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A POLYNOMIAL ANALYTICAL SOLUTION TO THE ONE-SPEED NEUTRON TRANSPORT EQUATION IN SLAB GEOMETRY UNDER INHERENTLY VERIFIED MARK-MARSHAK BOUNDARY CONDITIONS

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Boubaker polynomials are used to obtain analytical solutions to the one-speed neutron transport equation for strongly anisotropic scattering. The main advantage of the method lies in proposing solution terms which verify inherent symmetry and Mark-Marshak boundary conditions prior to resolution process. This original feature results in convergent and accurate solutions. Boubaker polynomials expansion scheme is further applied to homogeneous slab problem with strongly anisotropic scattering and vacuum boundaries. Parallel to the classical formulation, the kernels for scattered and fission neutrons are originally chosen on the basis of most realistic models. The results, expressed in terms of linear extrapolation distance d_e, are recorded and compared to those presented in the related literature.

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1. *Introduction*

During the past few decades, polynomial expansion analysis has played an important role in the methods for solving the one-speed neutron transport equation. The earliest known form of this equation has been presented by Davison [1] and treated by Case's singular eigenfunction expansion method (Case) [2, 3]. Consecutively, attempts to develop approximated solution have been performed by Bowden et al. [4], Bell and Glasstone [5] and many others.

In the present work, a polynomial expansion scheme is proposed in order to yield analytical solutions to the one-speed neutron transport equation. The main feature of the proposed protocol is verifying inherently and conjointly symmetry and Mark-Marshak boundary conditions. These conditions are ensured mainly prior to the resolution process, which makes this latter convergent and quicker than those proposed in the present literature.

2. Theory

2.1. The one-speed neutron transport equation in slab geometry

The considered system is a homogeneous slab extending, in one dimension, from $x = -a$ to $x = a$, bounded by a vacuum (Fig. 1).

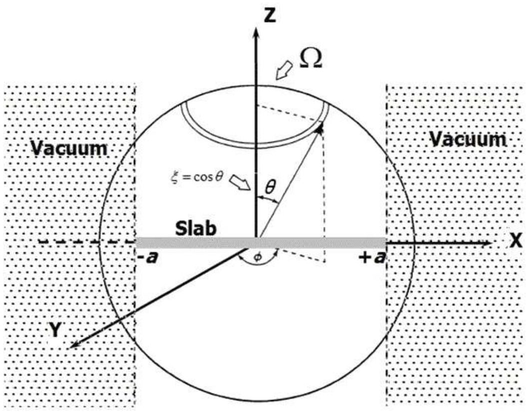

Fig. 1. Slab geometry.

In this plane geometry, the one-speed neutron transport equation (Davison) [1] is

$$\xi \frac{\partial \phi(x,\xi)}{\partial x} + \Omega_T \phi(x,\xi) = \Omega_S \int_{-1}^{1} \widetilde{k}_S(\xi,\xi')\phi(x,\xi')\mathrm{d}\xi' + \bar{\nu}\Omega_F \int_{-1}^{1} \widetilde{k}_F(\xi,\xi')\phi(x,\xi')\mathrm{d}\xi', \quad (1)$$

where x is the spatial coordinate, ξ the direction cosine of the angle between the neutron velocity and x-axis before scattering, ϕ the steady-state angular flux/flux density of neutrons, Ω_T the total cross section, Ω_S the scattering cross section, Ω_F the fission cross-section, $\bar{\nu}$ the mean number of neutrons emitted per fission, $\widetilde{k}_S$ the kernel for scattered neutrons, $\widetilde{k}_F$ kernel for fission neutrons and ξ' the direction cosine of the angle between the neutron velocity and x-axis after scattering.

$\widetilde{k}_F(\xi,\xi')$ represents the $2a$-thick slab one-dimensional fission kernel. Since the fission is supposed to be an isotropic event in local reference frames, this kernel is presumed to be constant (Yilmazer) [6]:

$$\widetilde{k}_F(\xi,\xi') = \frac{1}{2}\,. \tag{2}$$

The expression for $\widetilde{k}_S$,the kernel for scattered neutrons, is chosen according to the backward-forward-isotropic model (Yilmazer and Tombakoglu [7]; Yaşa [8]):

$$\widetilde{k}_S = \widetilde{k}_l + \widetilde{k}_f + \widetilde{k}_b,$$

where

$$\widetilde{k}_l = \frac{1}{2}(1-p_f-p_b)(1+3q\xi\xi')\,, \quad \widetilde{k}_f = \delta(\xi-\xi')\times p_f\,, \quad \widetilde{k}_b = \delta(\xi+\xi')\times p_b\,, \tag{3}$$

where p_f are the forward-scattering probabilities in a collision, p_b are the backward-scattering probabilities in a collision and q is the mean cosine of scattering angle.

In Eq. (3), $\widetilde{k}_l$ expresses linearly anisotropic scattering, while $\widetilde{k}_f$ and $\widetilde{k}_b$ represent the forward and backward scattering, respectively.

By affecting numerical values to the kernels and expressing both x and a in mean-free-path units, Eq. (1) becomes

$$\xi\frac{\partial\phi(x,\xi)}{\partial x} + \phi(x,\xi) = \int_{-1}^{1} h(\xi,\xi')\phi(x,\xi')\mathrm{d}\xi', \tag{4}$$

where

$$h(\xi,\xi') = \frac{\Omega_S}{\Omega_T}(0.08 + 0.42\delta(\xi-\xi') + 0.42\delta^2(\xi+\xi') + \frac{\nu\Omega_F}{2\Omega_T}\,.$$

In this way, the symmetry and Mark-Marshak boundary conditions have been imposed. The Mark-Marshak boundary conditions concern mainly the incoming current and the continuity of the angular flux at boundaries, which implies, among others, the continuity of all angular moments of the neutron flux across the vacuum edges ($x = \pm a$ planes),

$$\phi(x,\xi)\big|_{x=+a,\,\xi<0} = \phi(x,\xi)\big|_{x=-a,\,\xi>0} = 0\,. \tag{5}$$

It has been admitted that these conditions are difficult to simulate. Yilmazer and Tombakoglu [7] stated that even they can be replaced by imposing a zero incoming angular flux at the boundaries for some specific values of ξ.

On the other hand, the studied system symmetry imposes

$$\phi(-x,\xi)\big|_{x\in[-a,a]} = \phi(x,\xi)\big|_{x\in[-a,a]}\,. \tag{6}$$

2.2. Glossary and resolution historic

The earliest known approximated solution to the one-speed neutron transport equation is mostly attributed to Davison [1], followed by Case [2] and Case and Zweifel [3]. Their studies were the first attempts to convert the one-speed neutron transport equation to an algebraic set of eigenvalue equations within a spectral domain. Later, Bowden et al. [4] transformed the one-speed neutron transport integro-differential equation plane geometry into a singular integral equation. This transformation was used and enhanced by Bell and Glasstone [5], Kaper et al. [9], Greenberg et al. [10].

Several methods were proposed in the last two decades, particularly in the case of finite slabs, such as the diamond difference implicit trapezoidal (Barros et al.) [11], the two-region system for the scalar neutron flux (Garis) [12], the differential approximations (Su [13]) and the multiple collision (De Oliveira et al.) [14] methods.

Polynomial approximation methods for the solution of transport problems have been firstly applied by Conkie [15] for the solution in slab geometry. Some polynomial approximations have also been proposed by Levermore and Pomraning [16] and Pomraning et al. ([17 − 20]) who developed a flux-limited diffusion theory in models of radiation hydrodynamics, and Ganapol [21] who proposed the use of perturbation to develop a numerical method for solving the one-dimensional transport problem by polynomial reconstruction. In some recent studies (Anli et al., [22]; Yaşa et al. [23]), polynomials expansions have been successfully applied in eigenvalue spectrum calculations and criticality of bare/reflected slab geometries for isotropic scattering.

A complete glossary of the resolution methods has been detailed by Sahni and Sjöstrand [24]. The motivation of this panoply of attempts can be summarized through the sentence of Sahni [25]: "*...this problem is very complex and a rich source of interesting mathematical problems. Lot more work still remains to be done*".

2.3. Boubaker polynomials related properties

The Boubaker polynomials $B_m(X)$ have been established as-such by Oyedum et al. [26] and Zhang et al. ([27 − 29]). Their particularities have been exploited and discussed in several publications (Ghrib et al. [30]; Slama et al. [31]; Zhao et al. [32]; Awojoyogbe and Boubaker [33]; Ghanouchi et al. [34]; Fridjine et al. [35]; Tabatabaei et al. [36]; Belhadj et al. [37]; Lazzez et al. [38]; Guezmir et al. [39]; Yildirim et al. [40]; Dubey et al. [41]).

Zhang [29] and Ben Mahmoud [42] stated that $B_m(X)$ explicit monomial form raised some singularities for the indices $4q$. It has been demonstrated that for these indices, the $2q$-rank monomial term vanished in the manner that $B_{4m}(X)$ expression is reduced to have $2q-1$ effective terms. The corresponding $4q$th-order Boubaker polynomials are presented in Eq. (7) as a general form, and in Eq. (8)

the first functions,

$$B_{4q}(X) = 4\sum_{p=0}^{2q}\left[\frac{q-p}{4q-p}\,C_{4q-p}^{p}\right](-1)^p X^{2(2q-p)}\,. \tag{7}$$

So we have:

$$B_0(X) = 1\,,$$

$$B_4(X) = X^4 - 2\,,$$

$$B_8(X) = X^8 - 4X^6 + 8X^2 - 2\,,$$

$$B_{12}(X) = X^{12} - 8X^{10} + 18X^8 - 35X^4 + 24X^2 - 2\,, \tag{8}$$

$$B_{16} = X^{16} - 12X^{14} + 52X^{12} - 88X^{10} + 168X^6 - 168X^4 - 48X^2 - 2\,,$$

$$B_{20} = X^{20} - 16X^{18} + 102X^{16} - 320X^{14} + 455X^{12} - 858X^8 + 1056X^6 - 495X^4 + 80X^2 - 2\,.$$

Figure 2 presents the graphics of the first $4q$-order Boubaker polynomials. Zhao et al. [32] conjectured from these graphics that the number of real positive roots is $2q-1$, and that they are contained exclusively in the domain [0;2].

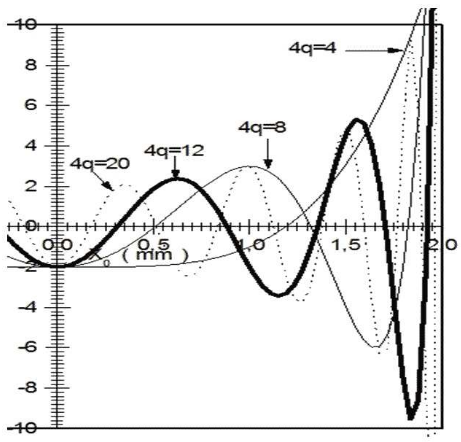

Fig. 2. Graphic representation of the first $4q$-order Boubaker polynomials.

Many arithmetical and differential properties of the Boubaker polynomials have been demonstrated (Zhao and Naing [43]), for example,

$$B_{4(q+1)} = (X^4 - 4X^2 + 2)B_{4q}(X) - B_{4(q-1)}(X) = B_4^*(X)B_{4q}(X) - B_{4(q-1)}(X), \tag{9}$$

$$B_{4q}^2(X)-B_{4(q-1)}(X)B_{4(q+1)}(X)=X^2(X^2-1)^2(3X^2+4)=B_8^*(X), \quad \forall q>1 \quad (10)$$

and

$$\sum_{q=1}^{n} B_{4q}^2(x) = \frac{1}{2x(2x^2-4)}\left[B'_{4(n+1)}(x)B_{4n}(x) - B'_{4n}(x)B_{4(n+1)}(x) - 4x^3\right]. \quad (11)$$

The existence of a specific generating function and a unique imaginary root has been demonstrated by Zhao and Naing [43] who demonstrated also that each $4q$-order Boubaker polynomial has exactly $4q-2$ real roots, contained exclusively in the domain [-2;2]. Tabatabaei et al. [36] and Khélia et al. [44] outlined the arithmetical properties of the $B_{4n}(X)$ minimal real positive root denoted α_n. These properties gave the fundaments of the Boubaker polynomials expansion scheme (BPES), which was used for the first time by S. Fridjine et al. (2009) [35] and S. Lazzez et al. [38] in different applied physics studies.

While solving a Cauchy boundary-type differential equation, the advantage of the BPES lies in embedding the exogenous boundary condition thanks to properties of $4q$-Boubaker polynomials:

i) Values at boundaries, in the reduced real domain $[0;\alpha_q]$

$$\sum_{q=1}^{N} B_{4q}(x)\Big|_{x=0} = -2N \neq 0\,, \qquad \sum_{q=1}^{N} B_{4q}(x)\Big|_{x=\alpha_q} = 0\,. \quad (12)$$

ii) first derivatives values at boundaries,

$$\sum_{q=1}^{N} \frac{\mathrm{d}B_{4q}(x)}{\mathrm{d}x}\Bigg|_{x=0} = 0\,, \qquad \sum_{q=1}^{N} \frac{\mathrm{d}B_{4q}(x)}{\mathrm{d}x}\Bigg|_{x=\alpha_q} = \sum_{q=1}^{N} H_q\,, \quad (13)$$

where

$$H_n = B'_{4n}(\alpha_n) = \frac{4\alpha_n(2-\alpha_n^2)\sum_{q=1}^{n} B_{4q}^2(\alpha_n)}{B_{4(n+1)}(\alpha_n)} + 4\alpha_n^3 \quad (14)$$

and

iii) second-derivative values at boundaries

$$\sum_{q=1}^{N} \frac{\mathrm{d}^2B_{4q}(x)}{\mathrm{d}x^2}\Bigg|_{x=0} = \frac{8}{3}N(N^2-1)\,, \qquad \sum_{q=1}^{N} \frac{\mathrm{d}^2B_{4q}(x)}{\mathrm{d}x^2}\Bigg|_{x=\alpha_q} = \sum_{q=1}^{N} G_q\,, \quad (15)$$

with

$$G_q = \frac{\mathrm{d}^2B_{4q}(x)}{\mathrm{d}x^2}\Bigg|_{x=\alpha_q} = \frac{3\alpha_q(4q\alpha_q^2+12q-2)H_q - 8q(24q^2\alpha_q^2+8q^2-3q+4)}{(\alpha_q^2-1)(12q\alpha_q^2+4q-2)}\,.$$

The last condition (iii) is deduced from the second-order differential equation established by Labiadh et al. [45]:

2.4. Resolution protocol

The standard formulation for the one-speed neutron transport equation, including the main boundary conditions, and as deduced from Eqs. (4) − (6), is

$$\xi \frac{\partial \phi(x,\xi)}{\partial x} + \phi(x,\xi) = \int_{-1}^{1} h(\xi,\xi')\phi(x,\xi')\mathrm{d}\xi', \tag{16}$$

where $\phi(x,\xi)\Big|_{x=\pm a, \xi<0} = 0\,, \qquad \phi(-x,\xi)\Big|_{x\in[-a,a]} = \phi(x,\xi)\,.$

According to the established definition (Zhao et al. [32]; Tabatabaei et al. [36]; Belhadj et al. [37]; Yildirim et al. [40]; Dubey et al. [41]), the $4n$-Boubaker polynomials expansion scheme (BPES) is applied to Eq. (16) by applying the expression

$$\phi(x,\xi) = \frac{1}{2N_0}\sum_{q=1}^{N_0} \omega_q B_{4q}(\left(x\frac{\alpha_q}{a}\right) B_{4N_0}(2\xi)\,, \tag{17}$$

where α_q is the $4q$-Boubaker polynomial minimal root, N_0 is a prefixed integer, and $\omega_q\big|_{q=1,\ldots,N_0}$ are unknown real coefficients.

The main advantage of this formulation consists undoubtedly in verifying inherently both symmetry and Mark-Marshak boundary conditions.

This way, Eq. (16) is equivalent to the unique equation

$$\xi \sum_{q=1}^{N_0} \omega_q \frac{\alpha_q}{a} \frac{\mathrm{d}\left\langle B_{4q}\left(x\alpha_q/a\right)\right\rangle}{\mathrm{d}x} B_{4N_0}(2\xi) + \sum_{q=1}^{N_0} \omega_q B_{4q}\left(x\frac{\alpha_q}{a}\right) B_{4N_0}(2\xi)$$

$$= \int_{-1}^{1} h(\xi,\xi') \sum_{q=1}^{N_0} \omega_q B_{4q}\left(x\frac{\alpha_q}{a}\right) B_{4N_0}(2\xi')\mathrm{d}\xi'\,, \tag{18}$$

which is equivalent, by integrating along the interval $[a,+a]$ for x and $[1,+1]$ for ξ, to the equation

$$\sum_{q=1}^{N_0} \omega_q A_q = \sum_{q=1}^{N_0} \omega_q A'_q\,, \tag{19}$$

with

$$A_q\Big|_{1\le q\le N_0} = \int_{-a}^{a}\left[\int_{-1}^{1}\left(\frac{\xi\alpha_q}{a}B'_{4q}\left(x\frac{\alpha_q}{a}\right) + B_{4q}\left(x\frac{\alpha_q}{a}\right)\right) B_{4N_0}(2\xi)\mathrm{d}x\right]\mathrm{d}\xi\,,$$

$$A'_q\Big|_{1\leq q\leq N_0} = \int\limits_{-a}^{a}\left[\int\limits_{-1}^{1}\left[\int\limits_{-1}^{1} h(\xi,\xi')B_{4q}\left(x\frac{\alpha_q}{a}\right)B_{4N_0}(2\xi')\mathrm{d}\xi'\right]\mathrm{d}\xi\right]\mathrm{d}x\,. \qquad (20)$$

These integrals are calculated thanks to the $4q$-Boubaker polynomial database along with the knowledge of the global kernel $h(\xi,\xi')$ (Eq. (3)). A solution to the main equation is obtained by determining the set of coefficients $\omega_q^{\mathrm{opt}}\big|_{q=1,\ldots,N_0}$ which minimises the function η_{N_0},

$$\eta_{N_0} = \left(\sum_{q=1}^{N_0}\omega_q^{\mathrm{opt}}A_q - \sum_{q=1}^{N_0}\omega_q^{\mathrm{opt}}A'_q\right)^2. \qquad (21)$$

The obtained solution is finally presented as a continuous and indefinitely derivable expression

$$\phi(x,\xi) = \frac{1}{N_0}\sum_{q=1}^{N_0}\omega_q^{\mathrm{opt}}B_{4q}\left(x\frac{\alpha_q}{a}\right)B_{4N_0}(2\xi)\,. \qquad (22)$$

Among the parameters deduced from the solution, like the eigenvalues spectrum, the extrapolated end point and slab critical size, the relevancy of the linear extrapolation distance d_e has been outlined by many studies (Yilmazer and Tombakoglu [7]; Yaşa [8]; Yilmazer [6]).

This parameter is defined as the distance outside the physical boundary at which a linear extrapolation reaches zero. From a mathematical point of view, there are many ways to define this extrapolation distance (Woznicka [46]; Dahl and Sjöstrand [47]; Pomraning and Szilard [48]. Most commonly, the linear extrapolated distance d_e is defined as the distance from a vacuum boundary at which the asymptotic flux (extended by its natural curvature with distance) vanishes (Fig. 3).

In the actual study, the linear extrapolation distance d_e is calculated as the absolute value of the ratio of the asymptotic flow to its derivative in the direction perpendicular to the surface,

$$d_e = \left|\left(\phi(x,\xi)\Big|_{x=0}\Big/\frac{\mathrm{d}\phi(x,\xi)}{\mathrm{d}x}\Big|_{x=0}\right)_{\xi=0}\right|. \qquad (23)$$

Since the remaining variable parameters in Eq. (4) are solely Ω_S, Ω_T, Ω_F and $\bar{\nu}$, the obtained values of d_e have been indexed on the synthetic parameter c which represents the mean number of secondary neutrons per collision

$$c = \frac{\Omega_S + \bar{\nu}\Omega_F}{\Omega_T}\,. \qquad (24)$$

The obtained values of d_e, for various values of c and for $N_0 = 7$ are presented in Fig. 4, along with the precedent results published by Yaşa [8] and Davison [1].

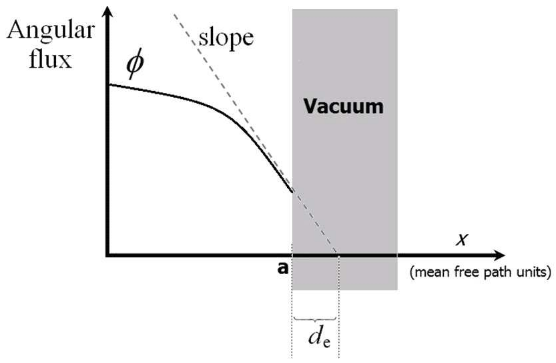

Fig. 3. The linear extrapolation distance d_e.

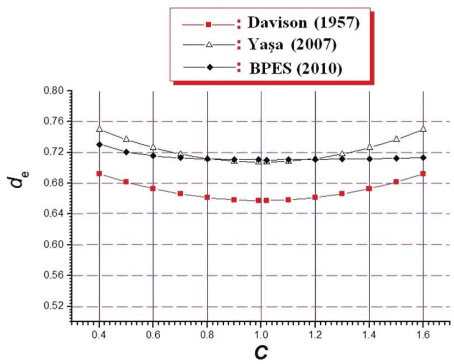

Fig. 4. Values of d_e versus c along with precedent results (Yaşa [8], Davison [1]).

3. Discussion and perspectives

Figure 4 presents calculated linear extrapolation distance d_e for various values of collision parameter c, in comparison with the integral transport results of Yaşa [8] and Davison [1] for the cases of strongly backward-forward and linearly anisotropic scattering.

A complete agreement with the results of Yaşa [8] can be observed for values of c around unity ($c \approx 1.0$) or in the diffusion limit for close backward and forward scattering probabilities. Inconsistencies encountered regarding the earliest solution Davison [1] have been discussed previously by Williams [49]. It has been stated that under the presumption of anisotropic fission kernel, approximations used by Davison [1] may not converge or converge slowly. More importantly, differences encountered at limiting cases of a highly reflecting ($c \approx 0.4$) or a purely absorbing ($c \approx 1.6$) medium, could easily be explained by the fact that scattering and fission kernels have been handled, by the referred model, as two independent parameters, far from the actual study's embedded kernels approach.

On the other hand, it should be remarked that the actually used polynomial procedure is in some sense an analytical ordinate one but in which symmetry and boundary conditions are definitely ensured before final resolution. This feature lightens drastically the resolution system size and hence avoids inaccuracies that discrete ordinate procedures encounter when the integrand is too ill-behaved (Bowden and Bullard [50]) to be approximated by a polynomial expansion. In this context, it could be mentioned that the "*difficulties in convergence encountered with polynomial methods*" evoked by Yildiz [51] and Williams [49], could have been avoided if boundary conditions were not forced at the same level as the main equation during the resolution process.

4. *Conclusion*

In this study, a recently proposed version of the Boubaker polynomials expansion scheme (BPES), which was used in several applied and theoretical physics problems, has been further developed to slab geometry for strongly anisotropic scattering. Backward-forward isotropic model has been chosen for the scattering kernel as a combination of linearly anisotropic and strongly backwardforward kernels. Further to that, the realistic approach of using an isotropic fission kernel in the transport equation has been implemented.

The obtained values of the linear extrapolation distance d_e are almost in complete agreement with the recent literature data except for some limiting cases. More importantly, it is observed that precedent models, which considered the same kernels for fission and scattering, yielded deviations in linear extrapolation distances in comparison with the values presented in the literature of the last decades.

Regarding the convergence and speed of the resolution process, it has been noted that the establishment of polynomials expansions which verify conjointly and inherently symmetry and Mark-Marshak boundary conditions reduces calculation systems size and produces faster convergent results.

The obtained results can easily be extended to the more general case where the scattering can be approximated functionally as a self-standing polynomial expansion expressing strongly backward/forward kernel components. This approximation awaits to be exploited later.

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POLINOMNO ANALITIČKO RJEŠENJE ZA JEDNOBRZINSKO RAZLAŽENJE NEUTRONA U SLOJU UZ PROVJERENO SADRŽANE MARK-MARSHAKOVE GRANIČNE UVJETE

Primjenjuju se Boubakerovi polinomi za dobivanje analitičkog rješenja jednadžbe za razlaženje neutrona jedne brzine pri jako anizotropnom raspršenju. Osnovna prednost metode sastoji se u traženju rješenja preko članova koji provjeravaju unutarnju simetriju i Mark-Marshakove granične uvjete prije postupka razvoja. Ta izvorna odlika vodi na konvregentna i točna rješenja. Boubakerova se polinomna shema razvoja zatim primjenjuje na problem jednolikog sloja s jako neizotropnim raspršenjem i granicama s vakuumom. Usporedo s klasičnim predstavljanjem, jezgre za raspršene i diobene neutrone se izvorno odabiru na osnovi najstvarnijih modela. Ishodi računa, izraženi preko linearne ekstrapolacijske duljine d_e, prikazuju se i uspoređuju s objavljenima.