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A HIGH-ORDER MOC INCLUDING A SPATIAL POLYNOMIAL EXPANSION FOR CROSS SECTIONS

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1 INTRODUCTION

The TDT (Two and Three Dimensional Transport) deterministic code of the APOLLO3® calculation platform utilises the Method of Characteristics (MOC) to solve the Boltzmann equation for neutrons. In order to reduce the bias and the errors of the current schemes, in the recent years the TDT application has been extended to three-dimensional extruded geometries [1], to provide a better representation of 3D environment effects also in view of a future one-step core calculation.
Even more recently, a polynomial description for the neutron flux has been introduced [2]: along the axial (extruded) direction a per-region constant ("step-constant") flux representation has been substituted by a description assigning to each region a set of coefficients for the polynomial expansion. At the price of a greater complication in the equations, this has permitted to reduce the number of axial meshes by a factor higher than 10, the memory required by a factor ~ 3 and the computation time by a factor ~ 2.
The present work constitutes the natural continuation of the one above, as the same treatment is given to both the neutron flux and the cross sections. The aim is to apply the polynomial expansion in the case of evolution calculations: as a matter of fact, the combination of a polynomial flux expansion and step-constant cross sections over extended axial meshes is highly inaccurate if non-zero burnup cases are considered, since a refined axial mesh is required to describe the modification of cross-section profiles due to nuclide depletion. A polynomial expansion for cross sections is therefore needed, together with the one for the flux, to fully utilize the MOC 3D polynomial method.

2 THE POLYNOMIAL EXPANSION

If a polynomial profile is assumed for their spatial dependence, the angular mono-group neutron flux $\psi(\vec{r},\vec{\Omega})$ and the arbitrary mono-group macroscopic cross section $\Sigma(\vec{r})$ can be written as

$$\begin{gathered}\psi(\vec{r},\vec{\Omega}) \sim \vec{P}(\vec{r})\cdot\vec{\psi}_r(\vec{\Omega}), \qquad \Sigma(\vec{r}) \sim \vec{P}(\vec{r})\cdot\vec{\Sigma}_r \\ \vec{P}(\vec{r}) = \{P_p(\vec{r}),\ p=0,N_p\}, \qquad \vec{\psi}_r(\vec{\Omega}) = \{\psi_{r,p}(\vec{\Omega}),\ p=0,N_p\} \qquad \vec{\Sigma}_r = \{\Sigma_{r,p},\ p=0,N_p\},\end{gathered} \tag{1}$$

where $\vec{P}$ is the set of expansion polynomials, and $\vec{\psi}_r(\vec{\Omega})$ and $\vec{\Sigma}_r$ the associated flux and cross-section coefficients, respectively. N_p is the chosen degree for the expansion. At least for a first implementation, the choice has been made to use the same expansion base for the two physical quantities, which seems reasonable given their close interdependence. As in [2], the polynomial representation is adopted only along the axial direction, while step-constant values characterize the radial one; moreover, exactly the same polynomials are employed:

$$\vec{P}(\tilde{z}_r) = \{(\tilde{z}_r)^p,\ p = 0, N_p\}, \qquad \tilde{z}_r = \frac{z_r - \bar{z}_r}{\Delta z_r/2}, \tag{2}$$

where r is the region index, $\bar{z}_r$ the region mid-height axial coordinate, Δz_r the region height and z_r the absolute axial coordinate ranging from the bottom to the top of region r. In this way, $(\tilde{z}_r)^p \in [-1, 1]$ for every region.

In order to highlight how this impacts the numerical problem, one may consider the mono-group integral transport equation evaluated along a characteristic line of direction $\vec{\Omega}$:

$$\psi(\vec{r}_0 + l\vec{\Omega}, \vec{\Omega}) = \psi(\vec{r}_0, \vec{\Omega})\, e^{-\tau(l)} + \int_0^l dt\, q(\vec{r}_0 + t\vec{\Omega}, \vec{\Omega})\, e^{\tau(t)-\tau(l)}, \tag{3}$$

l being the length of the considered chord and $\vec{r}_0$ the chord entry endpoint. According to Eq. (1), the optical path length corresponding to t, $\tau(t)$, reads

$$\begin{aligned}\tau(t) &= \int_0^t dt'\, \Sigma(\vec{r}(t')) = \int_0^t dt'\, \vec{P}(\tilde{z}_r(t')) \cdot \vec{\Sigma}_r = \sum_{p=0}^{N_p} \int_0^t dt' \left(\frac{z_r^{in} - \bar{z}_r + \mu t'}{\Delta z_r/2}\right)^p \Sigma_{r,p} \\ &= \sum_{i=0}^{N_p} \Lambda_{i0}\, t + \sum_{i=0}^{N_p-1} \Lambda_{i1}\, t^2 + \sum_{i=0}^{N_p-2} \Lambda_{i2}\, t^3 + \cdots + \Lambda_{0N_p}\, t^{N_p+1},\end{aligned} \tag{4}$$

where $\Lambda_{ij} = P_i(z_r^{in})\Sigma_{r,i+j}\left(\frac{2\mu}{\Delta z_r}\right)^j \frac{1}{j+1}\binom{j+i}{i}$, μ is the cosine of the polar component of $\vec{\Omega}$ and z_r^{in} is the axial component of $\vec{r}_0$. The angular dependence of the emission source $q(\vec{r}, \vec{\Omega})$ is classically expressed in terms of an expansion over real spherical harmonics, up to the chosen anisotropy order K: $q(\vec{r}, \vec{\Omega}) = \sum_{l=0}^{K} \sum_{m=-l}^{m=l} A_l^m(\vec{\Omega})\, q_l^m(\vec{r}) = \sum_{n=1}^{N_m} A_n(\vec{\Omega})\, q_n(\vec{r})$, where a single index is used to indicate the angular moments, whose number is $N_m = (K+1)^2$. The emission source for group g can therefore be written as

$$\begin{aligned} q^g(\vec{r}, \vec{\Omega}) &= \\ &= \sum_n A_n(\vec{\Omega}) \sum_{g'} \Sigma_{s,n}^{g'\to g}(\vec{r})\, \Phi_n^{g'}(\vec{r}) + \frac{1}{k_{eff}} \sum_i \chi_i^g \sum_{g'} \nu\Sigma_{f,i}^{g'}(\vec{r})\, \Phi_0^{g'}(\vec{r}) \\ &= \sum_n A_n(\vec{\Omega}) \sum_{g'} \vec{\Sigma}_{s,n,r}^{g'\to g} \Big(\vec{P}(\tilde{z}_r) \otimes \vec{P}(\tilde{z}_r)\Big) \vec{\Phi}_{n,r}^{g'} + \frac{1}{k_{eff}} \sum_i \chi_i^g \sum_{g'} \overrightarrow{\nu\Sigma}_{f,i,r}^{g'} \Big(\vec{P}(\tilde{z}_r) \otimes \vec{P}(\tilde{z}_r)\Big) \vec{\Phi}_{0,r}^{g'} \\ &= \vec{P}^{2N_p}(\tilde{z}_r) \cdot \vec{Q}_r^{2N_p,g}(\vec{\Omega}), \end{aligned} \tag{5}$$

where

$$\begin{aligned} \vec{Q}_r^{2N_p,g}(\vec{\Omega}) = \{Q_{r,p}^g(\vec{\Omega}),\ p = 0, 2N_p\}, \quad Q_{r,p}^g(\vec{\Omega}) &= \sum_n A_n(\vec{\Omega}) \sum_{g'} \sum_{k+l=p} \Sigma_{s,n,r,k}^{g'\to g} \Phi_{n,r,l}^{g'} \\ &+ \frac{1}{k_{eff}} \sum_i \chi_i^g \sum_{g'} \sum_{k+l=p} \nu\Sigma_{f,i,r,k}^{g'} \Phi_{0,r,l}^{g'}. \end{aligned} \tag{6}$$

In Eq. (5) the spatial behaviour of the angular flux moments $\{\Phi_n^g(\vec{r})\}$, of the average numbers of neutrons emerging from fission per unit path for each fissile isotope $\{\nu\Sigma_{f,i}^g(\vec{r})\}$ and of the coefficients of the scattering cross-section expansion over Legendre polynomials $\{\Sigma_{s,n}^{g'\rightarrow g}(\vec{r})\}$ is expressed in terms of the polynomials of Eq. (2). $\Sigma_{g'}$ and Σ_i represent the sums over energy groups and fissile isotopes, respectively, and the superscript $2N_p$ indicates that vectors contain the elements corresponding to polynomial orders from 0 to $2N_p$. Substituting the emission source into Eq. (3) (and omitting the energy index g), this latter results as

$$\psi(\vec{r}_0 + l\vec{\Omega}, \vec{\Omega}) = \psi(\vec{r}_0, \vec{\Omega})\, e^{-\tau(l)} + \sum_{k=0}^{2N_p} P_k(z_r^{in}) \sum_{p=k}^{2Np} Q_{r,p}^{2N_p}(\vec{\Omega}) \binom{p}{k} \left(\frac{2\mu}{\Delta z_r}\right)^{p-k} \int_0^l dt\, t^{p-k} e^{\tau(t)-\tau(l)}, \quad (7)$$

where $P_k(z_r^{in}) = \left(\frac{z_r^{in}-\bar{z}_r}{\Delta z_r/2}\right)^k$. The employment of the equation above requires knowing how to evaluate the integrals over the chord length, which, for how the optical path length is expressed (Eq. (4)), are of the kind

$$E_n(a_1, a_2, \ldots, a_{N_{p+1}}, l) = \int_0^l dt\, t^n e^{a_1(t-l)+a_2(t^2-l^2)+\ \ldots\ +a_{N_{p+1}}(t^{N_{p+1}}-l^{N_{p+1}})}. \quad (8)$$

Since no analytical solution is available for $N_p > 1$ and since it would be desirable to treat higher-order profiles (at least parabolic), we have decided to adopt a Prony approximation to express $e^{\tau(t)-\tau(l)}$ as

$$e^{a_1(t-l)+a_2(t^2-l^2)+\ \ldots\ +a_{N_{p+1}}(t^{N_{p+1}}-l^{N_{p+1}})} \approx \sum_{i=1}^{N_i/2} C_i e^{b_{iR}x} \begin{cases} cos(b_{iI}x) \\ sin(b_{iI}x) \end{cases}, \quad (9)$$

N_i being the chosen number of interpolation points. The presence of a cosine or a sine function depends on the b_i coefficients: for each pair of complex conjugates, there will be two subsequent terms having the same coefficient real parts (b_{iR} and b_{i+1R}) and imaginary parts (b_{iI} and b_{i+1I}), the former with the cosine function and the latter with the sine one.

3 FROM STEP-CONSTANT TO POLYNOMIAL CROSS SECTIONS

To obtain a first polynomial cross-section representation, we started translating a step-constant mesh into a polynomial one: for this purpose, we considered a set of macro-regions $\{r\}$, each one composed of a set of regions $\{i\}$ having constant cross-section values. To determine the coefficients $\{\Sigma_{r,p}, p = 0, N_p\}$ of the polynomial expansion within region r, one can first compute the cross-section moments with respect to the polynomials, which by definition read

$$'\vec{\Sigma}_r = \frac{1}{V_r}\int_r d\vec{r}\, \vec{P}(\tilde{z}_r)\Sigma(\vec{r}) = \frac{1}{\Delta z_r}\int_{z_r^{min}}^{z_r^{max}} dz\, \vec{P}(\tilde{z}_r)\Sigma(z) = \frac{1}{2}\int_{-1}^{1} d\tilde{z}_r\, \vec{P}(\tilde{z}_r)\Sigma(\tilde{z}_r), \quad (10)$$

V_r being the region volume. The integral over $\tilde{z}_r$ is equal to the sum of the contributions due to all the step-constant regions contained in r: therefore, the p^{th}-order moment can be written as

$$'\Sigma_{r,p} = \frac{1}{2}\sum_i \Sigma_i \int_{\tilde{z}_i^{low}}^{\tilde{z}_i^{up}} d\tilde{z}_r P_p(\tilde{z}_r) = \frac{1}{2(p+1)}\sum_i \Sigma_i \left[(\tilde{z}_i^{up})^{p+1} - (\tilde{z}_i^{low})^{p+1}\right], \quad (11)$$

where

$$\tilde{z}_i^{up} = \frac{\bar{z}_i - \bar{z}_r}{\Delta z_r/2} + \frac{\Delta z_i}{\Delta z_r}, \qquad \tilde{z}_i^{low} = \frac{\bar{z}_i - \bar{z}_r}{\Delta z_r/2} - \frac{\Delta z_i}{\Delta z_r}. \tag{12}$$

Once the moments have been the computed, the expansion coefficients can be retrieved as

$$\vec{\Sigma}_r = \bar{\bar{\mathcal{P}}}^{-1\prime}\vec{\Sigma}_r, \tag{13}$$

where the elements of matrix $\bar{\bar{\mathcal{P}}}$ read

$$\mathcal{P}_{ij} = \frac{1}{V_r}\int_r d\vec{r}\, P_i(\tilde{z}_r)P_j(\tilde{z}_r) = \frac{1}{\Delta z_r}\int_{\bar{z}_r-\Delta z_r/2}^{\bar{z}_r+\Delta z_r/2} dz_r \left(\frac{z_r - \bar{z}_r}{\Delta z_r/2}\right)^{i+j} = \begin{cases} \frac{1}{i+j+1} & for\ i+j\ even \\ 0 & for\ i+j\ odd \end{cases}. \tag{14}$$

Applying this to a cell of the ASTRID reactor [3], for an expansion of order 2 we have obtained the results shown in Fig. 1 for the fissile region (15 cm) and the fertile one above (10 cm). Figures refer to the energy group #1896 in a library of 1968 groups, in the case of burnup = 37500 MWd/t. The choice of this group is due both to the relatively strong variation it undergoes during evolution and to the relatively high values of the first- and second-order coefficients required for the polynomial expansion.

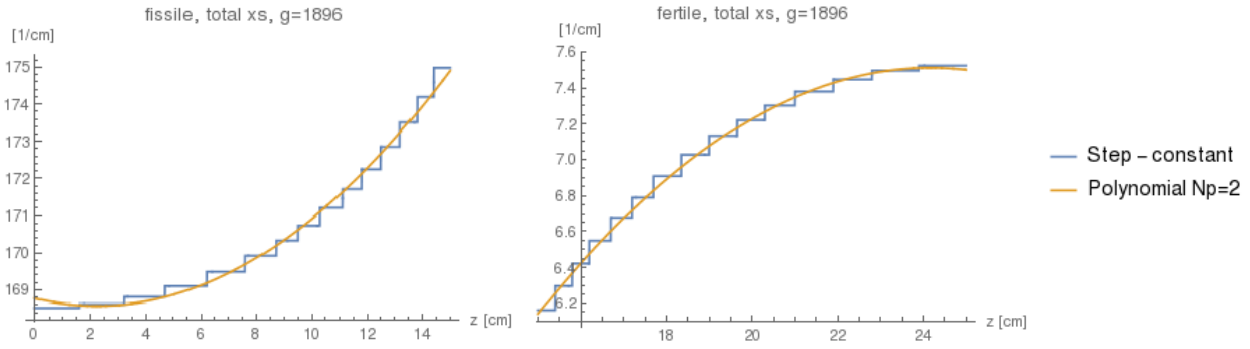

Figure 1: Total cross section plots for the fissile (left) and the fertile region (right).

4 PERSPECTIVES

The described method is currently being implemented in TDT, where Eq. (7) will be used as transmission equation for the trajectory sweep, at the inner iteration level of the power method. The problem will be closed by a suitable formulation of a balance equation, which has not been reported here because of lack of space and that will also be implemented. Once the code supports the polynomial cross-section environment, it will be necessary to accelerate the simulation.

REFERENCES

[1] S. Santandrea, D. Sciannandrone, R. Sanchez, L. Mao, L. Graziano, "A Neutron Transport Characteristics Method for 3D Axially Extruded Geometries Coupled with a Fine Group Self-Shielding Environment," *Nuclear Science and Engineering*, **186**, pp. 239-276 (2017).

[2] S. Santandrea, L. Graziano, D. Sciannandrone, "Accelerated polynomial axial expansions for full 3D neutron transport MOC in the APOLLO3® code system as applied to the ASTRID fast breeder reactor," *Annals of Nuclear Energy*, **113**, pp. 194-236 (2017).

[3] B. Fontaine, N. Devictor, P. Le Coz, A. Zaetta, D. Verwaerde, J.-M. Hamy, "The french R&D on SFR core design and ASTRID project," In: Global. Makuhari, Japan (2011).