Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

ON THE DEVELOPMENT OF AN EXPLICIT POLYNOMIAL FORM FOR HIGHER-ORDER ACCURATE QUANTIFICATION OF PERTURBATION EFFECTS IN NUCLEAR SYSTEMS

R. van Geemert, F. Tani
Paul Scherrer Institute, Nuclear Energy and Safety Research Department
CH-5232 Villigen PSI, Switzerland
rene.vangeemert@psi.ch, filippo.tani@psi.ch

ABSTRACT

A methodology is presented that allows a higher order accurate treatment of system perturbations that are assumed to have a substantial magnitude and therefore also a substantial effect on response quantities. Examples are localized material choice variations, burnable poison density variations at lattice level, complete fuel assembly permutations at core level, or specific uncertainties defined in the system composition. For these cases, it is necessary to raise the accuracy of the estimated responses above what can be achieved using first-order perturbation methods only, of course preferably without having to simply pursue expensive exact recalculations for each case, if the effects of many variations or uncertainties are to be assessed. Focussing on the neutronics of multiplying systems (without thermal-hydraulic feedback mechanisms incorporated), the setup of an explicit, noniterative, nonrecursive polynomial form for quantification of the perturbation effects is pursued. This form features the property that a response quantity change, caused by variations in certain parameters localised in space and energy, can be expanded polynomially up to higher order accuracy, with the variations themselves as functional arguments. Numerical results, showing the validity of the method, are reported, and possible application areas are discussed.

Key Words: generalized perturbation theory, uncertainty analysis, design optimization

1. INTRODUCTION

Adequate quantification of the effects of nuclear system parameter variations, as well as of material composition perturbations, on response quantities like eigenvalues and localised power densities, is of importance in various areas in nuclear technology. Examples are nuclear uncertainty analysis, sensitivity analysis for reactor transients and design optimization (i.e. fuel lattice design optimization, control rod movement planning, shielding design or in-core fuel management optimization). In a number of previous studies, where emphasis was put on assessing the effects of uncertainties in scalar system parameters, first order methodologies [1,2,3] were shown to generate adequate predictions of the effects of those uncertainties on different response quantities of relevance. The development presented in this paper is aimed essentially at a methodology that allows a higher order accurate treatment of localised material composition changes or uncertainties that may in fact have a substantial magnitude as well as a substantial effect on response quantities (such as material choice variations, burnable poison density variations at lattice level, or complete fuel assembly permutations at core level). For these cases, it is necessary to raise the accuracy of the results above what can be achieved using first-order methods only, of course preferably without having to simply pursue expensive exact recalculations for each case if the effects of many uncertainties or variations are to be assessed. In previous studies, acquisition of higher-order accurate perturbed results either entailed the use of preconditioned iterative methods [4,5,6], or required the

availability of an extensive set of higher order reference eigensolutions [7] of the system equations. This paper is focussed on the development of a methodology, focussed on the neutronics of multiplying systems (without thermal-hydraulic feedback mechanisms incorporated), that enables the setup of an explicit, noniterative, nonrecursive *polynomial* form. This form features the property that the effect on a response quantity, caused by variations in certain parameters localised in space and energy, can be expanded polynomially up to higher order accuracy, with the variations themselves as functional arguments.

2. OBJECTIVES OF THE DEVELOPMENT

The particular goal of the development presented here is to enable an expansion, in polynomial form, of the perturbation in *flux shape* caused by a prespecified perturbation distribution in the material composition field characterizing a certain reactor configuration. We emphasize again that, in this particular study, the focus is on the neutronics equations, with no thermal-hydraulic feedback mechanisms incorporated. With the spatial flux shape we adopted a rather ambitious choice for the response function, but generally the formalism can be set up for less ambitious choices for the response function as well (like, for example, the integral reactivity, the power produced by a prespecified subregion in the system, or a detector response). The convenience requirement for this expansion is that it is to satisfy the property of *not* containing any a-priori unknown quantities like the eigenvalue change and the flux change itself. Methods reported previously [4,5,6] have departed from this feature, as a result of which the developed numerical schemes leading to higher-order accurate solutions were still *iterative* in nature, though significantly accelerated. However, for various purposes it would be absolutely preferable to avail of an explicit, non-iterative expansion that gives the response function perturbation simply as a *polynomial* function of the parameter variations, with the order of the polynomial determined by the accuracy requirement on the result. In this way it is, for example, also possible to isolate a flux in a specific position and energy group as a *single* response quantity, and still be able to compute, for only this particular isolated response quantity, the perturbed value with higher-order accuracy, *without* the necessity of having to compute the perturbed entire flux solution (that is, for every position and energy group), as is in fact the case for the previously reported methodologies. In the next section, the classical neutronic system equations are recalled, followed by the systematic derivation of the expressions for polynomial expansion of the spatial effect on the flux distribution caused by local parameter variations.

3. GENERALIZED PERTURBATION THEORY FOR MULTIPLYING SYSTEMS

Throughout this study, we assume the standard form for the neutronics eigenvalue equation, determining the spatial flux shape $\underline{\psi}$ and the eigenvalue λ, which can be written compactly as

$$(\mathbf{M} - \lambda\mathbf{F})\,\underline{\psi} = \underline{0} \tag{1}$$

with $\mathbf{M}$ and $\mathbf{F}$ the neutron loss and production operator, respectively. The normalisation requirement for the spatial neutron flux shape, adopted in this study, is

$$\langle \underline{1} | \underline{\psi} \rangle \stackrel{\text{def}}{=} \int_{\mathrm{V}} \int_{0}^{\infty} \int_{4\pi} \psi(\underline{\mathrm{r}}, \mathrm{E}, \underline{\Omega}) \mathrm{d}\Omega \mathrm{d}\mathrm{E} \mathrm{d}\mathrm{V} = 1 \tag{2}$$

In order to initiate the formalism aimed at arriving at a polynomial form for perturbation calculations, we consider the response functional $\underline{\mathcal{R}}$, consisting of the flux $\underline{\psi}$ as a response vector, minus the system equations premultiplied with associated Lagrange multipliers $\underline{\underline{\Gamma}}^*$ and $\underline{\Phi}^*$:

$$\underline{\mathcal{R}} = \underline{\psi} - \langle \underline{\underline{\Gamma}}^* | \mathbf{M} - \lambda\mathbf{F} | \underline{\psi} \rangle - \underline{\Phi}^* (\langle \underline{1} | \underline{\psi} \rangle - 1) \tag{3}$$

Clearly, if $\lambda, \underline{\psi}$ satisfies the unperturbed system equations, then $\underline{\mathcal{R}} = \underline{\psi}$. Likewise, if the perturbed solution $\lambda', \underline{\psi}'$, perturbed due to operator changes $\mathbf{M}\rightarrow\mathbf{M}'=\mathbf{M}+\Delta\mathbf{M}$, $\mathbf{F}\rightarrow\mathbf{F}'=\mathbf{F}+\Delta\mathbf{F}$, satisfies the perturbed version of the system equations, then $\underline{\mathcal{R}}' = \underline{\psi}'$ and thus $\Delta\underline{\mathcal{R}} = \Delta\underline{\psi}$. In accordance with previously reported approaches, the $\underline{\underline{\Gamma}}^*$ and $\underline{\Phi}^*$ are chosen such that the particular 1^{st}-order terms which contain $\Delta\lambda$ and $\Delta\underline{\psi}$ in the development of $\Delta\underline{\mathcal{R}}\,[\Delta\mathbf{M}, \Delta\mathbf{F}, \Delta\lambda, \Delta\underline{\psi}]$ are conveniently conditioned to vanish. Writing $\Delta\underline{\psi}$ as $\langle\underline{\underline{\delta}}|\Delta\underline{\psi}\rangle$, with $\underline{\underline{\delta}}$ the unity tensor, subtracting the unperturbed from the perturbed response functional, using the adjoint operator property $\langle\underline{\underline{\Gamma}}^*|\mathbf{M}\Delta\underline{\psi}\rangle = \langle\mathbf{M}^*\underline{\underline{\Gamma}}^*|\Delta\underline{\psi}\rangle$ and ordering the terms, the following development for the response functional change is obtained:

$$\begin{aligned}\Delta\underline{\mathcal{R}} = &-\langle\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi}\rangle \;\left(\,1^{\text{st}}\text{ order },\ \text{a priori } \textit{known}\right)\\ &-\langle(\mathbf{M}^* - \lambda\mathbf{F}^*)\underline{\underline{\Gamma}}^* + \underline{\Phi}^*\underline{1} - \underline{\underline{\delta}}|\Delta\underline{\psi}\rangle + \Delta\lambda\langle\underline{\underline{\Gamma}}^*|\mathbf{F}\underline{\psi}\rangle \;\left(\,1^{\text{st}}\text{ order },\ \text{a priori } \textit{un}\text{known}\right)\\ &-\langle\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\Delta\underline{\psi}\rangle + \Delta\lambda\langle\underline{\underline{\Gamma}}^*|\Delta(\mathbf{F}\underline{\psi})\rangle \;\left(\,2^{\text{nd}}, 3^{\text{rd}}\text{ order },\ \text{a priori } \textit{un}\text{known}\,\right)\end{aligned} \tag{4}$$

The *a priori un*known 1^{st}-order terms in Eq.(4) can be conditioned to vanish, regardless of $\Delta\lambda$, $\Delta\underline{\psi}$, if the Lagrange multiplier $\underline{\underline{\Gamma}}^*$ is made to satisfy

$$(\mathbf{M}^* - \lambda\mathbf{F}^*)\,\underline{\underline{\Gamma}}^* = \underline{\underline{\delta}} - \underline{\Phi}^*\underline{1} \overset{\text{def}}{=} \underline{\underline{\mathrm{Q}}}^* \ , \tag{5}$$

with λ following from Eq.(1) and thus fixed here (the source $\underline{\underline{\mathrm{Q}}}^*$ can be interpreted here as a ***flux importance source distribution***), and if the uniqueness of $\underline{\underline{\Gamma}}^*$ is determined by the orthogonality condition

$$\langle\underline{\underline{\Gamma}}^*|\mathbf{F}\underline{\psi}\rangle = \underline{0} \tag{6}$$

How to numerically realize this combined objective, with the operator $(\mathbf{M}^* - \lambda\mathbf{F}^*)$ being singular, is discussed extensively in previously published studies [4,5,6]. These studies indicate that, since the operator $(\mathbf{M}^* - \lambda\mathbf{F}^*)$ is singular, meaning here that any arbitrary multiple of the fundamental adjoint flux $\underline{\psi}^*$ (the fundamental solution of the homogeneous adjoint equation $(\mathbf{M}^* - \lambda\mathbf{F}^*)\,\underline{\psi}^* = \underline{0}$) added to a particular solution will yield another valid solution to Eq.(5). However, since Eq.(6) can be satisfied only ([6]) if $\underline{\underline{\Gamma}}^*$ is numerically conditioned to be completely free of any traces of the fundamental adjoint flux $\underline{\psi}^*$, the uniqueness of $\underline{\underline{\Gamma}}^*$ is dictated in this way. By adding case-dependent traces of $\underline{\psi}^*$ to $\underline{\underline{\Gamma}}^*$, leaving the validity of Eq.(5) intact, any alternative orthogonality condition can be realized. The convenience of this property will become obvious in section 4, in which adding a trace of $\underline{\psi}^*$ is shown to enable the satisfaction of perturbed orthogonality conditions. The choice for the multiplier $\underline{\Phi}^*$ is determined by the fact that Eqs.(5) and (6) specify that $\langle\underline{\psi}|\underline{\underline{\mathrm{Q}}}^*\rangle = \underline{0}$. This can be clarified by analysing the inner product $\langle\underline{\psi}|\underline{\underline{\mathrm{Q}}}^*\rangle = \underline{0}$:

$$\langle\underline{\psi}|\underline{\underline{\mathrm{Q}}}^*\rangle = \langle\underline{\psi}|\mathbf{M}^* - \lambda\mathbf{F}^*|\underline{\underline{\Gamma}}^*\rangle = \langle(\mathbf{M} - \lambda\mathbf{F})\underline{\psi}|\underline{\underline{\Gamma}}^*\rangle = \langle\underline{0}|\underline{\underline{\Gamma}}^*\rangle = \underline{0} \tag{7}$$

Hence, $\underline{\Phi}^*$ is given by

$$\underline{\Phi}^* \;=\; \langle\underline{\underline{\delta}}|\underline{\psi}\rangle \;=\; \underline{\psi} \tag{8}$$

If Eqs.(5),(6),(8) are satisfied by $\underline{\underline{\Gamma}}^*$ and $\underline{\Phi}^*$, the expression for the response function change reduces to

$$\Delta\underline{\mathcal{R}} = \Delta\underline{\psi} = -\langle\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi} + \Delta\underline{\psi}\rangle + \Delta\lambda\,\langle\underline{\underline{\Gamma}}^*|\Delta\left(\mathbf{F}\underline{\psi}\right)\rangle \tag{9}$$

Inconveniently, $\Delta\lambda$ and $\Delta\underline{\psi}$ are still present in Eq.(9), giving rise to second and higher order terms in the expression that cannot be known a priori and will be negligible only in case of very small perturbations. The principal result of (first-order) generalized perturbation theory (GPT), with the flux distribution as the

choice for the response vector, is the *first-order* expression for the flux change as a function of the operator changes $\Delta\mathbf{M}$ and $\Delta\mathbf{F}$:

$$\Delta^{(1)}\underline{\psi} = -\langle\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi}\rangle \tag{10}$$

This kind of expression is at the basis of any sensitivity analysis methodology that is aimed at the qualitative differentation between response function effects due to different variations/uncertainties to be assessed. However, for applications where *accuracy* is important as well, the accuracy associated with this expression is acceptable only in case of very small localised uncertainties or variations. Hence, in the generalized case of not so small localised variations, a clear interest in the availability of an optimally efficient higher-order methodology can be identified. In theory, one can apply a methodology [7] featuring the use of higher mode (direct and adjoint) solutions of Eq.(1) for this purpose. However, the numerical practise of acquiring an extensive, well-converged set of higher modes for non-analytical cases, as required for application and reliability of such an approach, has proven quite nontrivial in our experience, especially where the issues of computational effort and feasible accuracy for high modes are concerned. Therefore, we invested in the development of an alternative methodology which does lead to a polynomial form but does not require higher modes explicitly. Since in Eq.(5), λ is a fixed scalar multiplier (since it followed from solving λ, $\underline{\psi}$ from Eq.(1) for the unperturbed, reference state of the system), expansion of $\underline{\underline{\Gamma}}^*$ in terms of an independent but finite set of basic flux importance vectors (solved for the same reference state) is a possibility that provides convenience under a number of numerical scenarios, as will become clear in sections 5 and 6. The description of this development is pursued in the next sections.

4. TOWARDS A POLYNOMIAL FORMULATION OF GPT

We now move forward towards developing a higher-order accurate polynomial expansion that does *not* contain $\Delta\lambda$ and $\Delta\underline{\psi}$ anymore, as in Eq.(9). Regarding $\Delta\lambda$, one can, perturbation-case dependently, make the response functional *higher-order* insensitive with respect to the eigenvalue change $\Delta\lambda$, that is, adjust $\underline{\underline{\Gamma}}^*$ slightly by allowing a trace $\Delta\underline{\alpha}\,\underline{\psi}^*$ of the fundamental adjoint mode $\underline{\psi}^*$ in the adjoint field $\underline{\underline{\Gamma}}^*$:

$$\underline{\underline{\Gamma}}^* \rightarrow \underline{\underline{\Gamma}}^{*\prime} = \underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* \ , \tag{11}$$

leaving, of course, the validity of Eq.(5) intact (since $(\mathbf{M}^* - \lambda\mathbf{F}^*)\underline{\psi}^* = \underline{0}$) but enabling the satisfaction of the *perturbed* orthogonality condition

$$\langle\underline{\underline{\Gamma}}^{*\prime}|\mathbf{F}\underline{\psi}\rangle + \langle\underline{\underline{\Gamma}}^{*\prime}|\Delta(\mathbf{F}\underline{\psi})\rangle = \langle\underline{\underline{\Gamma}}^{*\prime}|\mathbf{F}'\underline{\psi}'\rangle = 0 \tag{12}$$

rather than the reference condition $\langle\Gamma^*|\mathbf{F}\underline{\psi}\rangle = 0$ satisfied by the reference field $\underline{\underline{\Gamma}}^*$. Implementing the adjustment $\underline{\underline{\Gamma}}^{*\prime} = \underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^*$ in Eq.(12), in order to force the multiplier connected to $\Delta\lambda$ in Eq.(9) to vanish, we obtain the following dependence for $\Delta\underline{\alpha}$:

$$\Delta\underline{\alpha} = \frac{\langle\underline{\underline{\Gamma}}^{*\prime} \mid \mathbf{F}' \mid \underline{\psi}'\rangle}{\langle\underline{\psi}^* \mid \mathbf{F}' \mid \underline{\psi}'\rangle} \ , \tag{13}$$

in which case the development for $\Delta\underline{\mathcal{R}}$ reduces to the following form that does not contain $\Delta\lambda$ anymore:

$$\Delta\underline{\mathcal{R}} = -\langle\underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi} + \Delta\underline{\psi}\rangle \tag{14}$$

Obviously, Eq.(14) will represent an exactly valid relationship $\Delta\underline{\mathcal{R}} = \Delta\underline{\psi}$ *only* if a method is available for generating $\Delta\underline{\psi}$ which is, in this case, the response vector itself. Hence, with the response quantity

occurring on both the left- and right-handside of the equation, previously reported studies [4,5,6] have proposed a *preconditioned iterative* method for this. In this study however, we are interested in having a *polynomial* rather than iterative form for $\Delta\underline{\mathcal{R}}$, in which the explicit dependence on $\Delta\underline{\psi}$ is conveniently conditioned to vanish by case-dependent further correction of the sensitivity operator $\underline{\underline{\Gamma}}^*$, *without* a need for availing of many higher eigenmodes for the unperturbed case. Now, for setting up a polynomial expansion, featuring the absence of the a priori unknown term $\Delta\underline{\psi}$, we propose the following perturbation-case dependent adjustment of $\underline{\underline{\Gamma}}^*$:

$$\underline{\underline{\Gamma}}^* \rightarrow \underline{\underline{\Gamma}}^{*'} \;=\; \underline{\underline{\Gamma}}^* \;-\; \Delta\underline{\alpha}\,\underline{\psi}^* + \Delta\underline{\underline{\Gamma}}^* \;+\; \Delta^2\underline{\underline{\Gamma}}^* \;+\; \Delta^3\underline{\underline{\Gamma}}^* + \ldots \tag{15}$$

Utilizing this perturbation-case dependent adjustment in the development for $\Delta\underline{\mathcal{R}}$, with Eqs.(5),(6) still satisfied, and pre-assuming that the condition (12) can still be satisfied, we obtain:

$$\begin{aligned}
\Delta\underline{\mathcal{R}} = -\langle \underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi}\rangle \\
- [\langle \underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \Delta\underline{\psi}\rangle + \langle \Delta\underline{\underline{\Gamma}}^* | \mathbf{M} - \lambda\mathbf{F} | \Delta\underline{\psi}\rangle] \\
- \langle \Delta\underline{\underline{\Gamma}}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi}\rangle \\
- [\langle \Delta\underline{\underline{\Gamma}}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \Delta\underline{\psi}\rangle + \langle \Delta^2\underline{\underline{\Gamma}}^* | \mathbf{M} - \lambda\mathbf{F} | \Delta\underline{\psi}\rangle] \\
- \langle \Delta^2\underline{\underline{\Gamma}}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi}\rangle \\
- [\langle \Delta^2\underline{\underline{\Gamma}}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \Delta\underline{\psi}\rangle + \langle \Delta^3\underline{\underline{\Gamma}}^* | \mathbf{M} - \lambda\mathbf{F} | \Delta\underline{\psi}\rangle] \\
- \langle \Delta^3\underline{\underline{\Gamma}}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi}\rangle \\
- [\,\ldots \;+\; \ldots\,] \\
- \ldots \quad ,
\end{aligned} \tag{16}$$

which can be written in expansion notation, using the adjoint operators $\mathbf{M}^*$ and $\mathbf{F}^*$, as

$$\begin{aligned}
\Delta\underline{\mathcal{R}} = -\langle \underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi}\rangle - \sum_{\mathrm{n}=1}^{\infty} \left\langle \Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^* \middle| \Delta\mathbf{M} - \lambda\Delta\mathbf{F} \middle| \underline{\psi} \right\rangle \\
- \langle (\mathbf{M}^* - \lambda\mathbf{F}^*)\Delta\underline{\underline{\Gamma}}^* + (\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)(\underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^*) | \Delta\underline{\psi}\rangle \\
- \sum_{n=1}^{\infty} \left\langle (\mathbf{M}^* - \lambda\mathbf{F}^*)\Delta^{(n)}\underline{\underline{\Gamma}}^* + (\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)\Delta^{(n-1)}\underline{\underline{\Gamma}}^* \middle| \Delta\underline{\psi} \right\rangle
\end{aligned} \tag{17}$$

We see that all the terms containing the a-priori unknown $\Delta\underline{\psi}$ (which is the response vector itself), can be conveniently conditioned to vanish by imposing the following relationship between the consecutive (n-1)$^{\mathrm{th}}$ and n$^{\mathrm{th}}$ order sensitivity operator correction terms $\Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^*$ and $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$:

$$(\mathbf{M}^* - \lambda\mathbf{F}^*)\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^* = -(\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)\Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^* \stackrel{\mathrm{def}}{=} \Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^* \;\;, \tag{18}$$

with the n$^{\mathrm{th}}$ importance correction source $\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^*$ defined as

$$\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^* \stackrel{\mathrm{def}}{=} -(\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)\Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^* \tag{19}$$

The relationship between the consecutive $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$ is initiated by setting

$$\Delta^{(1)}\underline{\underline{Q}}^* = -(\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)[\underline{\underline{\Gamma}}^* - \Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*] \tag{20}$$

with $\Delta\underline{\tilde{\alpha}}$ the best *a priori* calculational estimate for $\Delta\underline{\alpha}$. Obviously, since $\Delta\underline{\alpha}$ is both at the root (through Eq.(20)) and at the end of the sequential determination of the expansion (through Eq.(13)), it formally plays the role of an outer iterative parameter. However, in sections 5 and 6 it will be argued that $\Delta\underline{\alpha}$, which is generally quite small and represents a minor term in the case-dependent corrected sensitivity operator $\underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* + \sum_{\mathrm{n}=1}^{\infty}\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$, can be assessed more than adequately enough in a non-iterative way. Because of this, it is possible to have an *explicit* rather than implicit (i.e., iterative or recursive) expansion that, as shown in section 8, features higher-order accuracy even in cases where substantial perturbations, of magnitudes larger than characteristic of control rod movements in an LWR-core, are imposed. If Eqs.(13),(18) and (20) are satisfied, we obtain the polynomial expansion

$$\Delta\underline{\mathcal{R}} = -\langle\underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi}\rangle - \sum_{\mathrm{n}=1}^{\infty}\langle\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi}\rangle \tag{21}$$

In sections 5 and 6, a semi-explicit (recursive) as well as an explicit (non-recursive) method are presented for fast calculation of the case-dependent, higher order components $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$ and the orthogonality correction term $\Delta\underline{\tilde{\alpha}}$ in the case-dependent sensitivity operator $\underline{\underline{\Gamma}}^* - \Delta\underline{\tilde{\alpha}}\,\underline{\psi}^* + \sum_{\mathrm{n}=1}^{\infty}\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$. Both $\Delta\underline{\tilde{\alpha}}$ and $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$ can be written as polynomial expressions with $\Delta\mathbf{M}$ and $\Delta\mathbf{F}$ as fuctional arguments. Due to this, $\Delta\underline{\mathcal{R}}$ can also be written as a polynomial expression with $\Delta\mathbf{M}$ and $\Delta\mathbf{F}$ as fuctional arguments. In section 6, it will be argued that the resulting form is similar to one where the dependence of a response vector $\underline{f}$ with respect to parameter variations, grouped in the variation vector $\Delta\underline{\mathrm{x}} = [\,\mathrm{x}_1\;\mathrm{x}_2\;\cdots\;\mathrm{x}_\mathrm{P}\,]^\mathrm{T}$, can be written as a functional expansion up to arbitrary order:

$$\underline{f}(\Delta\underline{\mathrm{x}}) = \frac{\partial\underline{f}}{\partial\underline{\mathrm{x}}}\Delta\underline{\mathrm{x}} + \frac{1}{2!}\frac{\partial^2\underline{f}}{\partial\underline{\mathrm{x}}^2}\Delta\underline{\mathrm{x}}^2 + \frac{1}{3!}\frac{\partial^3\underline{f}}{\partial\underline{\mathrm{x}}^3}\Delta\underline{\mathrm{x}}^3 \;+\; \ldots \tag{22}$$

with the expansion matrices $\frac{\partial\underline{f}}{\partial\underline{\mathrm{x}}}$, $\frac{\partial^2\underline{f}}{\partial\underline{\mathrm{x}}^2}$, $\ldots$ of general validity and independent of the choice for the components in the variation vector $\Delta\underline{\mathrm{x}}$. Obviously, Eq.(21) can be rewritten as

$$\Delta\underline{\mathcal{R}} = -\left\langle\underline{\underline{\Gamma}}^* - \Delta\underline{\alpha}\,\underline{\psi}^* + \sum_{\mathrm{n}=1}^{\infty}\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*\middle|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}\middle|\underline{\psi}\right\rangle \;, \tag{23}$$

indicating of course that the adjusted sensitivity field $\underline{\underline{\Gamma}}^{*'}$, constructed through expansion in conformity with Eq.(15), in fact satisfies the *perturbed* flux importance equation. Rewriting Eq.(4) as

$$\Delta\underline{\mathcal{R}} = -\langle\underline{\underline{\Gamma}}^*|\Delta\mathbf{M} - \lambda\Delta\mathbf{F}|\underline{\psi}\rangle \;-\; \langle(\mathbf{M}^{*\prime} - \lambda\mathbf{F}^{*\prime})\underline{\underline{\Gamma}}^* + \underline{\Phi}^*\underline{1} - \underline{\underline{\delta}}|\Delta\underline{\psi}\rangle + \Delta\lambda\langle\underline{\underline{\Gamma}}^*|\mathbf{F}'\underline{\psi}'\rangle \;, \tag{24}$$

it becomes clear that the converged $\underline{\underline{\Gamma}}^{*'}$ satisfies a perturbed flux importance equation that nevertheless has the same importance source distribution as the unperturbed flux importance equation:

$$\left(\mathbf{M}^{*\prime} - \lambda\mathbf{F}^{*\prime}\right)\underline{\underline{\Gamma}}^{*'} \;=\; \left(\mathbf{M}^* - \lambda\mathbf{F}^*\right)\underline{\underline{\Gamma}}^* \;=\; \underline{\underline{\delta}} - \underline{\Phi}^*\underline{1} \;, \tag{25}$$

so that the choice for $\underline{\Phi}^*$ as expressed in (8) can be preserved. Further, through the addition of the trace $\Delta\underline{\alpha}$ of the fundamental adjoint flux $\underline{\psi}^*$, $\underline{\underline{\Gamma}}^{*\prime}$ can be conditioned (with thereby its uniqueness determined as well) to satisfy the perturbed orthogonality condition:

$$\langle\underline{\underline{\Gamma}}^{*'}|\mathbf{F}'\underline{\psi}'\rangle = \underline{0} \tag{26}$$

Since the multiplier λ in these perturbed equations is, of course, still the one that followed from solving the unperturbed eigenvalue equation (1) for the unperturbed system, and thus fixed, Eq.(25) can be solved efficiently by polynomial expansion, with the operator changes as functional arguments, utilizing a finite set of basic flux importance vectors (solved for the same reference state), as will be shown in sections 5 and 6. In case of *very* large perturbations imposed in the system, the expansion may *diverge* in an oscillating way, which is a phenomenon that has been encountered before, and investigated in a previously published study [5] for the case of iterative higher-order perturbation theory. This behaviour can be briefly commented on here by noting that the condition number η for quantification of the convergence in scheme (18), written more explicitly as

$$(\mathbf{M}^* - \lambda\mathbf{F}^*)\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^* \;=\; -(\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*)\Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^* \;, \tag{27}$$

can be expressed as

$$\eta \;\approx\; \frac{\parallel (\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*) \parallel}{\parallel (\mathbf{M}^* - \lambda\mathbf{F}^*) \parallel} \tag{28}$$

Hence, the smaller $\Delta\mathbf{M}$ and $\Delta\mathbf{F}$, the faster the magnitudes of the higher order correction terms $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$ will descend to zero. However, should $\parallel (\Delta\mathbf{M}^* - \lambda\Delta\mathbf{F}^*) \parallel$ exceed $\parallel (\mathbf{M}^* - \lambda\mathbf{F}^*) \parallel$, the $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^*$ will diverge in an oscillating way, with the sign fluctuations being caused by the minus sign in Eq.(18). In section 8 it will be argued, partially through a numerical example, that for practical cases the perturbation regime that still preserves convergence of the expansion can be expected to be generously broad. This implies that the methodology is generally not constrained to the treatment of only small perturbations, and can in fact generate higher order accurate results for rather substantial localised system composition variations. Due to this, an interesting potential exists for its application in uncertainty propagation and design optimization studies where higher order accurate assessments of rather substantial uncertainties and localised material density changes are required.

5. RECURSIVE EXPANSION IN THE COEFFICIENT SPACE

For establishing computational efficiency in case of the envisaged need for quick but accurate evaluation of the effects of *many* different individual cases of localised perturbation distributions, a worthwile effort is to first numerically acquire a set of base solutions, $\underline{\gamma}^*_{\mathrm{kg}}$, associated with spatial region k and neutron energy group g, satisfying (with λ following from the solution of Eq.(1) for the unperturbed system, and thus fixed here):

$$(\mathbf{M}^* - \lambda\mathbf{F}^*)\underline{\gamma}^*_{\mathrm{kg}} = \underline{\delta}_{\mathrm{kg}} \tag{29}$$

with the components of the unity tensor $\underline{\delta}_{\mathrm{kg}}$ defined as

$$\left[\underline{\delta}_{\mathrm{kg}}\right]_{\mathrm{k,g;k',g'}} = \begin{cases} 1 & \text{if k' = k , g' = g} \\ 0 & \text{otherwise} \end{cases} \tag{30}$$

The physical interpretation of these solutions can be formulated by argueing that the space- and energy-dependent components of $\underline{\gamma}^*_{\mathrm{kg}}$ represent the relative, renormalized *importance* of localised, space- and energy-dependent parameter changes for any arbitrary response quantity defined in the particular phase space point k,g. Writing every adjoint source vector $\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^*$ that is defined in Eq.(19), as a sum over its

space- and energywise constituents that act as weight coefficients for the different orthonormal base vectors $\underline{\delta}_{\mathrm{kg}}$:

$$\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^{*}=\sum_{\mathrm{k}}\sum_{\mathrm{g}}\Delta^{(\mathrm{n})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}\underline{\delta}_{\mathrm{kg}}=\sum_{\mathrm{g}}\left\{\Delta^{(\mathrm{n})}\underline{\mathrm{q}}^{*}_{1\mathrm{g}}\begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}+\Delta^{(\mathrm{n})}\underline{\mathrm{q}}^{*}_{2\mathrm{g}}\begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}+\ldots\right\}\underline{\delta}_{\mathrm{g}}\ , \tag{31}$$

and applying the additivity property

$$(\mathbf{M}^{*}-\lambda\mathbf{F}^{*})\begin{bmatrix}\underline{\gamma}^{*}_{\mathrm{kg}}\\ \underline{\gamma}^{*}_{\mathrm{k'g'}}\end{bmatrix}=\begin{bmatrix}\underline{\delta}^{*}_{\mathrm{kg}}\\ \underline{\delta}^{*}_{\mathrm{k'g'}}\end{bmatrix}\ \Longrightarrow\ (\Delta\mathbf{M}^{*}-\lambda\Delta\mathbf{F}^{*})[\mathrm{c}_{\mathrm{kg}}\,\underline{\gamma}^{*}_{\mathrm{kg}}+\mathrm{c}_{\mathrm{k'g'}}\,\underline{\gamma}^{*}_{\mathrm{k'g'}}]=\mathrm{c}_{\mathrm{kg}}\,\underline{\delta}^{*}_{\mathrm{kg}}+\mathrm{c}_{\mathrm{k'g'}}\,\underline{\delta}^{*}_{\mathrm{k'g'}}\ , \tag{32}$$

the solution of Eq.(18) can be expanded as

$$\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}=\sum_{\mathrm{k}}\sum_{\mathrm{g}}\Delta^{(\mathrm{n-1})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}\,\underline{\gamma}^{*}_{\mathrm{kg}} \tag{33}$$

Now, instead of solving each $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}$ iteratively as a function of its predecessor $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}$, it is possible to define a *recursive* solution of Eq.(18) *in the coefficients space*, enabling a computationally much more efficient and quicker way for determining $\underline{\underline{\Gamma}}^{*'}=\underline{\underline{\Gamma}}^{*}-\Delta\underline{\alpha}\,\underline{\psi}^{*}+\Delta\underline{\underline{\Gamma}}^{*}+\Delta^{2}\underline{\underline{\Gamma}}^{*}+\ldots$, by using the fact that *any* field $\underline{\underline{\Gamma}}^{*'}$ can be represented *entirely* and *uniquely* by its *expansion coefficients* in case of utilizing the set $\{\underline{\gamma}^{*}_{\mathrm{kg}}\}$. Defining

$$\Delta\underline{\zeta}^{*}_{\mathrm{kg}}=(\Delta\mathbf{M}^{*}-\lambda\Delta\mathbf{F}^{*})\underline{\gamma}^{*}_{\mathrm{kg}}\ , \tag{34}$$

we can rewrite Eq.(18) as

$$(\mathbf{M}^{*}-\lambda\mathbf{F}^{*})\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}=-\sum_{\mathrm{k}}\sum_{\mathrm{g}}\left\langle\Delta^{(\mathrm{n-1})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}\middle|\Delta\underline{\underline{\zeta}}^{*}\right\rangle_{\mathrm{kg}}\underline{\delta}_{\mathrm{kg}}\ , \tag{35}$$

with the (k,g)-component of the inner product $\langle\Delta^{(\mathrm{n-1})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}|\Delta\underline{\underline{\zeta}}^{*}\rangle_{\mathrm{kg}}$ defined as

$$\left\langle\Delta^{(\mathrm{n-1})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}\middle|\Delta\underline{\underline{\zeta}}^{*}\right\rangle_{\mathrm{kg}}=\sum_{\mathrm{k'}}\sum_{\mathrm{g'}}\Delta^{(\mathrm{n-1})}\mathrm{q}^{*}_{\mathrm{kg}}(\mathrm{k'},\mathrm{g'})\ \Delta\zeta^{*}_{\mathrm{kg}}(\mathrm{k'},\mathrm{g'}) \tag{36}$$

Realizing that $\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}=\sum_{\mathrm{k}}\sum_{\mathrm{g}}\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{q}}}^{*}_{\mathrm{kg}}\,\underline{\gamma}^{*}_{\mathrm{kg}}$ and thus

$$(\mathbf{M}^{*}-\lambda\mathbf{F}^{*})\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*}=\sum_{\mathrm{k}}\sum_{\mathrm{g}}\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{q}}}^{*}_{\mathrm{kg}}\,\underline{\delta}_{\mathrm{kg}}\ , \tag{37}$$

and combining this result with Eq.(35), we arrive at

$$\Delta^{(\mathrm{n})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}=-\left\langle\Delta^{(\mathrm{n-1})}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}\middle|\Delta\underline{\underline{\zeta}}^{*}\right\rangle_{\mathrm{kg}} \tag{38}$$

Using Eq.(38), one can define a recursive solution scheme in the coefficient space only. Once the $\underline{\gamma}^{*}_{\mathrm{kg}}$ and thus the $\Delta\underline{\zeta}^{*}_{\mathrm{kg}}$ are known, this recursion can be done by a simple program external to the neutronics code. This means that, with the $\underline{\gamma}^{*}_{\mathrm{kg}}$ available and the response quantity choice reflected in the zeroeth coefficients $\underline{\mathrm{q}}^{*}_{\mathrm{kg}}=\Delta^{(0)}\underline{\mathrm{q}}^{*}_{\mathrm{kg}}$, it is possible to *automate* the setup of a higher-order accurate sensitivity database for various quantities of interest, without requiring further iterative calculations by the neutronics code.

6. EXPLICIT POLYNOMIAL EXPANSION

We now move towards an explicit, non-recursive expression. For application in lattice and shielding design, as well as in core loading pattern design, having an explicit form provides better conditions for pursuing optimization studies. We assume that we have macroscopic cross-section perturbations (for example, due to isotope density uncertainties/variations or due to nuclear data uncertainties), defined in P different cells. For the notations that follow, we emphasize that the energy group dependence, though not written explicitly, is incorporated *implicitly* in the expressions. In this case, we can write

$$\Delta^{(\mathrm{n})}\underline{\underline{\mathrm{Q}}}^{*} = -\sum_{\mathrm{p}_0=1}^{\mathrm{P}} \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^{*}(\mathrm{p}_0)\underline{\delta}_{\mathrm{p}_0} \quad , \tag{39}$$

with '(A)' indicating 'absorption' and '(F)' indicating 'fission', leading, according to Eq.(33), to the result

$$\Delta^{(\mathrm{n})}\underline{\underline{\Gamma}}^{*} = -\sum_{\mathrm{p}_0=1}^{\mathrm{P}} \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \Delta^{(\mathrm{n}-1)}\underline{\underline{\Gamma}}^{*}(\mathrm{p}_0)\underline{\gamma}_{\mathrm{p}_0}^{*} \tag{40}$$

Writing, for the first sensitivity operator correction, the expansion form

$$\Delta^{(1)}\underline{\underline{\Gamma}}^{*} = \sum_{\mathrm{p}_0=1}^{\mathrm{P}} \underline{\underline{\vartheta}}_1\left[\mathrm{p}_0\right] \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \quad , \tag{41}$$

we obtain for the first expansion coefficient matrix $\underline{\underline{\vartheta}}_1\left[\mathrm{p}_0\right]$, associated with the perturbation p_0,

$$\underline{\underline{\vartheta}}_1\left[\mathrm{p}_0\right] = -\left[\underline{\underline{\Gamma}}^{*}(\mathrm{p}_0) - \Delta\underline{\tilde{\alpha}}\,\psi^{*}(\mathrm{p}_0)\right]\underline{\gamma}_{\mathrm{p}_0}^{*} \quad , \tag{42}$$

with $\Delta\underline{\tilde{\alpha}}$ the intitial estimate for $\Delta^{(\mathrm{n})}\underline{\alpha}$, defined by the expression:

$$\Delta\underline{\tilde{\alpha}} = \frac{\langle \underline{\underline{\Gamma}}^{*} \mid \mathbf{F}' \mid \underline{\psi} + \Delta^{(1)}\underline{\psi}\rangle}{\langle \underline{\psi}^{*} \mid \mathbf{F}' \mid \underline{\psi} + \Delta^{(1)}\underline{\psi}\rangle} \quad , \tag{43}$$

using the reference $\underline{\underline{\Gamma}}^{*}$ and the directly calculable first-order estimate (10) for the change in flux distribution. Implementing Eq.(42) in Eq.(40) for obtaining $\Delta^{(2)}\underline{\underline{\Gamma}}^{*}$, we get

$$\begin{aligned}
\Delta^{(2)}\underline{\underline{\Gamma}}^{*} &= -\sum_{\mathrm{p}_0=1}^{\mathrm{P}} \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \Delta^{(1)}\underline{\underline{\Gamma}}^{*}(\mathrm{p}_0)\underline{\gamma}_{\mathrm{p}_0}^{*} \\
&= -\sum_{\mathrm{p}_0=1}^{\mathrm{P}} \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \left\{-\sum_{\mathrm{p}_1=1}^{\mathrm{P}} [\underline{\underline{\Gamma}}^{*}(\mathrm{p}_1) - \Delta\underline{\tilde{\alpha}}\,\psi^{*}(\mathrm{p}_1)]\gamma_{\mathrm{p}_1}^{*}(\mathrm{p}_0) \left(\Delta\Sigma_{\mathrm{p}_1}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_1}^{(\mathrm{F})}\right)\right\}\underline{\gamma}_{\mathrm{p}_0}^{*} \\
&= \sum_{\mathrm{p}_0=1}^{\mathrm{P}} \sum_{\mathrm{p}_1=1}^{\mathrm{P}} \underline{\underline{\vartheta}}_2\left[\mathrm{p}_0, \mathrm{p}_1\right] \left(\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_0}^{(\mathrm{F})}\right) \left(\Delta\Sigma_{\mathrm{p}_1}^{(\mathrm{A})} - \lambda\Delta\Sigma_{\mathrm{p}_1}^{(\mathrm{F})}\right) \quad ,
\end{aligned} \tag{44}$$

with the second order expansion coefficient matrix $\underline{\underline{\vartheta}}_2\left[\mathrm{p}_0, \mathrm{p}_1\right]$, associated with the perturbations p_0 and p_1, given by

$$\underline{\underline{\vartheta}}_2\left[\mathrm{p}_0, \mathrm{p}_1\right] = (-1)^2[\underline{\underline{\Gamma}}^{*}(\mathrm{p}_1) - \Delta\underline{\tilde{\alpha}}\,\psi^{*}(\mathrm{p}_1)]\gamma_{\mathrm{p}_1}^{*}(\mathrm{p}_0)\underline{\gamma}_{\mathrm{p}_0}^{*} \tag{45}$$

Generalizing to $\Delta^{(n)}\underline{\underline{\Gamma}}^*$, we obtain

$$\Delta^{(n)}\underline{\underline{\Gamma}}^* = \sum_{p_0=1}^{P}\sum_{p_1=1}^{P}\cdots\sum_{p_{n-1}=1}^{P}\underline{\underline{\vartheta}}_n\,[p_0,p_1,\ldots,p_{n-1}]\prod_{i=0}^{n-1}\left(\Delta\Sigma_{p_i}^{(A)}-\lambda\Delta\Sigma_{p_i}^{(F)}\right)\ , \tag{46}$$

with the expression for the n^{th} order expansion coefficient matrix $\underline{\underline{\vartheta}}_n\,[p_0,p_1,\ldots,p_{n-1}]$, associated with the perturbations $p_0,\ \ldots,\ p_{n-1}$, given by

$$\underline{\underline{\vartheta}}_n\,[p_0,p_1,\ldots,p_{n-1}] = (-1)^n[\underline{\underline{\Gamma}}^*(p_{n-1})-\Delta\underline{\tilde{\alpha}}\,\psi^*(p_{n-1})]\gamma^*_{p_n}(p_{n-1})\gamma^*_{p_{n-1}}(p_{n-2})\cdots\gamma^*_{p_1}(p_0)\underline{\gamma}^*_{p_0}$$

which can be written more formally as

$$\underline{\underline{\vartheta}}_n\,[p_0,p_1,\ldots,p_{n-1}] = (-1)^n[\underline{\underline{\Gamma}}^*(p_{n-1})-\Delta\underline{\tilde{\alpha}}\,\psi^*(p_{n-1})]\left\{\prod_{i=1}^{n-1}\gamma^*_{p_{n-i}}(p_{n-i-1})\right\}\underline{\gamma}^*_{p_0} \tag{47}$$

Obviously, afterwards we still need to update $\Delta\underline{\tilde{\alpha}}\ \rightarrow\ \Delta^{(n)}\underline{\alpha}$, such that we can really enforce $\langle\underline{\underline{\Gamma}}^{*'}|\mathbf{F}'\psi'\rangle = 0$. Now, from Eq.(13) we obtain

$$\left\langle\underline{\underline{\Gamma}}^*+\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*_i-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*\ \middle|\ \mathbf{F}'\ \middle|\ \underline{\psi}+\sum_{i=1}^{n}\Delta^{(i)}\underline{\psi}\right\rangle-\Delta^{(n)}\alpha\left\langle\underline{\psi}^*\ \middle|\ \mathbf{F}'\ \middle|\ \underline{\psi}+\sum_{i=1}^{n}\Delta^{(i)}\underline{\psi}\right\rangle=\underline{0} \tag{48}$$

With $\sum_{i=1}^{n}\Delta^{(i)}\underline{\psi}$ pre-estimated by $\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle$, we get

$$\Delta^{(n)}\underline{\alpha} = \frac{\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*+\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*_i\ |\ \mathbf{F}'\ |\ \underline{\psi}+\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle}{\langle\underline{\psi}^*\ |\ \mathbf{F}'\ |\ \underline{\psi}+\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle} \tag{49}$$

Further, incorporating the case-independent orthogonality property $\langle\underline{\underline{\Gamma}}^*|\mathbf{F}\underline{\psi}\rangle = \underline{0}$, we obtain

$$\Delta^{(n)}\underline{\alpha} = \frac{\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*|\Delta\mathbf{F}\underline{\psi}+\mathbf{F}\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle}{\langle\underline{\psi}^*\ |\ \mathbf{F}'\ |\ \underline{\psi}+\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle}$$

$$+\ \frac{\langle\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*_i\ |\ \mathbf{F}'\ |\ \underline{\psi}+\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle}{\langle\underline{\psi}^*\ |\ \mathbf{F}'\ |\ \underline{\psi}+\langle\underline{\underline{\Gamma}}^*-\Delta\underline{\tilde{\alpha}}\,\underline{\psi}^*-\sum_{i=1}^{n}\Delta^{(i)}\underline{\underline{\Gamma}}^*|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle} \tag{50}$$

with $\Delta\underline{\tilde{\alpha}}$ defined by Eq.(43). The denominators in Eq.(50) allow further explicit expansion by application of the Taylor formula

$$\frac{1}{1-\Delta x} = 1\ +\ \Delta x\ +\ \Delta x^2\ +\ \Delta x^3\ +\ \ldots\ +\ \Delta x^n\ +\ O(\Delta x^{n+1}) \tag{51}$$

for a renormalized variation Δx. Numerical experience, also in the case of substantial perturbations, has pointed out that this direct procedure of non-iterative computation of $\Delta^{(n)}\underline{\alpha}$ can hardly be improved by still reinitializing $\Delta\underline{\tilde{\alpha}}\ :=\ \Delta^{(n)}\underline{\alpha}$ and repeating the procedure (effectively pursuing an outer iterative loop), in the sense that the 'new' result for $\Delta^{(n)}\underline{\alpha}$ has been observed hardly to differ from the 'old' $\Delta^{(n)}\underline{\alpha}$, also in case of substantial perturbations. Therefore, in acquiring the numerical results that are presented in section

8, no such outer iteration was performed. Summarizing, the complete explicit polynomial form of order n for the flux change, due to a set of P simultaneous perturbations, amounts to

$$\begin{aligned}\left[\Delta\underline{\psi}\right]^{(\mathrm{n})} &= -\langle\underline{\underline{\Gamma}}^{*\prime}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle \\ &= \Delta^{(1)}\underline{\psi} + \underbrace{\Delta^{(\mathrm{n})}\underline{\alpha}\langle\underline{\psi}^{*}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle}_{\text{orthogonality correction}} - \underbrace{\sum_{\mathrm{i}=1}^{\mathrm{n}}\langle\Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}^{*}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle}_{\text{explicit higher order terms}}\end{aligned} \quad , \tag{52}$$

with the following explicit expressions for $\Delta^{(\mathrm{n})}\underline{\alpha}$, $\Delta^{(\mathrm{i})}\psi$ and $\Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}^{*}$:

$$\begin{cases} \Delta^{(\mathrm{n})}\underline{\alpha} = \frac{\langle\underline{\underline{\Gamma}}^{*}-\Delta\tilde{\underline{\alpha}}\,\underline{\psi}^{*}+\sum_{\mathrm{i}=1}^{\mathrm{n}}\Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}_{\mathrm{i}}^{*}\,|\,\mathbf{F}'\,|\,\underline{\psi}+\langle\underline{\underline{\Gamma}}^{*}-\Delta\tilde{\underline{\alpha}}\,\underline{\psi}^{*}-\sum_{\mathrm{i}=1}^{\mathrm{n}}\Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}^{*}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle}{\langle\underline{\psi}^{*}\,|\,\mathbf{F}'\,|\,\underline{\psi}+\langle\underline{\underline{\Gamma}}^{*}-\Delta\tilde{\underline{\alpha}}\,\underline{\psi}^{*}-\sum_{\mathrm{i}=1}^{\mathrm{n}}\Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}^{*}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle\rangle} \ , \text{ with} \\ \Delta\tilde{\underline{\alpha}} = \frac{\langle\underline{\underline{\Gamma}}^{*}\,|\,\mathbf{F}'\,|\,\underline{\psi}+\Delta^{(1)}\underline{\psi}\rangle}{\langle\underline{\psi}^{*}\,|\,\mathbf{F}'\,|\,\underline{\psi}+\Delta^{(1)}\underline{\psi}\rangle} \ , \\ \Delta^{(1)}\underline{\psi} = -\langle\underline{\underline{\Gamma}}^{*}|\Delta\mathbf{M}-\lambda\Delta\mathbf{F}|\underline{\psi}\rangle \ \text{ and} \\ \Delta^{(\mathrm{i})}\underline{\underline{\Gamma}}^{*} = \sum_{\mathrm{p}_0=1}^{\mathrm{P}}\cdots\sum_{\mathrm{p}_{\mathrm{i}-1}=1}^{\mathrm{P}}\underline{\underline{\vartheta}}_{\mathrm{i}}\left[\mathrm{p}_0,\mathrm{p}_1,\ldots,\mathrm{p}_{\mathrm{i}-1}\right]\prod_{\mathrm{j}=0}^{\mathrm{i}-1}\left(\Delta\Sigma_{\mathrm{p}_\mathrm{j}}^{(\mathrm{A})}-\lambda\Delta\Sigma_{\mathrm{p}_\mathrm{j}}^{(\mathrm{F})}\right) \ , \text{ with} \\ \underline{\underline{\vartheta}}_{\mathrm{i}}\left[\mathrm{p}_0,\mathrm{p}_1,\ldots,\mathrm{p}_{\mathrm{i}-1}\right] = (-1)^{\mathrm{i}}\left[\underline{\Gamma}^{*}(\mathrm{p}_{\mathrm{i}-1})-\Delta\tilde{\underline{\alpha}}\,\psi^{*}(\mathrm{p}_{\mathrm{i}-1})\right]\left\{\prod_{\mathrm{j}=1}^{\mathrm{i}-1}\gamma_{\mathrm{p}_{\mathrm{i}-\mathrm{j}}}^{*}\left(\mathrm{p}_{\mathrm{i}-\mathrm{j}-1}\right)\right\}\underline{\gamma}_{\mathrm{p}_0}^{*} \end{cases} \tag{53}$$

As one can check in the expressions listed in Eqs.(53),(52), all the input required for application of the expansion (i.e., $\underline{\underline{\Gamma}}^{*}$, $\underline{\underline{\gamma}}^{*}$, $\underline{\psi}^{*}$, $\underline{\psi}$ and λ) will be known *a priori*. Thus, in case of the P perturbations $\Delta\Sigma_{\mathrm{p}}^{(\mathrm{A})}$, $\Delta\Sigma_{\mathrm{p}}^{(\mathrm{F})}$, the resulting flux change distribution $\Delta\underline{\psi}$ can, with higher-order accuracy, be written as a polynomial function, up to arbitrary order n, with case-independent j^{th}-order expansion coefficients $\underline{\omega}_{\mathrm{j}}\left[\mathrm{p}_0,\ldots,\mathrm{p}_{\mathrm{j}-1}\right]$ and with the variations $\Delta\mathrm{x}_{\mathrm{p}_\mathrm{i}} \stackrel{\mathrm{def}}{=} (\Delta\Sigma_{\mathrm{p}_\mathrm{i}}^{(\mathrm{A})}-\lambda\Delta\Sigma_{\mathrm{p}_\mathrm{i}}^{(\mathrm{F})})$ as functional arguments:

$$\left[\Delta\underline{\psi}\right]^{(\mathrm{n})} = \sum_{\mathrm{j}=1}^{\mathrm{n}}\left\{\sum_{\mathrm{p}_0=1}^{\mathrm{P}}\cdots\sum_{\mathrm{p}_{\mathrm{j}-1}=1}^{\mathrm{P}}\underline{\omega}_{\mathrm{j}}\left[\mathrm{p}_0,\ldots,\mathrm{p}_{\mathrm{j}-1}\right]\prod_{\mathrm{i}=1}^{\mathrm{j}-1}\Delta\mathrm{x}_{\mathrm{p}_\mathrm{i}}\right\} \tag{54}$$

The offdiagonal elements in $\underline{\omega}_{\mathrm{j}}\left[\mathrm{p}_0,\ldots,\mathrm{p}_{\mathrm{j}-1}\right]$ give rise to *cross-terms* in the expansion. These cross-terms reflect the mutual influence (neutronic coupling) of different positions with regard to their contribution to the n^{th}-order effect in the response quantity (which, in this case, is the flux distribution). Obviously, the number of cross-terms grows drastically with both the number of perturbations P and the expansion order n. However, it will generally be possible to pre-classify part (and often: most) of the cross-terms as being of such small magnitude that they will hardly contribute to the expansion, and therefore can be omitted without seriously affecting the final result of the expansion. In particular, this property applies when, in the product $\prod_{\mathrm{i}=1}^{\mathrm{n}-1}\gamma_{\mathrm{p}_{\mathrm{n}-\mathrm{i}}}^{*}(\mathrm{p}_{\mathrm{n}-\mathrm{i}-1})$ (which occurs in Eq.(47) for the definition of the higher order expansion coefficients $\underline{\underline{\vartheta}}_{\mathrm{n}}\left[\mathrm{p}_0,\mathrm{p}_1,\ldots,\mathrm{p}_{\mathrm{n}-1}\right]$), many combinations $\mathrm{p}_{\mathrm{n}-\mathrm{i}}$,$\mathrm{p}_{\mathrm{n}-\mathrm{i}-1}$ occur for which $\gamma_{\mathrm{p}_{\mathrm{n}-\mathrm{i}}}^{*}(\mathrm{p}_{\mathrm{n}-\mathrm{i}-1})$ is very small. These will then give rise to a product chain containing many small numbers that thus cause a very small final value of the product. This is especially the case when the different perturbations are spatially somewhat farther apart in the system. Hence, if the calculation approach for setting up the expansion is conditioned adequately, a possible transition from computational gain to computational loss, related to the existence of many higher-order cross-terms, can be avoided.

7. COMPUTATIONAL INVESTMENTS AND PROFITS

The computational effort, involved in determining the base set according to Eq.(29), is typically two or even three orders of magnitude larger than the effort associated with a single standard iterative calculation, depending on system size, mesh and adopted number of energy groups. This picture would change slightly when one avails of a massively *parallel* machine, as is described in more detail in one of the studies [6] pursued previously. Since the calculation of the base set can be parallellized straightforwardly, it would be possible to reduce the wall clock time for its acquisition by typically two orders of magnitude (depending on the number of available parallel processors). In this way, one could lower the wall clock time barrier significantly for the subsequent use of the base set in sequentially programmed procedures. In any case, this computational investment will pay off in terms of a reduced overall wall clock time when the effects of *many* variations are to be assessed, regardless of whether the base set is computed parallelly or sequentially. In case of typically thousands or more assessments, the computational gain will be rewarding indeed. However, when one is interested in quantifying the effect on, for example, the power distribution and/or the reactivity of only a *limited* number of possible uncertainties or parameter variations, it is more recommendable simply to assess these effects by a number of repetitions of the standard calculational (i.e. iterative) procedure, and perform a limited sensitivity study in that way.

The *real* merit of the presented methodology starts to surface when one wants to pursue an automated *extensive* sensitivity study that is meant to include information on the influences on a response function (reaction rate distributions, reactivity, or detector responses) exerted by *many* different known or potential uncertainty sources and to make a reliable, higher-order accurate ranking of the importance of different potential error sources, or when one aims at performing a *design optimization study*. Especially in the latter case, the power of the method is related to the enabled use of more sophisticated mathematical optimization methods that utilize the higher-order gradient information. In this way, application of the polynomial form, with the possibility to compute the expansion coefficients $\underline{\omega}_{\mathrm{j}}\left[\mathrm{p}_0,\ldots,\mathrm{p}_{\mathrm{j}-1}\right]$ explicitly, may be expected to lead to either a significant acceleration of the nuclear design optimization process or/and, more importantly, to lead to better final designs. Further, in case of variation/discrepancy propagation studies, a possibility to pursue the relatively time-economous setup of a polynomial expansion *external* to the neutronics code is a desirable property from a programming efficiency point of view, which would facilitate the efficient generation of extensive higher-order accurate sensitivity databases in validation and sensitivity studies. In the next section, two numerical validation tests will be presented.

8. NUMERICAL VERIFICATION OF THE METHODOLOGY

The method has been tested on a nodal neutronics model for a fictitious PWR core, containing 96 fuel elements per quadrant. As a numerical test, a substantial material composition change was introduced quadrant-symmetrically in one of the fuel elements, amounting to a single localised $\mathrm{k}_{\mathrm{inf}}$-decrease of 25%. Naturally, such a perturbation gives rise to a spatial disturbance in the power distribution in the core (as shown in Fig.1), especially in the perturbation position itself, but also in its direct and more distant surroundings.

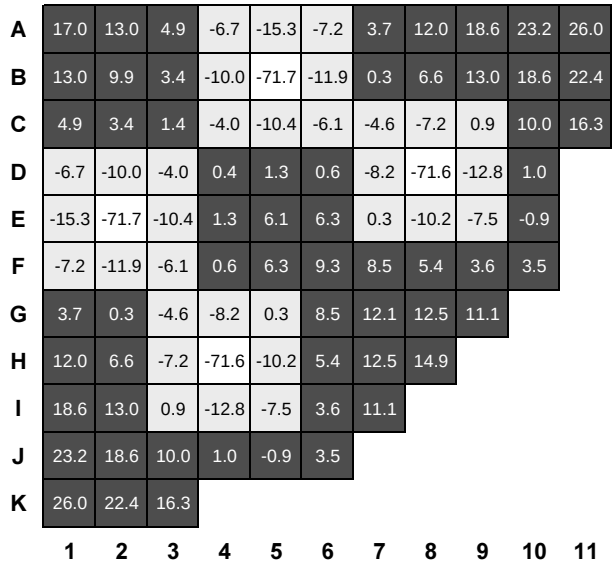
Using the polynomial form, it was possible to compute, within short time compared to pursuing simply a new standard iteration for the perturbed case, the spatial power disturbance with higher-order accuracy. In Fig.2, the agreement between the prediction of polynomial GPT and the exact perturbed nodal powers is illustrated as a function of the expansion order n. In this figure, it is interesting to observe that, by low order expansion only, more distant (and thus smaller) power changes can be better captured than the power

	1	2	3	4	5	6	7	8	9	10	11
A	6.0	5.1	3.5	1.3	-1.1	-3.7	-5.8	-7.2	-7.8	-7.9	-7.8
B	6.2	5.3	3.6	1.3	-1.7	-5.1	-7.9	-9.0	-9.0	-8.7	-8.4
C	6.5	5.6	3.9	1.2	-2.6	-7.9	-13.2	-12.9	-11.2	-10.1	-9.4
D	7.0	6.1	4.3	1.5	-2.9	-10.4	-21.4	-16.7	-12.9	-11.3	
E	7.7	6.8	5.1	2.2	-1.8	-7.2	-13.3	-13.7	-12.3	-11.4	
F	8.4	7.5	5.9	3.5	0.2	-3.5	-7.0	-9.1	-9.9	-10.3	
G	9.1	8.3	7.0	4.9	2.2	-0.7	-3.4	-5.6	-7.2		
H	9.7	9.2	8.0	6.3	4.1	1.6	-0.8	-3.0			
I	10.4	9.9	8.9	7.5	5.6	3.4	1.2				
J	10.8	10.4	9.6	8.3	6.7	4.8					
K	11.0	10.7	10.1								

Figure 1. Spatial disturbance in the power distribution (expressed in % with respect to the unperturbed nodal power distribution), due to a localised material composition perturbation, causing a -25% k_{inf}-perturbation in element D7.

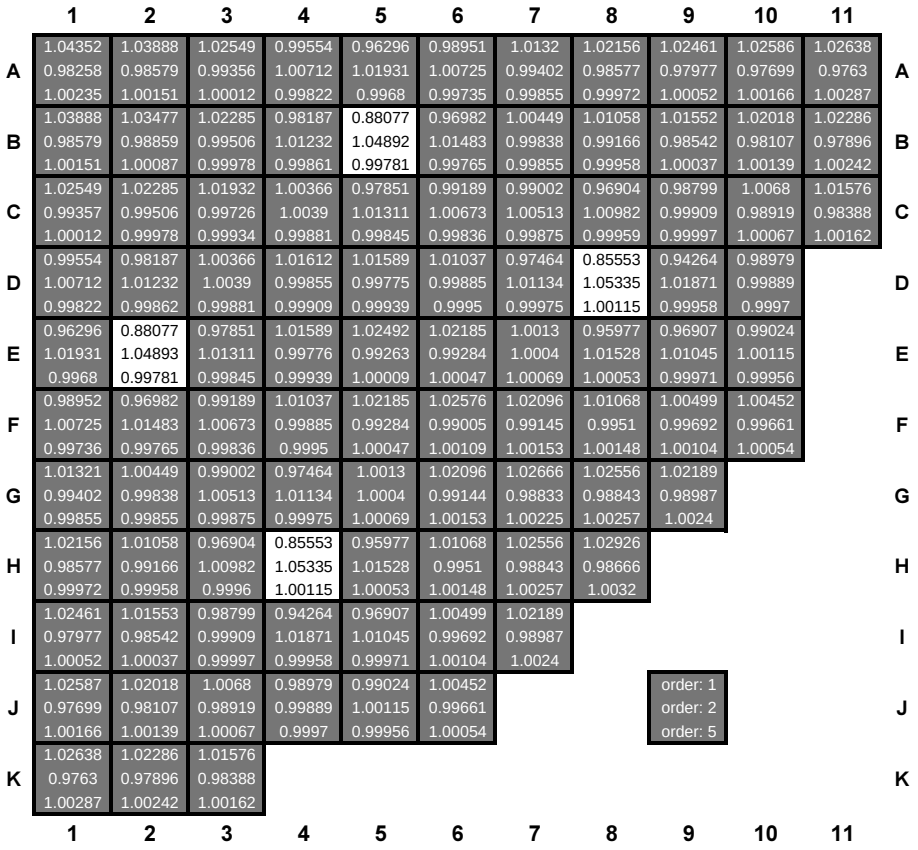
	1	2	3	4	5	6	7	8	9	10	11	
A	1.0123 0.9934 0.9986	1.0109 0.9946 0.9990	1.0083 0.9967 0.9999	1.0045 0.9997 1.0010	0.9999 1.0031 1.0023	0.9948 1.0069 1.0036	0.9906 1.0104 1.0050	0.9882 1.0128 1.0061	0.9877 1.0143 1.0071	0.9882 1.0148 1.0076	0.9886 1.0150 1.0078	A
B	1.0125 0.9931 0.9983	1.0110 0.9942 0.9988	1.0082 0.9963 0.9996	1.0040 0.9994 1.0007	0.9981 1.0034 1.0020	0.9907 1.0081 1.0033	0.9844 1.0123 1.0047	0.9825 1.0147 1.0060	0.9839 1.0156 1.0069	0.9856 1.0156 1.0074	0.9868 1.0156 1.0077	B
C	1.0128 0.9924 0.9979	1.0113 0.9935 0.9983	1.0083 0.9957 0.9992	1.0033 0.9991 1.0003	0.9951 1.0040 1.0016	0.9819 1.0108 1.0029	0.9667 1.0180 1.0040	0.9697 1.0189 1.0055	0.9768 1.0177 1.0066	0.9811 1.0169 1.0071	0.9838 1.0164 1.0075	C
D	1.0133 0.9914 0.9974	1.0118 0.9925 0.9978	1.0088 0.9948 0.9986	1.0033 0.9984 0.9997	0.9935 1.0037 1.0009	0.9733 1.0127 1.0020	0.9344 1.0278 1.0023	0.9554 1.0230 1.0046	0.9704 1.0192 1.0059	0.9767 1.0178 1.0066		D
E	1.0140 0.9903 0.9968	1.0126 0.9915 0.9972	1.0096 0.9936 0.9980	1.0044 0.9971 0.9991	0.9958 1.0020 1.0003	0.9822 1.0087 1.0015	0.9645 1.0166 1.0024	0.9650 1.0183 1.0038	0.9713 1.0177 1.0050	0.9753 1.0173 1.0058		E
F	1.0147 0.9893 0.9962	1.0134 0.9904 0.9967	1.0108 0.9923 0.9974	1.0064 0.9954 0.9984	1.0000 0.9995 0.9997	0.9919 1.0042 1.0008	0.9835 1.0088 1.0019	0.9789 1.0121 1.0031	0.9779 1.0139 1.0041	0.9778 1.0152 1.0050		F
G	1.0155 0.9882 0.9957	1.0145 0.9892 0.9961	1.0123 0.9910 0.9968	1.0088 0.9936 0.9977	1.0040 0.9970 0.9989	0.9984 1.0007 1.0001	0.9928 1.0043 1.0012	0.9881 1.0076 1.0022	0.9846 1.0101 1.0032			G
H	1.0163 0.9873 0.9952	1.0155 0.9881 0.9956	1.0137 0.9896 0.9962	1.0111 0.9918 0.9970	1.0074 0.9947 0.9981	1.0030 0.9979 0.9993	0.9985 1.0011 1.0004	0.9942 1.0041 1.0014				H
I	1.0170 0.9865 0.9948	1.0163 0.9871 0.9951	1.0150 0.9884 0.9957	1.0129 0.9903 0.9965	1.0099 0.9928 0.9975	1.0063 0.9957 0.9986	1.0025 0.9986 0.9996					I
J	1.0175 0.9860 0.9946	1.0169 0.9866 0.9949	1.0158 0.9877 0.9954	1.0141 0.9893 0.9961	1.0117 0.9914 0.9970	1.0088 0.9939 0.9979				order: 1 order: 2 order: 3		J
K	1.0177 0.9858 0.9945	1.0173 0.9863 0.9947	1.0165 0.9871 0.9951									K
	1	2	3	4	5	6	7	8	9	10	11	

Figure 2. Evolution of the node-wise agreement between the prediction of polynomial GPT and the exact perturbed nodal powers for the case shown in Fig.1, as a function of the expansion order n.



	1	2	3	4	5	6	7	8	9	10	11
A	17.0	13.0	4.9	-6.7	-15.3	-7.2	3.7	12.0	18.6	23.2	26.0
B	13.0	9.9	3.4	-10.0	-71.7	-11.9	0.3	6.6	13.0	18.6	22.4
C	4.9	3.4	1.4	-4.0	-10.4	-6.1	-4.6	-7.2	0.9	10.0	16.3
D	-6.7	-10.0	-4.0	0.4	1.3	0.6	-8.2	-71.6	-12.8	1.0	
E	-15.3	-71.7	-10.4	1.3	6.1	6.3	0.3	-10.2	-7.5	-0.9	
F	-7.2	-11.9	-6.1	0.6	6.3	9.3	8.5	5.4	3.6	3.5	
G	3.7	0.3	-4.6	-8.2	0.3	8.5	12.1	12.5	11.1		
H	12.0	6.6	-7.2	-71.6	-10.2	5.4	12.5	14.9			
I	18.6	13.0	0.9	-12.8	-7.5	3.6	11.1				
J	23.2	18.6	10.0	1.0	-0.9	3.5					
K	26.0	22.4	16.3								

Figure 3. Spatial disturbance in the power distribution (expressed in % with respect to the unperturbed nodal power distribution), due to four simultaneous localised material composition perturbations, causing a -60% k_{inf}-perturbation in the elements B5, E2, D8 and H4.



	1	2	3	4	5	6	7	8	9	10	11
A	1.04352 0.98258 1.00235	1.03888 0.98579 1.00151	1.02549 0.99356 1.00012	0.99554 1.00712 0.99822	0.96296 1.01931 0.9968	0.98951 1.00725 0.99735	1.0132 0.99402 0.99855	1.02156 0.98577 0.99972	1.02461 0.97977 1.00052	1.02586 0.97699 1.00166	1.02638 0.9763 1.00287
B	1.03888 0.98579 1.00151	1.03477 0.98859 1.00087	1.02285 0.99506 0.99978	0.98187 1.01232 0.99861	0.88077 1.04892 0.99781	0.96982 1.01483 0.99765	1.00449 0.99838 0.99855	1.01058 0.99166 0.99958	1.01552 0.98542 1.00037	1.02018 0.98107 1.00139	1.02286 0.97896 1.00242
C	1.02549 0.99357 1.00012	1.02285 0.99506 0.99978	1.01932 0.99726 0.99934	1.00366 1.0039 0.99881	0.97851 1.01311 0.99845	0.99189 1.00673 0.99836	0.99002 1.00513 0.99875	0.96904 1.00982 0.99959	0.98799 0.99909 0.99997	1.0068 0.98919 1.00067	1.01576 0.98388 1.00162
D	0.99554 1.00712 0.99822	0.98187 1.01232 0.99862	1.00366 1.0039 0.99881	1.01612 0.99855 0.99909	1.01589 0.99775 0.99939	1.01037 0.99885 0.9995	0.97464 1.01134 0.99975	0.85553 1.05335 1.00115	0.94264 1.01871 0.99958	0.98979 0.99889 0.9997	
E	0.96296 1.01931 0.9968	0.88077 1.04893 0.99781	0.97851 1.01311 0.99845	1.01589 0.99776 0.99939	1.02492 0.99263 1.00009	1.02185 0.99284 1.00047	1.0013 1.0004 1.00069	0.95977 1.01528 1.00053	0.96907 1.01045 0.99971	0.99024 1.00115 0.99956	
F	0.98952 1.00725 0.99736	0.96982 1.01483 0.99765	0.99189 1.00673 0.99836	1.01037 0.99885 0.9995	1.02185 0.99284 1.00047	1.02576 0.99005 1.00109	1.02096 0.99145 1.00153	1.01068 0.9951 1.00148	1.00499 0.99692 1.00104	1.00452 0.99661 1.00054	
G	1.01321 0.99402 0.99855	1.00449 0.99838 0.99855	0.99002 1.00513 0.99875	0.97464 1.01134 0.99975	1.0013 1.0004 1.00069	1.02096 0.99144 1.00153	1.02666 0.98833 1.00225	1.02556 0.98843 1.00257	1.02189 0.98987 1.0024		
H	1.02156 0.98577 0.99972	1.01058 0.99166 0.99958	0.96904 1.00982 0.9996	0.85553 1.05335 1.00115	0.95977 1.01528 1.00053	1.01068 0.9951 1.00148	1.02556 0.98843 1.00257	1.02926 0.98666 1.0032			
I	1.02461 0.97977 1.00052	1.01553 0.98542 1.00037	0.98799 0.99909 0.99997	0.94264 1.01871 0.99958	0.96907 1.01045 0.99971	1.00499 0.99692 1.00104	1.02189 0.98987 1.0024				
J	1.02587 0.97699 1.00166	1.02018 0.98107 1.00139	1.0068 0.98919 1.00067	0.98979 0.99889 0.9997	0.99024 1.00115 0.99956	1.00452 0.99661 1.00054			order: 1 order: 2 order: 5		
K	1.02638 0.9763 1.00287	1.02286 0.97896 1.00242	1.01576 0.98388 1.00162								

Figure 4. Evolution of the node-wise agreement between the prediction of polynomial GPT and the exact perturbed nodal powers for the case shown in Fig.3, as a function of the expansion order n.

changes at the perturbation position itself and its direct surroundings. Other cases, involving simultaneous, even larger perturbations in various fuel nodes, have been investigated as well. As an example, we imposed four large material composition changes, amounting to localised k_{inf}-perturbations of -60%, in the four octant-symmetric positions B5, E2, D8 and H4. This situation covers a perturbation range that is larger than the range of perturbations induced by substantial movements of *control rods* in multiple LWR lattice positions. As expected, this multi-perturbation gave rise to a significant spatial disturbance in the power distribution in the core (shown in Fig.3). In Fig.4, the agreement between the prediction of polynomial GPT and the exact perturbed nodal powers is illustrated as a function of the expansion order n. Generally of course, the larger the perturbations, the higher the required order of the polynomial expansion for establishing a prespecified accuracy level, and also the longer the required calculation time. With a higher-order accurate prediction for the perturbed eigensolution (the perturbed flux field), it is possible as well to acquire a higher-order accurate estimate for the perturbed *eigenvalue*, using the well-known expression [4,5,6]

$$[\Delta\lambda]^{(n)} = \frac{\langle \underline{\psi}^* | \Delta\mathbf{M} - \lambda\Delta\mathbf{F} | \underline{\psi} + \Delta^{(n)}\underline{\psi} \rangle}{\langle \underline{\psi}^* | \mathbf{F}' | \underline{\psi} + \Delta^{(n)}\underline{\psi} \rangle} \tag{55}$$

In Table I, values of $[\Delta\lambda]^{(n)}/\Delta\lambda$, as a function of the expansion order n, obtained in this way, are listed for the cases illustrated in Figs.1 and 2 (case 1) and in Figs.3 and 4 (case 2).

Table I. Values of $[\Delta\lambda]^{(n)}/\Delta\lambda$, as a function of the expansion order n, for the cases illustrated in Figs.1 and 2 (case 1) and in Figs.3 and 4 (case 2).

case	n=1	n=2	n=3	n=4
1	0.93377	1.01985	0.99359	1.00076
2	0.84527	1.06566	0.95867	1.00353

In Table II, an overview is given of the wall clock times required for establishing the agreements as illustrated in Figs.2 and 4.

Table II. Comparison of CPU-time requirements between the polynomial n^{th}-order expansion (ΔT_{poly}) and standard, nonconditioned iteration (ΔT_{iter}, for the cases illustrated in Figs.1 and 2 (case 1) and in Figs.3 and 4 (case 2).

case	n	ΔT_{poly} (s)	ΔT_{iter} (s)
1	3	0.037	0.45
2	5	0.071	0.46

Obviously, from these tests it becomes clear that the formalism can handle rather substantial spatial material composition perturbations at reactor core level, enabling, in any case, a very efficient spatial perturbation propagation formalism featuring higher-order accuracy. In addition, a clear potential emerges for application in planning and design optimization studies where the assessment of the effects of large variations plays a role (for example, in-core fuel management optimization and control rod movement planning). Divergence behaviour for the expansion, the possible occurence of which has been indicated at the end of section 6, has been observed to start in our test model, for example, in case of repeating the case of perturbing the positions B5, E2, E8 and H5, with k_{inf}-perturbations of -70 %. However, the range of perturbations within which the methodology will allow the assessment of variations, in the framework of fuel design, core loading pattern or reactor control planning optimization studies, is more than sufficient for expecting a rewarding application potential.

The pre-classification technique for limiting the number of necessarily present higher-order cross-terms in the polynomial expansion, as discussed at the end of section 6, was applied to prevent a drastic growth of the computational effort as a function of the expansion order n. As becomes obvious from Table II, in both cases a higher-order accurate prediction/reconstruction of the power change distribution was established in less time than required by a forward unconditioned re-iteration with similar accuracy. We emphasize that, in case of smaller perturbations, or in case of an interest in only scalar response functions, of lower dimensionality than the flux distribution (like the reactivity or a local detector response), a higher computational gain could have been reported. Further, we point out that, in case of perturbation calculations at the level of, for example, a highly heterogeneous fuel lattice, higher-order expansions are expected to be required in order to establish degrees of accuracy similar to the ones reported here.

9. CONCLUSIONS

A methodology has been developed that enables expansion, in polynomial form, of the effect on a prespecified response function distribution (in this study, the *flux shape* was chosen), caused by perturbations in the material composition field characterizing a nuclear system. The presented formalism was designed specifically to allow a higher order accurate treatment of localised material composition changes or uncertainties that may in fact have a substantial magnitude and therefore also a substantial effect on response quantities (such as material choice variations, burnable poison density variations at lattice level, or complete fuel assembly permutations at core level). For these cases, it is necessary to raise the accuracy of the results above what can be achieved using first-order methods only, of course preferably without having to simply pursue expensive exact recalculations for each case if the effects of many uncertainties or variations are to be assessed.

The developed expansion expressions have the convenient property of not containing a-priori unknown quantities. Previously reported methods departed from this feature, as a result of which the developed numerical schemes, leading to higher-order accurate solutions, were still *iterative* in nature, though noticeably accelerated. The explicit, non-iterative expansion, developed in this study, gives the response function perturbation as a *polynomial* function of the parameter variations, with the order of the expansion determined by the accuracy requirement on the result. In this way it is, for example, also possible to isolate a flux in a specific position and energy group as a *single* response quantity, and still be able to compute, for only this particular isolated response quantity, the perturbed value with higher-order accuracy, *without* the necessity of having to compute the perturbed *entire* flux distribution (that is, for every position and energy group) as featured by previously reported methodologies. In the study presented here, we adopted a rather ambitious choice for the response function, which was the entire spatial flux distribution. Generally

however, the formalism can be set up for numerically less ambitious choices for the response function as well (like, for example, the integral reactivity, the power produced by a prespecified subregion in the system, or a detector response).

It has been argued that for practical cases the perturbation regime that still preserves convergence of the expansion can be expected to be generously broad. This implies that the methodology is generally not constrained to the treatment of only small perturbations, and can in fact handle rather substantial localised system composition changes. Due to this, a clear potential emerges for application in planning and design optimization studies where the assessment of the effects of large variations plays a role (for example, in-core fuel management optimization and control rod movement planning). In these cases, the polynomial form would enable superior optimization conditions for quantification of the system effects of parameter variations during the optimization process, as well as create opportunities for application of more advanced mathematical optimization methods that require the availability of higher-order gradient information. Further examples of areas that may benefit from the application of this methodology, are nuclear uncertainty and sensitivity analysis. Where sensitivity studies involving *many* different parameter variations are concerned, polynomial GPT can serve very adequately to raise the accuracy level beyond first order, without a drastic increase in required computational effort.

REFERENCES

[1] D.G. Cacuci, C.F. Weber, E.M. Oblow, J.H. Marable, “Sensitivity Theory for General Systems of Nonlinear Equations”, *Nuclear Science and Engineering* **75**, pp.88–110 (1980).

[2] D.G. Cacuci, P.J. Maudlin, C.V. Parks, “Adjoint Sensitivity Analysis of Extremum-Type Responses in Reactor Safety”, *Nuclear Science and Engineering* **83**, pp.112–135 (1983).

[3] L.A. Belblidia, J.M. Kallfelz, D.G. Cacuci, “Generalized Perturbation Theory with Derivative Operators for Power Density Investigations in Nuclear Reactors”, *Nuclear Science and Engineering* **84**, pp.206–225 (1983).

[4] G.I. Maldonado, P.J. Turinsky, D.J. Kropaczek, “Employing Nodal Generalized Perturbation Theory for the Minimization of Feed Enrichment during Pressurized Water Reactor In-Core Nuclear Fuel Management Optimization”, *Nuclear Science and Engineering* **121**, pp.312–325 (1995).

[5] B.R. Moore, P.J. Turinsky, “Higher Order Generalized Perturbation Theory for Boiling Water Reactor In-Core Fuel Management Optimization”, *Nuclear Science and Engineering* **130**, pp.98–112 (1998).

[6] R. van Geemert, J.E. Hoogenboom, “Development of Parallellized Higher-Order Generalized Perturbation Theory for Application in Equilibrium Cycle Optimization”, *Annals of Nuclear Energy* **28**, Issue 14, pp.1377-1411 (2001).

[7] A. Gandini, “Implicit and Explicit Higher Order Perturbation Methods for Nuclear Reactor Analysis”, *Nuclear Science and Engineering* **67**, pp.347-355 (1978).