



Application of the inverse generalized perturbation theory to the optimization of fuel assembly design



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ABSTRACT

Many methods have been proposed to optimize fuel assembly design, most of them based on metaheuristic techniques. The method presented here is based on the inverse perturbation theory. Parameters to be optimized are some isotope densities, such as Gd, ^{235}U , ^{239}Pu . The optimization is constrained to some target values of relevant reactor observables, such as the breeding ratio, the reactivity loss rate during the fuel cycle, the maximum reactivity, the spectral index. The method is fit to solve multi-objective problems. In the examples, 2 or 3 simultaneous objectives are determined.

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1. Introduction

Fuel assembly design optimization can be done in two main ways: in one hand, determining the value of some integral parameters constrained to an integral observable or, in the other hand, determining the spatial distribution of some local parameters constrained to a local observable. In the first class of problems we can find the gadolinium density that enables to match a target reactivity loss rate, or the plutonium density that enables to match a target breeding ratio. In the second class we can find the determination of the position of gadolinia pins that enable to minimize the local peaking factor.

Many methods have been introduced to solve this kind of problem. They are based either on a pure mathematical framework or on metaheuristic techniques that mimic some natural phenomena. In the first class of methods we find the Newton–Raphson method and the perturbation methods (Gandini et al., 1969; Dall'Osso, 2009). In the second class we can find the simulated annealing (Rogers, 2008; Galloway et al., 2008), the neural networks (Ortiz et al., 2006), the genetic algorithms (Yilmaz, 2005). Several other methods belong to the second class. They have mainly been devoted to reload pattern optimization (François et al., 2013).

The method presented here is based on the inverse perturbation theory. As Ronen (1979) suggested, whilst perturbation theory enables determining the effect of a known perturbation on a given

physical system, inverse perturbation theory enables determining the perturbation that causes a known effect. The inverse generalized perturbation theory has been presented in detail in a previous article (Dall'Osso, 2009) and only the basic methodology framework is recalled here, in Section 2.1. In Section 2.2 an improvement based on the application of the method to special observables is presented. Examples are presented in Section 3. Some aspects of the method are discussed in Section 4. Conclusions are provided in Section 5.

2. Method

We present hereafter the approach for the case of simple observables such as the spectral index or the breeding ratio, and for special cases where the observables are derivatives of the reactivity. This later case is useful to determine maxima or minima.

2.1. General case

Let us consider an observable quantity f in the system, expressed as the ratio of linear functionals of the neutron flux Φ :

$$f = \frac{\langle h_1, \Phi \rangle}{\langle h_2, \Phi \rangle}, \quad (1)$$

where h_1 and h_2 are linear operators and the product $\langle h, \Phi \rangle$ is defined as $\int \int \int h \Phi d^3r dE d\Omega$.

For instance, if the observable f is the spectral index (defined as the ratio between the fast and the thermal flux), we have:

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$$h_1 = \begin{cases} 1, & E > E_c \\ 0, & \text{otherwise} \end{cases} \quad (2)$$

$$h_2 = 1 - h_1,$$

where E_c is the cut energy, i.e. the energy separating the thermal from fast energy domain, typically $E_c = 0.625$ eV.

Our problem is to determine the change in a parameter p (e.g. ^{239}Pu density) in order to achieve the target value of f and satisfying the neutron balance equation, in steady state:

$$A\Phi = \frac{1}{k_{\text{eff}}} F\Phi, \quad (3)$$

where A and F are the absorption–scattering and the fission production operators respectively, and k_{eff} is the effective multiplication factor.

At the basis of the inverse perturbation method there is the importance Ψ_0^* (Gandini, 1967) associated to the observable f , in the initial state of the system (indicated by the subscript 0). The importance is the solution of the equation:

$$A_0^* \Psi_0^* = \frac{1}{k_{\text{eff},0}} F_0^* \Psi_0^* + S_0^*, \quad (4)$$

where the term S_0^* is the source of the generalized importance associated to the functional appearing in Eq. (1), defined as:

$$S_0^* = \frac{h_{1,0}}{\langle h_{1,0}, \Phi_0 \rangle} - \frac{h_{2,0}}{\langle h_{2,0}, \Phi_0 \rangle}. \quad (5)$$

By definition, the term S_0^* is orthogonal to the flux (i.e. $\langle S_0^*, \Phi_0 \rangle = 0$). This condition allows a solution to the problem defined in Eq. (4).

After some manipulations on Eqs. (3) and (4) and using the definitions in Eqs. (1) and (5) we obtain (Dall'Osso, 2009):

$$-\langle \Psi_0^*, \delta A \Phi \rangle + \frac{1}{k_{\text{eff}}} \langle \Psi_0^*, \delta F \Phi \rangle + \left(\frac{1}{k_{\text{eff}}} - \frac{1}{k_{\text{eff},0}} \right) \langle \Psi_0^*, F_0 \Phi \rangle - \frac{\langle (f \delta h_2 - \delta h_1 + \delta h_{2,0}), \Phi \rangle}{\langle h_{1,0}, \Phi_0 \rangle} = 0, \quad (6)$$

where we have introduced the following definitions: $\delta A = A - A_0$, $\delta F = F - F_0$ and $\delta f = f - f_0$.

If we indicate with δp the variation that must be applied to the global parameter p in order to attain the desired value of the observable f , Eq. (6) can be rewritten, neglecting second order dependencies, as:

$$\delta p \left\langle \Psi_0^*, \left(\frac{\partial A}{\partial p} - \frac{1}{k_{\text{eff}}} \frac{\partial F}{\partial p} \right) \Phi \right\rangle - \left(\frac{1}{k_{\text{eff}}} - \frac{1}{k_{\text{eff},0}} \right) \langle \Psi_0^*, F_0 \Phi \rangle + \delta p \frac{\left\langle \left(f \frac{\partial h_2}{\partial p} - \frac{\partial h_1}{\partial p} \right), \Phi \right\rangle}{\langle h_{1,0}, \Phi_0 \rangle} + \delta f \frac{\langle h_{2,0}, \Phi \rangle}{\langle h_{1,0}, \Phi_0 \rangle} = 0. \quad (7)$$

In the general case, the partial derivative $\partial/\partial p$ is approximated by the ratio between the variations of the operators (A , F , h_1 and h_2) and the independent parameter p into two states, for instance

$$\frac{\partial A}{\partial p} \approx \frac{A(p+\delta p) - A(p)}{\delta p}.$$

In case the independent parameter is the nuclide density of an isotope, the elements of matrix $\partial A/\partial p$ are the microscopic absorption and scattering cross sections and the elements of matrix $\partial F/\partial p$ are the microscopic production cross sections. It can be shown that in this case the h operators are linear combinations of the microscopic cross sections (Dall'Osso, 2009).

In more general situations, several constraints must be satisfied on several observables f_j ($j = 1, \dots, N_C$) and the same number of parameters p_i ($i = 1, \dots, N_C$) has to be determined. In such cases, Eq. (7) can be reformulated by adding the subscript j in $h_{j,1,0}$, $h_{j,2,0}$ and $\Psi_{j,0}^*$, in order to distinguish the operators and importance related to the different observables:

$$\sum_{i=1}^{N_C} \delta p_i \left\langle \Psi_{j,0}^*, \left(\frac{\partial A}{\partial p_i} - \frac{1}{k_{\text{eff}}} \frac{\partial F}{\partial p_i} \right) \Phi \right\rangle - \left(\frac{1}{k_{\text{eff}}} - \frac{1}{k_{\text{eff},0}} \right) \langle \Psi_{j,0}^*, F_0 \Phi \rangle + \sum_{i=1}^{N_C} \delta p_i \frac{\left\langle \left(f_j \frac{\partial h_{j,2}}{\partial p_i} - \frac{\partial h_{j,1}}{\partial p_i} \right), \Phi \right\rangle}{\langle h_{j,1,0}, \Phi_0 \rangle} + \delta f_j \frac{\langle h_{j,2,0}, \Phi \rangle}{\langle h_{j,1,0}, \Phi_0 \rangle} = 0. \quad (8)$$

Eq. (8) constitutes a set of N_C equations in N_C unknowns. Solving it with respect to δp_i we obtain the values of the parameters enabling matching the target values f_j of the observables. Since the flux Φ in Eq. (8) is not known, the determination of the constrained parameters p_i is done by an iterative process:

- Compute the fluxes solving Eq. (3).
- Determine δp_i solving Eq. (8), where the target values of f_j are imposed.
- Continue until a fixed residual error is reached.

Approaching to the convergence, the error due to neglecting second order dependencies and the error on the evaluation of the derivatives become smaller and smaller. It has to be pointed out that Eqs. (7) and (8) have been derived using the exact perturbation theory (not approximated to first order), therefore they are valid for any amount of the variation and with only one calculation of the adjoint functions (at the initial state).

In case the j th observable to be controlled is k_{eff} , the related equation is derived from the classical perturbation theory and becomes (Dall'Osso, 2008):

$$\sum_{i=1}^{N_C} \delta p_i \left\langle \Phi_0^*, \left(\frac{\partial A}{\partial p_i} - \frac{1}{k_{\text{eff}}} \frac{\partial F}{\partial p_i} \right) \Phi \right\rangle - \left(\frac{1}{k_{\text{eff}}} - \frac{1}{k_{\text{eff},0}} \right) \langle \Phi_0^*, F_0 \Phi \rangle = 0, \quad (9)$$

instead of Eq. (8), with Φ_0^* the adjoint flux in the initial configuration.

Examples of this problem are the determination of isotope densities, such as the triple search presented in Section 3.1, where the ^{239}Pu , ^{10}B and the H_2O densities are constrained to breeding ratio, criticality and spectral index.

2.2. Special case: reactivity derivatives as target observables

In some problems the observable that has to be optimized is a derivative of the reactivity, such as a sensitivity, or a reactivity coefficient (e.g. the Doppler coefficient). In this case the derivative can be expressed using the classical perturbation theory. The expression can be obtained using Eq. (9) for a single parameter p_i that we indicate with symbol q , and taking the limit for $\delta q \rightarrow 0$, which implies that the initial state becomes equal to the final state ($\Phi_0^* \rightarrow \Phi^*$ and $F_0 \rightarrow F$):

$$\frac{\partial \rho}{\partial q} = - \frac{\left\langle \Phi^*, \left(\frac{\partial A}{\partial q} - \frac{1}{k_{\text{eff}}} \frac{\partial F}{\partial q} \right) \Phi \right\rangle}{\langle \Phi^*, F \Phi \rangle}. \quad (10)$$

Taking into account that by definition of adjoint operator $\langle \Phi^*, A \Phi \rangle = \langle A^* \Phi^*, \Phi \rangle$ and $\langle \Phi^*, F \Phi \rangle = \langle F^* \Phi^*, \Phi \rangle$, this means that the operators h_1 and h_2 associated to the observable defined in Eq. (10) are:

$$h_1 = - \left(\frac{\partial A^*}{\partial q} - \frac{1}{k_{\text{eff}}} \frac{\partial F^*}{\partial q} \right) \Phi^*, \quad (11)$$

$$h_2 = F^* \Phi^*.$$

In this kind of problem the perturbation theory is used twice: to compute the h operators and to solve the optimization problem.

Examples of this problem are the determination of the gadolinium density constrained to the reactivity loss rate (Section 3.2) and the determination of the water density maximizing the multiplication factor (Section 3.3).

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