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IMPROVEMENTS AND CORE APPLICATIONS OF THE MIGRATION MODE METHOD

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ABSTRACT

The problem to achieve detailed information in energy for the neutron flux with reasonable computational time has always been of great interest. Commonly, this aim is pursued with calculations in multigroup theory using many energy groups, although this disregards the goal of fast computations. Recently, some energy treatments have been developed to overcome this drawback, thus giving good approximation of the neutron spectrum. Among them, the migration mode method shows interesting features. Its derivation as a spectral synthesis method is discussed in the paper. New choices for the test weighting function sets allow the solution reproducing integral properties of the analyzed system. The multigroup method is obtained following the same approach of synthesis too. Applications to 3D full core calculations are studied in stationary conditions solved by an upgraded version of the code SMART. The MMM is compared here with the standard 2 MGM, usually chosen to model neutronically industrial cores. A simple system, for which an analytical solution is possible, is drawn to check consistency and robustness of the implemented code. Then results pertaining to a PWR core follow.

Key Words: Spectral Methods, Migration Mode Method, Criticality, Core Analysis.

1. INTRODUCTION

The standard procedure for the energy treatment in nuclear chain reactors is based on the application of the multigroup theory. Detailed calculations in fine multigroup neutron transport determine the flux distribution in reflected assemblies, which is used to collapse and homogenize cross sections in a few-group structure. Further simpler problems, like neutron diffusion, are run to compute flux distribution in the full core.
Moving to a smaller energy mesh leaves out information on the neutron spectrum. Although the multigroup method (MGM) allows preserving reaction rates over energy ranges, a fine reproduction of the flux along the energy axis cannot be achieved. Solutions to reduce the loss of information in collapsing a detailed neutron spectrum into a broad representation have been proposed with spectral synthesis methods (SSMs) [1]. Here, the energy dependence is studied employing different spectral modes which analyze the problem. Among them, the MGM can be placed, which simply divides the energy axis in non-overlapping regions imposing constant solutions herein [2].

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Other methods do not consider any partition of the energy axis. The modal expansion method was one of the first to be introduced [3]. Its application was mainly proposed for fast reactors, sustaining hard neutron spectra which can be sufficiently treated only with many-group fine, but computationally expensive, MGM [4].
Several improvements have been done to allow the MGM to compute with better accuracy the neutron spectrum. One notable approach avoids the step variation of the flux using linear form functions inside the groups [5]. Recently then, a generalized MGM condensation theory has extended this approach, advancing complete orthogonal set of polynomials to describe in-group fluxes [6]. This attempt relaxes the intrinsic discontinuity of the MGM, but the use of polynomials introduces potential flux oscillations, undergoing into negative values. If analytical forms for cross sections exist, more sophisticated methods may be advanced. Among them, an interesting one uses the Laplace transform to finally compute the neutron spectrum in homogeneous infinite media [7]. The Migration Mode Method (MMM) expands the neutron flux with a superposition of functions in energy, called the migration modes [8]. This particular SSM presents common aspects with the modal expansion method, but its application was originally introduced for light water reactors (LWRs). Here the available fundamental knowledge of the physics of the system is used to describe the behavior of neutrons, migrating in the energy domain. In this paper improvements of the MMM are presented with particular attention to possible weighting procedures employed to close the final linear system for the migration mode coefficients. Use of the generalized importance as weighting functions allows the MMM solution to conserve some integral properties of the original reference problem. Applications to 3D core calculations follow in stationary conditions, amply showing MMM features. The studied MMM is compared here with the standard 2 MGM, usually chosen to model neutronically industrial nuclear cores.

2. THE MIGRATION MODE METHOD

SSMs have been largely applied to solve partial differential equations (PDEs) rather successfully to obtain good computational results. Such methods consist of all the techniques in which an approximate solution $\varphi(x, y)$ is expected as:

$$\varphi(x, y) = \sum_{i=1}^{N} \omega_i(x)\psi_i(x, y) \tag{1}$$

where x and y belong to disjoint subsets of independent variables; the N ψ_i are the known trial functions, or also called base functions, and ω_i are the combining coefficients. The adoption of a set of trial functions ψ_i which does not constitute a base for its space, move Eq. (1) to an approximation. The solving strategy introduces Eq. (1) into the governing PDE, then integrating over y the resulting expressions with new test wheighting functions $\zeta_i(x, y)$. The dependence on the x variable can then be treated with numerical approaches. This procedure allows the computation of the expansion coefficients ω_i by solving ensued linear systems. This method converts a continuous operator problem to a discrete one. A special case arises when test and trial functions are the same, thus speaking of Galerkin SSM.
In MGM, the angular flux $\varphi(\mathbf{r}, E, \mathbf{\Omega}, t)$ is assumed to be composed by terms separable into prod-

ucts of functions depending on energy only, $\psi_g(E)$, and other functions $\varphi_g(\mathbf{r}, \mathbf{\Omega}, t)$:

$$\varphi(\mathbf{r}, E, \mathbf{\Omega}, t) = \sum_{g=1}^{G} \varphi_g(\mathbf{r}, \mathbf{\Omega}, t)\psi_g(E),$$

$$\psi_g(E) = \begin{cases} \dfrac{\phi_{ref}(E)\theta_g(E)}{\displaystyle\int_{E_{g+1}}^{E_g} \phi_{ref}(E)dE}, & E \in [E_g, E_{g+1}) \\ 0, & \text{otherwise} \end{cases} , g = 1, 2, ..., G. \tag{2}$$

θ_g are non overlapping rectangle functions null everywhere but in specified g-th intervals according to a specified energy mesh and ϕ_{ref} is a collapsing spectrum of reference. The test functions are the θ_g themselves. An attempt to describe the solution in energy with higher accuracy suggests replacing θ_g with:

$$\theta_g(E) = \sum_j \alpha_{g,j} P_{g,j}(E), \tag{3}$$

where $P_{g,j}$ may build a polynomial base on the *g*-th energy group.
The MMM avoids the restriction of a particular energy mesh and considers trial functions defined uniquely over the whole energy range. These functions are solutions of particular physical problems in infinite media, characterizing the studied system. Generally, they do not form a complete set of eigenfunctions. Therefore no requirements exist for them, but that to be at least $\mathcal{C}^1(\mathbb{R})$. After having selected M migration modes Q_m, the MMM adopts the following assumption for the neutron angular flux φ:

$$\varphi(\mathbf{r}, E, \mathbf{\Omega}, t) = \sum_{m=1}^{M} a_m(\mathbf{r}, \mathbf{\Omega}, t)\, Q_m(\mathbf{r}, E, \mathbf{\Omega}, t), \tag{4}$$

where the migration mode coefficients a_m are the new unknowns. The order M of expansion limits the physical achievable knowledge of the system and fixes the computational burden.

2.1. Trial Function Set

With the introduction of migration modes Q_m as trial functions, Eq. (4) contains a strong physical interpretation. Thus considering that neutrons can be classified in migrating particles under the influence of thermal vibration of structure atoms at equilibrium, neutrons migrating suffering collisions during their slowing down, neutrons migrating under the only emitters influence, neutrons migrating under a specific resonance depression, etc., the definition of the modes Q_m become straightforward [8]. Considering negligible the distorsions of the spectrum modes Q_m in space and angle, only their dependece on the energy variable is kept. This can limit the amount of data while solving the problem in multidimensional spaces featuring real practical problems.
Considering neutron spectra evaluated in homogenized fuel assemblies of LWRs, three main components are clearly observable:

- a Maxwellian distribution representing the thermal equilibrium of scattered neutrons with the moderator material;

- a slowing down distribution of the kind $1/E$ characterizing the neutron stream in epithermal energy range;
- a fission emitted neutron distribution.

A Maxwellian spectrum can be evaluated by:

$$Q_M = (kT_n)\tilde{E}\exp\tilde{E}, \quad \text{with } \tilde{E} = E/(kT_n), \tag{5}$$

where k is the Boltzmann's constant, $\tilde{E}$ is an adimensioned quantity representing energy, scaled at the thermal energy of motion for vibrating nuclei at neutron temperature T_n. This last can be calculated through correlations, starting form the absorption cross section and the wall temperature T_w, i.e. that measured at the external surface of the rod cladding. Here, this was assumed to be close to the moderator temperature T_{mod}. In epithermal regions collisions and resonance absorptions affect the neutron slowing down. Different base functions have been proposed to fit real spectra, obtained in infinite media by the high resolution transport code APOLLO2-A. A simple option suggests to search a shape close to $E^{-b_{SD}}$ for 6 eV $< E <$ 1 MeV with b_{SD} close to 1, depending on self-shielding. Correlations of different physical problems can determine an optimum value. To avoid the singular behavior at very low energies, a more suitable formula was proposed by Dall'Osso [8]:

$$Q_{SD} = C_{SD}\frac{E\exp(b_{SD1}/\sqrt{E})}{(E+E_{SD})^{b_{SD2}}}, \tag{6}$$

where C_{SD} is a normalization constant. Another function has been formulated by Gandini et Al. involving directly cross sections as indipendent variables to fit better reference slowing down spectra [9]:

$$\begin{aligned} Q_{SD} &= C'_{SD}\frac{\tilde{\chi}^{\vartheta}(E)p^{\alpha}(E)}{E^{\beta}\Sigma_t^{\gamma}(E)}, \\ \tilde{\chi}(E) &= \int_E^{\infty}\chi(E')dE', \\ p(E) &= \exp\left[-\int_E^{\infty}\frac{\Sigma_a(E')}{\xi\Sigma_s(E')}\frac{dE'}{E'}\right]. \end{aligned} \tag{7}$$

In Eq.s (7) C'_{SD} is again a normalization constant, Σ_t, Σ_s and Σ_a are respectively the total, scattering and absorption macroscopic cross sections, while ξ is the mean lethargy gain per neutron collision. $\tilde{\chi}(E)$ is the complement to the cumulative fission emission spectrum and $p(E)$ resembles the resonance escape probability. α, β, γ and ϑ take into account for possible adjustments like tuning parameters. This formula allows a fine description of the reference slowing down spectrum, but limits the general character assumed by its migration mode.
Neutrons produced by fission appear at E, around dE, with probability $\chi(E)dE$. The emission probability density function $\chi(E)$ is evaluated as:

$$\chi(E) = 0.771\sqrt{E}\exp(-0.776E). \tag{8}$$

The mode Q_{SE} in Eq. (8) depends on the nuclear fuel material and its numerical coefficients refer to uranium fuel enriched at less than 10% in mass. But this dependence very slightly modifies the related coefficients and then it is assumed as a general mode.
To keep a similar computational effort in comparing MMM to 2G MGM, the set of migration

modes is bounded to 2 combining linearly, with a coefficient f_{em}, Q_{SD} and Q_{SE}, which often shows certain coupling in many reference calculations.

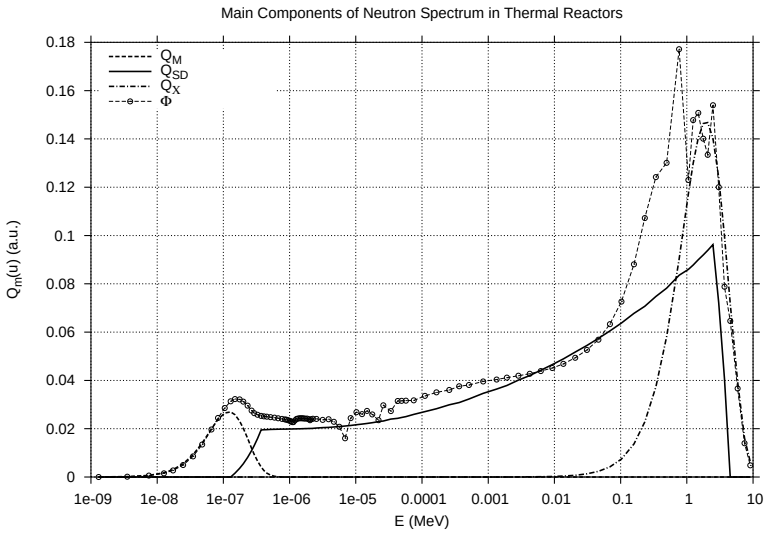

Figure 1: **Migration modes and a real reference spectrum of a PWR fuel assembly, enriched at 3.5% in ^{235}U. Q_{SD} refers to Eq. (6)**

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2.2. Test Function Set

Any problem in neutron transport theory can be generally described by mathematical operators as:

$$1/v\ \partial_t\varphi + \hat{L}\varphi = \hat{M}\varphi + S, \tag{9}$$

where $\hat{L}$ and $\hat{M}$ are the removal and the inner production operators, respectively, S counts external sources and v specifies the velocity modulus of migrating neutrons. Studying critical stationary systems means getting homogeneous problems, then splitting the production operator into its scattering component $\hat{T}$ and its fission emission one $\hat{F}$, the Boltzmann operator $\hat{H}$ becomes:

$$\left[\hat{L} - \hat{T} - \hat{F}/k_{eff}\right]\varphi = \hat{H}\varphi = 0. \tag{10}$$

Being the MMM a SSM, an unavoidable error of approximation $\delta\varphi$ enters the balance Eq. (10). To neglect it and compute only the MMM flux $\tilde{\varphi}$, a particular coefficient, named equivalence factor f_S, is introduced as:

$$\hat{H}(\tilde{\varphi} + \delta\varphi) = \left[\hat{L} - f_S\hat{T} - \hat{F}/k_{eff}\right]\tilde{\varphi}. \tag{11}$$

This new eigenvalue is a measure of the disregarded information about the neutron migration in the performed synthesis. f_S acts on the scattering contribution because the error of this modeling was found to be almost proportional to the application of the scattering operator onto the neutron

flux.
To determine M mode coefficient a_m, the MMM carries the projection of Eq. (11) over M test functions U_l, $l = 0, ..., M-1$. These operations evidence integral quantities, to which peculiar physical meaning may be attributed. The choice of a test function set is completely arbitrary, but each U_l can make the solution showing a particular feature. Taking formerly step constant U_l, the MMM solution is forced to satisfy the global neutron balance over specified regions of its phase space. This implies for the synthesis error $\delta\varphi$:

$$\langle \hat{H}\delta\varphi \rangle = (1 - f_S)\langle \hat{T}\tilde{\varphi} \rangle, \tag{12}$$

where $\langle ... \rangle$ means integration over the portion of phase space where U_l is not vanishing.
Identifying integral quantities, it is possible then to conceive test functions in the sense of importance functions. Considering proper initial and boundary conditions for the adjoint flux $\varphi^\dagger$, the adjoint problem for Eq. (10), is:

$$\left[\hat{L}^\dagger - \hat{T}^\dagger - \hat{F}^\dagger/k_{eff}\right]\psi^\dagger = \hat{H}^\dagger\psi^\dagger = S^\dagger, \tag{13}$$

as the conjugate $k^*_{eff} = k_{eff}$ being a real number. The condition for $\psi^\dagger$ to be adjoint to φ, solution of Eq. (10), requires the orthogonality between φ and $S^\dagger$, thus $\langle \varphi | S^\dagger \rangle = 0$. Giving importance to the asymptotic level of power, so using the adjoint flux $\varphi^\dagger$ with a vanishing $S^\dagger$, f_S becomes identically unitary:

$$\begin{aligned} \langle \varphi^\dagger | \left[\hat{L} - \hat{T} - \hat{F}/k_{eff}\right](\tilde{\varphi} + \delta\varphi)\rangle &= \langle \left[\hat{L}^\dagger - f^*_S\hat{T}^\dagger - \hat{F}^\dagger/k_{eff}\right]\varphi^\dagger | \tilde{\varphi}\rangle, \\ \langle \hat{H}^\dagger\varphi^\dagger | \delta\varphi\rangle &= (1 - f^*_S)\langle \varphi^\dagger | \hat{T}\tilde{\varphi}\rangle, \\ \text{generally,}\quad \langle S^\dagger | \delta\varphi\rangle &= (1 - f^*_S)\langle \psi^\dagger | \hat{T}\tilde{\varphi}\rangle. \end{aligned} \tag{14}$$

A null $S^\dagger$ makes the MMM solution computing the same k_{eff} of the reference problem. Furthermore, $f_S = 1$ implies also $\hat{H}\delta\varphi = 0$. Eq. (14) allows to conserve more properties including other generalized importance functions $\psi^\dagger$ among the test functions. A $\psi^\dagger$ is defined with respect to a unique observable s. The relation between s and $S^\dagger$ follows from their definitions:

$$s = \frac{\langle h_1\varphi\rangle}{\langle h_2\varphi\rangle}, \quad S^\dagger = \frac{h_1}{\langle h_1\varphi\rangle} - \frac{h_2}{\langle h_2\varphi\rangle} \tag{15}$$

where h_1 and h_2 are new operators applying on φ. As the MMM solves the problem $\hat{H}\tilde{\varphi} = 0$, the projection over $\psi^\dagger$ conserves its correspondent s:

$$\left\langle S^\dagger \middle| \tilde{\varphi} \right\rangle = \frac{\langle h_2\tilde{\varphi}\rangle}{\langle h_2\varphi\rangle} - \frac{\langle h_1\tilde{\varphi}\rangle}{\langle h_1\varphi\rangle}, \quad s = \frac{\langle h_1\tilde{\varphi}\rangle}{\langle h_2\tilde{\varphi}\rangle} = \tilde{s}. \tag{16}$$

$h_1(E) = 1$ for $E \geq E_c$, null otherwise, and $h_2 = 1 - h_1$ allow computing the spectral index SI; normally the cut energy E_c is fixed at 0.0625 eV. An attempt to overcome the hard task of finding a suitable slowing down mode in the resonance regions suggests to save other characteristic integral quantities. In the present work, the conservation of ^{235}U and ^{238}U absorption probabilities per fission emitted neutron were investigated. These coefficients are evaluated selecting microscopic absorption cross section for h_1 and macroscopic fission production one for h_2.
When the trial functions Q_m constitute a base and show orthogonality, a good choice for U_l is the same trial function set. In fact, possible computational speed enhancements may be sought thanks

to simple formulae evaluating their norms. Assuming physical modes (see Sec.2.1), orthogonality seems far to be found and weighted results are necessary keeping mixed mode projected terms. Noticing that on the lethargy domain, spectra seem to show a polynomial shape, the adoption of a shifted Legendre polynomial base, modulated correctly, has been proposed [6]. Adopting functions of simple bases is mathematically very practical but under the computing point of view less straightforward, because such functions do not contain as much information as the physical ones. As a result, it requires many more trial functions in the description of a good quality neutron flux.
Eventually, by a variational approach, to minimize the error in the system equation, Eq. (11), in a least square sense, $\langle(\hat{H}\delta\varphi)^2\rangle$, $U_l = Q_l\hat{H}^\dagger$, while regarding the one in the solution, $\langle(\delta\varphi)^2\rangle$, $U_l = Q_l\hat{H}^{-1}$ [3].

3. MMM DIFFUSION MODEL

The MMM was implemented in the AREVA NP nodal diffusion code SMART to compare its performance with respect to the present 2G MGM version. In order to provide reference results, a general MGM version of the code has been developed too. Diffusion theory can be derived by P_1 transport under the assumptions of an isotropic external source and stationary conditions, for which the neutron scalar flux ϕ and its current **J** are:

$$\begin{gathered}\varphi(\mathbf{r},E,\mathbf{\Omega}) = \frac{1}{4\pi}\left[\phi(\mathbf{r},E) + 3\mathbf{\Omega}\cdot\mathbf{J}(\mathbf{r},E)\right],\\ \phi(\mathbf{r},E) = \oint_{4\pi}\varphi(\mathbf{r},E,\mathbf{\Omega})\,d\mathbf{\Omega}, \mathbf{J}(\mathbf{r},E) = \oint_{4\pi}\mathbf{\Omega}\,\varphi(\mathbf{r},E,\mathbf{\Omega})\,d\mathbf{\Omega}.\end{gathered} \tag{17}$$

With the mentioned assumptions, P_1 verifies Fick's law and neutron balance equation leads to the diffusion model for neutrons, which in multigroup form becomes:

$$\left\{\begin{array}{rcl}\nabla_{\mathbf{r}}\cdot\mathbf{J}_g(\mathbf{r}) + \Sigma_{t,g}\phi(\mathbf{r}) &=& \displaystyle\sum_{g'=1}^{G}\left[\Sigma_{s,g'\to g}(\mathbf{r}) + \frac{\chi_g(\mathbf{r})}{k_{eff}}\nu\Sigma_{f,g'}(\mathbf{r})\right]\phi_{g'}(\mathbf{r}),\\ \mathbf{J}_g(\mathbf{r}) &=& -D_g(\mathbf{r})\nabla_{\mathbf{r}}\phi_g(\mathbf{r}),\ \text{with}\\ \phi_g(\mathbf{r}) = \displaystyle\int_{E_{g+1}}^{E_g}\phi(\mathbf{r},E)\,dE,\ \chi_g(\mathbf{r}) &=& \displaystyle\int_{E_{g+1}}^{E_g}\chi(\mathbf{r},E)\,dE.\end{array}\right. \tag{18}$$

MGM cross sections of Eq. (18) for the nuclear reaction X are collapsed as:

$$\begin{gathered}\Sigma_{X,g}(\mathbf{r}) = \left[\int_{E_{g+1}}^{E_g}\Sigma_X(\mathbf{r},E)\phi(\mathbf{r},E)dE\right]\Big/\phi_g(\mathbf{r}),\\ \Sigma_{s,g'\to g}(\mathbf{r}) = \left[\int_{E_{g+1}}^{E_g}dE\int_{E_{g'+1}}^{E'_g}\Sigma_s(\mathbf{r},E'\to E)\phi(\mathbf{r},E')dE'\right]\Big/\phi_{g'}(\mathbf{r}).\end{gathered} \tag{19}$$

The diffusion coefficient D_g follows the same treatment when preparing cross section sets for homogenized regions. The MMM form requires the substitution of Eq. (4) in the original diffusion

equation showing:

$$\begin{cases} \nabla_{\mathbf{r}} \cdot \mathbf{J}_l(\mathbf{r}) &= \sum_{m=1}^{M} \left[\Sigma_{s,lm}(\mathbf{r}) + \frac{\chi_l(\mathbf{r})}{k_{eff}} \nu\Sigma_{f,m}(\mathbf{r}) - \Sigma_{t,lm}(\mathbf{r}) \right] a_m(\mathbf{r}), \\ \mathbf{J}_l(\mathbf{r}) &= -\sum_{m=1}^{M} D_{lm}(\mathbf{r}) \nabla_{\mathbf{r}} a_m(\mathbf{r}), \text{ with} \end{cases} \tag{20}$$

$$\nu\Sigma_{f,m}(\mathbf{r}) = \int_0^\infty dE\, \nu\Sigma_f(\mathbf{r}, E)\, Q_m(E),\ \chi_l(\mathbf{r}) = \int_0^\infty dE\, U_l(E)\, \chi(\mathbf{r}, E).$$

The other material constants are similarly evaluated as:

$$\begin{aligned} \Sigma_{t,lm}(\mathbf{r}) &= \int_0^\infty dE\, U_l(E)\, \Sigma_t(\mathbf{r}, E)\, Q_m(E), \\ \Sigma_{s,lm}(\mathbf{r}) &= \int_0^\infty dE\, U_l(E) \int_0^\infty dE'\, \Sigma_s(\mathbf{r}, E' \to E)\, Q_m(E'). \end{aligned} \tag{21}$$

The MMM needs a new treatment for cross sections, avoiding use of spectra to collapse successively from finer energy mesh to broader ones, as the MGM requires. This advantage is limited if adjoint fluxes are employed as test functions. Post-processing modules suitable for the transport code APOLLO2-A were also designed to produce MMM cross sections in infinite homogenized media for full core applications.

Comparing Eq. (18) and Eq. (20), MMM presents denser solving matrices after common numerical procedure to treat the spatial variable, especially for the streaming term. Eq. (11) is then solved by a nodal expansion method (NEM) in 3D which correct directional currents evaluated on surfaces of a spatial coarse mesh. The coupling among core nodes is then entrusted by a finite difference method mounted on a checkerboard scheme iteratively solved in a Jacobi-like algorithm. Then, although the reduced sparsity, the small rank of solving matrices does not demand much more comptutational time in the MMM. In the MGM the boundary conditions on the flux ϕ apply directly to ϕ_g, while for the MMM these conditions must be converted into a_m relations. For zero flux at boundaries, a homogeneous Dirichlet boudary condition simply states:

$$\begin{gathered} \phi_g^{bnd} = 0, g = 1, ..., G \text{ and} \\ \int_0^\infty dE\, U_l(E)\, \phi^{bnd}(E) = \sum_{m=1}^{M} Q_{lm}\, a_m^{bnd}, l = 0, ..., M-1; \\ \text{then, } \mathbf{Q} \cdot \left| a_m^{bnd} \right\rangle = 0, a_m^{bnd} = 0, m = 1, ..., M \end{gathered} \tag{22}$$

with $\mathbf{Q}$ being non singular. When zero incoming current is found, the flux ϕ becomes proportional to the current at the boundary according to a Robin relation:

$$\phi^{bnd} \mp \zeta\, \mathbf{J}^{bnd} \cdot \mathbf{n} = 0, \tag{23}$$

where $\mathbf{n}$ is the outcoming versor at the boundary surface and ζ is a simple constant. Marshak condition suggests $\zeta = 2$ [2]. In SMART a more accurate value of 2.13129 is proposed using the transport relation for the extrapolated distance $d = 0.71\lambda_{tr}$, where λ_{tr} is the trasport mean free path $\lambda_{tr} = 3D$ [10]. As it is well-known, the MGM form adds to Eq. (23) the subscript of the g-th group. d extrapolates the flux outside the boundary to its zero value. In the MMM, the quadrature over the test function U_l ends in an eigenvalue system, which after some algebra becomes:

$$\zeta\, \mathbf{D}^{-1}\mathbf{Q} \cdot \left| a_m^{bnd} \right\rangle = d \left| a_m^{bnd} \right\rangle. \tag{24}$$

The d series is inferiorly limited, this bound is the one with phisical meaning able to sustain a positive flux in the whole domain. A unique d is selected for all mode coefficients, in contrast with G d_g of MGM. M d_m cannot be achieved by an arbitrary choice of $\{U_l\}$.
Finally, in case of a reflective boundary where $\mathbf{J}_g^{bnd} \cdot \mathbf{n} = 0$, for the MMM this condition is relaxed to $\nabla_{\mathbf{r}}\, a_m^{bnd} = 0, \forall m$.

4. APPLICATIONS

Several benchmark cases are proposed to validate the upgraded version of SMART. Performed tests compare 2M MMM to 2G MGM pointing out its advantages. Reference calculations are in 99G MGM. Material constants employed in multidimensional systems are calculated in infinite medium condition as stated by the standard approach in reactor physics. Different versions of MMM are analyzed changing the slowing down mode and its coupling with the fission spectrum to reproduce better reference spectra of infinite media. Different envisaged options are:

- MMM1: Q_{SD} by Gandini et al., Eq. (7);
- MMM2: Q_{SD} by Dall'Osso, Eq. (6);
- MMM3: Heuristic Q_{SD}, this mode is numerically defined as the difference between the reference spectrum and Q_M;
- MMM4: again Eq. (6) with $b_{SD,1}$ and $b_{SD,2}$ fitted by the ordinary least square technique (OLS).

Still, MMMi.2 implies a special optimization on f_{em} fixing the ratio between Q_{SD} and $Q_{SE} = \chi$ capable to gain the reference SI. Only MMM1 and MMM2 represent the slowing down by physical laws. MMM3, MMM4 and the optimization MMM*i*.2 are attemps to have a better description of the reference spectrum in the infinite medium. In the implemented modules $b_{SD1} = 4.5E-4$, $b_{SD2} = 1.8965$ and $E_{SD} = 8.0E-8$ MeV. ξ is the mean lethargy gain per neutron collision, fixed at 0.92 for moderating water [10]; α, β, γ and ϑ are all unitary.
A first benchmark (ANBM) presents a bare homogeneous regular parallelepiped (210x210x220 cm), for which an analytical solution exists. Its volume is discretized in a coarse 7x7x8 mesh. Dirichlet, zero flux boundary conditions are assumed everywhere. An exact asymptotic spatial solution provides a geometrical buckling B^2 and allows studying the only energy approximations. However, a continuous treatment of energy is not available and the best approximation with a fine MGM induces the denomination of semi-analytical (SA).
Table I shows k_{eff} evaluations for homogenized macroscopic cross sections of a fuel assembly, type UO_2 17x17 enriched at 3.5 % of ^{235}U at hot zero power condition (HZP): core configured at thermal equilibrium relative to water temperature of 286 °C and density of 0.7538 g/cm^3 with boron concentration of 1236 PPM. Test functions are $U_0(E) = 1$, $\forall E$, and $U_1(E) = \phi^{\dagger}(E)$. In Table II different versions of MMM are tested by their evaluated k_{eff}.

Table I: **ANBM: Numerical and Semi-Analytical k_{eff} comparisons, reference $k_\infty = 1.07848$.**

	k_{eff}			Δk (pcm)		
	FDM	NEM	SA	(FDM - *Ref*)	(NEM - *Ref*)	(SA - *Ref*)
99G	1.038395	1.037746	1.037719	67.6	2.7	0.0
2G	1.038957	1.038445	1.038285	123.8	72.6	56.6
MMM1	1.037672	1.037149	1.036992	-4.7	-57.0	-72.7
MMM1.2	1.039346	1.038841	1.038689	162.7	112.2	97.0
MMM2	1.035288	1.034732	1.034565	-243.1	-298.7	-315.4
MMM2.2	1.038626	1.038113	1.037958	90.7	39.4	23.9
MMM3	1.038588	1.038076	1.037921	86.9	35.7	20.2
MMM4	1.038320	1.037805	1.037649	60.1	8.6	-7.0
MMM4.2	1.038909	1.038401	1.038248	119.0	68.2	52.9

As displayed, good performances in the infinite medium description achieve generally a better reproduction of the system multiplication. Fluxes integrated over the nodes are reported in Table II; here, data refer to extreme working conditions at moderator density of 0.2 g/cm^3, where neutron spectra harden strongly. Then, light negative fluxes in thermal regions come, due to unaccuracy in the thermal mode. Although this, the condensed thermal flux is correctly evaluated. MMM flux reconstruction achieves correctly the proportional reproduction of the spectrum from the center to outer regions of the system in Fig. 2. Fig. 3 checkes the MMM flux at the core center and at HZP against a computed 99G reference.

Table II: **ANBM: in order SA fluxes (a.u.), 99G, 2G, 2M MMM2.2 relative errors (%) of node fluxes follow at middle height NE quadrant; respectively condensed fast flux and thermal one are listed per each node.**

135.006	1.88462	121.636	1.69799	84.1747	1.17504	30.0416	0.41937
1.68	1.68	1.67	1.68	1.65	1.66	1.62	1.63
-2.62	7.17	-2.63	7.16	-2.65	7.14	-2.68	7.11
-1.79	4.54	-1.79	4.53	-1.81	4.51	-1.84	4.48
378.278	5.2806	340.817	4.75765	235.852	3.2924	84.1747	1.17504
1.71	1.72	1.70	1.71	1.68	1.69	1.65	1.66
-2.59	7.20	-2.60	7.19	-2.62	7.17	-2.65	7.14
-1.76	4.57	-1.76	4.56	-1.78	4.54	-1.81	4.51
546.627	7.63068	492.494	6.87501	340.816	4.75765	121.636	1.69799
1.73	1.74	1.72	1.73	1.70	1.71	1.67	1.68
-2.57	7.22	-2.58	7.22	-2.60	7.19	-2.63	7.16
-1.74	4.59	-1.74	4.58	-1.76	4.56	-1.79	4.53
606.711	8.46942	546.627	7.63068	378.278	5.28059	135.006	1.88462
1.73	1.74	1.73	1.74	1.71	1.72	1.68	1.68
-2.57	7.23	-2.57	7.22	-2.59	7.20	-2.62	7.17
-1.73	4.60	-1.74	4.59	-1.76	4.57	-1.79	4.54

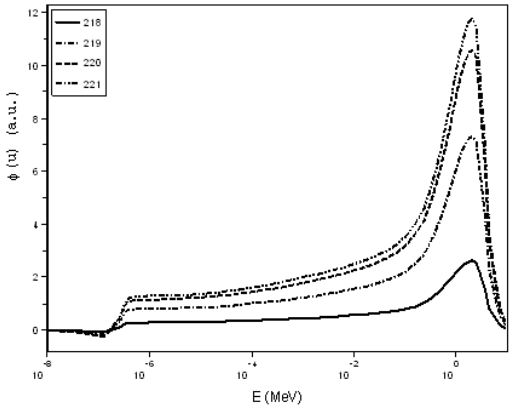

Figure 2: ANBM: MMM2.2 evaluated spectra at low moderator density in lethargy at specified nodes, $k_{eff} = 0.71559$, (see Table II, 1^{st} column).

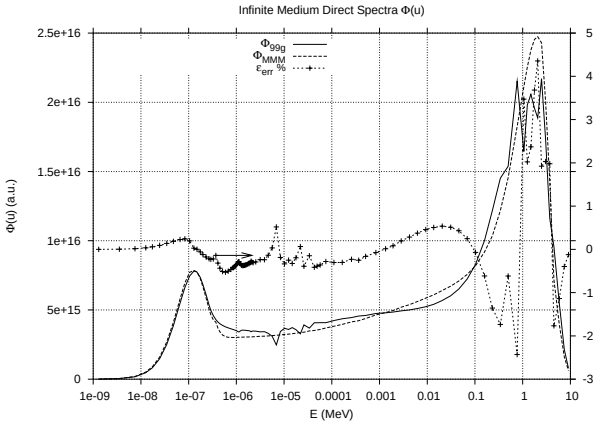

Figure 3: ANBM: MMM spectra at core center and HZP condition, $k_{eff} = 1.03811$.

The 900 MW PWR benchmark (PWRBM) presents many aspects combining complex geometry description and high material heterogeneity. The system sets up an industrial core, designed for thermal power production at beginning of cycle 1 (BOC). The core model is surrounded by a water reflector. Six different assembly types are employed, whose material constants are still referred to HZP conditions.

To collapse reflector cross sections the most representative spectrum obtained by a fine full core 99G MGM calculation and evaluated in the bottom reflector was used. Of course, the choice for the collapsing spectrum is critical. Table III reports k_{eff} computed at HZP with different boundary conditions. About the heterogeneity, it turns out that improvements in the description of the reference spectrum in infinite medium do not achieve the same benefit gained for homogeneous systems, as in ANBM. MMM3 confirms this statement.

Table III: **PWRBM: k_{eff} NEM results at HZP for zero incoming current and zero flux boundary condition, respectively ZFbc and ZICbc.**

	k_{eff}, ZICbc	Δk (pcm)	k_{eff}, ZFbc	Δk (pcm)
99G	0.989256	0.0	0.988841	0.0
2G	0.990511	125.5	0.989899	105.8
MMM1.2	0.990585	132.9	0.989744	90.3
MMM2.2	0.989485	22.9	0.989141	30.0
MMM3	0.987547	-170.9	0.987305	-153.6
MMM4.2	0.989393	13.7	0.98901	16.9

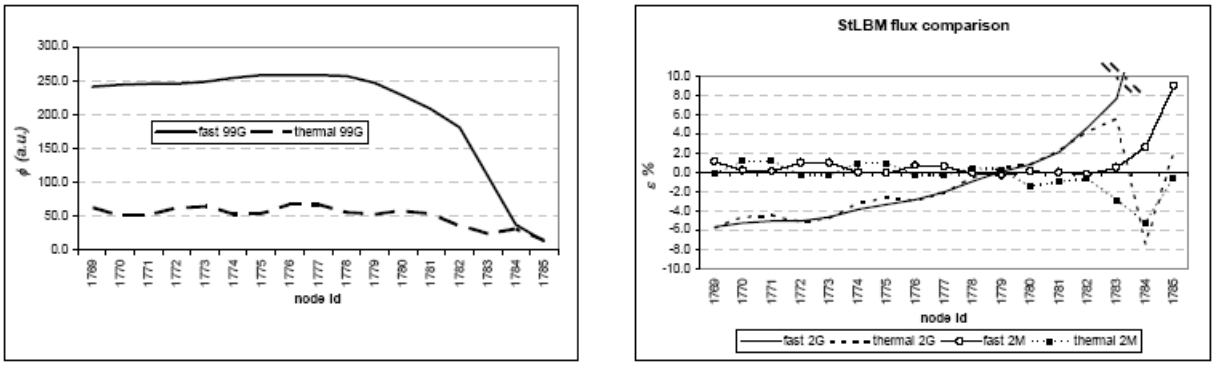

Figure 4: **99G flux evaluated radially at middle core height and condensed in its fast and thermal contributions, from core center node** 1769 **to the boarder (*left*), and MMM2.2 and 2G relative deviations (*right*)**

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Fig. 4 shows the flux distribution with correspondent MMM2.2 and 2G deviations. Imposed unitary discontinuity factors neglect the strong heterogeneity, introduced alternating fuel with and without burnable poisons. This causes errors in the flux distribution, but displays the MMM capability to detect spectrum variations. The implementation in SMART of the MMM gives consistency with a good matching between 2G and 2M results.
Since the MMM solution has the property to fit the neutron spectrum, it is expected a priori that it may partially consider spectrum changes due to local conditions shifts, such as moderator density variations. On the other hand, the MGM can deal with them only through the use of ordinary parameterized cross sections tables. A verification of this assertion has been done with a test case carried out varying the moderator density. In one of these tests the cross sections have been computed at 5 library points by a fine MGM APOLLO2-A and interpolated with polynomials between them. The results are shown in Fig. 5.

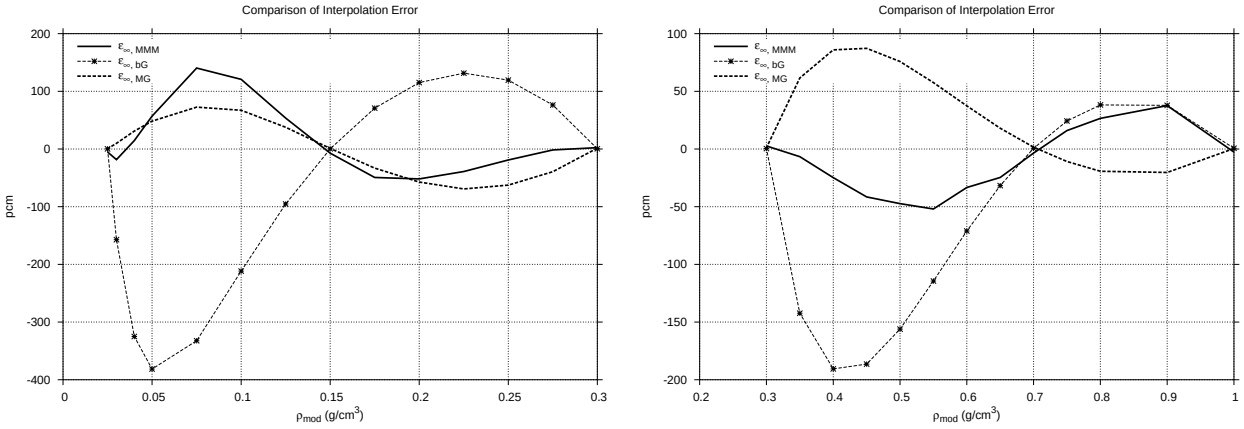

Figure 5: Interpolation error effects on k_∞ varying water moderator density; MMM, bG, MG mean respectively MMM2.2, 2G and 99G. The interpolation is parabolic in the sets: $0.025 - 0.15 - 0.3$ and $0.3 - 0.7 - 1.0$ g/cm ^{3}.

5. CONCLUSIONS

A better insight into the method has been achieved, mainly improving the theory of MMM. Above all, the benefit of using neutron importance as a weighting test function deserves a particular attention. This new feature allows predicting quite accurately specific observables, like the k_{eff}, in multidimensional system, without using any equivalence factor, which was formerly needed in MMM applications. Different MMM versions have been conceived to study spectrum distorsions moving from infinite medium condition to real multidimensional systems. Results suggest adopting MMM2.2 as the reference MMM choice. The method can get wider energy information on the flux in complex 3D structures exporting the synthesis done in infinite media for the cross section processing.
New modules to produce cross sections in MMM and MGM theory have been implemented in FORTRAN90, treating APOLLO2-A's output files. SMART has been upgraded with a MMM 3D static solver and a general group MGM one, keeping all the functionalities of the existing 2G MGM, counting accelerations and symmetries.
Test cases show that the slowing down mode needs to be carefully modeled, as thermalization for very hard spectra. A physical study on neutron migration in energy is on-going. Due to the physical meaning of modes, the MMM is able to make synthesis of any system, provided that a proper mode set has been identified. This comment advances MMM applications also to other nuclear cores (BWR, FBR, ...).

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