 1986). The numerical results generated by the ED method for one-speed S_2 problems in slab geometry are absolutely free from all spatial truncation errors. In 1990, a new method was introduced by Barros and Larsen (1990): the spectral Green's function (SGF) nodal method. In that work they described and tested the method for one-group slab-geometry S_N problems with linearly anisotropic scattering and a prescribed interior source and generated solutions that were completely free from spatial truncation errors. Two years later, the authors extended the method to generate solutions in two-dimensional Cartesian geometry (Barros and Larsen, 1992). Therefore, the SGF method developed for solving S_N problems in slab- geometry was generalized to solve the one-dimensional transverse-integrated nodal equations. Here, a "constant" approximation was used for the transverse leakage terms. The resulting SGF-Constant Nodal (SGF-CN) method has proved to be very accurate for deep penetration transport problems. The SGF-CN method treats the scattering source terms exactly and the only approximations involve the transverse leakage terms. For X-Y geometry, the authors (Barros and Larsen, 1991) tried an alternative treatment for the transverse-leakage terms by introducing the Expontential SGF (SGF-ExpN) method for homogeneous problems. In that work, the transverse-leakage terms were approximated by exponential functions. The exponential functions were chosen based on the physics of deep penetration problems, where

the neutron flux attenuates exponentially with increasing distance from the source. Later on, Mello and Barros (2002) generalized the SGF-ExpN method for calculations in heterogeneous domains considering a "partial anisotropy" in the exponential approximations. The present work appears as a preliminary investigation of a new proposal for handling transverse-leakage terms, based on a polynomial approach for the exponential approximations. Here we approximate the exponential and hyperbolic functions which are necessary for calculating the transfer functions (the Green's functions of the auxiliary equations of the SGF method) for monoenergetic linearly anisotropic scattering S_N equations in slab geometry, and we use Rational Functions – so called Padé approximants and we compare the results with the standard SGF method – already compared with the Diamond Difference (DD) results (Lewis and Miller Jr., 1993) by Barros and Larsen (1990) for the scalar flux.

2. MATHEMATICAL PRELIMINARIES

Let us consider the S_N equations in a slab-geometry with linearly anisotropic scattering [8]:

$$\begin{aligned}
&\mu_m \frac{d}{dx}\psi_m(x) + \sigma_t(x)\psi_m(x) = \frac{1}{2}\sigma_{s,0}\sum_{n=1}^{M}\psi_n(x)\,\omega_n + \frac{3}{2}\mu_m\sigma_{s,1}\sum_{n=1}^{M}\mu_n\psi_n(x)\,\omega_n + Q(x), \\
&m=1,...,N, \quad x \in D=\{x \in \mathbf{R} / 0 \le x \le a\}, \\
&\psi_m(0) = f_m, \quad \mu_m>0, \\
&\psi_m(a) = g_m, \quad \mu_m<0.
\end{aligned} \tag{1}$$

where we assume that source and cross sections are piecewise constant functions in *D*:

(x) Є D, 1≤ m ≤ M with M = N(N+2)/2

N = order of the angular quadrature

$\sigma_T(x)$ *= macroscopic total cross section*

$\sigma_{s,0}(x)$ *= zero'th component of the macroscopic differential scattering cross section*

$\sigma_{s,1}(x)$ *= first-order component of the macroscopic differential scattering cross section*

f_m *,* g_m *are prescribed incident fluxes on the outer boundaries of D.*

Q(x) = isotropic neutron source in D

2.1. The SGF method

Let consider the uniform grid Ω represented in Fig.1

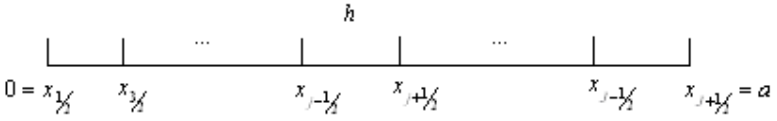

Figure 1. Grid Ω on a homogeneous slab.

h denote the width of the j'th spatial cell

Hold an arbitrary cell, one can think of $\psi_{m,j}$ as the interior cell-average angular flux in direction *m* due to the incoming cell-edge fluxes, $\psi_{n,j-\frac{1}{2}}$ for $\mu_m > 0$ and $\psi_{n,j+\frac{1}{2}}$ for $\mu_m < 0$, and the interior source *Q*. The auxiliary equation having the following form (Barros and Larsen, 1990)

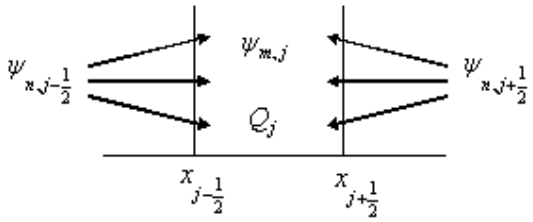

Figure 2. Arbitrary j'th cell

$$\psi_{m,j} = \sum_{n=1}^{N/2} \theta_{m,n} \psi_{n,j-\frac{1}{2}} + \sum_{n=N/2+1}^{N} \theta_{m,n} \psi_{n,j+\frac{1}{2}} + G_m(Q) \qquad (2)$$

where the $\theta_{m,n}$ play the role of the Green's function.

Our goal now is to test a polynomial approximation for the exponential and hyperbolic functions that appear in the calculation of the transfer functions (Green's functions) in the standard SGF one-dimensional problems. The transfer functions calculation are made through following system equations (see Barros and Larsen, 1990).

$$\left(\frac{2a_m(\nu_k)\nu_k}{h\sigma_t}\right)\sinh\left(\frac{h\sigma_t}{2\nu_k}\right) = \exp\left(-\frac{h\sigma_t}{2\nu_k}\right)\sum_{n=1}^{N/2} a_n(\nu_k)\,\theta_{m,n} + \exp\left(+\frac{h\sigma_t}{2\nu_k}\right)\sum_{n=\frac{N}{2}+1}^{N} a_n(\nu_k)\,\theta_{m,n} \qquad (3)$$

where ν_k and $a_n(\nu_k)$ are, respectively, eigenvalues and eigenvectors that appears in the standard one-dimensional SGF method.

2.2. The Padé Approximant

In general, the evaluation of an arbitrary function f(x) can be made when we seek to determine another function R(x) so that, for any desired value "x", the value of R(x) will be close enough to f(x) for the desired purpose. In this work, our purpose is to evaluate the exponential and hyperbolic functions in the equation (3). The arguments $(-\frac{h\sigma_t}{2\nu_k})$ of these functions indicates its spatial dependence through one-dimensional cell midpoint $\overline{x}_i \equiv (h_i / 2)$ as well as its dependence with the both material parameter σ_T and eigenvalues ν_k (k = 1, 2,..., N).
Thus, we can represent the exponential and hyperbolic functions "f(x)" as a polynomial expansion, using for Padé Approximant (Burden and Faires, 1985), this task

$$R(x) \equiv \frac{\sum_{k=0}^{M} a_k x^k}{1+\sum_{k=1}^{N} b_k x^k} \quad , \tag{4}$$

where $R(x)$ is the Padé approximant to the series and $M+N$ is the order of $R(x)$.

A Padé approximant, so called, is that rational function, of a specified order, whose power series expansions agrees with a given power series to the highest possible order. To find the "better" order for apply we tested some orders on Maple V Release computational program.

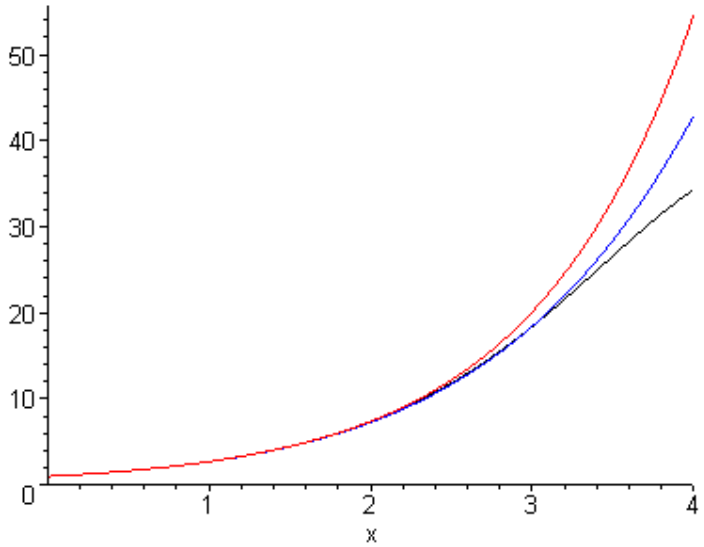

Figure 3. Representative curves for the exponential function, Mclaurin series and Padé Approximant.

The red curve indicate the exponential function; the black curve indicate the Padé Approximant for the exponential function by 5th order; the blue curve indicate the McLaurin series for the exponential function, by order 5th.

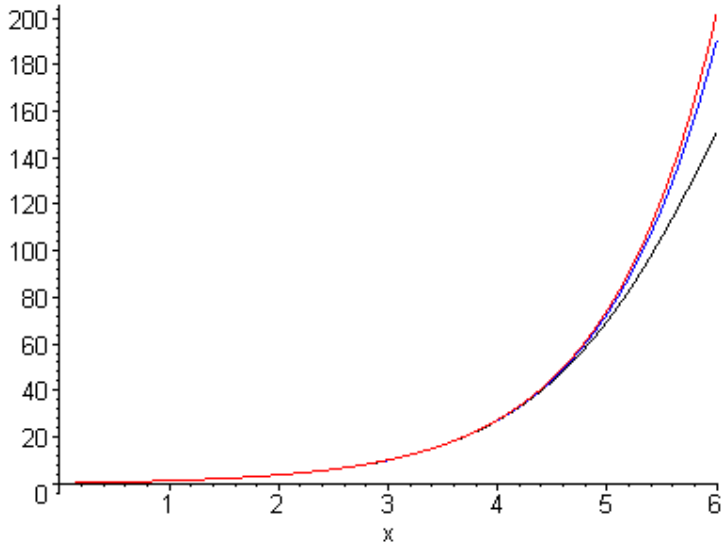

Figure 4. Representative curves for the hyperbolic function, Mclaurin series and Padé Approximant.

The Figure 4 shows the hyperbolic function aproximated use Pade Approximant by 9^{th} order. Here, we can see the "better" approximation for the hyperbolic function when we used a high-order to Padé Approximant.

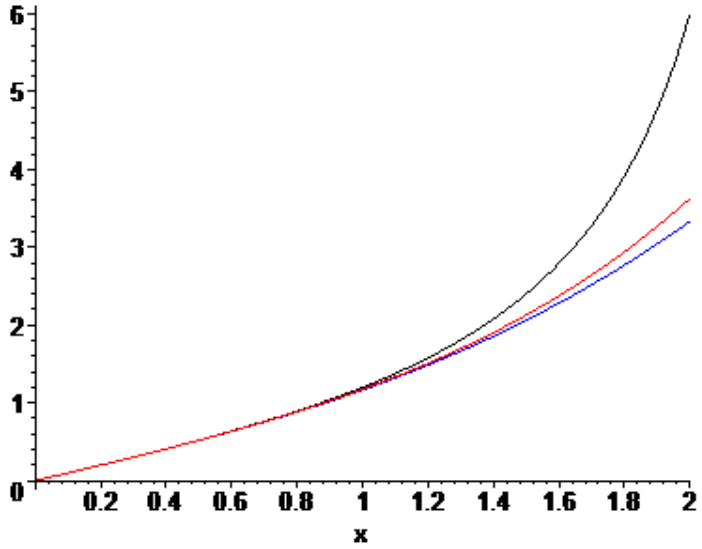

Figure 5. Representative curves for the hyperbolic function, McLaurin series and Padé Approximant in low-order.

When we used a low-order, as see in Figure 5, the representative curve (black curve) of Padé Approximant apply on the hyperbolic function results the "bad" approximation.

3. NUMERICAL RESULTS

In this paper we will consider only spatial homogeneous problems in the slab with total width a = 100cm and we will solve them using the S_2 Gauss-Legendre quadrature set, with varying number of spatial cells (2, 4, 10, 20, 50 and 100). The homogeneous slab has the following parameters:

Table 1. Material parameters of homogeneous slab.

Material	σ_T	σ_{S0}	σ_{S1}
1	1.0	0.99	0.80

The dimensions of all cross sections are in cm^{-1} .

We will use Padé Approximant to approximate the exponential and hyperbolic functions which are presents in equation (3) to obtain the values for the Green's functions, $\theta_{m,n}$. This values are very important just because its approximation gives us the response for this preliminary investigation about the Rational Functions approximation. We define the spatial domain $D=\{x \in R / 0 \leq x \leq a\}$ and construct on D an uniform grid Ω with $j = 1,2,..,J$ spatial cells, where the *j'th* spatial cell is denoted by Ω_j and h_j represents its width. Thus, the boundaries will be always $x = x_{1/2} = 0$ and $x = x_{J+1/2} = a$ and the interfaces for Ω_j belongs to the interval $[x_{j-1/2}, x_{j+1/2}]$. Clearly the Ω_j midpoint is $\overline{x}_j = [(x_{j-1/2} + x_{j+1/2})]/2 = x_{j-1/2} + (h_j / 2)$. The boundary conditions (written here for an arbitrary S_N quadrature set) are $\Psi_m(0) = 1.0$ for $\mu_m > 0$ (m = 1,2,...,N/2) and $\Psi_m(100) = 0.$ for $\mu_m < 0$ (m = (N/2)+1,..., N), and we consider there's no internal source (Q = 0) in all spatial domain.

Table 2. Numerical values for the Green's functions – 7th order Padé Approximant for exponential function and 9th order for hiperbolic function

Cell numbers	Padé approximant		SGF standard method	
	$\Theta_{1,1}$	$\Theta_{1,2}$	$\Theta_{1,2}$	$\Theta_{1,2}$
2	0.250722E+00	0.157094E+00	0.250756E+00	0.157114E+00
4	0.419785E+00	0.241998E+00	0.419785E+00	0.241998E+00
10	0.619854E+00	0.260343E+00	0.619854E+00	0.260343E+00
20	0.739759E+00	0.207417E+00	0.739759E+00	0.207417E+00
50	0.861331E+00	0.119716E+00	0.861331E+00	0.119716E+00
100	0.921463E+00	0.694601E-01	0.921463E+00	0.694601E-01

Table 3. Numerical values for the Green's functions – 5th order Padé Approximant for exponential function and 9th order for hiperbolic function

Cell numbers	Padé approximant		SGF standard method	
	$\Theta_{1,1}$	$\Theta_{1,2}$	$\Theta_{1,2}$	$\Theta_{1,2}$
2	0.252296E+00	0.158054E+00	0.250756E+00	0.157114E+00
4	0.419824E+00	0.242015E+00	0.419785E+00	0.241998E+00
10	0.619854E+00	0.260343E+00	0.619854E+00	0.260343E+00
20	0.739759E+00	0.207417E+00	0.739759E+00	0.207417E+00
50	0.861331E+00	0.119716E+00	0.861331E+00	0.119716E+00
100	0.921463E+00	0.694601E-01	0.921463E+00	0.694601E-01

Table 4. Numerical values for the Green's functions – 4th order Padé Approximant for exponential function and 7th order for hiperbolic function

Cell numbers	Padé approximant		SGF standard method	
	$\Theta_{1,1}$	$\Theta_{1,2}$	$\Theta_{1,1}$	$\Theta_{1,2}$
2	0.261993E+00	0.163954E+00	0.250756E+00	0.157114E+00
4	0.420260E+00	0.242207E+00	0.419785E+00	0.241998E+00
10	0.604631E+00	0.253946E+00	0.619854E+00	0.260343E+00
20	0.739759E+00	0.207417E+00	0.739759E+00	0.207417E+00
50	0.861331E+00	0.119716E+00	0.861331E+00	0.119716E+00
100	0.921463E+00	0.694601E-01	0.921463E+00	0.694601E-01

Table 5. Numerical values for the Green's functions – 3th order Padé Approximant for exponential function and 5th order for hiperbolic function

Cell numbers	Padé approximant		SGF standard method	
	$\Theta_{1,1}$	$\Theta_{1,2}$	$\Theta_{1,1}$	$\Theta_{1,2}$
2	0.213828E+00	0.134471E+00	0.250756E+00	0.157114E+00
4	0.415962E+00	0.240312E+00	0.419785E+00	0.241998E+00
10	0.619692E+00	0.260368E+00	0.619854E+00	0.260343E+00
20	0.739743E+00	0.207426E+00	0.739759E+00	0.207417E+00
50	0.861330E+00	0.119717E+00	0.861331E+00	0.119716E+00
100	0.921463E+00	0.694601E-01	0.921463E+00	0.694601E-01

4. CONCLUSIONS

The results presented in Tables 2, 3, 4 and 5, demonstrate the accuracy of the Rational Function use Pade Approximant poynomial method for our pourpose that were appoximate the exponential and hyperbolic functions that go before the Green's functions calculations through the linear system given by equation (3). The Rational Function were implemented through Padé Approximant (Burden and Faires, 2001). In the Tables 2, 3, 4 and 5, the shaded lines indicate the "bad" results. Increasing these orders, even for coarse meshes, we obtain better results, as see in Table 2. It is very important accentuate that Green's functions has directly impact on the scalar flux calculations. Note that, the order for aproximated the

hiperbolic function is very important. Low-order results in "bad" aproximation for this function. We hope in future work use the Padé Aproximant approach presented here associated with the leakage terms in the one-dimensional transverse-integrated S_N equations for X-Y Cartesian problems.

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