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ON PROGRESS OF THE SOLUTION OF THE STATIONARY 2-DIMENSIONAL NEUTRON DIFFUSION EQUATION: A POLYNOMIAL APPROXIMATION METHOD WITH ERROR ANALYSIS

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ABSTRACT

Recently the stationary neutron diffusion equation in heterogeneous rectangular geometry was solved by the expansion of the scalar fluxes in polynomials in terms of the spatial variables (x, y), considering the two-group energy model. The focus of the present discussion consists in the study of an error analysis of the aforementioned solution. More specifically we show how the spatial subdomain segmentation is related to the degree of the polynomial and the Lipschitz constant. This relation allows to solve the 2-D neutron diffusion problem for second degree polynomials in each subdomain. This solution is exact at the knots where the Lipschitz cone is centered. Moreover, the solution has an analytical representation in each subdomain with supremum and infimum functions that shows the convergence of the solution. We illustrate the analysis with a selection of numerical case studies.

1. INTRODUCTION

The neutron diffusion problem is until now predominantly solved by means of numerical procedures, traditionally by finite differences (FDM) and finite elements techniques (FEM). Several examples of these solutions can be found in references [3, 4, 5]. In other way, the authors of [1, 2] solved the neutron diffusion equation in analytical way. Following this direction, in previous works the authors presented a solution in analytical representation to one dimensional diffusion and kinetics problems [6, 7]. This approach is extended to the stationary neutron diffusion equation in heterogeneous rectangular geometry considering the two-group energy model. The procedure to solve the equation system is based on a segmentation of the domain, where in each segment the solution is approximated by the expansion of the scalar fluxes in polynomials in terms of the spatial variables (x, y). As this expansion is local and centered at the element center (where the series truncation provides no error), it's secure to say that the complete solution for the neutron scalar flux is exact for a finite set of points. Also, due to its direct applicability

on the algorithm itself, it's convenient to state that the expression for the neutron scalar flux has a legit error control scheme, securing the convergence by the mesh size control. Therefore, the focus of the present discussion consists in the study of an error analysis of the aforementioned solution. More specifically we show how the spatial subdomain segmentation is related to the degree of the polynomial and the Lipschitz constant. This relation allows to solve the 2-D neutron diffusion problem for second degree polynomials in each subdomain. This solution is exact at the knots where the Lipschitz cone is centered. Moreover, the solution has an analytical representation in each subdomain with supremum and infimum functions that shows the convergence of the solution. In the following we illustrate the analysis with a selection of numerical case studies.

2. THE NEUTRON DIFFUSION PROBLEM

The starting point for the forthcoming discussion is given by the multi-group neutron diffusion equation considering two cartesian dimensions and constant nuclear parameters,

$$-D_g\left(\frac{\partial^2\phi_g}{\partial x^2}+\frac{\partial^2\phi_g}{\partial y^2}\right)+\Sigma_{r_g}\phi_g-\sum_{g'=1}^{g-1}\Sigma_{s_{g'\to g}}\phi_{g'}=\frac{1}{k_{eff}}\chi_g\sum_{g'=1}^{G}\nu_{g'}\Sigma_{f_{g'}}\phi_{g'}\ . \tag{1}$$

Here $g=1,2\ldots G$ are the energy groups, D_g represents the diffusion coefficient, Σ_{r_g}, Σ_{f_g} and $\Sigma_{s_{g'\to g}}$ are the macroscopic cross sections for removal, for fission and for scattering from energy group g' into group g. Further, χ_g is the integrated spectra of fission, ν_g is the average number of neutrons generated by fission for energy group g and k_{eff} is the effective multiplication factor.

In order to solve the eigenvalue problem the power method is used [8]. The power method is a numerical method to find the dominant eigenvalue of an eigenvalue problem, together with its respective eigenfunction (or eigenvector). It uses an initial guess for the eigenvalue and eigenfunction, then it's used as an input source term into the eigenvalue problem (for all energies), and its solution will provide a new eigenfunction. The normalization of this eigenfunction will weight the new eigenvalue, and the new eigenvalue and eigenfunction are used at the construction of the new source term. This procedure is repeated until some stop criterion.

2.1. The polynomial approximation method

In this section we show the methodology for the approximate solution with error control. This methodology construct an approximate low order polynomial solution for the neutron scalar flux ϕ. If this Taylor series expansion converges to the actual ϕ, we can truncate it and still have a precise approximation of the neutron scalar flux. The truncation of this local expansion has a validity limited by its convergence radius, which is the highest distance from the series center that will provide a precise solution under some error. This convergence error is the parameter that will bound the size of the segmentation radius, and the motivation for a segmented domain. This way, each region has a different polynomial approximation, in other words, ϕ inside certain region named $[i,j]$ is approximated by its polynomial approximation $\phi^{[i,j]}$. Boundary and interface conditions, together with the

differential equation, are used to find the values of the coefficients forming an algebraic system, solved by the iterative method of Gauss-Seidel [9].

That said, to solve the neutron diffusion problem we are going to approximate the function ϕ as a low order polynomial, but to find this expression it's necessary to express it in a complete Taylor series, as follows,

$$\phi^{[i,j]} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} F_{m,n}^{[i,j]} x^m y^n \ , \tag{2}$$

for $i = 1, 2 \ldots I$ and $j = 1, 2 \ldots J$, where $\phi^{[i,j]} = \phi^{[i,j]}(x, y)$ is the unknown ϕ valid for the region $[i, j]$; $F_{m,n}$ is an unknown constant coefficient of $x^m y^n$ at the Taylor series expansion of $\phi^{[i,j]}$; and i and j indicate the region of the domain segmentation. It's important to emphasize that here, x and y refer to the local positions, being $x = 0$ and $y = 0$ the center of the particular segment $[i, j]$.

Substituting the expansion (2) in the differential equation (1), we obtain,

$$\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\Big[-D^{[i,j]}\Big((m+2)(m+1)F_{m+2,n}^{[i,j]} + (n+2)(n+1)F_{m,n+2}^{[i,j]}\Big) + \Sigma_r^{[i,j]} F_{m,n}^{[i,j]}\Big] x^m y^n = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} S_{m,n}^{[i,j]} x^m y^n \ . \tag{3}$$

Note that the equation (3) generates an index equation, which makes explicit the dependance between the terms $F_{m,n}$ and the terms of order $F_{m+2,n}$ and $F_{m,n+2}$. Considering this, it is reasonable to consider a truncation order of at least 2 for both m and n series to use the index equation (3) at least once, since it represents the contribution of the differential equation on the results. We chose to use the index equation once, so the truncation order is 2.

This consideration also imply that the error control is now made through the segment size alone. So, the methodology closes the problem using the equation (3) for $m = n = 0$:

$$\left(-2D^{[i,j]}\right) F_{2,0}^{[i,j]} + \left(-2D^{[i,j]}\right) F_{0,2}^{[i,j]} + \left(\Sigma_r^{[i,j]}\right) F_{0,0}^{[i,j]} = S_{0,0}^{[i,j]} \ . \tag{4}$$

By substituting the truncated expansion in the boundary and interface conditions we obtain an algebraic system which is solved using a "block-by-block" form of the Gauss-Seidel method [9].

As the polynomial order is fixed, the error control is made by analysing the size of each region. This is the reason to subdivide the domain and connect the local solutions through the boundary and interface conditions. It is important to note that expression (4) establishes a relation for some terms of the equation (3) truncated at its second term. It means that, while the equation (4) establishes a relation for $F_{2,0}^{[i,j]}$, $F_{0,2}^{[i,j]}$ and $F_{0,0}^{[i,j]}$, the other terms have their values bound by the error control.

2.2. Convergence

Convergence of the equation (3) is ensured by the fact that the polynomial is differentiable at any arbitrary point in the interval and is limited in the interval that allows us to use the Lipschitz criterion, that usually indicates a function as continuous, as a measure for the difference of the correct and the approximate solution.

$$|\phi(x_i) - \phi(x_j)| \leq \kappa \, |x_i - x_j| \, . \tag{5}$$

If this inequality is satisfied on a determined interval of x, then $\phi(x)$ is called "Lipschitz continous". Lipschitz continuous functions are uniformly continuous, which implies that for any $\hat{\epsilon} > 0$ exists $\delta > 0$ such that if $|x - x_i| < \delta$ then $|\phi(x) - \phi(x_i)| < \hat{\epsilon}$. In our work, using this assures convergence of the series, for:

$$|\phi(x_{max}, y) - \phi(x_{min}, y)| \leq \kappa \, |x_{max} - x_{min}| = 2\kappa\Delta x = \hat{\epsilon}, \tag{6}$$

and,

$$|\phi(x, y_{max}) - \phi(x, y_{min})| \leq \kappa \, |y_{max} - y_{min}| = 2\kappa\Delta y = \hat{\epsilon}. \tag{7}$$

Thus, the Lipschitz implies in an implicit equation that allows to estimate Δx and Δy, so we can find an expression to establish a relation between the Lipschitz constant κ and the mesh size. Note, that the way of obtaining the Δx and Δy is not direct, after having a solution one has to check whether the choice is compatible with the Lipshitz inspired criterion. In this sense the criterion is not an explicit one such as the Cauchy reasoning, or others, so that one has to determine a solution and do a self-consistency test afterwards. In general experimenting with polynomial degrees and segmentation sizes already yields values compatible with the implicit criterion cited above, especially if a low polynomial degree is used. For instance a polynomial of degree 2 may have either a true maximum or one on the segment boundary, which is straightforward to check. Note, that κ is related to an error estimate, since the expansion of a function in a Taylor series coincides with its exact value at the point where the Lipschitz cone is centred. Thus, the Lipshitz cone defines a supremum and an infimum for possible values of the true solution in a specific segment, which upon taking the limits $\Delta x \to 0$ and $\Delta y \to 0$ converge towards the exact solution. Note, that this reasoning makes only sense if the solution is given as a continuous function. In other words, this convergence criterion based on the Lipschitz condition is not applicable for discrete solutions, where no finite and discrete set of exact values of the solution exist.

3. NUMERICAL RESULTS

The methodology is applied to a test case, which is an eigenvalue problem with homogeneous boundary conditions, and considering two energy groups: $g = 1$ indicates the fast energy group and $g = 2$, the thermal. As mentioned before, we are considering two dimensional cartesian geometry with orthogonal regions and boundaries with homogeneous

meshing. The results are normalized at percentages of maximum of the fast neutron scalar flux (maximum value of ϕ_1 is 100%), with positions for the peaks of both fast and thermal fluxes, together with the converged value of k_{eff}. The stop criteria for the power method and block-by-block iterations are $\bar{\epsilon} = \varepsilon = 10^{-6}$. For this test the boundary conditions are null flux for all boundaries, and $\Delta x = \Delta y = 4\ cm$. Nuclear data for this case is shown in Table 1 and the geometry data is shown in Figure 1.

The Figures 2 and 3 show the results for the fast and the thermal neutron flux. The maximum fast neutron scalar flux happened at the (x, y) positions $(44, 76)$, $(44, 84)$, $(76, 44)$, $(76, 116)$, $(84, 44)$, $(84, 116)$, $(116, 76)$ and $(116, 84)$, in centimeters; and the maximum thermal neutron scalar flux happened at the (x, y) positions $(68, 68)$, $(68, 92)$, $(92, 68)$ and $(92, 92)$, in centimeters. The maximum eigenvalue is $k_{eff} = 1.017405$. Numerical comparisons are not reported in this work because the discussed solution is analytical in the knots of the segmented domain, as well the error of the analytical continuous representation for the solution encountered inside each segment is controlled by the Lipshitz constant.

Table 1: Nuclear parameters

	D_1 $[cm]$	D_2 $[cm]$	Σ_{r_1} $[cm^{-1}]$	Σ_{r_2} $[cm^{-1}]$	$\nu_1\Sigma_{f_1}$ $[cm^{-1}]$	$\nu_2\Sigma_{f_2}$ $[cm^{-1}]$	$\Sigma_{s_{1\to2}}$ $[cm^{-1}]$
R1	1.4	1.4	0.02	0.15	0.0167511	0.4786031	0.01
R2	1.4	1.4	0.02	0.143	0.0167511	0.4786031	0.01
R3	1.3	0.5	0.018	0.05	0.0071790	0.1435809	0.01

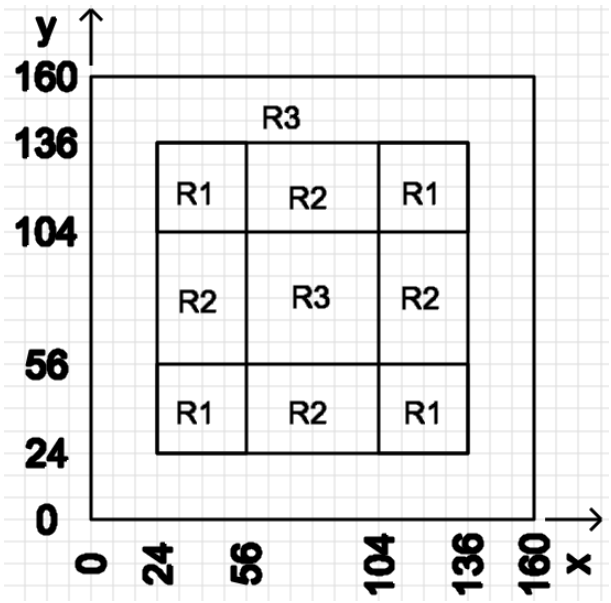

Figure 1: Geometry, in cm.

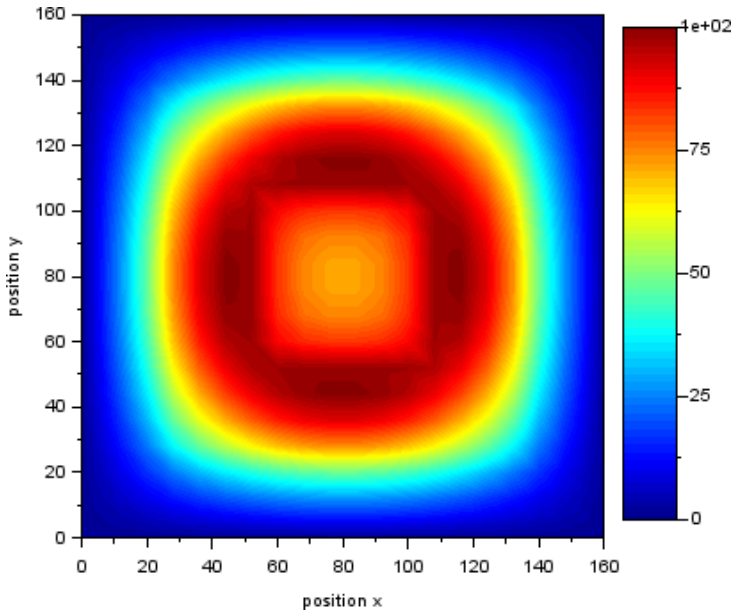

Figure 2: Fast neutron scalar flux in $cm^{-2}s^{-1}$.

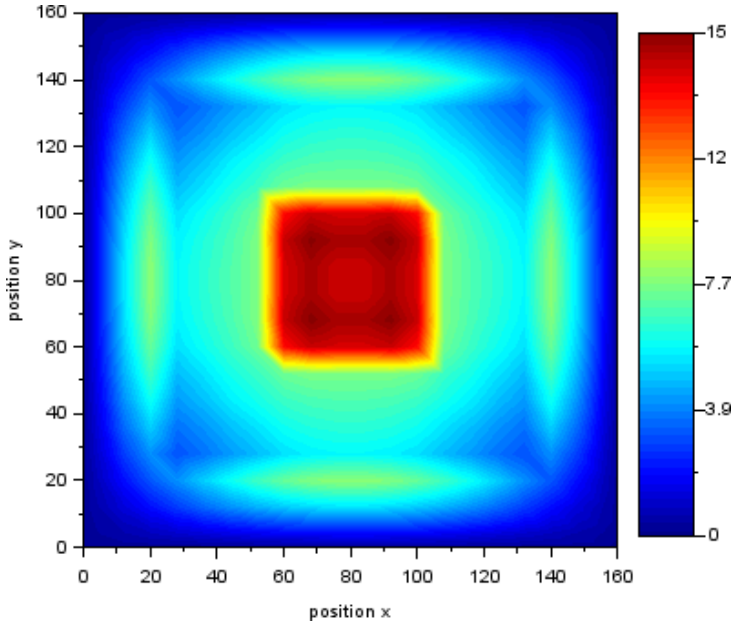

Figure 3: Thermal neutron scalar flux in $cm^{-2}s^{-1}$.

4. CONCLUSIONS

In the present work is shown a simple method to solve the multi-group neutron diffusion equation in a heterogeneous rectangle. The principal feature of the elaborated method is that generates a continuous solution with error control, and that is exact on a finite set of discrete points in the segmented domain. This method represents from a computational point of view the same simplicity as the finite difference method but preserving a continuous dependence of the space time variables in the solution and moreover without approximating the differentiation operators. Note, that the space domain is not discrete, the connection of the respective solutions of each domain is made by analytical continuation that allows to construct the global solution for the heterogeneous domain of the problem in a continuous fashion. The size of each sub-domain is related to the truncation of the Taylor expansion and the precision of the solution, respectively. It is noteworthy, that the solution is exact at each knot, since the relation of the coefficients is established by the differential equation together with initial and boundary conditions, in other words only exact relations are used to get the numerical values of those coefficients. Each knot defines the centre of a Lipshitz cone that has the true solution in its interior, and in this sense provides an estimate for the error. It is noteworthy, that the extension to time dependent problems is straightforward and in a future work we focus our attention in this direction.

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