HIGHER ORDER HGPT METHODOLOGY APPLICATION FOR BNCT DOSIMETRY RELATED SENSITIVITY ANALYSIS

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ABSTRACT

A sensitivity analysis relevant to Boron Neutron Capture Therapy (BNCT) through the use of the Heuristically Based Generalized Perturbation Theory (HGPT) coupled to the 1D neutron transport and diffusion code TRUCO is presented in this work. While previous practical applications of this methodology were limited to the first order, a more detailed aproximation to realistic dosimetry problems with phantom heads gives rise to the need of second and higher order expansions. This work has been focused on the second order and the generalization to importance functions and higher order expansions is being under development. Sensitivity coefficients for given functional responses obtained by using both the HGPT formalism and the response surface generated by direct calculations with the computer code TRUCO were calculated and several results in 1D spherical geometry are given. As expected, comparison of the results obtained show an excellent agreement with relative errors minors than 5% and 1% in all cases at first and second order, respectively, encouraging the implementation of this methodology as a useful tool for sensitivity analysis in the development of epithermal beams for BNCT.

1. INTRODUCTION

The sensibility of the results of integral magnitudes calculations to the model and data used is generally difficult to evaluate and the most common method used is the first order perturbation theory, a very important tool to make extensive and low-cost parametric studies. On the other hand, higher order expansions are needed when strong perturbations are under consideration. Also, the approximation to the sensitivity analysis proposed in the Heuristically based Generalized Perturbation Theory or HGPT, adopted first by Usachev[1] and then extensively used by Gandini,[2,3] makes an exclusive use of the importance conservation concept and has been widely verified and extensely used, been its derivation simple and elegant. This paper presents, for the first time, the use of first and second order HGPT coupled to the 1D neutron transport and diffusion code TRUCO[4,5] for sensitivity analysis relevant to BNCT.

1.1 THE BNCT PROJECT

As one of the branches of the priority line in the Argentinean national nuclear energy program, a project of Tumor Therapy based on Boron Neutron Capture (BNCT) is currently being developed at the RA-6 (a 500kW MTR nuclear research reactor) in Bariloche. At present, the epithermal beam is under design and near future activities include the computational dosimetry validation through relative and absolute macroscopic dose measurements in phantoms and comparison with MCNP calculated values. Hence, once the neutron-photon coupled source is characterized in this facility, phantom heads will be used to carry out dose measurements and slow, expensive and many times impracticable, due to the big computer expenses, Monte Carlo source re-evaluation must possibly be done. Then, a fast and reliable technique for optimization of the source and for computational dosimetry validation through sensitivity analysis would be very useful. In this paper, we propose an alternative and very appealing strategy for the sensitivity analysis through the use of the HGPT methodology that drastically reduces the number of transport calculations to be performed.

Referring the therapy methodology, optimum therapy for cancer would involve killing tumor cells without seriously damaging normal tissues. BNCT is a binary treatment modality where each of the 2 components can be manipulated separately. Only when both come together will a therapeutic effect on tumor tissue - or a detrimental effect on healthy tissue - occur. The first component is a stable isotope of boron (boron 10) that can be concentrated in tumor cells. The second is a beam of low energy neutrons that produces short-range radiation when absorbed or “captured” by the boron. The combination of these two conditions at the site of a tumor releases radiation that can destroy malignant tissues. If the treatment proceeds as intended, the destructive effects of the capture reaction would occur primarily in those cancer cells that have accumulated boron 10. Normal cells with low concentrations of boron would be spared.

The aim of this work is oriented to the sensitivity analysis of response functions such as the partial and total dose received by a hypothetical spherical tumor at the center of such phantom heads in a simulated tumor-brain-neutron source system due to variations in boron concentration inside the tumor. To this objective, the Heuristically based Generalized Perturbation Theory (HGPT) methodology[2,3] has been used in relation to the BNCT technique, after having implemented it into

the neutron diffusion/transport TRUCO code.[4,5] To verify the validity of the resulting sensitivity coefficients, a comparison has been made with the same coefficients obtained by direct runs and analytically when possible.

Good results to first order on simple one-dimensional models were shown in a previous work,[6] encouraging the use of more complicated models and geometries as carried out in this work.

The TRUCO code version complemented with the HGPT capability has been so far limited to the diffusion option in 1D geometry. An improvement is envisaged for extending this capability to the S_N transport option (already available in the TRUCO standard code).

2. THEORY

2.1 HGPT METHODOLOGY

Consider a generic physical model defined by a system of K non-linear coupled equations. The system is formally written as

$$\vec{m}\,(\,\vec{f}\,(\vec{r}),\vec{p}) = \vec{0}\ , \tag{1}$$

where $\vec{m}$ includes linear as well as nonlinear operators related to the phase-space variables. The vector field

$$\vec{f}\,(\vec{r}) = [f_1(\vec{r}), f_2(\vec{r}), \ldots, f_K(\vec{r})]^T\ , \tag{2}$$

depends on the position vector in the phase-space

$$\vec{r} = [r_1, r_2, \ldots, r_I]^T\ , \tag{3}$$

and the components m_k (k=1,2,...,K) are functions, not necessarily linear, of $\vec{f}$ and of the vector representing the set of independent parameters

$$\vec{p}\,(\vec{r}) = [\,p_1(\vec{r})\,, p_2(\vec{r})\,, \ldots, p_I(\vec{r})\,]^T\ . \tag{4}$$

The boundary conditions of system (1) can be formally written as

$$\vec{C}\,(\,\vec{f}\,(\vec{r}^{\,s})\,,\vec{p}) = \vec{0}\ , \tag{5}$$

where $\vec{r}^{\,s}$ is a point on the boundary surface of the phase-space.

Consider now a response of interest, or functional $R(\vec{f}\,(\vec{r}),\vec{p})$ given by

$$R(\vec{f}(\vec{r}),\vec{p}) = <\vec{S}^{+}(\vec{r})\ \vec{f}(\vec{r})> , \tag{6}$$

where $\vec{S}^{+}$ is an assigned vector function while brackets < > represent integration over the phase-space.

In a sensibility analysis we are interested in the evaluation of the variation δR of the response R in terms of perturbations δp_i (i=1,2,...,I) of the system parameters. The variation of R, obtained from Eq. (6), is given by

$$\delta R = \sum_{i=1}^{I} \delta p_i [< \vec{S}^{+}_{/i}\ \vec{f} > + < \vec{S}^{+}\ \vec{f}_{/i} >] + O_2 , \tag{7}$$

where O_2 is a second or higher order term

$$O_2 = \frac{1}{2!}\sum_{i,j=1}^{I} \delta p_i \delta p_j \left[<\vec{f}\,\vec{S}^{+}_{/ij}> + 2<\vec{f}_{/j}\vec{S}^{+}_{/i}> + <\vec{f}_{/ij}\vec{S}^{+}>\right] + \ldots , \tag{8}$$

and

$$\vec{f}_{/i} = \frac{\partial \vec{f}}{\partial p_i} , \tag{9}$$

$$\vec{f}_{/ij} = \frac{\partial^2 \vec{f}}{\partial p_i \partial p_j} , \tag{10}$$

$$\vec{S}^{+}_{/i} = \frac{\partial \vec{S}^{+}}{\partial p_i} , \tag{11}$$

$$\vec{S}^{+}_{/ij} = \frac{\partial^2 \vec{S}^{+}}{\partial p_i \partial p_j} . \tag{12}$$

Then, the evaluation of $\vec{f}_{/i}$ and $\vec{f}_{/ij}$ is necessary to obtain δR to first and second order, respectively.

Expanding the perturbed equation,

$$\vec{m}'(\vec{f}', \vec{p}') = \vec{0} , \tag{13}$$

around a reference solution $\vec{f}$ we obtain

$$\delta\vec{m} = \vec{m}'(\vec{f}',\vec{p}') - \vec{m}(\vec{f},\vec{p}) = \sum_{i=1}^{I} \delta p_i \left[\frac{\partial \vec{m}}{\partial p_i} + \underline{H} \frac{\partial \vec{f}}{\partial p_i} \right] +$$
$$+ \frac{1}{2!} \sum_{i,j=1}^{I} \delta p_i \delta p_j \left[\vec{m}_{/ij} + \underline{\Xi}_i \vec{f}_{/j} + \underline{\Xi}_j \vec{f}_{/i} + \sum_{k=1}^{K} \underline{D}\left(\vec{f}_{/j}^{(k)}\right) \underline{\Omega}^{(k)} \vec{f}_{/i} + \underline{H} \vec{f}_{/ij} \right] + \ldots = \vec{0} \,, \tag{14}$$

where $\underline{H}$ represents the operator

$$\underline{H} = \frac{\bar{\partial} \vec{m}}{\partial \vec{f}} = \begin{vmatrix} \frac{\bar{\partial} m_1}{\partial f_1} & \frac{\bar{\partial} m_1}{\partial f_2} & \cdots & \frac{\bar{\partial} m_1}{\partial f_N} \\ \frac{\bar{\partial} m_2}{\partial f_1} & \frac{\bar{\partial} m_2}{\partial f_2} & \cdots & \frac{\bar{\partial} m_2}{\partial f_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\bar{\partial} m_N}{\partial f_1} & \frac{\bar{\partial} m_N}{\partial f_2} & \cdots & \frac{\bar{\partial} m_N}{\partial f_N} \end{vmatrix} , \tag{15}$$

by $\frac{\bar{\partial}}{\partial f_i}$ denoting a Fréchet derivative[7,8,9] and where

$$\underline{\Xi}_i = \begin{vmatrix} \frac{\bar{\partial}^2 m_1}{\partial p_i \partial f_1} & \frac{\bar{\partial}^2 m_1}{\partial p_i \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_1}{\partial p_i \partial f_N} \\ \frac{\bar{\partial}^2 m_2}{\partial p_i \partial f_1} & \frac{\bar{\partial}^2 m_2}{\partial p_i \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_2}{\partial p_i \partial f_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\bar{\partial}^2 m_N}{\partial p_i \partial f_1} & \frac{\bar{\partial}^2 m_N}{\partial p_i \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_N}{\partial p_i \partial f_N} \end{vmatrix} , \tag{16}$$

while $\underline{\Omega}^{(k)}$ represents the double operator

$$\underline{\Omega}^{(k)} = \begin{vmatrix} \frac{\bar{\partial}^2 m_1}{\partial f_1^{(k)} \partial f_1} & \frac{\bar{\partial}^2 m_1}{\partial f_1^{(k)} \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_1}{\partial f_1^{(k)} \partial f_N} \\ \frac{\bar{\partial}^2 m_2}{\partial f_2^{(k)} \partial f_1} & \frac{\bar{\partial}^2 m_2}{\partial f_2^{(k)} \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_2}{\partial f_2^{(k)} \partial f_N} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\bar{\partial}^2 m_N}{\partial f_N^{(k)} \partial f_1} & \frac{\bar{\partial}^2 m_N}{\partial f_N^{(k)} \partial f_2} & \cdots & \frac{\bar{\partial}^2 m_N}{\partial f_N^{(k)} \partial f_N} \end{vmatrix} . \tag{17}$$

Notation $\vec{w}^{(k)}$ represents a vector obtained from $\vec{w}$ by up-shifting its components by (k-1) positions and $\underline{D}(\vec{w})$ denotes the diagonal matrix

$$\underline{D}(\vec{w}) = \text{diag}\,[w_1, w_2, ..., w_N]\ . \tag{18}$$

Since in Eq. (14) the parameters p_i and their changes δp_i have been assumed to be independent from each other, it must follow

$$\underline{H}\,\vec{f}_{/i} = \vec{S}_{(i)}\ , \tag{19}$$

$$\underline{H}\,\vec{f}_{/ij} = \vec{S}_{(ij)}\ , \tag{20}$$

where

$$\vec{S}_{(i)} = -\frac{\partial \vec{m}}{\partial p_i}\ , \tag{21}$$

$$\vec{S}_{(ij)} = -\left[\frac{\partial^2 \vec{m}}{\partial p_i\,\partial p_j} + \underline{\Xi}_i \vec{f}_{/j} + \underline{\Xi}_j \vec{f}_{/i} + \sum_{k=1}^{K} \underline{D}\left(\vec{f}_{/j}^{(k)}\right)\underline{\Omega}^{(k)}\vec{f}_{/i}\right]. \tag{22}$$

The boundary condition for Eq. (19) can be obtained in analogous form from Eq. (5)

$$\frac{\partial \vec{C}}{\partial p_i} + \frac{\bar{\partial}\vec{C}}{\partial \vec{f}}\cdot\frac{\partial \vec{f}}{\partial p_i} = 0 \quad (\vec{r} = \vec{r}^{\,s})\ . \tag{23}$$

To first order expansion, Eq. (19) and the boundary condition given by Eq. (23) allow us to evaluate $\vec{f}_{/i}$ and, substituting into Eq. (7) would give us the variation δR. However, this procedure is not used because despite Eq. (19) is linear ($\underline{H}$ depends on $\vec{f}$, but not on $\vec{f}_{/i}$), its drawback is its dependence on parameter p_i and therefore it has to be solved I times. A similar drawback is found for second order expansions. To avoid this difficulty, an equivalent formulation will be used making use of the so called importance function, as described in the following.

2.2 IMPORTANCE FUNCTION

The HGPT formalism is based on the concept of *importance* relevant to a (particle) density field and to its *conservation principle*. Along with the HGPT formalism, the importance function, $\vec{f}^{\,*}$, is defined, obeying the reciprocity relationship[2]

$$<\vec{f}_{/i}\ \vec{S}^{+}> = <\vec{f}^{\,*}\ \vec{S}_{(i)}>\ , \tag{24}$$

$$<\vec{f}_{/ij}\ \vec{S}^{+}> = <\vec{f}^{\,*}\ \vec{S}_{(ij)}>\ . \tag{25}$$

with $\vec{S}_{(i)}$ and $\vec{S}_{(ij)}$ given by Eqs. (21) and (22), respectively.

The HGPT procedure can be schematized as follows

a) Inclusion of the initial and boundary conditions within the governing equations through the use of Dirac's delta functions,

b) Definition of the equation governing the derivative functions

$$\underline{H}\ \vec{f}_{/i} = \vec{S}_{(i)} , \tag{26}$$

where the boundary conditions are built within $\underline{H}$,

c) Definition of the equation governing the importance function

$$\underline{H}^{*}\ \vec{f}^{*} = \vec{S}^{+} , \tag{27}$$

with boundary conditions

$$\vec{C}^{*}(\vec{f}^{*}) = \vec{0} , \tag{28}$$

coming directly from Eq. (27).

Equation (24) can be rewritten as

$$< \vec{f}_{/i}\ \underline{H}^{*}\ \vec{f}^{*} > = < \vec{f}^{*}\ \underline{H}\ \vec{f}_{/i} > . \tag{29}$$

Recalling that in the HGPT method the boundary conditions for the real calculation are included into the operator $\underline{H}$, and consequently, into operator $\underline{H}^{*}$ for the importance function calculation, this relationship shows the general equivalence between the importance and the so called adjoint function concepts. With the HGPT methodology, operator $\underline{H}^{*}$ is obtained from $\underline{H}$ making use of the ***reversion rules*** resulting, in some significant cases, from the comparison between the balance equations governing the **real** and the **importance** functions. These reversal operations need, in some cases, the application of the so called "coordinate dependence complementation",[3] so that each variable will depend on all the field coordinates (and time). This rule is necessary for obtaining the correct operator $\underline{H}^{*}$ (inclusive of the elements relevant to the boundary conditions).

Finally, substituting Eq. (24) in Eq. (7) we obtain

$$\delta R = \sum_{i=1}^{I} \delta p_i \left[< \vec{f}\ \vec{S}^{+}_{/i} > + < \vec{f}^{*}\ \vec{S}_{(i)} > \right] + O_2 . \tag{30}$$

The first term at right side corresponds to the so called, easy to calculate, direct term, and the second order term O_2 is, substituting Eqs. (22) and (25) in Eq. (8)

$$O_2 = \frac{1}{2!}\sum_{i,j=1}^{I} \delta p_i \delta p_j \left[<\vec{f}\,\vec{S}^{+}_{/ij}> + 2<\vec{f}_{/j}\vec{S}^{+}_{/i}> + <\vec{f}^{*}[\frac{\partial^2 \vec{m}}{\partial p_i \partial p_j} + 2\underline{\Xi}_i \vec{f}_{/j} + \sum_{k=1}^{K} \underline{D}\left(\vec{f}^{(k)}_{/j}\right)\underline{\Omega}^{(k)}\vec{f}_{/i}]> \right] . \quad (31)$$

We have here limited here the formulation to second order, but higher order expressions could be obtained as well following a similar procedure.

3. CODE TRUCO

The one dimensional neutron diffusion S_N transport code TRUCO (TRansporte Unidimensional. Código Optimizado S_N)[4] solves the multigroup neutron-gamma transport equation. It was developed to replace the ANISN code[10,11] as a calculational tool.

3.1 CHARACTERISTICS

Principal features of this code are summarized as follows:

- 1D Geometries: Slab, Cylindrical and Spherical.
- Approximations: S_N and Diffusion [Finite Differences].
- Problems solved: Eigenvalue (k_{eff}) and Source-Driven.
- Direct and Adjoint solutions.
- General Anisotropic Scattering treated by Legendre Polynomials expansion, where the polynomial expansion limit is given only by cross sections sets availability.

3.2 MAIN OPTIONS

The code was developed to deal with two kinds of problems:

a) *External Source Calculation (Q^{ext}).* Flux convergence is searched for any of the following source-driven cases:

Distributed isotropic Q^{ext}: L=0.
Shell anisotropic Q^{ext}: group and angular-wise in-coming angular flux.
Anisotropic Q^{ext} by group, angle and interval.

b) *Eigenvalue Calculation (k_{eff}).* The λ-mode equation is solved. ($Q^{ext}_{lg}=0 \ \forall$ l,g).

The following accelerations were implemented to improve overall performance:

- Inner Iterations: Diffusion Synthetic Acceleration (DSA)
- Outer Iterations: Chebyshev Polynomials
- Thermal Iterations: Group by Group Rebalance

3.3 1D-FORMALISM

Consider the stationary Boltzmann transport equation in matrix form

$$\underline{B}\,\vec{n} + \vec{S} = \vec{0}\ , \tag{32}$$

where $\underline{B}$ is the Boltzmann operator applied to the neutronic density n ($n=\psi v^{-1}$) and $\vec{S}$ is a neutron constant source.

In the diffusion approximation the code solves for each region, assuming in it constant cross sections, the equation

$$-D_g\left[\frac{d^2\phi_g(r)}{dr^2} + \frac{\xi}{r}\frac{d\phi_g(r)}{dr}\right] + \Sigma_g^R(r)\,\phi_g(r) = S_g(r)\ , \tag{33}$$

with $\xi=0$ for slab, $\xi=1$ for cylinder and $\xi=2$ for sphere, and where D_g is the diffusion coefficient, Σ_g^R is the total remotion cross section (absorption including buckling correction and group out-scattering), and the source term is defined as

$$S_g(r) = \sum_{h\neq g}\Sigma_{hg}^s\phi_h(r) + \chi_g\sum_{h=1}^{G}[\nu\Sigma_f]_h\,\phi_h(r) + Q_g(r)\ , \tag{34}$$

with $1\leq(g,h)\leq G$.

3.4 ADJOINT FLUX CALCULATION

To obtain the importance function (n^*), TRUCO solves the adjoint form of system (32)

$$\underline{B}^*\,\vec{n}^* + \vec{S}^+ = \vec{0}\ , \tag{35}$$

by transposing in energy the scattering matrix and the fission source of the source term.

In Eq. (34), instead of the fission source term

$$\chi_g(x)\sum_{h=1}^{G}[\nu\Sigma_f(x)]_h\,\phi_h(x)\ , \tag{36}$$

we have

$$[\nu\Sigma_f(x)]_g\sum_{h=1}^{G}\chi_h(x)\,\phi_h^*(x)\ . \tag{37}$$

The matrix associated with the treatment of the leakage terms of the **Diffusion** equation is self adjoint, so it is not transposed.

The matrix associated with the treatment of the leakage terms of the **Transport** equation is not transposed either. Rather, because angular directions sets are assumed to be symmetric, the adjoint calculation of the leakage operator proceeds as in the direct calculation; but the results of the adjoint calculation are identified with $-\Omega_m$. For example, the boundary condition of no-incoming flux in an adjoint problem is interpreted as a condition of no-outgoing flux.

Difference equations are exactly adjoint in plane geometry. The discretization error in curved geometries is small and decreases with decreasing size of the space-angle mesh.

In addition to transposing the scattering cross section matrix, TRUCO inverts the group order of the cross sections, the source (if any), the fission spectrum and speeds, and the input flux guess. This inversion is a convenience, because the adjoint of a *downscatter* problem is a more time-consuming *upscatter* problem. By proceeding in inverse group order, the *upscatter* problem becomes, once more, of the same difficulty of a *downscatter* problem.

Adopting the point-wise convergence test, we obtain the same k_{eff} in both direct and adjoint calculations in all multiregion, multigroup problems considered.

4. APPLICATIONS

We present in this work the sensitivity analysis of response functions such as the partial and total dose received by a hypothetical spherical tumor at the center of the phantom heads due to boron concentration inside the tumor and in healthy tissue in a source driven system with an external uniform surface current representing the neutron source from the core.

4.1 SOURCE DRIVEN SYSTEMS

Consider now a source driven system at stationary conditions. The general HGPT formulation obtained can be adopted for studies concerning dose problems. In these cases, the neutron density is assumed to obey the (linear) equation

$$\underline{B}\,\vec{n} + \vec{S} = \vec{0} \ . \tag{38}$$

Given then a response $R = <\vec{S}^{+}\,\vec{n}>$, typically a neutron dose quantity, the perturbation expression is, at first order

$$\delta R = \sum_{i=1}^{I} \delta p_i [<\vec{S}^{+}_{/i}\vec{n}> + <\vec{\psi}^{*}(\vec{B}_{/i}\vec{n} + \vec{S}_{/i})>] \ , \tag{39}$$

with $\vec{n}$ representing the unperturbed neutron density and function $\vec{\psi}^{*}$ obeying equation

$$\underline{B}^{*}\,\vec{\psi}^{*} + \vec{S}^{+} = \vec{0}\ . \tag{40}$$

4.1.1 *Homogeneous Sphere.* To be used in calculations referring tumors therapy by means of the Boron Neutron Capture Technique, we studied the variation of the dose received in the tumor due to changes in the tumor size and in the boron concentration in the system.

As a first approximation to the solution of the flux for this problem, we simulate the tumor as a homogeneous sphere of radius R_e, diffusion coefficient D and absorption cross section Σ_a, with an external uniform surface current j^{ext} taken from core calculations. From Eq. (33) the diffusion monoenergetic 1D spherical equation to solve is

$$-D\left[\frac{d^2\phi(r)}{dr^2}+\frac{2}{r}\frac{d\phi(r)}{dr}\right] + \Sigma_a\,\phi(r) = 0\ , \tag{41}$$

or

$$m = -\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi(r)}{dr}\right)+ K^2\,\phi(r) = 0 \quad , \quad K^2=\frac{\Sigma_a}{D}\ , \tag{42}$$

with boundary conditions (BC)

- symmetry at the center of the sphere, i.e.

$$\left.\frac{d\phi(r)}{dr}\right|_{r=0} = 0\ , \tag{43}$$

- in-current j^{ext} at the external surface

$$\left(\frac{\phi(r)}{4}+\frac{D}{2}\frac{d\phi(r)}{dr}\right)\Bigg|_{r=R_e} = j^{ext}\ . \tag{44}$$

We rewrite Eq.(42) including BC

$$m=-\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\phi(r)}{dr}\right)+K^2\phi(r)-R_e^2\frac{d\phi(r)}{dr}\frac{\delta(r)}{r^2}-R_e^2\left(\frac{\phi(r)}{4D}+\frac{d\phi(r)}{2\,dr}-\frac{j^{ext}}{D}\right)\frac{\delta(r-R_e)}{r^2}=0\ , \tag{45}$$

where δ is the Dirac's delta function.

The derived equation can be written as $H\,\phi_{/i} = S_{(i)}$, with

$$H = \frac{\bar{\partial} m}{\partial \phi} = -\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d(.)}{dr} \right) + K^2(.) - R_e^2 \frac{d(.)}{dr}\frac{\delta(r)}{r^2} - R_e^2 \left[\frac{(.)}{4D} + \frac{1}{2}\frac{d(.)}{dr} \right] \frac{\delta(r - R_e)}{r^2} \quad , \tag{46}$$

and

$$S_{(i)} = -\frac{\partial m}{\partial p_i} = -2KK_{/i}\phi + R_e^2 \left[\frac{D_{/i}}{D^2}\left(j^{ext} - \frac{\phi}{4} \right) - \frac{1}{D} j_{/i}^{ext} \right] \frac{\delta(r - R_e)}{r^2} \quad . \tag{47}$$

The importance function equation has the form $H^* \phi^* = S^+$, with

$$H^* = -\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d(.)}{dr} \right) + K^2(.) + R_e^2 \frac{d(.)}{dr}\frac{\delta(r)}{r^2} + R_e^2 \left[\frac{1}{2}\frac{d(.)}{dr} - \frac{(.)}{4D} \right] \frac{\delta(r - R_e)}{r^2} \quad , \tag{48}$$

where BC $\left.\frac{d\phi^*}{dr}\right|_{r=0} = 0$ and $\left.\left(\frac{D}{2}\frac{d\phi^*}{dr} - \frac{\phi^*}{4}\right)\right|_{r=R_e} = 0$ are derived from Eq. (48).

If we consider a response $R = < S^+ \phi >$ such as the average flux in the sphere

$$R = \bar{\phi} = \frac{1}{V}\int_V \phi(r)\, d^3\vec{r} \quad \Rightarrow \quad S^+ = \frac{1}{V} \quad . \tag{49}$$

Taking $p_i = \Sigma_a$ ($S_{/i}^+ = 0$), the sensitivity coefficient is, from Eq. (30) and Eq. (47)

$$\frac{\partial R}{\partial p_i} = < \phi^* S_{(i)} > = < \phi^* 2KK_{/i}\phi > - R_e^2 < \phi^* \left[\frac{D_{/i}}{D^2}\left(j^{ext} - \frac{\phi}{4} \right) - \frac{j_{/i}^{ext}}{D} \right] \frac{\delta(r - R_e)}{r^2} > \quad . \tag{50}$$

If the response is the total absorption reaction rate in the sphere $R = \int_V \Sigma_a \phi(r)\, d^3\vec{r}$, then $S^+ = \Sigma_a$.

Taking $p_i = \Sigma_a$ ($S_{/i}^+ = 1$), the sensitivity coefficient is, from Eq. (30)

$$\frac{\partial R}{\partial p_i} = < \phi > + < \phi^* S_{(i)} > = < \phi > + < \phi^* 2KK_{/i}\phi > - R_e^2 < \phi^* \left[\frac{D_{/i}}{D^2}\left(j^{ext} - \frac{\phi}{4} \right) - \frac{j_{/i}^{ext}}{D} \right] \frac{\delta(r - R_e)}{r^2} > \quad . \tag{51}$$

4.2.2 *Concentric Spheres.* As a better approximation to the problem, we simulated the tumor (boroned water) and the surrounding brain (water) as two concentric spheres. We assume the same BC as in the first example, adding the following conditions

- flux and current continuity at the interface ($r = r_B$) of media 1(boron-water) and 2 (water), i.e.

$$\phi_1(r_B) = \phi_2(r_B) \quad ; \quad D_1 \frac{d\phi_1(r)}{dr} = D_2 \left.\frac{d\phi_2(r)}{dr}\right|_{(r=r_B)} \quad . \tag{52}$$

A similar derivation can be extracted for a second order expansion, where Eq. (19) must first be solved for $\phi_{/i}$ for every $p_{/i}$ considered.

4.2. RESULTS

For first order, Eq. (41) is solved by TRUCO in order to find the direct flux ϕ. The code was modified to solve Eq. (40) with the respective importance source, given by Eq. (49). A FORTRAN program coupled to TRUCO was developed to calculate the sensibility coefficients of Eqs. (50) and (51).

We are interested in the sensitivity coefficients defined by Eqs. (50) and (51), assuming the following constants for thermal neutrons for the reference state

Table I. Reference State Constants

Material	Σ_a [cm^{-1}]	Σ_s [cm^{-1}]	D [cm]	R^a [cm]
Boron Water	0.03	3.4	0.1	3^b
Water	0.02	3.4	0.1	10

a. External radius.
b. Concentric Spheres case only.

An external incoming current of j^{ext}=1.0 n/(cm^2.s) was taken for both cases.

Results for first order are shown in Table II for the homogeneous sphere and in Table III for the concentric spheres, where the analytical solution for each case is of the type $\phi(r)=A\sinh(\alpha r)/r$, being α the material buckling and A a level constant defined by j^{ext}. Changes of 10, 50 and 100% of Σ_a^B are considered as perturbations and, while perturbated flux can be calculated either analytically or by direct runs, one value of the sensitivity coefficient is given by means of HGPT due to its dependence on unperturbed flux only.

For second order expansions, Eq. (19) is solved by an auxiliary program to TRUCO for each parameter p_i. A comparison of first and second order results are shown in Table IV for the reconstruction of the variation of the average flux in the concentric spheres, where a second order expansion analysis seems useful a priori.

Table II. First Order Sensitivity Coefficients ($\partial R/\partial \Sigma_a^B$) for the Homogeneous Sphere

Response Functional **R**	Analytical	HGPT	Direct	Rel. Error (%) 100*[1-(HGPT)/(DIR)]
$<V^{-1}\phi>$ [n/cm^2.s] (Aver. Flux)	-8.19962 E+02	-8.259 E+02 [n/cm .s]	+10% [a] -8.210 E+02	- 0.6
	-8.16883 E+02		+50% -8.177 E+02	-1.0
	-8.10389 E+02 [n/cm .s]		+100% -8.112 E+02 [n/cm .s]	-1.8
$<\Sigma_a^B\phi>$ [n/cm^3.s] (Total Dose)	3.17509 E+05	3.195 E+05 [n/cm^2.s]	+10% 3.180 E+05	- 0.4
	3.16583 E+05		+50% 3.169 E+05	-0.8
	3.14485 E+05 [n/cm^2.s]		+100% 3.148 E+05 [n/cm^2.s]	-1.5

a. Perturbation of parameter Σ_a^B.

Table III. First Order Sensitivity Coefficients ($\partial R/\partial \Sigma_a^B$) for the Concentric Spheres

Response Functional **R**	Analytical	HGPT	Direct	Rel. Error (%) 100*[1-(GPT)/(DIR)]
$<V^{-1}\phi>$ [n/cm^2.s] (Aver. Flux)	-2.21389 E+01	-2.235 E+01 [n/cm .s]	+10% [a] -2.220 E+01	- 0.7
	-2.19749 E+01		+50% -2.206 E+01	-1.3
	-2.16558 E+01 [n/cm .s]		+100% -2.174 E+01 [n/cm .s]	-2.8
$<\Sigma_a^B\phi>$ [n/cm^3.s] (Total Dose)	8.57274 E+03	8.629 E+03 [n/cm^2.s]	+10% 8.578 E+03	- 0.6
	8.39680 E+03		+50% 8.402 E+03	-2.7
	8.25996 E+03 [n/cm^2.s]		+100% 8.265 E+03 [n/cm^2.s]	-4.4

a. Perturbation of parameter Σ_a^B.

As shown in Table II, sensitivity coefficients are obtained for the average flux and total dose for the homogeneous case with errors minors than 2% in all cases.

Results for the concentric spheres shown in Table III give a maximum relative error of –4.4 % for tumor total dose when duplicating the boron concentration in the ill tissue.

Table IV. Reconstruction of δR for the Concentric Spheres

Response Functional **R**	Method	$\delta\Sigma_a^B$	δR	Rel. Error (%) 100*[1-(GPT)/(DIR)]
$\langle V^{-1}\phi\rangle$ [n/cm^2.s] (Aver. Flux)	Analytical	+10%	-6.64167 E-02	
	Direct		-6.660 E-02	
	HGPT Order 1		-6.705 E-02	-0.70
	HGPT Order 2		-6.680 E-02	-0.30
$\langle V^{-1}\phi\rangle$ [n/cm^2.s] (Aver. Flux)	Analytical	+50%	-3.32961 E-01	
	Direct		-3.309 E-01	
	HGPT Order 1		-3.352 E-01	-1.30
	HGPT Order 2		-3.325 E-01	-0.48
$\langle V^{-1}\phi\rangle$ [n/cm^2.s] (Aver. Flux)	Analytical	+100%	-6.4965 E-01	
	Direct		-6.522 E-01	
	HGPT Order 1		-6.705 E-01	-2.80
	HGPT Order 2		-6.579 E-01	-0.87
$\langle\Sigma_a^B\phi\rangle$ [n/cm^3.s] (Total Dose)	Analytical	+10%	2.57182 E+01	
	Direct		2.573 E+01	
	HGPT Order 1		2.589 E+01	-0.60
	HGPT Order 2		2.581 E+01	-0.31
$\langle\Sigma_a^B\phi\rangle$ [n/cm^3.s] (Total Dose)	Analytical	+50%	1.25952 E+02	
	Direct		1.260 E+02	
	HGPT Order 1		1.294 E+02	-2.70
	HGPT Order 2		1.266 E+02	-0.47
$\langle\Sigma_a^B\phi\rangle$ [n/cm^3.s] (Total Dose)	Analytical	+100%	2.47797 E+02	
	Direct		2.479 E+02	
	HGPT Order 1		2.588 E+02	-4.40
	HGPT Order 2		2.502 E+02	-0.93

Second order expansion results for the reconstruction of the variations in the average flux and total dose shown in Table IV give a maximum relative error of 0.87 % and 0.93 % when duplicating the boron concentration in the ill tissue for the average flux and tumor total dose, respectively.

CONCLUSIONS

An application of the HGPT methodology for sensibility analysis relevant to the BNCT technique was made.

Comparisons between sensitivity coefficients obtained by perturbation and direct calculations show excellent agreement with relative errors less than 5 % and 1% at first and second order expansions, respectively, proving the efficiency of the involved methodologies.

Good results to first and second order on simple models are shown, encouraging the use of more complicated models and geometries to take into account uncertainties associated to measures also in tumor size. Higher order HGPT expansions are envisaged in further developments to account for large parameter changes and for future use in sensitivity analysis related to Photon Radiation Therapy with Cobalt 60, where an accurate calculation of dose of 1 to 3 % error is required.

Future work is oriented towards the application of this methodology in the multigroup case to perform sensitivity analysis related to the epithermal beam characterization where the source spectra will be taken from direct core calculations.

Also, computer time savings of at least one order of magnitude were observed due to the lack of iterative schemes in the HGPT methodology and also to the quickness and efficiency of the methodologies involved. This time saving becomes crucial when long parametric studies in the design of an irradiation facility are involved.

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