SECOND ORDER PERTURBATION THEORY FOR NONLINEAR TIME-DEPENDENT PROBLEMS: APPLICATION TO A SIMPLIFIED COUPLED TRANSIENT

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ABSTRACT

In this paper a second-order perturbation technique for nonlinear time-dependent problems is presented and applied to a simplified multi-physics model. This method is developed by using the properties of the adjoint problem which allows calculating the set of first and second order coefficients by solving a number of linear systems.

As an illustrative example the adjoint procedure is applied to a reference transient problem, represented by a coupled point-kinetic/lumped-parameters model, and used to calculate the sensitivity coefficients of a safety related response with respect to a set of input parameters. The results obtained are compared with the values given by a direct sampling of the forward nonlinear problem. A way to reduce the number of calculations required for the application of second order adjoint techniques is also discussed.

Our first results show that the procedure provides good estimations in presence of higher order perturbation components, being able to reconstruct the responses of interest even in presence of non-Gaussian probability density functions. Furthermore, the use of reduced second order information decreases the computational requirements of the method, making it appealing for possible large scale applications.

Key Words: Second Order perturbation theory, Coupled problems

1. INTRODUCTION

Perturbation techniques are commonly used to perform sensitivity analysis and uncertainty propagation in simulations. They have been used extensively over the last decades in the reactor physics field in particular for criticality problems, where such techniques can be used to calculate the perturbation of an output quantity (i.e., the fundamental eigenvalue or any functional of the flux) following a perturbation in the input cross-sections [1].

This is usually done by using adjoint-based techniques such as the Generalized Perturbation theory [2] which rely on a first order approximation of the perturbed quantities and on the definition of an adjoint problem used to reduce the number of calculations required to perform a perturbation analysis for quantities of interest. In general these techniques can be extended to any kind of differential problems by using more general derivations of the adjoint theory such as the Adjoint Sensitivity Analysis Procedure [3]. The application to time-dependent problems however
has been much more limited: some examples can be found for fuel depletion calculations [1], kinetic problems [4], thermal-hydraulics transients [5] or simplified coupled problems [6].

An important drawback of adjoint techniques is their usual first order approximation which makes the method less accurate when dealing with large input perturbations. In order to overcome this issue, an adjoint based approach for the calculation of higher order perturbation components was first proposed by Greenspan [7] with the application to source driven systems. For linear time-dependent problems a similar approach was presented by Gandini [8], who derived an expression for the Taylor expansion coefficients of any functional response, obtained by solving a new adjoint problem together with a linearized system for each of the input parameters.

In the present work we apply this Second Order Adjoint based perturbation technique to a nonlinear time-dependent problem, represented by a coupled point-kinetic/lumped-parameters system. The first part of the paper contains the introduction of the Adjoint Sensitivity Analysis procedure together with the derivation of the Second Order Adjoint problem used to perform the second order perturbation analysis. In the second section the theory is then applied to the coupled time-dependent problem used to describe a positive reactivity insertion transient. We consider a safety related response, the maximum temperature reached by the fuel during the transient, with respect to which first and second order perturbation theory are applied.

Finally, a method to reduce the number of calculations by neglecting part of the second order information is suggested and its validity in terms of uncertainty quantification is compared to a standard Monte Carlo prediction.

2. FIRST AND SECOND ORDER ADJOINT THEORY FOR NONLINEAR TIME-DEPENDENT PROBLEMS

We start with the introduction of a generic formulation of a nonlinear time-dependent problem.

\[
\frac{du}{dt} = L(\alpha, u) \\
u(0) = u_{in}(\alpha)
\]  

(1)

where \(L\) is the nonlinear operator depending on the set of input parameters \(\alpha\) and acting on the unknown vector \(u\) and \(u_{in}\) is the vector which defines the initial conditions which is assumed to depend on the set of input parameters. Once the solution of this system is known one may be interested in quantities (responses) which depend on it through functional relations. This is the case when dealing for example with integral parameters or minimum or maximum points such as averaged or peak temperatures. A general way to express these responses is by using the following functional

\[
R = \langle f(\alpha, t), u(t) \rangle
\]  

(2)

where we used the bra-ket notation to write the time integral

\[
\langle a, b \rangle = \int_{0}^{t_f} a \cdot b dt
\]
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We assume for sake of simplicity the response functional to be linear with respect to the solution and we introduce a weight function $f$ used to define the response of interest. We also assume that $f$ is linear with respect to the input parameters.

The first order variation of the response corresponding to a variation of any of the input parameters can be calculated using the Adjoint Sensitivity Analysis Procedure (ASAP) derived in [3]. The first step to implement the procedure is by introducing the following perturbation notation

$$u = u_0 + \delta u$$
$$\alpha = \alpha_0 + \delta \alpha$$

where the subscript 0 refers to the reference value of the quantity or, in other words, the mean value of the input parameters and corresponding nonlinear solution. According to the theory, the first order variation of the functional $R$ can be defined, using the bra-ket notation, as

$$\delta R \approx \left\langle \frac{\partial f}{\partial \alpha} \delta \alpha, u_0 \right\rangle + \left\langle u^*, \frac{\partial L}{\partial \alpha} (\alpha_0, u_0) \delta \alpha \right\rangle + u^*(0) \cdot \delta u_{in}$$

(3)

The first term on the right-hand side, known as the direct component, defines the variation caused by a perturbation of the weight function $f$ while the second term defines the contribution caused by the perturbation of the nonlinear operator. This depends on the operator $\frac{\partial L}{\partial u}$ which is the Gateaux Derivative (GD) of the nonlinear operator $L$ taken in the direction of the parameters perturbation, and on $u^*$ which is an adjoint function solving the following problem

$$-\frac{du^*}{dt} = \left( \frac{\partial L}{\partial u}(\alpha_0, u_0) \right)^* u^* + \nabla_u R$$
$$u^*(t_f) = 0$$

(4)

The operator $\frac{\partial L}{\partial u}$ is the adjoint of the GD of the original nonlinear operator taken in the direction of the solution. This operator is therefore linear and depends on the reference solution of Equation 1. The definition of the adjoint problem is completed for a particular response by introducing the inhomogeneous term $\nabla_u R$ and the proper boundary conditions. Once this problem is solved for the response $R$ one can therefore calculate its variation by solving a simple inner product. The third term of the expression 3 includes the effects of a change in the initial boundary value of the time problem on the response. The most important approximation present by this formulation is introduced by neglecting any higher order term, which means that there is a range of validity for the prediction of the variation of the response. In other words, if we consider the Taylor expansion

$$\delta R = \sum_{i=1}^{K} \left( \frac{\partial R}{\partial \alpha_i} \right)_{\alpha_0, u_0} \delta \alpha_i + \frac{1}{2} \sum_{i=1}^{K} \sum_{j=1}^{K} \left( \frac{\partial^2 R}{\partial \alpha_i \partial \alpha_j} \right)_{\alpha_0, u_0} \delta \alpha_i \delta \alpha_j +$$
$$+ \frac{1}{3!} \sum_{i=1}^{K} \sum_{j=1}^{K} \sum_{k=1}^{K} \left( \frac{\partial^3 R}{\partial \alpha_i \partial \alpha_j \partial \alpha_k} \right)_{\alpha_0, u_0} \delta \alpha_i \delta \alpha_j \delta \alpha_k + O(\delta \alpha^4)$$
calculating the response variation with the first order adjoint theory means truncating this expansion to the first term. In the next section a method to estimate the second order terms of the expansion is introduced, the method is based on re-using the same adjoint approach used for the first order contribution (thereby reducing the computational requirement).

2.1. Adjoint Theory for second order perturbation components

The aim of the second order adjoint theory is to define a way to obtain the second order perturbation components for the response of interest using the adjoint properties already introduced for the first order propagation. The first step is to express each of the second order mixed derivatives of the expansion as

$$\frac{\partial^2 R}{\partial \alpha_i \partial \alpha_j} = \frac{\partial}{\partial \alpha_i} \left[ \frac{\partial R}{\partial \alpha_j} \right]$$

The first order adjoint theory allows to represent first order derivatives as functionals, it is therefore possible to write the second order information as a first order variation of these functionals. If we consider the adjoint formulation of the first order variation of the response with respect to the parameter $\alpha_i$ and we perturb this quantity in the direction $\delta \alpha_j$ we are able to determine the derivative information we need. This corresponds to estimating the following variation

$$\frac{\partial^2 R}{\partial \alpha_i \partial \alpha_j} \delta \alpha_j \delta \alpha_i = \frac{\partial}{\partial \alpha_i} \left[ \frac{\partial R}{\partial \alpha_j} \delta \alpha_j \right] \delta \alpha_i = \frac{\partial}{\partial \alpha_i} \left[ \left\langle \frac{\partial f}{\partial \alpha_j}, \delta \alpha_j, \mathbf{u}_0 \right\rangle + \left\langle \mathbf{u}^* \frac{\partial L}{\partial \alpha_j}(\alpha_0, \mathbf{u}_0) \right\rangle + \mathbf{u}^* \cdot \frac{\partial \mathbf{u}_m}{\partial \alpha_j} \right] \delta \alpha_j \delta \alpha_i$$

where we used Equation 3 to express the first order variation of $R$ with respect to $\alpha_j$. Taking into account that we are assuming the weight function $f$ to be linear with respect to the input parameters, the GD of the previous expression in the direction $\alpha_i$ can be written as

$$\frac{\partial^2 R}{\partial \alpha_i \partial \alpha_j} \delta \alpha_j \delta \alpha_i = \left\langle \mathbf{u}^* \frac{\partial L}{\partial \alpha_j}(\alpha_0, \mathbf{u}_0), \delta \alpha_j \right\rangle \delta \alpha_i +$$

$$+ \left\langle \delta \mathbf{u}^*(\delta \alpha_i), \frac{\partial L}{\partial \alpha_j}(\alpha_0, \mathbf{u}_0) \right\rangle \delta \alpha_j +$$

$$+ \left\langle \mathbf{u}^*, \frac{\partial}{\partial \mathbf{u}} \left( \frac{\partial L}{\partial \alpha_j}(\alpha_0, \mathbf{u}_0) \right) \delta \mathbf{u}(\delta \alpha_i) \right\rangle \delta \alpha_j +$$

$$+ \delta \mathbf{u}^*(\delta \alpha_i, t = 0) \cdot \frac{\partial \mathbf{u}_m}{\partial \alpha_j} \delta \alpha_j$$

The unknown quantities in this expression, denoted with $\delta \mathbf{u}(\delta \alpha_i)$ and with $\delta \mathbf{u}^*(\delta \alpha_i)$, are, respectively, the first order variation of the forward and the adjoint solution caused by the variation $\delta \alpha_i$. Once these quantities are known (together with the Hessian of the linear operator with respect to the input parameters) the second order information can be calculated by performing the usual inner products. These first order variations can be evaluated by linearizing the forward and the adjoint problem and solving with respect to the perturbation considered. If we
consider for example the nonlinear forward problem this linearization procedure leads to the following system

$$\frac{d\delta u(\delta \alpha_i)}{dt} = \left( \frac{\partial L}{\partial u}(\alpha_0, u_0) \right) \delta u(\delta \alpha_i) + \left( \frac{\partial L}{\partial \alpha_i}(\alpha_0, u_0) \right) \delta \alpha_i$$

(6)

$$\delta u(0) = \frac{\partial u_{in}}{\partial \alpha_i} \delta \alpha_i$$

which is defined by the partial GD of the original operator and by a source term and a set of initial conditions which depend on the perturbation considered. Due to its linearity and the fact that we are dealing with perturbations that are constant in time, this system needs to be solved once for each of the perturbed parameters independently of the perturbation magnitude. The solution of this problem is then used to evaluate the third term of Eq. 5. The same linearization has to be applied to the adjoint system, applying the GD to the system described in Eq. 4 with respect to \(\alpha_i\) leads to

$$-\frac{d\delta u^*(\delta \alpha_i)}{dt} = \left( \frac{\partial L}{\partial u}(\alpha_0, u_0) \right)^* \delta u^*(\delta \alpha_i) + \frac{\partial}{\partial \alpha_i} \left[ \left( \frac{\partial L}{\partial u}(\alpha_0, u_0) \right)^* u^* \right] \delta \alpha_i +$$

$$+ \frac{\partial}{\partial u} \left[ \left( \frac{\partial L}{\partial u}(\alpha_0, u_0) \right)^* u^* \right] \delta u(\delta \alpha_i)$$

$$\delta u^*(t_f) = 0$$

(7)

where we have introduced the Gateaux Differentials of the first order adjoint problem. This operation defines a new system of ODEs used to estimate the variation of the adjoint solution with respect to any of the input perturbations. The main operator of the system is the same as the original adjoint problem 4, the only difference is represented by the two inhomogeneous terms arising from the application of the GD. Both terms depend on the adjoint solution while the second one introduces a dependency on the first order variation of the forward problem. The term is caused by the perturbation of the part of the adjoint operator which depends on the forward solution, this means that we can solve the system for each of the input perturbations only after we obtained the corresponding solution of problem 6.

After we solved problems 6 and 7 for all perturbed parameters, corresponding to a total of \(2N\) calculations (where \(N\) is the number of perturbed input parameters) to add to the original adjoint used for the first order information, we can substitute the solutions obtained in Eq. 5 to reconstruct the Hessian matrix containing the second order derivatives of the response. It must be pointed out that, being the Hessian a symmetric matrix, changing the indices in Eq. 5 should not affect the value of the second order derivative.

In the next section the theory introduced so far is applied to a simplified coupled problem used to model a nonlinear transient in a point-reactor.
3. APPLICATION TO A SIMPLIFIED NEURONICS/ THERMAL-HYDRAULICS PROBLEM

The problem considered for the application of the second order perturbation techniques introduced in the previous section consists of a system of a coupled ODE modeling the time-dependent behavior of a simplified reactor. The model is derived using a point-kinetic approximation for the neutron population [9] together with a lumped parameter description for the reactor temperatures. These assumptions allow the elimination of the spatial dependencies and therefore to focus on the time-dependent part. The point-kinetic system is

\[
\frac{dP}{dt} = \frac{\rho(T_f, T_c, t) - \beta P}{\Lambda} + \sum_{k=1}^{6} \lambda_k C_k
\]

\[
\frac{dC_k}{dt} = -\lambda_k C_k + \frac{\beta_k P}{\Lambda}
\]

where \(P\) is the reactor power, \(\Lambda\) the mean generation time, \(C_k\) the concentration of the \(k\)th precursor group, \(\beta_k\) and \(\lambda_k\) the delayed neutrons fraction and the decay constant for the \(k\)th precursor group and \(\beta\) the total delayed neutrons fraction. The thermo-kinetics/thermal-hydraulics equations, needed to describe the removal of the heat by the coolant, are approximated using a lumped parameter model, i.e. averaging the unknown values over the whole domain. Assuming the reactor is divided into a fuel and a coolant region, their time-dependent average temperatures are described by the equations

\[
M_f c_p f \frac{dT_f}{dt} = P + H(T_c - T_f)
\]

\[
M_c c_p c \left[ \frac{dT_c}{dt} + v \frac{T_c - T_{in}}{L} \right] = H(T_f - T_c)
\]

where \(M_f\) and \(M_c\) are the fuel and coolant mass respectively, \(H\) the total heat transfer coefficient, \(v\) the coolant flow velocity, \(L\) the channel length and \(T_{in}\) the inlet temperature of the coolant. The coupling between these two equations is given by the presence of the power production term \(P\) and by the time-dependent reactivity \(\rho(t)\) in the point kinetic equation, defined as the contribution of three different terms

\[
\rho(t) = \rho_{ext} + \alpha_D [T_f - T_f(0)] + \alpha_c [T_c - T_c(0)]
\]

where \(\rho_{ext}\) represents an external reactivity insertion, \(\alpha_D\) and \(\alpha_c\) are the Doppler and the coolant feedback reactivity coefficients respectively, and \(T_f(0)\) and \(T_c(0)\) are the initial system temperatures. We assume that the system starts from the following initial conditions

\[
P(0) = P_0
\]

\[
C_k(0) = \frac{\beta_k}{\lambda_k} P_0
\]

\[
T_f(0) = T_c(0) + \frac{P_0}{H}
\]

\[
T_c(0) = T_{in} + \frac{P_0 L}{M_c c_p c v}
\]
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The parameters used for the model are included in Table I. These data have been obtained using a Sodium Fast Reactor as a reference, the kinetic and heat transfer parameters can be found in [10].

Starting from these initial conditions, we consider a transient triggered by a positive reactivity insertion. This external step reactivity is described by a step function which is positive ($0.5\$) between the initial time and $t = 0.5$ and negative ($-1\$) for ($t > 0.5s$). This reference problem has been solved by using a Matlab built-in ODE solver, the solution is presented in Fig. 1. As seen from the figure, the power starts to increase after the reactivity insertion until the Doppler reactivity is sufficiently strong to compensate the external amount. Then the introduction of the negative step (after $0.5s$) brings the system to a power level lower than the initial value.

Regarding the fuel temperature, this negative insertion represents the point when it reaches its maximum (with the coolant temperature following with a small delay). To illustrate the application of perturbation techniques to time-dependent problems we decided to use the fuel temperature at this point of the transient as the response with respect to which the methods introduced before are applied.

### Table I. Parameter values and uncertainties used in the coupled model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P$ (MW)</td>
<td>1800</td>
</tr>
<tr>
<td>$\Lambda$ (s)</td>
<td>$4 \times 10^{-7}$</td>
</tr>
<tr>
<td>$M_f$ (kg)</td>
<td>9675</td>
</tr>
<tr>
<td>$M_c$ (kg)</td>
<td>1168</td>
</tr>
<tr>
<td>$c_{pf}$ (J/kgK)</td>
<td>500</td>
</tr>
<tr>
<td>$c_{pc}$ (J/kgK)</td>
<td>1200</td>
</tr>
<tr>
<td>$H$ (kW/K)</td>
<td>$2.5 \times 10^6$</td>
</tr>
<tr>
<td>$v$ (m/s)</td>
<td>7.5</td>
</tr>
<tr>
<td>$\alpha_d$ (pcm/K)</td>
<td>-0.687</td>
</tr>
<tr>
<td>$T_{in}$ ($^\circ C$)</td>
<td>380</td>
</tr>
<tr>
<td>$\alpha_c$ (pcm/K)</td>
<td>0.123</td>
</tr>
<tr>
<td>$\rho_{ext}$</td>
<td>0.5$</td>
</tr>
</tbody>
</table>

3.1. Application of the first and second order adjoint perturbation theory

Once the response of interest is defined (as the fuel temperature at $t = 0.5s$), the application of the first and second order perturbation techniques introduced in Section 2 requires the solution of a set of adjoint and perturbed equations. First, the adjoint Equation 4 was solved and used in 3 in order to obtain the first order sensitivity information for the response. We limited the present perturbation analysis to five parameters: the two reactivity coefficients, the total heat transfer coefficient $H$, the inlet temperature $T_{in}$ and the magnitude of the positive reactivity insertion $\rho_{ext}$. The left part of Figure 2 contains the first order sensitivity coefficients for this set of parameters. The interpretation of these coefficient is quite straightforward and does not need an extensive discussion: increasing the heat transfer coefficient reduces the maximum fuel temperature during the transient while increasing both the inlet temperature and the magnitude of the reactivity step would have the opposite effect. At the same time a stronger Doppler coefficient reduces the maximum power reached during the transient (and therefore the temperature), while the contribution of the coolant coefficient is negligible.
Figure 1. Reference transient describing the response of the system to a step reactivity insertion. The value of the step reactivity is $\rho_{\text{ext}} = 0.5$ for $0 < t \leq 0.5 \text{s}$ and $\rho_{\text{ext}} = -1$ for $t > 0.5 \text{s}$.

In order to determine the second order derivatives (Hessian matrix) of the response with respect to these 5 parameters, 10 further calculations were required (5 perturbed forward problems and 5 perturbed adjoint calculations). The right part of Figure 2 shows the Hessian matrix calculated using these solutions in Eq. 5. This matrix is symmetric as one would expect and defines the second order correction to the response variation given any input perturbation. The off-diagonal terms of this matrix represent the cross-correlation between the different parameters: for example the effect of perturbing the Doppler coefficient will be higher if the heat transfer coefficient is perturbed at the same time.

The response surfaces with respect to the input parameters obtained using a first and a second order estimation are presented in Figure 3 where they are compared with the surfaces obtained by running the full model for the different realizations of the input parameters. This comparison shows, as one would expect analyzing the Hessian matrix, that for the current response there are some parameters whose perturbation introduces a considerable second order correction. This the case, for example, for the total heat transfer coefficient (top surfaces). If a numerical approximation (like finite difference) was used instead of the adjoint method to calculate the coefficients of the Taylor expansion one would need $N^2 + 2N + 1$ runs of the full model [11] in order to estimate the first and second order sensitivity coefficients. This is in contrast with the $2N + 2$ calculations needed by the adjoint theory when dealing with a response localized in time. However, for large perturbation sets the computational requirement would become eventually too
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Figure 2. First (left) and second (right) order sensitivity coefficients for the fuel temperature at \( t = 0.5s \). The coefficients are expressed in terms of relative variation of the output corresponding to a relative variation of the inputs.

expensive considering that each response analyzed would need a set of new calculations.

A way to reduce the number of calculations needed to reconstruct the Hessian matrix would be simply by neglecting part of it. As can be seen from Figure 2 many of the diagonal and off-diagonal terms of this matrix are negligible, the problem would be determining “a priori” which elements (and therefore calculations) can be discarded. A first criterion could be based on the magnitude of the first order derivatives while a second one could be, when dealing with uncertainty quantification, the standard deviation associated to the input parameters (as it was suggested in [8]). In the next section an example of optimization of the second order perturbation theory when dealing with an uncertainty quantification problem is presented.

3.2. Application to an uncertainty quantification problem

Let’s assume we are dealing with an uncertainty propagation problem: we want to estimate the probability density function of the response given a set of probability density functions for the input parameters. We consider these pdfs to be log-normally distributed (in order to exclude non-physical realizations of the input parameters) with two different relative standard deviations: 5% for the external reactivity and 10% for the rest of the parameters.

The probability density function of the response can be obtained by sampling the response for a large number of realizations of the input parameters set. We performed this sampling procedure calculating the realization of the response in the following ways
Figure 3. Response surfaces of the fuel temperature at \( t = 0.5 \text{s} \) with respect to different input parameters, comparison between first and second order estimation and exact variation

- using the full model.
- using a first order Taylor expansion obtained with the first order adjoint theory. (2 calculations)
- using a second order expansion obtained with the second order adjoint theory. (12 calculations)
- using a reduced second order expansion obtained by including only 4 elements of the Hessian matrix. (6 calculations)

The Hessian elements used for the reduced second order model were chosen according to the magnitude of the corresponding first order coefficient and taking into account the value of the standard deviation of the input parameters. This led (as it can be seen from Figure 2) to the choice of the elements corresponding to the total heat transfer coefficient and to the inlet temperature while the second order contribution due to a change in external reactivity was discarded considering that its standard deviation is half the value of the other two. Figure 4 shows the comparison of the pdf obtained by sampling these different approximations of the response. The responses obtained with a Taylor expansion have been sampled \( 10^6 \) times in order to reduce the statistical noise while the one obtained using the full model has been sampled \( 10^5 \) times because of computational restrictions. As it can be seen from the shape of the pdf the full model propagates higher order perturbation components which are responsible for the tail towards...
higher temperature values. This information is lost by the first order propagation while the pdf reconstructed using second order expansion coefficients is much closer to the real one. It is also interesting to point out that the pdf sampled with reduced second order model is not far from the one containing the full Hessian information despite the fact that we neglected 21 of the 25 coefficient of the matrix. This translates to a reduced number of calculations required, 6 instead of 12. The main challenge from this point of view is the mathematical definition of a ranking criterion that can be used to select the second order information “a priori”, therefore reducing the computational requirement of the second order adjoint propagation.

4. CONCLUSIONS AND FUTURE WORK

In this paper we presented the application of a second order adjoint perturbation technique to a simplified coupled time-dependent problem. The mathematical definition of this second order perturbation technique is very similar to the first order procedure, the main difference being the number of adjoint and perturbed calculations required to reconstruct the Hessian matrix.

The application of the technique to a reference transient shows how this second order propagation can be very important for an accurate reconstruction of the statistical moments of interest for a safety related response. The main challenge is the reduction of the number of calculations required by the method. Although the mathematical definition of a ranking criterion still needs to be defined, we have shown how the number of second order calculations can be reduced by carefully selecting part of the Hessian information.
As a future work we will study a way to determine a priori which part of the second order information needs to be evaluated in order to perform an accurate propagation. After this task is completed the application of the theory can be extended to more complex problems like the uncertainty analysis of large scale systems.

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REFERENCES