

ADVANCES IN HEURISTICALLY BASED GENERALIZED PERTURBATION THEORY

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ABSTRACT

A distinctive feature of heuristically based generalized perturbation theory (HGPT) methodology consists in the systematic use of importance conservation concepts. As well known, this use leads to fundamental reciprocity relationships. Instead, the alternative variational and differential one approaches make a consistent use of the properties of the adjoint function. The equivalence between the importance and the adjoint functions have been demonstrated in important cases. There are some instances, however, in which the commonly known operator reversal rules to determine the operator governing the adjoint function are not adequate. In this paper ways proposed to generalize these rules, as adopted with the HGPT methodology, are illustrated. When applied to the neutron/nuclide field characterizing the core evolution in a power reactor system, in which also an intensive control variable (ρ) is defined, these rules lead to an orthogonality relationship connected to this same control variable. A set of ρ -mode eigenfunctions may be correspondingly defined and an extended concept of reactivity (generalizing that commonly associated with the multiplication factor) proposed as more directly indicative of the "controllability" of a critical reactor system.

INTRODUCTION

Since the beginning of nuclear reactor physics studies, perturbation theory has played an important role. As well known, it was first proposed by Wigner [1] as early as 1945 to study fundamental quantities such as the reactivity worths of different materials in the reactor core. It is also well known that this first formulation, today widely used by reactor analysts, makes a consistent use of the adjoint flux concept.

The advantage of using perturbation theory lies in the fact that instead of making a new, often lengthy direct calculation of the eigenvalue (and then of real flux) for every perturbed system configuration, a simple integration operation is required in terms of unperturbed quantities, of the type $\langle \mathbf{f}^* \delta B \mathbf{f} \rangle$.

It is interesting that as early as 1948 Soodak [2] associated to the adjoint flux the concept of importance, viewing it as proportional to the contribution of a neutron inserted in a given point of a critical system to the asymptotic power.

Along with the introduction of the concept of importance and, parallel to it, along with the development of calculational methods and machines, from the early 60's a flourishing of perturbation methods, at first in the linear domain and then in the nonlinear one, have been proposed for the analysis of reactor core, shielding, nuclide evolution, thermohydraulics.

The perturbation formulations proposed by various authors may be subdivided into three main categories, according to the approach followed in their derivation:

1. The heuristic approach, making exclusive use of importance conservation concepts, adopted first by Usachev [3] and then extensively used by Gandini [4-7]. It will be referred to, in the following, as heuristic generalized perturbation theory (HGPT) method.

2. The variational approach adopted, in particular, by Lewins [8], Pomraning [9], Stacey [10], Harris and Becker [11] and Williams [12].

3. The differential method, proposed by Oblov [13] and extensively developed by Cacuci [14], based on a formal differentiation of the response considered.

Each of the above methods has its own merit, although all of them can be shown equivalent to each other [15,23].

Basing on a long experience, it is our belief that the GPT approach can be easily grasped by the reactor engineers, due to the inherent simplicity and elegance of the heuristic derivation.

As mentioned above, a distinctive feature of heuristically based generalized perturbation theory (HGPT) methodology consists in the systematic use of importance conservation concepts. As well known, this use leads to fundamental reciprocity relationships. Instead, the variational and the differential derivations make a consistent use of the properties of the adjoint function (which only a posteriori is interpreted as importance). The equivalence between the importance and the adjoint functions have been demonstrated in most cases of interest. There are some instances, however, in which the commonly known operator reversal rules to determine the operator governing the adjoint function are not adequate. In this paper a generalization of these rules, as adopted with the HGPT methodology, is illustrated in relation to a number of significant cases.

THE HGPT METHOD

In the HGPT method the importance function is uniquely defined in relation to a given system response, for example, a neutron dose, the quantity of plutonium in the core at end of cycle, the temperature of the outlet coolant.

The HGPT method was first derived in relation to the linear neutron density field. Then it was extended to other (assumed) linear density ones, in particular:

- to the nuclides, relevant to core evolution problems
- to the enthalpies, relevant to thermohydraulics.

For all these density fields the equations governing the importance functions were obtained directly by imposing that on average the contribution to the chosen response from a particle [a neutron, or a nuclide, or an energy carrier (phonon)] introduced at a given time in a given phase space of the system is conserved through time (importance conservation principle). Obviously such importance will result dependent on the time, position, and in certain cases, energy and direction, of the inserted particle.

Consider a response Q of the type

$$Q = \int_{t_0}^{t_F} \langle s^+, f \rangle dt \equiv \langle\langle s^+, f \rangle\rangle, \quad (1)$$

with s^+ given and f being the density function. Weighting all particles inserted into the system, let's assume a source s , with the corresponding importance (f^*) will obviously give the response itself, i.e.,

$$\langle\langle f^*, s \rangle\rangle \equiv Q = \langle\langle s^+, f \rangle\rangle, \quad (2)$$

which represents an important reciprocity relationship. This relationship may be shown to correspond to that defining the fundamental property of the adjoint function (See Appendix 1).

From these first derivations the rules for determining the equation governing the importance f^* function were learned. They implied, in relation to the equation governing f^* :

- change of sign of the odd derivatives,
- transposing matrix elements,
- inverting the order of operators,
- substitution of the source s with s^+ .

The first three operations will be generally called "operator reversal" operations.

The HGPT method was then extended to any field governed by linear operators for which the rules for their reversal were known. In particular it was extended to the derivative fields, obtained from expanding to first order, around a given starting solution, a number of important nonlinear equations, in particular:

- the coupled neutron/nuclide field, relevant to core evolution problems
- the temperature field, relevant to thermohydraulics.

GENERAL FORMULATION

Consider a generic physical model defined by a number of parameters p_j ($j=1,2,\dots,J$) and described by an N -component vector field f obeying equation

$$m(f|p) = 0. \quad (3)$$

Vector $f(q,t)$ generally depends on the phase space coordinates q and time t . Vector p represents the set of independent parameters p_j ($j=1,2,\dots$) fully describing the system and entering into equation (3). Their value generally determines physical constants, initial conditions, source terms, etc. Equation (3) can be viewed as an equation comprising linear, as well as nonlinear, operators and is assumed to be derivable with respect to parameters p_j and (in the Frechet sense) component function f_n ($n=1,2,\dots,N$).

Consider now a response of interest, or functional Q as given by Eq.(1). In the following, we shall look for an expression giving perturbatively the change δQ of the response Q in terms of perturbations δp_j of the system parameters. In particular, expressions giving the sensitivity coefficients relevant to each parameter p_j will be obtained.

Expanding equation (3) around a reference solution gives the equation governing the derivative function $f/j [= \frac{df}{dp_j}]$

$$\sum_{j=1}^J (Hf/j + m/j)\delta p_j + O_2 = 0 \quad (4)$$

where O_2 is a second, or higher order term, and where $m/j = \frac{\partial m}{\partial p_j}$.

Operator H is given by the expression

$$H = \begin{pmatrix} \frac{\partial m_1}{\partial f_1} & \frac{\partial m_1}{\partial f_2} & \dots & \frac{\partial m_1}{\partial f_N} \\ \frac{\partial m_2}{\partial f_1} & \frac{\partial m_2}{\partial f_2} & \dots & \frac{\partial m_2}{\partial f_N} \\ \dots & \dots & \dots & \dots \\ \frac{\partial m_N}{\partial f_1} & \frac{\partial m_N}{\partial f_2} & \dots & \frac{\partial m_N}{\partial f_N} \end{pmatrix} \quad (5)$$

where by $\frac{\partial}{\partial f_n}$ we have indicated a Frechet derivative [16].

Since in equation (3) the parameters p_j , and their changes δp_j have been assumed to be independent from each other, it must follow

$$Hf/j + m/j = 0, \quad (6)$$

which represents the (linear) equation governing the derivative function f/j . The source term m/j is here intended to account also, via appropriate delta functions, for the initial and, if the case, boundary conditions.

Consider now functional

$$Q_j = \langle\langle h^+, f/j \rangle\rangle. \quad (7)$$

Adopting the concept of importance associated with field f/j , if we weight with it space- and time-wise the source term m/j (including delta functions to accomodate initial conditions), this amounts to a result equivalent to functional Q_j , i.e.,

$$Q_j = \langle\langle f^*, m/j \rangle\rangle, \quad (8)$$

where f^* is the importance function obeying equations

$$H^* f^* + h^+ = 0, \quad (9)$$

H^* being obtained by reversing operator H . As we have seen above, this implies transposing matrix elements, changing sign of the odd derivatives, inverting the order of operators.

We can easily see that the sensitivities s_j ($j=1,2,\dots,J$) of system parameters can be written

$$s_j = \langle\langle \frac{\partial h^+}{\partial p_j}, f \rangle\rangle + \langle\langle f^+, \frac{\partial m}{\partial p_j} \rangle\rangle, \quad (10)$$

where the first term on the right-hand side represents the so called, easy to calculate, direct term.

The overall change δQ due to the perturbation δp_j ($j=1,2,\dots,J$) of system parameters can be written

$$\delta Q = \sum_{j=1}^J \delta p_j [\langle\langle \frac{\partial h^+}{\partial p_j}, f \rangle\rangle + \langle\langle f^+, \frac{\partial m}{\partial p_j} \rangle\rangle]. \quad (11)$$

Coordinate complementation Rule

It may occur, in certain circumstances, that one or more components (e.g., f_2) of the vector field f do not depend on a given space-time coordinate (e.g., x). Without alteration of the problem specifications and results, this, or these variables may be interpreted as averaged quantities and then replaced by the proper averaging operator [e.g., $\langle \cdot \rangle_{(x)/V_x}$] applied to the corresponding extended variable [so replacing, to exemplify, f_2 with $\langle f_2(x) \rangle_{(x)/V_x}$]. These extended variables will then be assumed dependent also on this coordinate, although only their average values with respect to it are of interest and no further specification for them is required. This rule is referred to as "coordinate dependence complementation". Its use is required in order that a correct operation reversal is made to obtain the operator governing the importance function.

NUCLIDE EVOLUTION FIELD

A GPT related perturbation methodology relevant to the nuclide field has been first developed in 1975 [17]. Kallfelt et al. [18] coupled it with the GPT methodology relevant to the neutron field to account for nonlinear effects inherent in burnup problems. Other efforts in the nonlinear domain have been made by Harris and Becker [11], who arrived at a still crude formulation, and, successively, by Williams [12] and Gandini [6,7].

Williams used variational techniques starting from the time-wise discretized neutron and nuclide density equations, along with the quasi-static approximation.

Gandini used the heuristically based GPT method after having formally extended the neutron and nuclide densities to a control (intensive) variable. A rule which has played a crucial role for simply determining the operator governing the importance function with this latter method has been that of the variable dependence complementation mentioned before. The equations obtained governing the (time-wise continuous) importance function are relevant to the physical solution. Different integration schemes can then be defined [19,20].

Typical quantities which can be analysed with these methodologies are:

- the amount of a material specified in a given region at the end of the reactor life cycle;

- the d.p.a. of a specific material and at a given position;
- the residual reactivity at the end of the reactor life cycle.

Formulation of the Problem

To the neutron and fuel nuclide densities, represented by vectors $n(r,t)$ $c(r,t)$, respectively, defined in the reactor lifetime (t_0, t_F) , a specified intensive control variable, $\rho(t)$, is associated in order to maintain the overall power history, $W(t)$, assigned. Vector n represents the space- and time-dependent neutron density in a multigroup energy form, whereas vector c the space- and time-dependent density of the various fuel nuclide species (generally, inclusive also of the fission products). The intensive, time-dependent, control variable $\rho(t)$ may represent, for instance, the overall control rod bank penetration into the core (not their relative movement, which is generally described by parameters p_j), or the average neutron poison material density. The nonlinear governing equations can then be represented as

$$m_{(n)}(n, c, r | p) = -\frac{\partial n}{\partial t} + B(c, \rho | p) n + s_n(p) = 0 \quad (12)$$

$$m_{(c)}(n, c | p) = -\frac{\partial c}{\partial t} + E(n | p) c + s_c(p) = 0 \quad (13)$$

$$m_{(\rho)}(n, c | p) = \langle c, S(p)n \rangle - W(p) = 0 \quad (14)$$

where B is the neutron diffusion, or transport, matrix operator, E the nuclide evolution matrix, s_n and s_c are given source terms (s_n generally assumed zero during burnup, except a delta-like source at t_0 to represent initial conditions, whereas s_c is generally given by a sum of delta functions defined at t_0 and at each fuel feed operation), S is a matrix containing the microscopic fission cross-sections $\sigma_{f,g}^m$ (m and g being indexes of materials and groups, respectively).

If we introduce the field

$$f(r, t) = \begin{vmatrix} n(r, t) \\ c(r, t) \\ \rho(t) \end{vmatrix} \quad (15)$$

the system of Eqs.(15), (16) and (17) may be represented in the compact symbolic form, Eq.(1), and the GPT methodology described above applied.

Consider a functional

$$Q = \int_{t_0}^{t_F} \langle s_n^+ s_c^+ s_\rho^+ \left| \begin{vmatrix} n(r, t) \\ c(r, t) \\ r(t) \end{vmatrix} \right\rangle dt \quad (16)$$

Q may represent, for instance, the amount of a given nuclide built up at time t_F [in this case $s_n^+ = 0$ and s_c^+ includes a delta function $\delta(t - t_F)$], or the fluence at a specific point \vec{r} [in this case $s_c^+ = 0$ and s_n^+ includes a delta function $\delta(r - \vec{r})$]. The importance function

$$f^*(r, t) = \begin{vmatrix} n^*(r, t) \\ c^*(r, t) \\ \rho^*(t) \end{vmatrix} \quad (17)$$

can then be defined, governed by Eq.(10). More explicitly, it results

$$\begin{vmatrix} \left(\frac{\partial}{\partial t} + B^*\right) & \left[\frac{\partial(Ec)}{\partial n}\right]^T & S^T c \\ \left[\frac{\partial(Bn)}{\partial c}\right]^* & \left(\frac{\partial}{\partial t} + E^T\right) & S n \\ \langle n, \left(\frac{\partial B}{\partial \rho}\right)^* (\cdot) \rangle & 0 & 0 \end{vmatrix} \begin{vmatrix} n^* \\ c^* \\ \rho^* \end{vmatrix} + \begin{vmatrix} s_n^+ \\ s_c^+ \\ s_\rho^+ \end{vmatrix} = 0 \quad (18)$$

The bottom row equation of system, Eq.(21) corresponds to a relationship between n^* and n , i.e.,

$$\langle n, \left(\frac{\partial B}{\partial \rho}\right)^* n^* \rangle = s_\rho^+ . \quad (19)$$

In case $s_\rho^+ = 0$, Eq. (22) corresponds to an orthogonality relationship. A set of ρ -mode eigenfunctions may be correspondingly defined and an extended concept of reactivity (generalizing that commonly associated with the multiplication factor) proposed as more directly indicative of the "controllability" of a critical reactor system (See Appendix 2).

From Eq. (21) a solution scheme can be directly obtained. It can be shown that the type of equations to be solved reduce to the types:

$$B^* n^* + h_n^+ = 0 \quad (20)$$

$$E^T c^* + h_c^+ = 0 \quad (21)$$

where h_n^+ and h_c^+ are known source terms. Therefore, existing, well established codes can be used for their solution.

THERMOHYDRAULIC FIELD

The applicability of the HGPT technique was demonstrated [21] in relation to the calculation of sensitivity coefficients required when analysing (generally nonlinear) multichannel thermohydraulic systems. The application of sensitivity methods to the thermohydraulic field has been first proposed by Oblov [22] using the so called differential method [13]. The application of the HGPT to this field [6,7] was proposed to overcome a number of difficulties inherent with sensitivity methods, in particular, that of writing the importance function related to the response of interest (typically, a temperature, or pressure, in a given space-time point) with its proper boundary conditions. Under this respect, the HGPT method allows a rather straightforward procedure. The equivalence between the HGPT and the differential method has been shown by Andrade Lima and Marques Alvim [23].

A major effort is presently underway using HGPT methodology [24,25], aiming at constructing a code by which a multi-channel thermohydraulic problem can be perturbatively analysed. These equations

have been written in the form of a nonlinear matrix operator governing, within each channel, the compound field including fuel, clad, coolant and wall temperatures, coolant pressure and density, and cross-flow. Adopting the simple rules for reversing the Jacobian matrix has made it possible to obtain the equation governing the importance function relevant to the response to be analysed.

A rule which also here played a crucial role has been that of the coordinate dependence complementation mentioned above. Interface and/or limit conditions between different regions have been accommodated in the governing equations by means of appropriate delta functions. This allows to arrive directly at the appropriate interface and/or limit conditions for the importance function.

Once this methodology is implemented, a number of applications can be foreseen, in particular,

- System analysis and optimization searches;
- Propagation of physical data errors in design quantities;
- Basic physical data adjustment on the basis of experimental information (for instance, temperature and pressure detections at specified positions in an experimental setup at different steady state conditions).

APPENDIX 1. IMPORTANCE AND ADJOINT FUNCTIONS

Consider the equations governing the neutron density n and the corresponding importance function n^*

$$\frac{\partial n}{\partial t} = B_T n + s \quad (1.1)$$

$$-\frac{\partial n^*}{\partial t} = B_T^* n^* + s^* \quad (1.2)$$

Multiplying on the left by n^* and n , respectively, integrating over space and time and subtracting, gives

$$\int_{t_0}^{t_F} \langle n^* (-\frac{\partial}{\partial t} + B_T) n \rangle dt + \int_{t_0}^{t_F} \langle n^* s \rangle dt = \int_{t_0}^{t_F} \langle n (\frac{\partial}{\partial t} + B_T^*) n^* \rangle dt + \int_{t_0}^{t_F} \langle n s^* \rangle dt \quad (1.3)$$

Making use of the source reciprocity relationship, Eq.(2), we obtain

$$\int_{t_0}^{t_F} \langle n^* (-\frac{\partial}{\partial t} + B_T) n \rangle dt = \int_{t_0}^{t_F} \langle n (\frac{\partial}{\partial t} + B_T^*) n^* \rangle dt \quad (1.4)$$

which corresponds to the relationship for the adjoint function.

At stationary condition we may write the well known property of the adjoint

$$\langle n^* B_T n \rangle = \langle n B_T^* n^* \rangle \quad (1.5)$$

We have then then demonstrated that operators B_T and B_T^* , this latter heuristically obtained by reversal operations, corresponds to the so called "real" and "adjoint" operators, respectively.

APPENDIX 2. THE GENERALIZED REACTIVITY

Consider a reactor system at critical conditions. The neutron density may be written as

$$Bn = 0 \quad (2.1)$$

where operator B depends on a intensive (and then space-independent) control parameter ρ (for instance corresponding to the average density of a poison, or the overall depth of the control rods, assumed zero at critical conditions). In order to explicit its dependence on this control parameter, we shall replace operator B with its linear expansion $B + \frac{\partial B}{\partial \rho} \rho$, where ρ assumes now the role of the eigenvalue. Equation (2.1) corresponds to the so called fundamental mode equation, to which the eigenvalue $\rho=0$ is associated. The equations governing the real and adjoint ℓ th ($\ell=1,2,\dots$) order mode can be written:

$$(B + \frac{\partial B}{\partial \rho} \rho) \phi_{\ell} = 0 \quad (2.2)$$

$$(B^* + \frac{\partial B^*}{\partial \rho} \rho) \phi_{\ell}^* = 0 \quad (2.3)$$

Clearly $\rho_1=0$ and $\phi_1=\alpha n$, α being an arbitrary coefficient. It is easy to show the orthogonality relation $\langle \phi_{\ell}^* \frac{\partial B}{\partial \rho} \phi_s \rangle = 0$ for $\ell \neq s$. Consider then the perturbation δp of a generic parameter p_j (e.g., a nuclide density) inducing a perturbation $\delta B (\equiv \frac{\partial B}{\partial p_j} \delta p_j)$ of the transport operator. Let us then assume that the criticality is reset by an appropriate change $\delta \rho = (\rho' - \rho)$ of the control parameter. Corresponding changes $\delta B_{\rho} (\equiv \frac{\partial B}{\partial \rho} \delta \rho)$ and $\delta n (\equiv n' - n)$ of operator B and density n will occur, respectively.

The function n' will be governed by the equation

$$(B + \delta B + \delta B_{\rho})n' = 0 \quad (2.4)$$

Multiplying this equation on the left by ϕ_1^* and Eq.(2.3) for $\ell=1$ by n' , we obtain,

$$\int_{\text{syst}} \phi_1^{*T} B n' dr - \int_{\text{syst}} n'^T B^* \phi_1^* dr + \int_{\text{syst}} \phi_1^{*T} (\delta B + \delta B_{\rho}) n' dr = 0 \quad (2.5)$$

By the property of the adjoint operators, the first two terms cancel. Recalling that

$$\delta B_{\rho} = \frac{\partial B}{\partial \rho} \delta \rho \quad (2.6)$$

we then obtain, setting for simplicity $\delta \rho = \delta \rho_1$,

$$\delta\rho = -\frac{\int_{\text{syst}} \phi_1^{*T} \delta B n' dr}{\int_{\text{syst}} \phi_1^{*T} \frac{\partial B}{\partial \rho} n' dr}, \quad (2.7)$$

which dropping terms of second or higher order may be written

$$\delta\rho = -\frac{\int_{\text{syst}} \phi_1^{*T} \delta B n dr}{\int_{\text{syst}} \phi_1^{*T} \frac{\partial B}{\partial \rho} n dr}. \quad (2.8)$$

If we consider as a fictitious control parameter the quantity $(\lambda-1)$ where λ is the coefficient (eigenvalue) multiplying the neutron source in the transport equation (recalling with obvious notation that $B \equiv A + \lambda F$, λ being 1 at criticality) the above equation may be written in the form

$$-\delta\lambda = \frac{\int_{\text{syst}} \phi_1^{*T} \delta B n dr}{\int_{\text{syst}} \phi_1^{*T} F n dr}, \quad (2.9)$$

i.e., corresponds to the well known equation for the reactivity $\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}$ ($\equiv -\delta\lambda$) induced into the system by a perturbation δB . We can then introduce the concept of generalized reactivity (GR) and define

$$\text{GR} = \frac{\int_{\text{syst}} \phi_1^{*T} \delta B n dr}{\int_{\text{syst}} \phi_1^{*T} \frac{\partial B}{\partial \rho} n dr} \quad (2.10)$$

amounting to the effect of the perturbation δB in terms of equivalent change (in the sense of resetting the criticality) of the control parameter ρ . This may have an interest in those cases in which a realistic value (such as an equivalent average neutron poison concentration change) is desired to represent the impact of a given perturbation. With little effort, programs apt to calculate $\frac{\delta k_{\text{eff}}}{k_{\text{eff}}}$ can be made apt to calculate also GR.

We observe that the values GR and the standard reactivity expression, Eq.(2.9), are related via normalization integrals, i.e.,

$$\text{GR} = \frac{\int_{\text{syst}} \phi_1^{*T} F n dr}{\int_{\text{syst}} \phi_1^{*T} \frac{\partial B}{\partial \rho} n dr} \frac{\delta k_{\text{eff}}}{k_{\text{eff}}}. \quad (2.11)$$

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