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SENSITIVITY ANALYSIS OF COUPLED CRITICALITY CALCULATIONS

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ABSTRACT

Perturbation theory based sensitivity analysis is a vital part of todays' nuclear reactor design. This paper presents an extension of standard techniques to examine coupled criticality problems with mutual feedback between neutronics and an augmenting system (for example thermal-hydraulics). The proposed procedure uses a neutronic and an augmenting adjoint function to efficiently calculate the first order change in responses of interest due to variations of the parameters describing the coupled problem.

The effect of the perturbations is considered in two different ways in our study: either a change is allowed in the power level while maintaining criticality (power perturbation) or a change is allowed in the eigenvalue while the power is constrained (eigenvalue perturbation). The calculated response can be the change in the power level, the reactivity worth of the perturbation, or the change in any functional of the flux, the augmenting dependent variables and the input parameters. To obtain power- and criticality-constrained sensitivities power- and k-reset procedures can be applied yielding identical results.

Both the theoretical background and an application to a one dimensional slab problem are presented, along with an iterative procedure to compute the necessary adjoint functions using the neutronics and the augmenting codes separately, thus eliminating the need of developing new programs to solve the coupled adjoint problem.

Key Words: Sensitivity analysis, adjoint sensitivity analysis procedure, coupled problems, Krylov methods

1. INTRODUCTION

Sensitivity analysis is a very useful tool in modern reactor design which provides means of calculating changes in responses of interest due to variations in parameters describing the system being investigated. In neutron transport calculations the most common responses are the critical eigenvalue and functionals of the flux, both for which perturbation methods are well established - perturbation theory for the critical eigenvalue and generalized perturbation theory (GPT) respectively [1–3]. These methods have the advantage that once an appropriate adjoint problem is solved and a specific adjoint function is obtained, the change in the response caused by any perturbation of the input parameters can be calculated by simply performing an integration over the phase-space, thus avoiding the need to solve the transport problem again and again. The drawback is that the predicted variation is only accurate up to first order (as higher order terms are usually neglected in the derivation of the perturbation formulas).

Sensitivity analysis for generic linear and non-linear problems has also been rigorously derived - first order changes in both linear and non-linear responses can be easily calculated by applying the adjoint sensitivity analysis procedure (ASAP) [4]. The same can be said for augmented, coupled systems, a general approach is well presented in [5] and applications are also known of (see for example [6]).

Regarding coupled reactor physics calculations sensitivity studies mainly focused on time-dependent problems. In depletion perturbation theory coupled neutron-nuclide fields are investigated [7,8] while in case of transient analyses usually adjoint techniques are applied to point-kinetics coupled with simplified thermal-hydraulics [9,10].

A few papers have been published on the sensitivity analysis of shielding problems as well [11–13]. In these usually fixed source coupled neutron-gamma transport is considered and the adjoint transport equation is solved to provide first order changes in responses. However most often there is only one-way coupling, i.e. only secondary photons induced by neutrons are taken into account and gamma-neutron reactions are neglected.

This paper focuses on the sensitivity analysis of steady-state coupled criticality calculations. In Section 2 the theoretical background is presented, Section 3 introduces a numerical method proposed to solve the equations, while Section 4 demonstrates the application to a one-dimensional slab model.

2. THEORY

2.1. Formulation of the Coupled Reactor Physics Problem

In criticality calculations the following problem is solved:

$$\hat{L}(\alpha_n)\phi(x) = \lambda \hat{F}(\alpha_n)\phi(x), \tag{1}$$

where $\hat{L}$ and $\hat{F}$ are the standard loss and production operators, $\alpha_n(x)$ represent the input parameters (cross sections, geometrical sizes, etc.), while $\phi(x)$ and λ are the unknown flux and critical eigenvalue. Equation 1 can represent any form of the transport equation (S_N or P_L approximation, diffusion, etc.) with arbitrary discretization (finite volume, finite element, etc.), x and ϕ are simply the appropriate independent and dependent variables (e.g. in case of a finite volume multigroup diffusion approach x represents spatial points and energy groups, ϕ the group fluxes in the volumes).

Equation 1 is an eigenvalue problem, hence the normalization of the flux is arbitrary and can be expressed in general as

$$\frac{\langle C_f(x), \phi(x)\rangle_\phi}{C} = 1,$$

where $\langle \quad , \quad \rangle_\phi$ indicates integration over the phase-space, while $C_f(x)$ and C are a constraint function and a preset constraint value. In this paper the constraint will be the system power ($C = P$) with an appropriate power function ($C_f(x) = P_f(x) = Q\Sigma_f(x)$), but other normalizations are also possible (a detector function and a detector response, a fission source of one neutron, etc.).

In coupled criticality calculations the above model is extended to account for physical processes other than neutron transport (for example thermal-hydraulics, xenon-poisoning, etc.). The extra phenomena are described by additional dependent variables $T(y)$ (which can depend on independent variables y different from x), input parameters $\alpha_T(y)$ and equations. The coupling between neutronics and the augmenting system is taken into account by allowing some of the original parameters α_n to depend on extra parameters and the augmenting dependent variable, moreover the flux and some of the neutronic parameters to enter the augmenting equations. For example if coupling to thermal-hydraulics is considered the augmenting variable can simply be the temperature and cross sections in the extended model can take the form of

$$\Sigma(T) = \Sigma(T_1) + \frac{\Sigma(T_2) - \Sigma(T_1)}{T_2 - T_1}(\overline{T} - T_1),$$

where $\overline{T}$ is some spatially averaged temperature (e.g. an average fuel temperature), whereas $\Sigma(T_1)$ and $\Sigma(T_2)$ are the cross sections evaluated at average temperatures T_1 and T_2. In such a case $\Sigma(T_1)$, $\Sigma(T_2)$, etc. would be the extra input parameters and the original parameter (α_n) would simply be the cross section evaluated at a certain average temperature.

The simplest way to describe the entire coupled system is to consider a full set of input parameters α, consisting of the neutronic parameters being unaffected by the augmentation process (for example geometrical sizes and cross sections not depending on the augmenting variables), the additional parameters describing the dependency of the neutronic parameters on the augmenting dependent variables ($\Sigma(T_1)$, $\Sigma(T_2)$, etc.) and the augmenting parameters (α_T).

With the above said the coupled criticality problem can be represented by Equations 2-4, where the independent variables have been omitted for simplicity:

$$\hat{L}(T, \alpha)\phi = \lambda \hat{F}(T, \alpha)\phi \tag{2}$$

$$\hat{N}(T, \phi, \alpha) = 0 \tag{3}$$

$$\frac{\langle C_f(T, \alpha), \phi \rangle_\phi}{C} = 1. \tag{4}$$

The loss and production operators now also depend on the augmenting variable and the additional parameters. The augmenting equations are indicated with a general operator $\hat{N}$ acting linearly or non-linearly on the augmenting variables, the flux and all the input parameters. Moreover the normalization of the flux is such that the constraint function C_f gives the constraint value C.

2.2. Power Perturbation

In reality the coupled problem described by Equations 2-3 has a unique solution, the true physical steady-state, for which criticality ($\lambda = 1$) is always ensured by the feedbacks and no arbitrary flux normalization is allowed. Hence the problem can be considered as

$$\hat{L}(T,\alpha)\phi = \hat{F}(T,\alpha)\phi$$
$$\hat{N}(T,\phi,\alpha) = 0,$$

and for a given parameter set α^0 the solution is ϕ^0 and T^0. The corresponding unique power (constraint) value is

$$P^0 = C^0 = \left\langle C_f(T^0,\alpha^0), \phi^0 \right\rangle_\phi = \left\langle P_f(T^0,\alpha^0), \phi^0 \right\rangle_\phi .$$

When perturbations are made to the input parameters ($\Delta\alpha$) a different steady-state is reached at a possibly different power level. To investigate the effects of such perturbations the standard adjoint sensitivity analysis procedure (ASAP) can be used [4]. Here only the final equations needed to be solved and the formulas to calculate response variations are presented (for the notations see APPENDIX A).

The relative change in the power level is given by

$$\begin{aligned}\frac{\Delta P}{P^0} &= \frac{1}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi + \frac{1}{P^0}\left\langle \left.\frac{\partial P_f}{\partial T}\right|_0 \Delta T, \phi^0 \right\rangle_\phi + \frac{1}{P^0}\left\langle P_f^0, \Delta\phi \right\rangle_\phi = \\ &= \frac{1}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi + \frac{1}{P^0}\left\langle \left(\left.\frac{\partial P_f}{\partial T}\right|_0\right)^* \phi^0, \Delta T \right\rangle_T + \frac{1}{P^0}\left\langle P_f^0, \Delta\phi \right\rangle_\phi . \end{aligned} \tag{5}$$

To evaluate the terms containing $\Delta\phi$ and ΔT (the indirect terms) in Equation 5 without having to recalculate the original coupled problem again and again for every perturbation of the input parameters the following adjoint problem needs to be solved:

$$\left(\hat{M}^0\right)^* w_\phi^0 + \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T^0 = \frac{w_P^0}{P^0} P_f^0 \tag{6}$$

$$\left(\hat{J}^0\right)^* w_\phi^0 + \left(\left.\frac{\partial \hat{N}}{\partial T}\right|_0\right)^* w_T^0 = \frac{w_P^0}{P^0} \left(\left.\frac{\partial P_f}{\partial T}\right|_0\right)^* \phi^0. \tag{7}$$

In Equations 6-7 we introduced $\hat{M}^0 = \hat{L}^0 - \lambda^0 \hat{F}^0$ and $\hat{J}^0 \Delta T = \left.\frac{\partial \hat{M}}{\partial T}\right|_0 \Delta T \phi^0$ (with $\lambda^0 = 1$), and w_P^0 can be arbitrarily chosen. The boundary conditions usually need a more detailed discussion, here it is only emphasized that they have to be chosen in a way that the bilinear terms coming from the definition of the adjoint operators vanish (or at least become dependent only on the unperturbed solution, the known parameters and the parameter changes [4]). In Equations 6-7 the coupled adjoint operator on the left hand side is similar to that presented in [14], where GPT is used to efficiently calculate loading pattern characteristics for boiling water reactors taking into account the coupling between neutronics and thermal-hydraulics. However here no a priori distinction is made between “strong” and “weak” unknowns, all augmenting variables are included.

Having obtained the adjoint functions w_ϕ^0 and w_T^0 (for a chosen w_P^0) the relative change in the power level is given by Equation 8.

$$\frac{\Delta P}{P^0} = \frac{1}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi - \frac{1}{w_P^0}\left\langle w_\phi^0, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi - \frac{1}{w_P^0}\left\langle w_T^0, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T. \quad (8)$$

For other response functionals $R(\phi, T, \alpha)$ the change caused by the perturbation of the input parameters can be written as

$$\Delta R = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha + \left\langle \left.\frac{\partial R}{\partial \phi}\right|_0, \Delta\phi \right\rangle_\phi + \left\langle \left.\frac{\partial R}{\partial T}\right|_0, \Delta T \right\rangle_T = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha + \Delta R_{indirect},$$

with an associated change (ΔP) in the power level. Again, to get rid of the indirect term an adjoint problem needs to be solved:

$$\left(\hat{M}^0\right)^* w_\phi^P + \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T^P = \left.\frac{\partial R}{\partial \phi}\right|_0 \quad (9)$$

$$\left(\hat{J}^0\right)^* w_\phi^P + \left(\left.\frac{\partial \hat{N}}{\partial T}\right|_0\right)^* w_T^P = \left.\frac{\partial R}{\partial T}\right|_0. \quad (10)$$

This leads to the following expression for the change in the response:

$$\Delta R = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha - \left\langle w_\phi^P, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi - \left\langle w_T^P, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T \quad (11)$$

In practice reactors are most often operated at a given power level, hence it may be desirable to investigate sensitivities when the power is constrained (or the preset constraint value C has to be met). This can be done by tuning an appropriate parameter (which we will call the control parameter and designate by α_c in the rest of this paper) to counterbalance the changes in the power caused by the perturbation of the (other) input parameters, so that:

$$\frac{\Delta P_{\Delta\alpha}}{P^0} = -\frac{\Delta P_{\Delta\alpha_c}}{P^0}.$$

This "power-reset" procedure is very much the same as the "k-reset" used in traditional GPT [3]. Equation 8 can be used to evaluate both sides, leading to the following formula for the change in the control parameter:

$$\Delta\alpha_c = -\frac{\frac{w_P^0}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi - \left\langle w_\phi^0, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi - \left\langle w_T^0, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T}{\frac{w_P^0}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha_c}\right|_0, \phi^0 \right\rangle_\phi - \left\langle w_\phi^0, \left.\frac{\partial \hat{M}}{\partial \alpha_c}\right|_0 \phi^0 \right\rangle_\phi - \left\langle w_T^0, \left.\frac{\partial \hat{N}}{\partial \alpha_c}\right|_0 \right\rangle_T}. \quad (12)$$

Using Equation 11 and Equation 12 the power-constrained response perturbation is given by Equation 13:

$$\Delta R_{P-reset} = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha + \left.\frac{\partial R}{\partial \alpha_c}\right|_0 \Delta\alpha_c - \left[\left\langle w_\phi^P, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi + \left\langle w_\phi^P, \left.\frac{\partial \hat{M}}{\partial \alpha_c}\right|_0 \Delta\alpha_c\phi^0 \right\rangle_\phi\right] - \ldots$$

$$-\left[\left\langle w_T^P, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T + \left\langle w_T^P, \left.\frac{\partial \hat{N}}{\partial \alpha_c}\right|_0 \Delta\alpha_c \right\rangle_T\right]. \tag{13}$$

2.3. Eigenvalue Perturbation

One can also be interested in the reactivity worth of perturbations, which is one of the main interests in pure reactor physics problems. In coupled criticality calculations such a response can be calculated if we constrain the flux normalization while perturbing the input parameters (here no control parameter is used yet). Hence the problem being investigated is:

$$\begin{aligned} \hat{L}(T,\alpha)\phi &= \lambda \hat{F}(T,\alpha)\phi \\ \hat{N}(T,\phi,\alpha) &= 0 \\ \frac{\langle P_f(T,\alpha),\phi\rangle_\phi}{P} &= 1, \end{aligned}$$

where P is the preset power (constraint) value that has to be met. The unperturbed system (characterized by a parameter set α^0) is critical, hence $\lambda^0 = 1$, the corresponding steady state solution is ϕ^0 and T^0, while the total system power is P^0. Perturbing the input parameters while constraining the flux normalization to the power of P^0, the eigenvalue will differ from one, this difference can be interpreted as the reactivity worth of the perturbation and can be calculated as

$$\Delta\lambda = \frac{\left[\left\langle w_\phi^0, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi + \left\langle w_T^0, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T - \frac{w_P^0}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi\right]}{\left\langle w_\phi^0, \hat{F}^0\phi^0 \right\rangle_\phi}. \tag{14}$$

In Equation 14 w_ϕ^0 and w_T^0 are the solution of Equations 6-7 for the arbitrarily chosen w_P^0. The derivation of Equation 14 and the corresponding adjoint problem is quite similar to that presented in [3] for pure criticality problems, moreover Equation 14 reduces to the standard eigenvalue perturbation formula when no coupling is present.

For responses other than the critical eigenvalue, the adjoint problem that needs to be solved is

$$\left(\hat{M}^0\right)^* w_\phi^\lambda + \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T^\lambda = \frac{w_P^\lambda}{P^0} P_f^0 + \left.\frac{\partial R}{\partial \phi}\right|_0 \tag{15}$$

$$\left(\hat{J}^0\right)^* w_\phi^\lambda + \left(\left.\frac{\partial \hat{N}}{\partial T}\right|_0\right)^* w_T^\lambda = \frac{w_P^\lambda}{P^0} \left(\left.\frac{\partial P_f}{\partial T}\right|_0\right)^* \phi_0 + \left.\frac{\partial R}{\partial T}\right|_0, \tag{16}$$

with the auxillary condition that

$$\left\langle w_\phi^\lambda, \hat{F}^0\phi^0 \right\rangle_\phi = 0.$$

The above condition is needed so that the term $\Delta\lambda \left\langle w_\phi^\lambda, \hat{F}^0\phi^0 \right\rangle_\phi$ in the derivation disappears. As in the coupled case the neutronic adjoint is unique (unless the coupled adjoint operator is singular), this can be done by the proper choice of w_P^λ. The final expression for the response variation is

$$\Delta R = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha - \left\langle w_\phi^\lambda, \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha\phi^0 \right\rangle_\phi - \left\langle w_T^\lambda, \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha \right\rangle_T + \frac{w_P^\lambda}{P^0}\left\langle \left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha, \phi^0 \right\rangle_\phi . \quad (17)$$

Just like in standard GPT, one can apply a ”k-reset” procedure to obtain criticality constrained sensitivities. Equation 14 can be used to evaluate both sides of

$$\left.\frac{\partial \lambda}{\partial \alpha}\right|_0 \Delta\alpha = -\left.\frac{\partial \lambda}{\partial \alpha_c}\right|_0 \Delta\alpha_c,$$

leading to the same formula for the control parameter change as Equation 12. Finally, Equation 17 can be used to evaluate the change in the response both due to the input parameter perturbations and the control parameter change, leading to the following expression for the criticality-constrained sensitivities (which coincide with the power-constrained sensitivities):

$$\Delta R_{k-reset} = \left.\frac{\partial R}{\partial \alpha}\right|_0 \Delta\alpha + \left.\frac{\partial R}{\partial \alpha_c}\right|_0 \Delta\alpha_c - \left\langle w_\phi^\lambda, \left[\left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 \Delta\alpha + \left.\frac{\partial \hat{M}}{\partial \alpha_c}\right|_0 \Delta\alpha_c\right]\phi^0 \right\rangle_\phi - \ldots$$

$$- \left\langle w_T^\lambda, \left[\left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 \Delta\alpha + \left.\frac{\partial \hat{N}}{\partial \alpha_c}\right|_0 \Delta\alpha_c\right] \right\rangle_T + \frac{w_P^\lambda}{P^0}\left\langle \left[\left.\frac{\partial P_f}{\partial \alpha}\right|_0 \Delta\alpha + \left.\frac{\partial P_f}{\partial \alpha_c}\right|_0 \Delta\alpha_c\right], \phi^0 \right\rangle_\phi . \quad (18)$$

3. NUMERICAL METHODS FOR SOLVING THE COUPLED ADJOINT PROBLEM

The different approaches and responses lead to very similar adjoint problems. When a reactivity worth, a power change or the control parameter change has to be calculated, Equations 6-7 have to be solved. When other responses are considered the adjoint problems (Equations 9-10 and Equations 15-16) are the same, only the source terms are different.

From the programming point of view the desired path to follow when dealing with these equations is not to solve the coupled problem as a whole, but to iteratively solve the separate adjoint problems (i.e. the adjoint transport equation and the adjoint augmenting equation) and take care of the coupling terms as sources. This way the already existing neutronics and augmenting codes capable of solving the respective adjoint problems with fixed sources can be used. One problem with this approach is that the adjoint transport operator $\left(\hat{M}^0\right)^*$ is singular, which means that equations like

$$\left(\hat{M}^0\right)^* w_\phi^{(k)} = S_\phi^* - \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T^{(k-1)}$$

can only be solved if the source on the right hand side is orthogonal to the solution of the forward problem (ϕ^0) [3], which is most probably not the case in every step of the iteration. This difficulty can be overcome by splitting the fission operator and recasting the adjoint problem in the following way:

$$\left(\hat{M}_l^0\right)^* w_\phi + \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T = S_\phi^* + \lambda^0 l \left(\hat{F}^0\right)^* w_\phi$$
$$\left(\hat{J}^0\right)^* w_\phi + \left(\left.\frac{\partial \hat{N}}{\partial T}\right|_0\right)^* w_T = S_T^*.$$

Here the non-singular operator $\hat{M}_l^0 = \hat{D}^0 - \lambda^0(1-l)\hat{F}^0$ was introduced. The above form of the coupled adjoint problem provides a natural iterative scheme for solution:

$$\left(\hat{M}_l^0\right)^* w_\phi^{(k+\frac{1}{2})} = S_\phi^* - \left(\left.\frac{\partial \hat{N}}{\partial \phi}\right|_0\right)^* w_T^{(k)} + \lambda^0 l \left(\hat{F}^0\right)^* w_\phi^{(k)} \tag{19}$$
$$\left(\left.\frac{\partial \hat{N}}{\partial T}\right|_0\right)^* w_T^{(k+\frac{1}{2})} = S_T^* - \left(\hat{J}^0\right)^* w_\phi^{(k+\frac{1}{2})} \tag{20}$$

$$w_\phi^{(k+1)} = w_\phi^{(k)} + r_\phi \left(w_\phi^{(k+\frac{1}{2})} - w_\phi^{(k)}\right)$$
$$w_T^{(k+1)} = w_T^{(k)} + r_T \left(w_T^{(k+\frac{1}{2})} - w_T^{(k)}\right),$$

where r_ϕ and r_T are some relaxation constants. Experience so far indicates that such methods work with strong enough under-relaxation regardless of the value of l, but are not too robust and can become unstable if the relaxation constants are too large. However they seem to be excellent preconditioners for Krylov methods [15] applied to the full coupled adjoint problem.

4. APPLICATION TO A ONE-DIMENSIONAL SLAB

The theory presented above was applied to a one-dimensional slab problem, characterized by two-group diffusion and heat conduction, both subject to zero boundary conditions (at $\pm a$):

$$-D_1\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_1(x) + \left(\Sigma_1^t(T) - \Sigma_{1\to 1}^{tr}\right)\phi_1(x) - \Sigma_{2\to 1}^{tr}\phi_2(x) - \lambda\chi_1\left[\nu\Sigma_1^f\phi_1(x) + \nu\Sigma_2^f\phi_2(x)\right] = 0$$
$$-D_2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_2(x) + \left(\Sigma_2^t - \Sigma_{2\to 2}^{tr}\right)\phi_2(x) - \Sigma_{1\to 2}^{tr}\phi_1(x) - \lambda\chi_2\left[\nu\Sigma_1^f\phi_1(x) + \nu\Sigma_2^f\phi_2(x)\right] = 0$$
$$h\frac{\mathrm{d}^2}{\mathrm{d}x^2}T(x) + Q\left[\Sigma_1^f\phi_1(x) + \Sigma_2^f\phi_2(x)\right] = 0$$
$$\int_{-a}^{a}\mathrm{d}x Q\left[\Sigma_1^f(x)\phi_1(x) + \Sigma_2^f(x)\phi_2(x)\right] = P.$$

A constant thermal conductivity (h) was supposed and feedback was present due to the dependence of the total cross section of group one on the average temperature of the slab, i.e.

$$\Sigma_1^t(T) = \Sigma_1^{t,1} + \Sigma_1^{t,2}\cdot\left(\overline{T} - 300\right) = \Sigma_1^{t,1} + \Sigma_1^{t,2}\cdot\left(\frac{1}{2a}\int_{-a}^{a}T(x)\mathrm{d}x - 300\right).$$

All the used parameter values are summarized in Table I. Under these conditions both the forward and the adjoint problem for the eigenvalue and the power (Equations 6-7) have an analytical solution, hence simple responses can be expressed as functions of the input parameters. Naturally for more complicated responses and perturbations only numerical solutions are possible, these were obtained by using finite difference discretization of the forward and the adjoint problem and solving the resulting equations in MATLAB with LU factorization. The iterative scheme described in Section 3 for the coupled adjoint problem was tested with different values of l and the relaxation constants and convergence could be reached with typically 100-200 iterations. When Equations 19-20 were applied as a preconditioner for the MATLAB GMRES algorithm less then 10 Krylov iterations were needed.

Table I. Input Parameter Values of the 1D Slab Problem

Parameter	Value	Parameter	Value	Parameter	Value	Parameter	Value
$\Sigma_1^{t,1}[cm^{-1}]$	0.04	$\Sigma_1^{t,2}[cm^{-1}]$	0.0004	$\Sigma_2^{t}[cm^{-1}]$	0.139		
$D_1[cm]$	0.0025	$\Sigma_1^{f}[cm^{-1}]$	0.005	$D_2[cm]$	0.001	$\Sigma_2^{f}[cm^{-1}]$	0.05
χ_1	0.9	ν_1	3	χ_2	0.1	ν_2	2.5
$\Sigma_{1\to1}^{tr}[cm^{-1}]$	0.0075	$\Sigma_{1\to2}^{tr}[cm^{-1}]$	0.02	$\Sigma_{2\to1}^{tr}[cm^{-1}]$	0.0	$\Sigma_{2\to2}^{tr}[cm^{-1}]$	0.015
$h[Wm^{-1}K^{-1}]$	1	$a[m]$	2	$Q[MeV]$	200		

4.1. Sample responses

Figure 1 shows the steady-state power as a function of the perturbation of the feedback coefficient (the temperature dependent part of the total cross section of group one, $\Sigma_1^{t,2}$) and the thermal conductivity. The power decreases with the total cross section, as criticality can only be ensured if the increased absorption due to the stronger feedback coefficient is counterbalanced by a lower temperature, which can only be met at a lower power level and smaller flux values. In contrast the increase of thermal conductivity increases the power, as criticality is always reached at the same temperature distribution, therefore the power level and the flux can be higher in case of better conduction. In this latter case the perturbation theory prediction is exact, as it can be shown analytically that the steady-state power level is linearly proportional to the thermal conductivity.

Figure 2 shows the change of fast fission rate ($R = \int_{-a}^{a} \Sigma_1^f \Phi_1(x)\mathrm{d}x$) due to the perturbation of the thermal conductivity. When the conductivity increases the temperature distribution at which the reactor is critical is reached at a higher power and flux, which increases the fission rate as well (again, when the power level is not constrained, the fission rate is linear in k). When power-reset is used (which was done by adjusting the group two total cross section, $\Sigma_2^{t,1}$) the increase is even bigger as the power decrease induced by the control parameter perturbation hardens the spectrum, the flux decrease in group two is accompanied by an increase in group one. As the response is non-linear when the power is reset, the prediction of Equation 13 is only accurate for small perturbations for which the linear approximation holds.

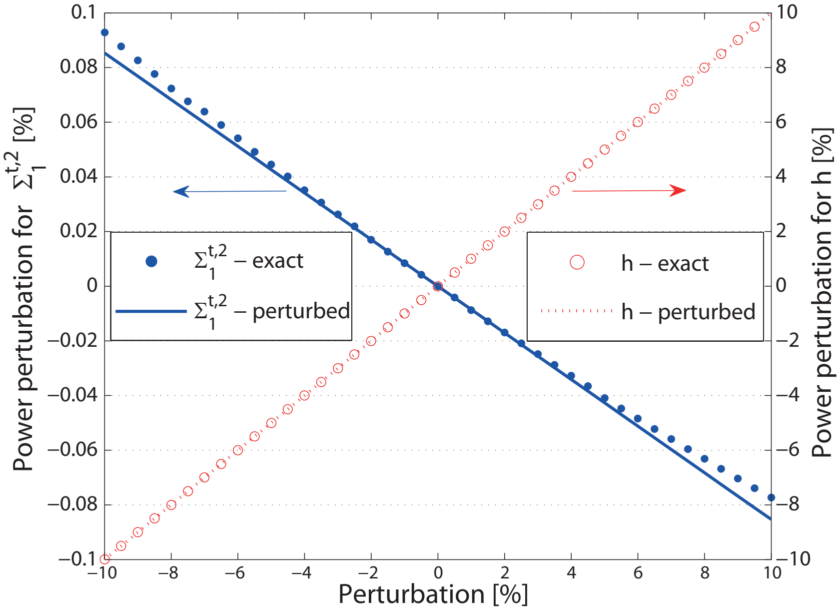

Figure 1. The Change of Power due to Perturbations. The increased conductivity makes it possible to reach higher powers at the same average temperature (as needed for criticality), whereas the increased absorption has to be counterbalanced by decreased temperatures (and hence power) to regain criticality.

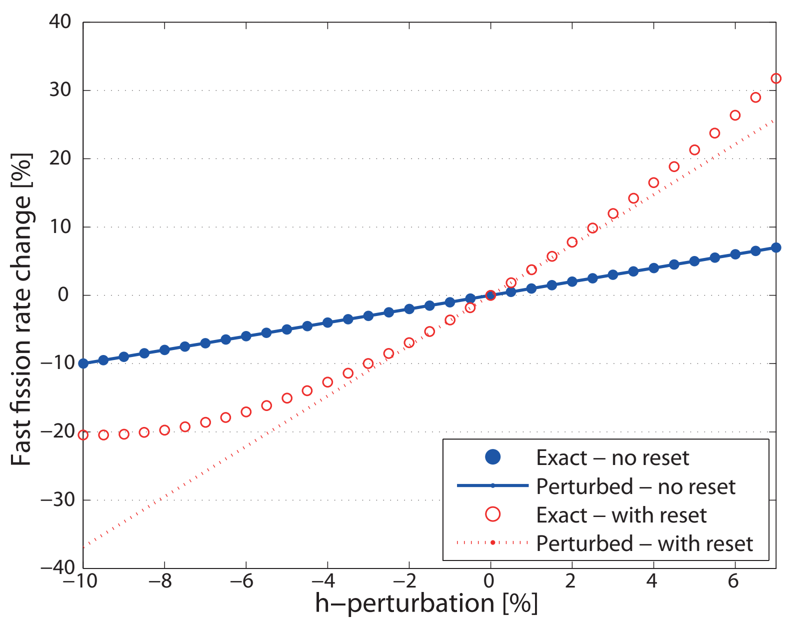

Figure 2. The Change of Fast Fission Reaction Rate due to the Thermal Conductivity Perturbation. When no power-reset is applied the fast fission rate increases as the power increases. When the power is reset by adjusting the group two total cross section ($\Sigma_2^{t,1}$) the spectral changes further increase the fast fission rate.

Figure 3 shows the multiplication factor as a function of the uniform perturbation of the thermal conductivity and the perturbation of the total cross section of group one between $\pm 0.8a$ (all other perturbations are uniform). When the power is constrained to the unperturbed value the increase of the thermal conductivity decreases the temperatures and increases the k-effective due to the negative feedback. When the absorption cross section is perturbed in the middle the power and temperature distributions are distorted (no longer cosine functions) and the difference between the reactivity effect predicted by the standard expression for $\Delta\lambda$ (considering only neutronics) and Equation 14 (taking into account the coupling) can be emphasized. In both cases the sensitivity is negative, however the pure neutronics prediction is significantly stronger than the coupled one, as in the latter case the increased absorption in the middle causes the power distribution to flatten out and the average temperature to decrease, which counterbalances the reactivity decrease somewhat.

Finally Figure 4 shows the number of outer Krylov iterations needed when solving Equations 6-7 with different values of l and different numbers of k during preconditioning (when Equations 19-20 were used as the preconditioner no underrelaxation was needed, hence $r_\phi = r_T = 1$ was chosen). The higher the value of l is the more the adjoint transport operator is distorted, hence the easier it gets to solve the adjoint transport problem (Equation 19), however the more Krylov iterations are needed. When the number of iterations in the preconditioning step is increased (k) the lower the number of the Krylov iterations gets, however the more times the adjoint transport and augmenting problem need to be solved. Obviously there is a trade-off between the number of Krylov iterations and the number of inner iterations, as well as the value of l in the preconditioning step.

5. Conclusions

This paper presented an extension of standard adjoint based sensitivity techniques making it possible to examine coupled criticality problems, in which physical processes other than neutron transport (e.g. thermal-hydraulics) are also taken into account. The proposed procedure uses appropriate adjoint functions and enables the efficient calculation of first-order changes in responses of interest due to perturbation of both the neutronic parameters and those describing the additional phenomena. To accommodate practical situations sensitivities can also be determined with a constraint on the power level or the criticality using the power- or k-reset procedures.

Numerical aspects of calculating the needed adjoint functions were also investigated and a possible iterative scheme was presented that relies on using the neutron transport and the augmenting codes separately in order to obtain the solution of the coupled adjoint problem. As was demonstrated on a one-dimensional slab model this method provides especially good convergence properties when used as a preconditioner for Krylov solvers. This makes the application of the technique to large-scale coupled problems promising, since Krylov algorithms are expected to be relatively easy to implement once the neutron transport and the augmenting codes together with their adjoints are available.

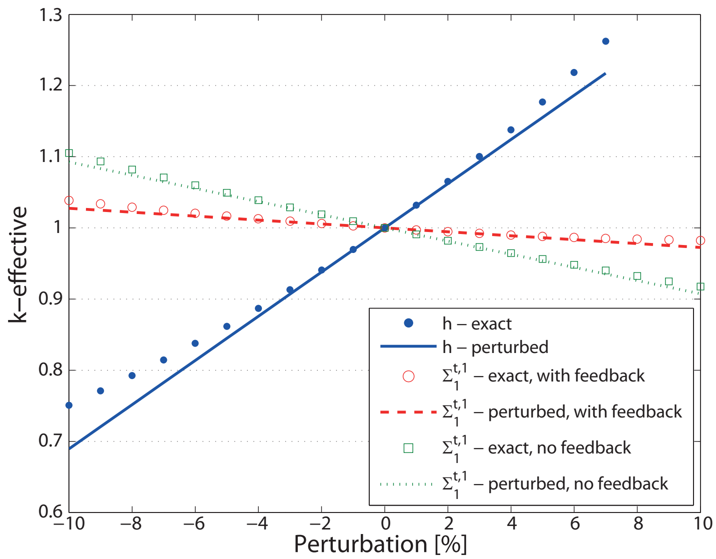

Figure 3. The Change of k-effective due to Perturbations. Due to the negative feedback the increased heat conduction has a positive reactivity worth. The increase of the total cross section in the middle of the slab decreases the k-effective, which is somewhat counterbalanced by the lower average temperature due to the changed power distribution in the coupled case.

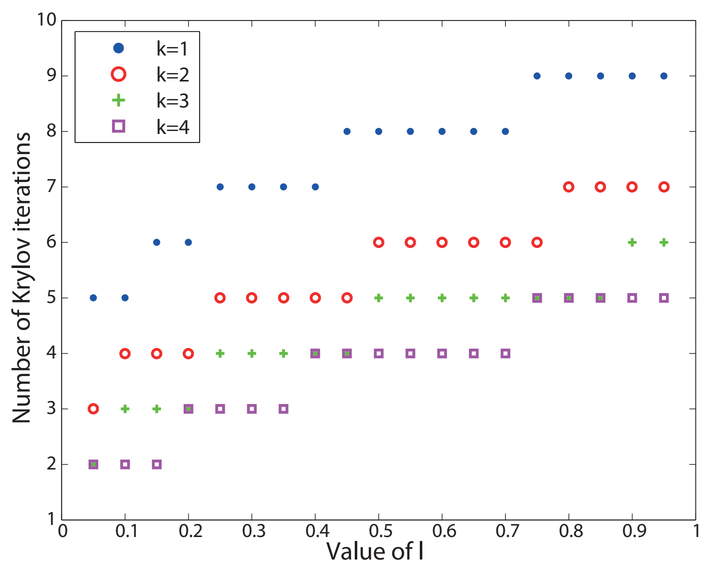

Figure 4. The Number of Krylov Iterations with Different Preconditioners. The number of Krylov iterations increases with l (but the solution of the adjoint transport problem becomes easier) and decreases with the number of iterations during preconditioning (but that increases the total number of transport and augmenting calculations).

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APPENDIX A. Notations

In this paper the following notations are used:

$$\hat{L}^0 = \hat{L}(T^0,\alpha^0) \qquad \hat{F}^0 = \hat{F}(T^0,\alpha^0) \qquad \hat{M}^0 = \hat{L}^0 - \lambda^0 \hat{F}^0$$

$$\left.\frac{\partial \hat{L}}{\partial T}\right|_0 = \left.\frac{\partial \hat{L}(T,\alpha)}{\partial T}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{F}}{\partial T}\right|_0 = \left.\frac{\partial \hat{F}(T,\alpha)}{\partial T}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{M}}{\partial T}\right|_0 = \left.\frac{\partial \hat{L}}{\partial T}\right|_0 - \lambda^0 \left.\frac{\partial \hat{F}}{\partial T}\right|_0$$

$$\left.\frac{\partial \hat{L}}{\partial \alpha}\right|_0 = \left.\frac{\partial \hat{L}(T,\alpha)}{\partial \alpha}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{F}}{\partial \alpha}\right|_0 = \left.\frac{\partial \hat{F}(T,\alpha)}{\partial \alpha}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{M}}{\partial \alpha}\right|_0 = \left.\frac{\partial \hat{L}}{\partial \alpha}\right|_0 - \lambda^0 \left.\frac{\partial \hat{F}}{\partial \alpha}\right|_0$$

$$\left.\frac{\partial \hat{L}}{\partial \alpha_c}\right|_0 = \left.\frac{\partial \hat{L}(T,\alpha)}{\partial \alpha_c}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{F}}{\partial \alpha_c}\right|_0 = \left.\frac{\partial \hat{F}(T,\alpha)}{\partial \alpha_c}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial \hat{M}}{\partial \alpha_c}\right|_0 = \left.\frac{\partial \hat{L}}{\partial \alpha_c}\right|_0 - \lambda^0 \left.\frac{\partial \hat{F}}{\partial \alpha_c}\right|_0$$

$$\hat{N}^0 = \hat{N}(T^0,\phi^0,\alpha^0) \qquad \left.\frac{\partial \hat{N}}{\partial T}\right|_0 = \left.\frac{\partial \hat{N}(T,\phi,\alpha)}{\partial T}\right|_{T^0,\phi^0,\alpha^0} \qquad \left.\frac{\partial \hat{N}}{\partial \alpha}\right|_0 = \left.\frac{\partial \hat{N}(T,\phi,\alpha)}{\partial \alpha}\right|_{T^0,\phi^0,\alpha^0}$$

$$\left.\frac{\partial \hat{N}}{\partial \alpha_c}\right|_0 = \left.\frac{\partial \hat{N}(T,\phi,\alpha)}{\partial \alpha_c}\right|_{T^0,\phi^0,\alpha^0} \qquad \left.\frac{\partial \hat{N}}{\partial \phi}\right|_0 = \left.\frac{\partial \hat{N}(T,\phi,\alpha)}{\partial \phi}\right|_{T^0,\phi^0,\alpha^0}$$

$$P_f^0 = P_f(T^0,\alpha^0) \qquad \left.\frac{\partial P_f}{\partial T}\right|_0 = \left.\frac{\partial P_f(T,\alpha)}{\partial T}\right|_{T^0,\alpha^0} \qquad \left.\frac{\partial P_f}{\partial \alpha}\right|_0 = \left.\frac{\partial P_f(T,\alpha)}{\partial \alpha}\right|_{T^0,\alpha^0}$$

$$\left.\frac{\partial P_f}{\partial \alpha_c}\right|_0 = \left.\frac{\partial P_f(T,\alpha)}{\partial \alpha_c}\right|_{T^0,\alpha^0}$$