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A 1st ORDER FORMULATION OF A REACTION RATE VARIATION FOR SPATIAL AND ENERGY COLLAPSING

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ABSTRACT

In this paper we present an extension of the Generalized Perturbation Theory (GPT) which enables accounting for a perturbation due to spatial and/or energy collapsing in the evaluation of a reaction rate variation. The proposed methodology could be proficiently and effectively adopted to appreciate the precision of the discretized, less refined calculation against an asymptotic, continuous space and energy one or a discretized, more refined calculation. A specific advantage of the proposed methodology is to be able to assign to each spatial mesh the weight of its contribution to the reaction rate variation, opening the way to a better understanding of the physical consequences of the collapsing and to a quantitative method to optimize a spatial grid.

Key Words: perturbation theory, cross sections collapsing, reaction rate, reactivity, optimization

1. INTRODUCTION

Since the beginning of the reactor development, the Classical Perturbation Theory, CPT, has been adopted and appreciated as a very powerful tool to evaluate, with high accuracy, the reactivity effects generated by small changes in the composition of a sample [1]. Very quickly, the method has been extended and generalized, under the name of Generalized Perturbation Theory (GPT), to the analysis of any kind of reaction-rates, either linear in the direct and adjoint fluxes or bi-linear in both them ([2], [3], [4]). With the introduction of the higher orders and the expansion on the harmonics of the neutron flux it is now likely reconstructing the reactivity and the reactions rates as accurately as desired in any perturbed condition ([5], [6]).

Conventionally, GPT have always accounted for cross-section variations in space and energy fixed conditions only, i.e., implicitly assuming that neither the number of energy groups nor the spatial meshing are modified when moving from the reference to the perturbed conditions.

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For the first time, in 2005, a work published by two authors of the present paper ([7]) suggested the adoption of a perturbation approach to evaluate the reactivity variation of a system as a consequence of the change in the energy group number and/or the spatial meshing. The present work, which is placed in the straight-line of the previous one, presents an extension of the methodology, which allows accounting for a variation of either the spatial mesh or the energy group number or both together, on both reactivity and reaction-rates, completing, that way, the set of variations which can be analyzed with the proposed methodology.

The development is founded on the awareness that any further discretization in space and energy generates a small error, compared to a either a continuous or a 'finer' asymptotic solution assumed as reference. It is then straightforward that the reactivity and the flux, obtained as result of a computation adopting collapsed cross-sections or coarser meshes, should be different from the original ones, due to the effect of the new meshing in space and energy.

Any difference between the reference and perturbed fluxes and reactivities can be seen as the 'source' of a small variation of the reaction rates. Thus, adopting a method derived from the 1st order Classical Perturbation Theory (CPT) [2], it is easy to quantify exactly not only the total variation, but also the asymptotic contribution of each individual region to the total reaction rate variation generated by the condensation-collapsing process.

The possibility to appreciate the weight of each spatial region is a major feature of the proposed method which can contribute significantly to improve understanding of the physical consequences of the collapsing and help developing a method to optimize a spatial grid. In this last sense, the new methodology can be part in the family of the so-called goal-oriented mesh adaptivity methods ([8]).

In the following, chapter 2 is aimed at presenting and discussing in some detail the development of the proposed new formulation; chapter 3 provides some numerical examples to show the physical consistency of the extended GPT methodology and, finally, chapter 4 sketches some conclusions and suggests possible fields of application.

2. THEORY

In this chapter, the proposed new method is fully and comprehensively derived. The first part of the chapter deals with the reactivity variation generated by space and energy collapsing and is mainly a recall of a previous work [7]. The second part is oriented to the description and the discussion of the methodology extension to set-out a relationship between the spatial/energy collapsing and a reaction rate variation.

2.1. Reactivity vs. Spatial/Energy Collapsing

Any generic reference system, which can be quoted as a 'fine-mesh' one, is governed by the homogeneous Boltzmann differential equation:

$$\left(A-\lambda_f F\right)\varphi_f = 0 \tag{1}$$

where A is the absorption + scattering + leakage operator and F is the fission production operator. Accordingly, any reaction rate can be defined as:

$$T_f = \frac{\langle \Sigma_1 \varphi_f \rangle}{\langle \Sigma_2 \varphi_f \rangle} \tag{2}$$

where, Σ_1 and Σ_2 are generic cross sections defined in the 'fine' space and, as usual, the symbol < > stands for integration in space and energy over the whole system.

If a flux-volume collapsing of the above-mentioned operators is performed, the system will be described by a new Boltzmann equation:

$$\left(\overline{A} - \lambda_c \overline{F}\right)\varphi_c = 0 \tag{3}$$

which admits the adjoint equation:

$$\left(\overline{A}^* - \lambda_c \overline{F}^*\right)\varphi_c^* = 0$$

In this new description, the generic Eq. (2) reaction-rate becomes:

$$T_c = \frac{\langle \overline{\Sigma}_1 \varphi_c \rangle}{\langle \overline{\Sigma}_2 \varphi_c \rangle} \tag{4}$$

where the collapsed cross-sections are obtained via the conventional weighting: $\overline{\Sigma} = \langle \Sigma\varphi \rangle / \langle \varphi \rangle$.
In any case, as a result of a mesh by mesh collapsing, the flux, the eigenvalue and the here above-defined new reaction rates shall be different from the original 'fine' ones due to the fine-structure information lost in the collapse.

If we assume that equation (3) has as solutions the eigenvalue λ_f and the collapsed flux $\overline{\varphi}_f$ (the true solutions that we hope for having after collapsing), generally, we will not obtain an homogeneous equation (as eq. 3) but an inhomogeneous one where the source term will be a new function that we call 'residual' function R and which is the remainder term originated from the collapsing itself:

$$\left(\overline{A} - \lambda_f \overline{F}\right)\overline{\varphi}_f = R \tag{5}$$

This equation can be viewed as an ordinary inhomogeneous differential equation (no more an eigenvalue equation but a one-solution equation) admitting as unique solution the flux $\overline{\varphi}_f$, depending on R, which contains some high-order harmonics.

Multiplying equation (3) by the adjoint solution of equation (5) (it is always possible to define an adjoint equation starting from a direct equation) and multiplying on both sides by the collapsed system adjoint flux φ_c^* [Eq. (5)], we obtain the system of constraints (actually, a couple of scalars because each one is an integral):

$$\left\langle \overline{\varphi}_f^* \middle| \left(\overline{A} - \lambda_c \overline{F}\right) \varphi_c \right\rangle = 0$$
$$\left\langle \varphi_c^* \middle| \left(\overline{A} - \lambda_f \overline{F}\right) \overline{\varphi}_f \right\rangle = \left\langle \varphi_c^* \middle| R \right\rangle$$

Subtracting them and remembering that an adjoint operator B is defined in such a way that $\left\langle f^* \middle| Bg \right\rangle = \left\langle B^* f^* \middle| g \right\rangle$, it is straightforward obtaining an expression for the eigenvalue variation engendered by the collapse. This relationship depends explicitly on the remainder function R:

$$\delta\lambda = \lambda_c - \lambda_f = \rho_f - \rho_c = -\delta\rho = \frac{\left\langle \varphi_c^* \middle| R \right\rangle}{\left\langle \varphi_c^* \middle| \overline{F}\overline{\varphi}_f \right\rangle} \tag{6}$$

This relationship can be viewed an application and a generalization of the Greenspan's lemma, derived for under-critical conditions [Refs. 9, 10].

According to the distributive property of the integral, any region-wise integrated term of $\left\langle \varphi_c^* \middle| R \right\rangle$ (divided by the whole integral $\left\langle \varphi_c^* \middle| \overline{F}\overline{\varphi}_f \right\rangle$) can be seen as the individual contribution of each spatial region to the total reactivity variation; in other words, the reactivity 'weight' of that region.

2.2. Reaction Rate vs. Spatial/Energy Collapsing

The same approach can be adopted to evaluate the impact of a collapsing on the reaction rates defined in equations (2) and (4).

At the 1st order, the relative difference between the reaction rate obtained with the flux issued from the collapsed equation and the original reaction rate can be written:

$$\frac{T_c - T_f}{T_f} \cong \frac{\left\langle \overline{\Sigma}_1 \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_1 \overline{\varphi}_f \right\rangle} - \frac{\left\langle \overline{\Sigma}_2 \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_2 \overline{\varphi}_f \right\rangle} \tag{7}$$

Where $\delta\varphi = \varphi_c - \overline{\varphi}_f$ is the difference between the flux issued from the collapsed equation (3) and the collapsed flux.

According to the Gandini's GPT heuristic approach [2], an adjoint source equation can be defined as follows:

$$\left(\overline{A} - \lambda_f \overline{F}\right)^* \Gamma^* = \frac{\overline{\Sigma}_1(x)}{\left\langle \overline{\Sigma}_1 \overline{\varphi}_f \right\rangle} - \frac{\overline{\Sigma}_2(x)}{\left\langle \overline{\Sigma}_2 \overline{\varphi}_f \right\rangle} \tag{8}$$

The solution Γ^* of equation (8) is usually called the *importance function*.

To obtain the relationship between the 1st order variation of the reaction rate (Eq. 7) and the importance function, Eq. 5 is to be written as:

$$\left(\overline{A} - \lambda_f \overline{F}\right)\delta\varphi = -R + \left(\overline{A} - \lambda_f \overline{F}\right)\varphi_c \tag{9}$$

Where we have used the definition: $\delta\varphi = \varphi_c - \overline{\varphi}_f$.

Let's now multiply the importance adjoint equation (8) by the flux variation $\delta\varphi$ and the flux variation direct equation (9) by the *importance function* Γ^*, after integration and subtraction (using the same methodology already shown in the previous paragraph), we obtain:

$$\frac{\left\langle \overline{\Sigma}_1 \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_1 \overline{\varphi}_f \right\rangle} - \frac{\left\langle \overline{\Sigma}_2 \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_2 \overline{\varphi}_f \right\rangle} = -\left\langle \Gamma^* \middle| R \right\rangle + \left\langle \Gamma^* \middle| \left(\overline{A} - \lambda_f \overline{F}\right)\varphi_c \right\rangle \tag{10}$$

But, from Eq. (3) and using $\delta\lambda = \lambda_c - \lambda_f$, we can write:

$$\left(\overline{A} - \lambda_f \overline{F}\right)\varphi_c = \left[\overline{A} - (\lambda_c - \delta\lambda)\overline{F}\right]\varphi_c = \delta\lambda\, \overline{F}\varphi_c \tag{11}$$

to finally obtain:

$$\frac{\left\langle \overline{\Sigma}_n \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_n \overline{\varphi}_f \right\rangle} - \frac{\left\langle \overline{\Sigma}_d \delta\varphi \right\rangle}{\left\langle \overline{\Sigma}_d \overline{\varphi}_f \right\rangle} = -\left\langle \Gamma^* \middle| R \right\rangle + \delta\lambda \left\langle \Gamma^* \middle| \overline{F}\varphi_c \right\rangle \tag{12}$$

We emphasize again that, compared to the conventional GPT [2], the integral $\left\langle \Gamma^* \middle| \overline{F}\varphi_c \right\rangle$ is not zero because the homogeneous equation associated to the source equation, Eq. (8), has only the obvious solution.

The main goal of the paper is demonstrating that, for each mesh in the system, the value of the function:

$$-\left\langle \Gamma^* \middle| R \right\rangle + \delta\lambda \left\langle \Gamma^* \middle| \overline{F}\varphi_c \right\rangle \tag{13}$$

accounts for the contribution of that specific mesh to the total reaction rate variation and, as it is the case for the reactivity variation, the function defined in Eq. (13) enables pointing out the space and energy region where the main discrepancies between the original 'fine' system and the new one originate.

This information is very useful when seeking for collapsing optimization and meshing procedures.

2.3. Comments

Before showing some numerical examples, it is worth to make some comments on Eq. (8) to point-out its features compared to the conventional GPT importance equation:

a. Even if Eq. (8) formally looks like the conventional GPT importance equation, a fundamental difference holds: in the present case, the *importance function* is computed through the collapsed (i.e., perturbed) equation and not from the original 'fine-mesh' reference (unperturbed) one, as it is always done for GPT;
b. The solution of the Eq. (8) is determined by the choice to impose the eigenvalue λ_f as multiplier of the collapsed production operator $\overline{F}$ (which means that equation $\left(\overline{A} - \lambda_f \overline{F}\right)^* \Psi = 0$ admits no solution except for the zero, obvious one);
c. As an immediate consequence of point b), the Γ^* function can be computed via an ordinary iterative sequence like:

$$A^*\Gamma^*_{i+1} = \lambda_f F^*\Gamma^*_i + \frac{\Sigma_1}{\left\langle \Sigma_1 \varphi_f \right\rangle} - \frac{\Sigma_2}{\left\langle \Sigma_2 \varphi_f \right\rangle}$$

without addition of any filtering as it is the case for conventional GPT, where a cleaning-up is necessary to clean the current solution up from the so-called "fundamental mode contamination" [2] [3] (actually, in GPT, Γ^*_{i+1} the fundamental mode is usually cleaned-up adopting a deflation technique:

$$\tilde{\Gamma}^*_{i+1} = \Gamma^*_{i+1} - \varphi^*_c \frac{\left\langle \overline{F}^*\Gamma^*_{i+1} \middle| \varphi_c \right\rangle}{\left\langle F^*\varphi^*_c \middle| \varphi_c \right\rangle}).$$

3. NUMERICAL EXAMPLES

In the following, a simple example is given where the meshes and the energy group number of a slab are modified. The sample computation geometry has two regions: fuel core and reflector. Boundary conditions are: reflection on the left (fuel side) and zero incoming current on the right (reflector). The slab has a thickness of 35 cm (30 cm fuel and 5 cm reflector). The reference spatial meshing is 0,25 cm (4 computation points per cm) and computation is performed at 2 energy groups using diffusion theory and finite difference method ([11]).

The target reaction rate is the ratio between the production reaction rate in the second half of the slab (boundary with the reflector) and the production reaction rate in the first one.

In the following table it is possible to see results for 3 perturbations:

1. mesh length goes from 0,25 to 1 cm,
2. energy groups go from 2 to 1,
3. both changes in a whole: from 4 to 1 computation points per cm and from 2 to 1 group.

Table I presents, on the one hand the reference values for the reactivity and the reaction rate (Exact 'fine' computation value), and on the other hand for the 3 collapsed cases the Exact 'coarse' computation value and the 1st order GPT value.

Table I. Numerical Examples and Results

Case	Reactivity (pcm)	Reaction Rate
Exact 'fine' computation value	19302	0,60791
Space collapsing: from 4 to 1 mesh par cm		
Exact 'coarse' computation value	19288	0,60456 (-0,55%)
'Coarse' value with 1st order GPT	19288	0,60452 (-0,56%)
Energy collapsing: from 2 to 1 group		
Exact 'coarse' computation value	20226	0,66564 (+9,50%)
'Coarse' value with 1st order GPT	20226	0,66577 (+9,52%)
Space and energy collapsing: from 4 to 1 mesh and from 2 to 1 group		
Exact 'coarse' computation value	20237	0,66707 (+9,73%)
'Coarse' value with 1st order GPT	20237	0,66722 (+9,76%)

These results point out that Eqs. (6) and (12) do well. Accordingly it can be claimed that the 1st order GPT is efficient for both reactivity variation (which was already known from [7]) as well as reaction rate variation, which is a fully new result. Figure 1 shows the mesh values of the integral (13) for the three cases here above. The same curve of the case '4 -> 1 mesh' is shown in Figure 2, with a different scale to enhance its trend.

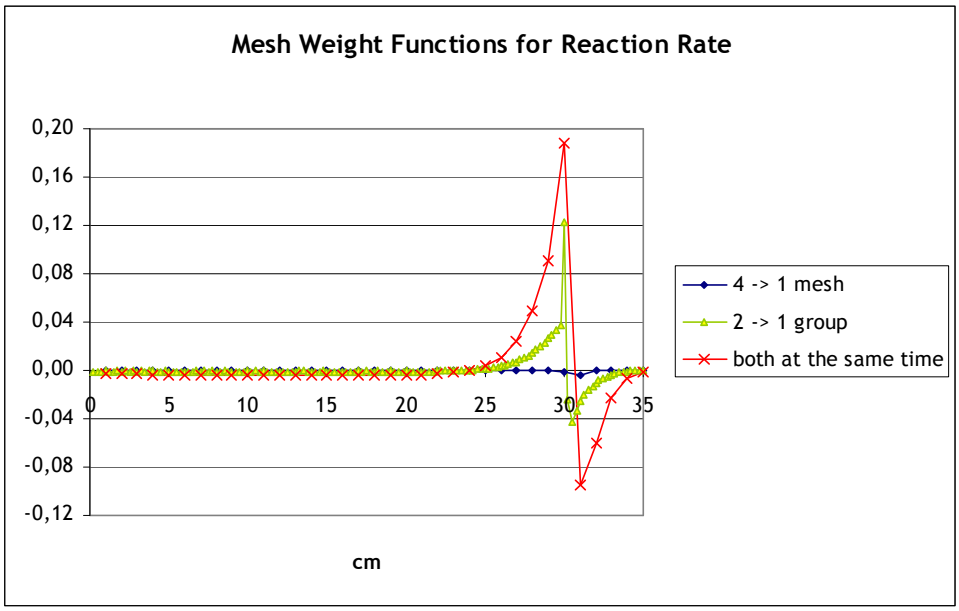

Figure 1. Mesh Weight Function for Reaction rate

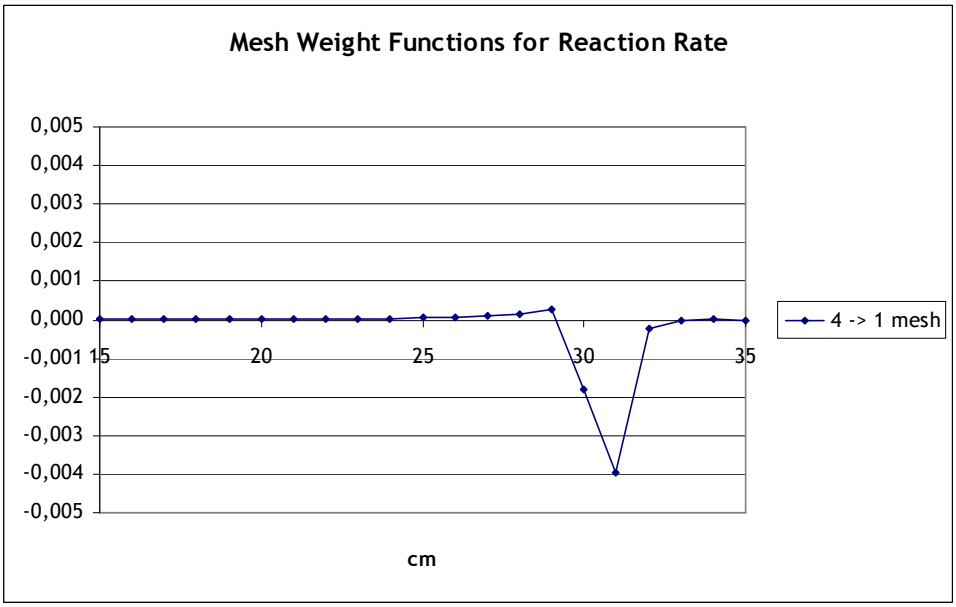

Figure 2. Focus on Mesh Weight Function for collapsing from 4 to 1 Mesh

The Figures 1 and 2 show that the source of the reaction rate variation, when a generic spatial collapsing is made, is located near the interface fuel-reflector. This is not surprising, and remains coherent with previous results obtained in the case of the reactivity variation, because the evaluation of the flux gradient is certainly more difficult with a 'coarse' spatial of energy grid than a 'finer' one. Anyway, we notice that the effects of the energy collapsing are still strong quite far from the boundary fuel-reflector and that the cumulated effects of energy and space collapsing are stronger than the simple sum of both.

This example gives a taste of the method effectiveness, but the demonstration should be completed and further validated, above all, in case of a larger number of energy groups. However, the method will probably continue be effective for any group number, because 2 / 1 group collapse at the fuel-moderator boundary means to loose information about the thermal part of the spectrum and it is a difficult problem to cope with.

4. CONCLUSIONS

The extension of the GPT proposed in this paper enlarges the field of applications of the perturbation theory to include a whole field, which has been impossible to cope with until now: conventional GPT could only match with problems such as the variation of either a microscopic cross section or an isotope concentration implicitly assuming that there is no change either in the spatial meshing or in the energy groups number.

The proposed approach of this paper enables evaluating, both qualitatively and quantitatively, the impact on the reactivity and on reaction rates of spatial meshing and/or energy group number variations. Moreover, it is also possible to assess rigorously the weight of each collapsed mesh to the calculation discrepancies on reactivity and reaction rate distribution.

This present paper describes the new theory and gives an example of numerical application to demonstrate the validity of the method and the physical consistency of the results.

This new capability could show-up very powerful and quite useful in many practical problems when the optimization of a spatial meshing required and when an optimum energy group splitting is to be searched for.

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