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Development of a hybrid method to improve the sensitivity and uncertainty analysis for homogenized few-group cross sections

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ABSTRACT

In the framework of two-step method of reactor core calculation, few-group homogenized cross sections generated by lattice-physics calculations are key input parameters for the three-dimensional full-core calculation. Conventional method for few-group cross-sections sensitivity and uncertainty (S&U) analysis related to the nuclear data was performed based on the effective self-shielding cross sections instead of the continuous-energy cross sections, which means resonance self-shielding effect (implicit effect) is neglected. Furthermore, the multi-group covariance data is generated from the continuous-energy cross sections. Therefore, in order to perform S&U analysis with respect to the continuous-energy cross sections for both accuracy and consistency, a hybrid method is proposed in this paper. The subgroup-parameter sensitivity-coefficients are calculated based on the direct perturbation (DP) method. The sensitivity-coefficients of the effective self-shielding cross sections and the responses (k_{eff} and few-group homogenized cross sections) are calculated based on the generalized perturbation theory (GPT). A boiling water reactor (BWR) pin-cell problem under different power conditions is calculated and analyzed. The numerical results reveal that the proposed hybrid method improves the sensitivity-coefficients of eigenvalue and few-group homogenized cross sections. The temperature effects on the sensitivity-coefficients are demonstrated and the uncertainties are analyzed.

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1. Introduction

Response sensitivity and uncertainty (S&U) analysis with respect to fundamental nuclear data is an important aspect in the framework of reactor numerical calculation. There are many applications based on S&U analysis. In the reactor design and safety analysis, design margin can be determined appropriately based on the S&U analysis, and additional efforts can also be found in order to reduce the uncertainties [1]. In the target accuracy assessment, when uncertainties cannot meet the safety parameter accuracy requirement, nuclear data uncertainties that need to be improved can be determined to solve a minimum problem based on the sensitivity-coefficients [2]. Nuclear-data adjustment is to minimize the uncertainties of safety parameters based on the integral experimental data and S&U analysis results [3]. S&U research has been receiving more and more attentions because of such significant applications. Accurate S&U evaluation is necessary under this circumstance.

In the conventional reactor physics 'two-step' scheme calculation, lattice-physics calculation is performed followed by core diffusion calculation. The few-group homogenized cross sections are the outputs of the lattice-physics calculation as well as the inputs of the core calculation. The uncertainties of fundamental nuclear data will be propagated to the core calculation results through few-group homogenized cross sections. Consequently, quantifying the uncertainties of fewgroup homogenized cross sections is a necessary step for the core calculation S&U analysis.

Conventional method for nuclear-data sensitivity analysis usually neglects resonance self-shielding effect [4]. However, resonance self-shielding is an important phenomenon in thermal reactors, which leads to the fact that implicit sensitivity arising from resonance calculation plays an important role in the S&U analysis of lattice-physic calculation [5–6]. In order to take into account the resonance self-shielding effect to improve the accuracy, the sensitivity analysis should be performed based on the continuous-energy cross sections rather than the effective self-shielding cross sections. On the other hand, nuclear-data covariance processing code, such as NJOY [7], calculates the covariance of multi-group cross sections at infinite dilution from the continuous-energy cross sections, instead of covariance of the effective self-shielding cross sections. From this perspective, it is appropriate to perform sensitivity analysis with respect to the continuous-energy counterparts of the multi-group cross sections to keep the consistency. Moreover, further analysis about the implicit effects on more responses beside the multiplication factor should be performed.

The subgroup method has been widely used for resonance calculation [8–9]. The subgroup parameters are calculated based on resonance cross-sectional tables or resonance integral tables, which are generated from continuous-energy cross sections off-line. The perturbation of continuous-energy cross sections will implicitly affect the final responses through the subgroup resonance calculation. Unlike the method to assess such implicit effect based on the conventional resonance calculated method [6,10], two problems will be encountered when the subgroup method is used. The first one is how to assess the effects on subgroup parameters when the continuous-energy cross sections are perturbed. The second one is how to assess the effects on the effective self-shielding cross sections when the subgroup parameters are perturbed. After these two problems are solved, the response sensitivity-coefficients with respect to the continuous-energy cross sections can be determined.

In our previous work [11], the implicit sensitivityanalysis method was developed for non-resonance nuclides, and only the eigenvalue implicit sensitivitycoefficients were studied. Though previous work demonstrated that the implicit sensitivity had a significant effect on the eigenvalue sensitivity-coefficients, more responses such as few-group homogenized cross sections were not investigated. Moreover, when the resonance nuclides are taken into account, the sensitivity-coefficient calculation method is not proposed when the continuous-energy cross sections are considered as the perturbation sources. In order to investigate the implicit effect on the fewgroup homogenized cross sections, and perform S&U analysis with respect to the continuous-energy cross sections with subgroup resonance calculation method being used for both accuracy and consistency, a new hybrid method is proposed in this paper. The subgroup-parameter sensitivity-coefficients with respect to the continuous-energy cross sections are calculated based on the direct perturbation (DP) method. The sensitivity-coefficients of effective self-shielding cross sections and the responses (k_{eff} and few-group homogenized cross sections) S&U analysis are calculated based on the generalized perturbation theory (GPT).

This paper is organized as follows. Theoretical models of this work are described in Section 2. The calculation flow chart is given in Section 3. Section 4 gives the verification and analysis based on a BWR fuel pin-cell under different power conditions. Finally, Section 5 summarizes and concludes the work.

2. Theoretical models

2.1. Sensitivity calculation

2.1.1. Sensitivity calculation for assembly homogenized few-group cross sections

Sensitivity-analysis method based on the GPT is proven to be very efficient when the amount of input parameters is far larger than that of the responses [12]. The method is well suitable for the sensitivity analysis of the reactor integral parameter R which has the following form:

$$R \equiv \frac{\langle \Phi^* H_1 \Phi \rangle}{\langle \Phi^* H_2 \Phi \rangle} \tag{1}$$

where H_1 and H_2 are the operators related to nuclear cross sections; Φ is the neutron angular flux and Φ^* is the adjoint neutron angular flux, which are the eigenvector solution of the neutron transport equation and adjoint neutron transport equation, respectively, which are given by Equations (2) and (3); $\langle \rangle$ denotes integration over appropriate phase space.

$$\begin{aligned} \mathbf{\Omega} \cdot \nabla \Phi + \mathbf{\Sigma}_{t}\left(\mathbf{r}, E\right) \Phi \\ &- \int_{0}^{\infty} dE' \int_{\mathbf{\Omega}'} \mathbf{\Sigma}_{s}\left(\mathbf{r}; E', \mathbf{\Omega}' \to E, \mathbf{\Omega}\right) \Phi(\mathbf{r}, E', \mathbf{\Omega}') d\mathbf{\Omega}' \\ &- \lambda \frac{\chi(E)}{4\pi} \int_{0}^{\infty} dE' \int_{\mathbf{\Omega}'} \nu \mathbf{\Sigma}_{f}(\mathbf{r}, E') \Phi(\mathbf{r}, E', \mathbf{\Omega}') d\mathbf{\Omega}' = 0 \end{aligned}$$

$$(2)$$

$$-\mathbf{\Omega} \cdot \nabla \Phi^* + \mathbf{\Sigma}_{t}(\mathbf{r}, E) \Phi^* -\int_{0}^{\infty} dE' \int_{\mathbf{\Omega}'} \mathbf{\Sigma}_{s}(\mathbf{r}; E, \mathbf{\Omega} \to E', \mathbf{\Omega}') \Phi^*(\mathbf{r}, E', \mathbf{\Omega}') d\mathbf{\Omega}' -\lambda \frac{\nu \mathbf{\Sigma}_{f}(\mathbf{r}, E)}{4\pi} \int_{0}^{\infty} dE' \int_{\mathbf{\Omega}'} \chi(E') \Phi^*(\mathbf{r}, E', \mathbf{\Omega}') d\mathbf{\Omega}' = 0$$
(3)

The operator forms of Equations (2) and (3) are given by Equations (4) and (5).

$$(L - \lambda F) \Phi = M\Phi = 0 \tag{4}$$

$$(L^* - \lambda F^*) \Phi^* = M^* \Phi^* = 0$$
 (5)

where F is the fission operator; L is the operator represents other terms; M is the Boltzmann transport operator; $\lambda = 1/k_{\text{eff}}$ is the minimum eigenvalue. F^* , L^* , and M^* are the corresponding adjoint operators.

The expression of the relative sensitivity-coefficient can be given by Equation (6) according to the definition:

$$S = \frac{\mathrm{d}R/R}{\mathrm{d}\alpha/\alpha}$$

$$= \alpha \left\{ \begin{pmatrix} \left\langle \Phi^* \frac{\mathrm{d}H_1}{\mathrm{d}\alpha} \Phi \right\rangle \\ \overline{\langle \Phi^* H_1 \Phi \rangle} - \frac{\left\langle \Phi^* \frac{\mathrm{d}H_2}{\mathrm{d}\alpha} \Phi \right\rangle}{\langle \Phi^* H_2 \Phi \rangle} \end{pmatrix} + \\ \left\langle \left(\frac{H_1^* \Phi^*}{\langle \Phi^* H_1 \Phi \rangle} - \frac{H_2^* \Phi^*}{\langle \Phi^* H_2 \Phi \rangle} \right) \frac{\mathrm{d}\Phi}{\mathrm{d}\alpha} \right\rangle + \\ \left\langle \left(\frac{H_1 \Phi}{\langle \Phi^* H_1 \Phi \rangle} - \frac{H_2 \Phi}{\langle \Phi^* H_2 \Phi \rangle} \right) \frac{\mathrm{d}\Phi^*}{\mathrm{d}\alpha} \right\rangle \right\}$$
(6)

where H_1^* and H_2^* are the adjoint operators of H_1 and H_2 correspondingly.

It can be found that the derivative of the flux needs to be calculated for each nuclear cross section to determine the sensitivity-coefficient, which leads to high computation cost. In order to avoid the calculation of the term $\frac{d\Phi}{d\alpha}$, a generalized adjoint equation should be established given by Equation (7) according to GPT:

$$M^*\Gamma^* = \frac{H_1^*\Phi^*}{\langle \Phi^*H_1\Phi\rangle} - \frac{H_2^*\Phi^*}{\langle \Phi^*H_2\Phi\rangle}$$
(7)

The second-term of the right hand of Equation (6) can be calculated alternatively by Equation (8):

$$\alpha \left\langle \left(\frac{\boldsymbol{H}_{1}^{*} \Phi^{*}}{\langle \Phi^{*} \boldsymbol{H}_{1} \Phi \rangle} - \frac{\boldsymbol{H}_{2}^{*} \Phi^{*}}{\langle \Phi^{*} \boldsymbol{H}_{2} \Phi \rangle} \right) \frac{\mathrm{d}\Phi}{\mathrm{d}\alpha} \right\rangle = -\alpha \left\langle \boldsymbol{\Gamma}^{*}, \frac{\mathrm{d}\boldsymbol{M}}{\mathrm{d}\alpha} \Phi \right\rangle$$
(8)

The third-term of the right hand of Equation (6) can be calculated with the similar method. With the transformation of the GPT-based method, the calculation of derivative of the flux and adjoint flux can be avoided. The sensitivity-coefficients can be obtained with respect to all nuclear cross sections once the corresponding adjoint flux is obtained. Therefore, this method is efficient for sensitivity calculation.

When *R* is a given few-group homogenized cross section of lattice-physics calculation, the expression is

$$\bar{\mathbf{\Sigma}}_{x,h} = \frac{\langle \mathbf{\Sigma}_x \Phi \rangle}{\langle \Phi \rangle} \tag{9}$$

where *x* is the cross-sectional type; *h* is the group index of few-group cross sections; $\bar{\Sigma}_{x,h}$ is the few-group cross sections; Σ_x is the multi-group macro cross sections.

The corresponding generalized adjoint equation is given as follows according to the above derivation [13–14]:

$$M^{*}\Gamma^{*} = \frac{\Sigma_{x}}{\langle \Sigma_{x} \Phi \rangle} - \frac{1}{\langle \Phi \rangle}$$
(10)

Then, the relative sensitivity-coefficients of fewgroup homogenized cross sections to multi-group cross sections can be evaluated as following:

$$S_{R,\sigma} = \frac{\mathrm{d}R/R}{\mathrm{d}\sigma/\sigma} = \sigma \frac{\langle (\mathrm{d}\boldsymbol{\Sigma}_x/\mathrm{d}\sigma) \,\Phi \rangle}{\langle \boldsymbol{\Sigma}_x \Phi \rangle} - \sigma \left\langle \boldsymbol{\Gamma}^* \frac{\mathrm{d}\boldsymbol{M}}{\mathrm{d}\sigma} \Phi \right\rangle$$
(11)

where σ is a specific multi-group cross section. *R* will represent arbitrary response which has the Equation (1) form hereinafter for simplification.

It should be noted that the sensitivity-coefficients obtained above are direct effects of the multi-group cross sections on the responses during the solution of multi-group neutron transport equation. However, resonance calculation is necessary before multi-group neutron transport calculation is performed. When continuous-energy cross sections are treated as the perturbation sources, the perturbation will influence the responses through resonance calculation indirectly, which is called implicit sensitivity [6]. Therefore, the total sensitivity-coefficient of the response R to the continuous-energy cross section can be expressed as follows:

$$S_{R,\alpha_{\omega,Eg}^{(k)}}^{\text{tot}} = \frac{\alpha_{\omega,Eg}^{(k)}}{R} \frac{\mathrm{d}R}{\mathrm{d}\alpha_{\omega,Eg}^{(k)}} = \frac{\alpha_{\omega,Eg}^{(k)}}{R} \sum_{x,g'} \frac{\partial R}{\partial \sigma_{x,g'}^{(k)}} \frac{\mathrm{d}\sigma_{x,g'}^{(k)}}{\mathrm{d}\alpha_{\omega,Eg}^{(k)}} \\ + \frac{\alpha_{\omega,Eg}^{(k)}}{R} \sum_{\substack{j,y,h \\ j \neq k}} \frac{\partial R}{\partial \sigma_{y,h}^{(j)}} \sum_{x,g'} \frac{\partial \sigma_{y,h}^{(j)}}{\partial \sigma_{x,g'}^{(k)}} \frac{\mathrm{d}\sigma_{x,g'}^{(k)}}{\mathrm{d}\alpha_{\omega,Eg}^{(k)}} \\ = \sum_{x,g'} S_{R,\sigma_{x,g'}^{(k)}}^{\exp} S_{\sigma_{x,g'}^{(k)},\alpha_{\omega,Eg}^{(k)}} \\ + \sum_{\substack{j,y,h \\ j \neq k}} S_{R,\sigma_{y,h}^{(k)}}^{\exp} \sum_{x,g'} S_{\sigma_{y,h}^{(j)},\sigma_{x,g'}^{(k)}} S_{\sigma_{x,g'}^{(k)},\alpha_{\omega,Eg}^{(k)}} \\ \end{cases}$$
(12)

where *x*, *y*, and ω are reaction indexes; *k* and *j* are nuclide indexes; *g*', *g*, and *h* are group indexes; α is the continuous-energy cross section; σ is the corresponding multi-group cross section; α with subscript *Eg* means the continuous-energy cross section in energy range of the *g*th energy group; $S_{R,\alpha}^{\text{tot}}$ is called total sensitivity-coefficient; $S_{R,\sigma}^{\text{exp}}$ is called explicit sensitivity-coefficient of *R* to the multi-group cross section σ ; $S_{\sigma_{x,g'}^{(j)},\sigma_{x,g'}^{(k)}}$ is the sensitivity-coefficient of the effective self-shielding cross section of nuclide *j* to the multi-group cross section $\sigma_{x,g'}^{(k)}$, and $S_{\sigma_{x,g'}^{(k)},\alpha_{\omega,Eg}}^{(k)}$ is the sensitivity-coefficient of the sensitivity-coefficient of nuclide *j* to the multi-group cross section $\sigma_{x,g'}^{(k)}$, and $S_{\sigma_{x,g'}^{(k)},\alpha_{\omega,Eg}}^{(k)}$ is the sensitivity-coefficient of the sensitivity-coefficient of $\sigma_{x,g'}^{(k)}$, and $S_{\sigma_{x,g'}^{(k)},\alpha_{\omega,Eg}}^{(k)}$.

Assuming that the effect of the continuous-energy cross section $\alpha_{\omega,Eg}^{(k)}$ on the multi-group cross sections of other energy groups is negligibly small, Equation (12) can be simplified as

$$S_{R,\alpha_{\omega,Eg}^{(k)}}^{\text{tot}} = \sum_{x} S_{R,\sigma_{x,g}^{(k)}}^{\exp} S_{\sigma_{x,g}^{(k)}} S_{\sigma_{x,g}^{(k)},\alpha_{\omega,Eg}^{(k)}} + \sum_{\substack{j, y, h \\ j \neq k}} S_{R,\sigma_{y,h}^{(j)}}^{\exp} \sum_{x} S_{\sigma_{y,h}^{(j)},\sigma_{x,g}^{(k)}} S_{\sigma_{x,g}^{(k)},\alpha_{\omega,Eg}^{(k)}}$$
(13)

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For resonance nuclides, the relationship between $\sigma_{x,g}^{(k)}$ and $\alpha_{\omega,Eg}^{(k)}$ is complicated because of the selfshielding phenomenon. $S_{\sigma_{x,g}^{(k)},\alpha_{\omega,Eg}^{(k)}}$ needs to be calculated, and $S_{\sigma_{y,h}^{(j)},\sigma_{x,g}^{(k)}}$ is also needed when resonance nuclide k participates in the resonance calculation process of other resonance nuclide j. However, for non-resonance nuclides, the multi-group cross section is always supposed to have a linear relationship with its continuousenergy cross section, because the weighting flux used to condense multi-group cross section is independent of the cross sections. Consequently, $S_{\sigma_{x,g}^{(k)},\alpha_{\omega,Eg}^{(k)}}$ is equal to 1.0 if reaction x is the same as reaction ω . If the selfshielding impact is neglected, the sensitivity-coefficient can be expressed as

$$S_{R,\alpha_{\omega,Eg}}^{\text{tot}} = S_{R,\sigma_{\omega,g}}^{\exp}$$
(14)

which can be calculated by Equation (11) directly.

According to the analysis above, the implicit sensitivity is indirectly aroused because of the resonance calculation. Consequently, it can be seen from Equation (13) that the key point to consider the implicit sensitivity is to obtain two terms. One is the sensitivity-coefficient of effective self-shielding cross section with respect to the continuous-energy cross section, $S_{\sigma_{x,g}^{(k)},\alpha_{x,Eg}^{(k)}}$, and the other one is the sensitivity-coefficient of effective selfshielding cross section with respect to that of other nuclide, $S_{\sigma_{y,h}^{(j)},\sigma_{x,g}^{(k)}}$.

2.1.2. Sensitivity calculation for effective self-shielding cross sections

The widely used subgroup resonance calculation method is applied in this paper, and the following derivation will be performed based on this method. Resonance cross section is divided into several bands (subgroups) from its minimum value to its maximum value in the subgroup resonance calculation method, which is shown in Figure 1 [9]. Each subgroup has the corresponding subgroup cross section and probability (collectively called subgroup parameters) defined as

$$\sigma_{x,g,i} = \frac{\int_{\Delta E_{g,i}} \sigma_x(E) \phi(E) dE}{\int_{\Delta E_{g,i}} \phi(E) dE}$$
(15)

$$p_{g,i} = \frac{\Delta E_{g,i}}{\Delta E_g} \tag{16}$$

where the subscript *i* stands for subgroup index; ΔE_g is the energy width of group *g*; $\Delta E_{g,i}$ is the energy range of the *i*th subgroup cross section, which is defined as $\Delta E_{g,i} \in \{E | \sigma_{g,i} < \sigma(E) \le \sigma_{g,i+1}\}.$

For the subgroup resonance calculation method, the resonance cross-sectional tables are built based on the continuous-energy cross sections. Subsequently, the subgroup parameters are calculated based on the resonance cross-sectional tables. And then the effective selfshielding cross section is defined as

$$\sigma_{x,g}\left(\boldsymbol{r}\right) = \frac{\sum\limits_{i=1,I} \sigma_{x,g,i}\left(\boldsymbol{r}\right)\phi_{g,i}\left(\boldsymbol{r}\right)}{\sum\limits_{i=1,I} \phi_{g,i}\left(\boldsymbol{r}\right)}$$
(17)

where *I* is the number of subgroup, and the weighting function of each subgroup, $\phi_{g,i}(\mathbf{r})$, is the solution of subgroup transport equation, which is the integration of the continuous-energy Boltzmann transport equation over a subgroup, as defined as follows:

$$\mathbf{\Omega} \cdot \nabla \phi_{g,i}(\mathbf{r}, \mathbf{\Omega}) + \mathbf{\Sigma}_{\mathrm{t},g,i}(\mathbf{r}) \phi_{g,i}(\mathbf{r}, \mathbf{\Omega}) = Q_{g,i}(\mathbf{r}, \mathbf{\Omega})$$
(18)

where the subgroup total cross section is given as

$$\boldsymbol{\Sigma}_{\mathsf{t},g,i} = N_a \sigma^a_{\mathsf{t},g,i} + \sum_{b \neq a} N_b \sigma^b_{\mathsf{t},g} \tag{19}$$

where *a* indicates the resonance nuclide that is performed resonance calculation currently, and *b* indicates the other nuclides, and N_a and N_b are the corresponding nuclide density. It can be found that for nuclide *b*, the subgroup cross sections for each band are just the multi-group cross sections.

In this study, $Q_{g,i}$ is equal to $\lambda p_i \Sigma_p$ based on intermediate resonance approximation. λ is the Goldstein– Cohen factor and Σ_p is the potential scattering cross section.

The corresponding operator form of Equation (18) is

$$L_g \phi_g = Q_g \tag{20}$$

The expression of Equation (17) is analogous to Equation (1), so it is easy to apply the GPT-based method to obtain effective self-shielding cross-sectional sensitivity-coefficients.

First, the generalized adjoint subgroup transport equation should be built

$$L_g^* \Gamma_g^* = Q_g^* \tag{21}$$

where L_g^* is the adjoint operator of L_g ; Q_g^* is the generalized adjoint source:

$$Q_{g,i}^{*} = \frac{\sigma_{x,g,i}}{\sum_{i=1,I} \int_{V} \int_{\Omega} \sigma_{x,g,i} \phi_{g,i}(\boldsymbol{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega} dV} - \frac{1}{\sum_{i=1,I} \int_{V} \int_{\Omega} \phi_{g,i}(\boldsymbol{r}, \boldsymbol{\Omega}) d\boldsymbol{\Omega} dV}$$
(22)

Then, the sensitivity-coefficient of the effective selfshielding cross section to the continuous-energy cross section can be expressed as follows according to the



Figure 1. Definition of subgroups in a broad energy group.

analogous Equation (11).

$$S_{\sigma_{xg},\alpha} = \alpha \left(\frac{\sum\limits_{i=1,I} \frac{\mathrm{d}\sigma_{x,g,i}}{\mathrm{d}\alpha} \phi_{g,i}}{\sum\limits_{i=1,I} \sigma_{x,g,i} \phi_{g,i}} - \left\langle \mathbf{\Gamma}_{x,g}^*, \left(\frac{\mathrm{d}L}{\mathrm{d}\alpha} \phi_g - \frac{\mathrm{d}Q_g}{\mathrm{d}\alpha} \right) \right\rangle \right)$$
$$= \frac{\sum\limits_{i=1,I} \sigma_{x,g,i} S_{\sigma_{x,g,i},\alpha} \phi_{g,i}}{\sum\limits_{i=1,I} \sigma_{x,g,i} \phi_{g,i}}$$
$$+ \sum\limits_{i=1,I} \int_V \int_{\mathbf{\Omega}} \mathbf{\Gamma}_{x,g,i}^* \left(Q_{g,i} S_{Q_{g,i},\alpha} - \alpha \frac{\mathrm{d}L}{\mathrm{d}\alpha} \phi_{g,i} \right) \mathrm{d}\mathbf{\Omega} \mathrm{d} \mathrm{V}$$
(23)

where $S_{\sigma_{x,g,i},\alpha}$ is the sensitivity-coefficient of the subgroup cross section to the continuous-energy cross section; $S_{Q_{g,i},\alpha}$ is the sensitivity-coefficient of the source term to the continuous-energy cross section. Because the source term is linearly dependent on the subgroup probability, $S_{Q_{g,i},\alpha}$ is equal to $S_{p_{g,i},\alpha}$.

There are two terms on the right side of Equation (23). The first one is the direct term, which accounts for the effect of the continuous-energy cross section α on the subgroup parameters directly. Only when α belongs to the same resonance nuclide as $\sigma_{x,g}$ will the direct term be non-zero. The second one is the indirect term, which accounts for the effect on the effective self-shielding multi-group cross section due to

the perturbation of weighting function (subgroup flux) caused by the change in continuous-energy cross section α . It should be noted that it is different compared to the conventional resonance calculation method. First, the subgroup parameters are used in the solving process of weighting flux. Therefore, the sensitivitycoefficients of effective self-shielding cross sections to subgroup parameters will be calculated by GPT first. And then the sensitivity-coefficients of effective selfshielding cross sections to continuous-energy cross sections can be calculated by combining the subgroupparameter sensitivity-coefficients. Second, for subgroup resonance calculation method, the effective selfshielding cross sections are region-dependent; therefore, the sensitivity-coefficients should be solved for each resonance region.

When α is not the cross section of the resonance nuclide involved in the current resonance calculation, the corresponding multi-group cross sections will participate in the resonance calculation according to Equation (19). Therefore, the sensitivity-coefficient of the effective self-shielding cross section with respect to the multi-group cross section can be obtained in this process, which are corresponding to the term $S_{\sigma_{xg}^{(k)},\sigma_{yh}^{(j)}}$ in Equation (13) and can be found in the previous study [11].

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When α is the cross section of the resonance nuclide involved in the current resonance calculation, the sensitivity-coefficient of the subgroup parameter to the continuous-energy cross section, $S_{\sigma_{x,g,i},\alpha}$ as shown in Equation (23), needs to be calculated.

2.1.3. Sensitivity calculation for subgroup parameter Several methods for subgroup-parameter generation have been studied and applied [15–16]. The fitting method [17–18] is employed for subgroup-parameter generation in this paper. The calculation is based on the resonance cross-sectional tables, which include the multi-group resonance cross sections under specific background cross section given as

$$\sigma_{x,g}(\sigma_b) = \frac{\int_{\Delta E_g} \sigma_x(E) \phi(E, \sigma_b) dE}{\int_{\Delta E_g} \phi(E, \sigma_b) dE}$$
(24)

where ΔE_g is the energy range of the *g*th group, and σ_b is the background cross section. $\phi(E, \sigma_b)$ is the weighting flux which is obtained with a continuous-energy method or a hyper-fine energy-group method.

The perturbation of the continuous-energy cross sections (point-wise cross sections) will affect both the cross sections and the weighting flux. As a result, the resonance cross-sectional tables and the subgroup parameters will be affected subsequently. The DP method can be used to obtain subgroup-parameter sensitivity-coefficients by perturbing the continuousenergy cross sections before the generation of resonance cross-sectional tables. Linear perturbation may be used approximately for the generation of the resonance cross-sectional tables if the weighting flux is deemed intact. The perturbed multi-group resonance cross section can be described as Equation (25) under this assumption:

$$\sigma_{x,g}'(\sigma_b) = \frac{\int_{\Delta E_g} (1 + \delta_x) \,\sigma_x(E) \,\phi(E, \sigma_b) \,dE}{\int_{\Delta E_g} \phi(E, \sigma_b) \,dE}$$
$$\approx (1 + \delta_x) \,\sigma_{x,g}(\sigma_b) \tag{25}$$

where δ_x is relative perturbation percent.

However, linear approximation may result in large errors when the weighting flux is closely related to the perturbation. The narrow resonance (NR) approximation was proposed in some previous studies [19–20]. The multi-group resonance cross section can be written as Equation (26) when the weighting flux is treated through the NR approximation:

$$\sigma_{x,g}(\sigma_b) = \frac{\int_{\Delta E_g} \frac{\sigma_x(E)}{\sigma_t(E) + \sigma_b} \frac{1}{E} dE}{\int_{\Delta E_g} \frac{1}{\sigma_t(E) + \sigma_b} \frac{1}{E} dE} = \frac{\int_{\Delta E_\mu} \frac{\sigma_x(\mu)}{\sigma_t(\mu) + \sigma_b} d\mu}{\int_{\Delta E_\mu} \frac{1}{\sigma_t(\mu) + \sigma_b} d\mu} (26)$$

When the continuous-energy cross sections have a relative perturbation of δ_x , the perturbed multi-group

resonance cross section can be given as

$$\sigma_{x,g}'(\sigma_b) = \frac{\int_{\Delta E_{\mu}} \frac{(1+\delta_x)\sigma_x(\mu)}{(1+\delta_t)\sigma_t(\mu)+\sigma_b} d\mu}{\int_{\Delta E_{\mu}} \frac{1}{(1+\delta_t)\sigma_t(\mu)+\sigma_b} d\mu}$$
$$= (1+\delta_x) \frac{\int_{\Delta E_{\mu}} \frac{\sigma_x(\mu)}{\sigma_t(\mu)+\sigma_b/(1+\delta_t)} d\mu}{\int_{\Delta E_{\mu}} \frac{1}{\sigma_t(\mu)+\sigma_b/(1+\delta_t)} d\mu}$$
$$= (1+\delta_x) \sigma_{x,g}(\sigma_b')$$
(27)

where $\sigma'_b = \sigma_b/(1 + \delta_t)$ and δ_t is the relative perturbation of $\sigma_t(\mu)$ for cross-sectional self-consistency when $\sigma_x(\mu)$ is perturbed. Equation (27) indicates that the perturbed multi-group resonance cross section obtained with the NR approximation is smaller than the value obtained with linear perturbation in case of $\delta_t > 0$ and $\delta_x > 0$ because the value of σ'_b is smaller than that of σ_b , which leads to the fact that the value of $\sigma_{x,g}(\sigma'_b)$ is smaller than that of $\sigma_{x,g}(\sigma_b)$. And when $\delta_t < 0$ and δ_x < 0, the situation is opposite.

This method, however, is valid only when the NR approximation is well satisfied. Therefore, a more accurate method is proposed in this paper as follows. The hyper-fine energy-group method is used to solve a neutron slowing-down equation for an infinite-homogeneous medium to generate the resonance cross-sectional tables in this study. The neutron slowing-down equation for an infinite-homogeneous medium is defined as [21]

$$\left[\boldsymbol{\Sigma}_{a}\left(E\right) + \boldsymbol{\Sigma}_{s}\left(E\right)\right]\phi\left(E\right) = Q_{s}$$
(28)

The point-wise cross sections within a specified energy group can be perturbed in the equation-solving process to capture the effect on the weighting flux to obtain the accurate perturbation of multi-group resonance cross sections. Then, the DP method can be applied to obtain the resonance cross-sectional sensitivity-coefficients with respect to the point-wise cross sections, which can be described as Equation (29):

$$S_{R,\beta} = \frac{\beta}{R} \frac{\mathrm{d}R}{\mathrm{d}\beta} = \frac{\beta}{R^0} \frac{\Delta R}{\Delta \beta}$$
(29)

where R^0 is the unperturbed response; β is a given input parameter; and ΔR and $\Delta \beta$ are the corresponding perturbed amount. In this specific case, R is the resonance cross section of a specified energy group and β is the point-wise cross section within this energy group.

It should be pointed out that an assumption is made that the continuous-energy cross sections (point-wise cross sections) are perturbed uniformly within the energy group to be perturbed. Uniform perturbation can obtain the resonance cross-sectional sensitivitycoefficients to all point-wise cross sections in this energy group and avoid the point-by-point calculation of the sensitivity-coefficients. Therefore, the resonance cross-section sensitivity-coefficients describe the relative perturbation of resonance multi-group cross sections with respect to the point-wise cross sections that are perturbed uniformly in the same energy group.

After the resonance cross-section sensitivitycoefficients are obtained, the perturbed subgroup parameters can be calculated subsequently. The DP method can be adopted to calculate the subgroupparameter sensitivity-coefficients with Equation (29).

2.2. Uncertainty calculation

The first moments of nuclear-data probability distributions were given in the early versions of evaluated nuclear-data libraries. With an increasing demand on the S&U analysis, the additional second moments of nuclear-data probability distributions were included starting from ENDF/B-IV [7]. The second moments, also called covariances, describe the information about the uncertainties of nuclear data and the correlations between them. The response uncertainties can be determined by combining the sensitivity-coefficients with the covariance. Suppose there is an approximate linear relationship between the response and the nuclear data:

$$R \approx R_0 + \sum_{n_1} \frac{\mathrm{d}R}{\mathrm{d}\alpha_{n_1}} \delta\alpha_{n_1} \tag{30}$$

The covariance between responses R_m and R_n can be computed using the identity:

$$\operatorname{cov}\left(R_{m}, R_{n}\right) \approx \sum_{n_{1}=1}^{NT} \sum_{n_{2}=1}^{NT} \left(\frac{\mathrm{d}R_{m}}{\mathrm{d}\alpha_{n_{1}}}\right) \operatorname{cov}\left(\alpha_{n_{1}}, \alpha_{n_{2}}\right) \left(\frac{\mathrm{d}R_{n}}{\mathrm{d}\alpha_{n_{2}}}\right)$$
(31)

where *m* and *n* are response indexes; $cov(\alpha_{n_1}, \alpha_{n_2})$ is the covariance between input parameters α_{n_1} and α_{n_2} . It is called the first-order uncertainty propagation formula.

Dividing the two sides of Equation (31) by the square of *R*, the first-order uncertainty propagation formula can be expressed in operator form:

$$\operatorname{rcov}(\mathbf{R}) \approx \mathbf{S}\mathbf{C}\mathbf{S}^{T}$$
 (32)

where rcov(R) is the relative covariance of the responses; *S* is the relative sensitivity-coefficient matrix; and *C* is the relative covariance of nuclear data.

3. Computational procedure

Based on the method proposed above, a code name COLEUS has been developed. The calculation flow chart is given in Figure 2. First, the resonance crosssectional sensitivity-coefficients are calculated based on the DP method off-line and the data are saved in the form of database for subsequent use. Second, in the calculation process of subgroup parameters, the DP method is applied to calculate the



Figure 2. The calculation flowchart for COLEUS.

subgroup-parameter sensitivity-coefficients. Third, the sensitivity-coefficients of the effective self-shielding cross section are calculated during the iteration process of subgroup resonance calculation. Fourth, a generalized adjoint neutron transport equation is solved for each type of response and the corresponding sensitivity-coefficients can be calculated. Finally, the uncertainty analysis is performed based on the firstorder uncertainty propagation formula.

4. Numerical results and discussions

Verification has been performed for COLEUS based on a BWR pin-cell case named PB-2 under different power conditions from the UAM benchmark [1]. One is under hot zero power (HZP) condition and the other one is under hot full power (HFP) condition. The calculations are carried out using the WIMS-D 69-group library based on ENDF/B-VII data, and the resonance energy groups are from the 15th group (5530.0–9118.0 eV) to the 27th group (4.0–9.877 eV). The covariance data library is created using NJOY [7] based on ENDF/B-VII.1 data. The S&U analysis for eigenvalue and two-group spatially homogenized cross sections are performed. The energy range of the first



Figure 3. The sensitivity-coefficients of resonance cross sections with respect to continuous-energy cross sections at different background cross sections.

group (fast group) is from 0.625 eV to 1.0×10^7 eV and the second group (thermal group) is from $1.0 \times 10-5$ eV to 0.625 eV.

4.1. Resonance cross-sectional sensitivity-coefficients

As described in Section 2, the DP method based on the hyper-fine energy-group method instead of the NR approximation and linear approximation is applied to obtain the resonance cross-sectional sensitivitycoefficients. In order to investigate the improvement, the comparisons of resonance cross-sectional sensitivity-coefficients calculated with three different methods at different background cross sections are given in Figure 3.

As shown in Figure 3, the sensitivity-coefficients of NR approximation and linear approximation have a good agreement with that of hyper-fine method at high energy groups (e.g. the 15th group (5530.0–9118.0 eV) and the 18th group (1425.1-2239.4 eV)), because the resonance peak at high energy can be well described by NR approximation, and linear approximation is also acceptable. On the other hand, good agreement can be also found at large background cross sections because the weighting flux will be affected decreasingly along with the increase of background cross section. However, large differences can be found within low-energy range (the 27th group (4.0-9.877 eV)) where the NR approximation is not well satisfied. The NR approximation or linear approximation will overestimate the resonance cross-sectional sensitivity-coefficients. Therefore, the sensitivity-coefficients can be improved by the proposed method.

4.2. Response sensitivity-coefficient verification and analysis

The DP method is considered as the reference method for response sensitivity-coefficient verification for the GPT-based method (GPT) used in this study. Because the implicit effect mainly occurs in the resonance energy-groups, the resonance energy-group regionintegrated relative total sensitivity-coefficients of some important responses calculated by those two methods are given and compared in Figures 4 and 5, and the explicit sensitivity-coefficients are given and compared in Figures 6 and 7. The subscript '1' stands for the first group (fast group) and '1-2' means the first to second group scattering. It can be found in the figures that the results of the GPT-based method agree well with the reference results. It proves the correctness of the proposed method.

Figures 8 and 9 give the comparisons of total sensitivity-coefficients and explicit sensitivitycoefficients under HZP and HFP conditions. It can be found that the proposed method can improve the response sensitivity-coefficients in different extents. For non-resonance nuclides such as ¹H, the positive perturbation of cross sections will always increase the resonance cross sections because of the fact that the resonance cross sections are monotonously increasing with the background cross-sectional increase. This phenomenon will lead to the negative implicit sensitivitycoefficients of $k_{\rm eff}$ in the ²³⁸U-dominated problem, where the resonance absorption is the dominated resonance reaction. Therefore, it can be found in Figure 8(a) that the explicit sensitivity-coefficients are always larger than total sensitivity-coefficients, which means that the explicit sensitivity-coefficients will overestimate the k_{eff} sensitivity-coefficients to non-resonance nuclides in such problems. Things are more complicated in the few-group parameters. First, the positive perturbation of σ_{elas} of ¹H will decrease the neutron in this energy group, which may decrease the corresponding few-group cross sections. On the other hand, the perturbation will increase the cross section itself and the resonance cross sections, which may increase the corresponding few-group cross sections. Consequently, the few-group cross-sectional sensitivity-coefficients are determined by those two terms. Positive implicit



Figure 4. The total sensitivity-coefficients of some important responses calculated by DP and GPT methods for PB-2 HZP case.



Figure 5. The total sensitivity-coefficients of some important responses calculated by DP and GPT methods for PB-2 HFP case.



Figure 6. The explicit sensitivity-coefficients of some important responses calculated by DP and GPT methods for PB-2 HZP case.



Figure 7. The explicit sensitivity-coefficients of some important responses calculated by DP and GPT methods for PB-2 HFP case.



Figure 8. The comparison of sensitivity-coefficients for σ_{elas} of ¹H.



Figure 9. The comparison of sensitivity-coefficients for σ_{ν} of ²³⁸U.



Figure 10. The relative covariance matrix and relative standard deviation of responses of PB-2 HZP case.

sensitivity can be found in Figure 8(b) while negative implicit sensitivity can be found in Figure 8(c,d) on the contrary.

For resonance nuclides such as ²³⁸U, the sensitivitycoefficients are also improved considerably, especially in the low-energy groups. Because the explicit sensitivity is approximated equivalent to the linear perturbation of continuous-energy cross section, which can be deduced from Equation (12) if the secondterm is deemed small, the resonance cross-sectional sensitivity-coefficients will be overestimated in this situation as demonstrated in Section 4.1. Therefore, smaller response total sensitivity-coefficients (absolute value) can be found in Figure 9 (a-d) for this reason if the proposed method is used.

4.3. Uncertainty analysis

The relative covariance matrices and relative standard deviations of different responses of PB-2 HZP case and HFP case are presented in Figures 10 and 11. It can be seen that the eigenvalue uncertainties are about 0.5%–0.6% for both the HZP case and the HFP case. Some uncertainties of few-group homogenized cross sections are more than 1%, such as the capture cross sections of both the first group and the second group

and the scattering cross sections of the first group. Considerable covariance can be found between different few-group homogenized cross sections. This phenomenon is caused by the fact that the different responses are impacted by the same nuclear data in the lattice-physics calculation. Therefore, it is necessary to take the covariance into account in the core S&U analysis.

In addition, interesting results can also be found. First, the fast-group homogenized cross-sectional uncertainties are usually larger than those of thermal group. Second, the uncertainties of the HFP case are larger than those of the HZP case generally. In order to investigate the reasons, the five most significant uncertainty contributors are listed in Tables 1-4 for some important responses. It can be found that uncertainty contributors vary for different responses. However, the σ_{γ} and σ_{inel} of ²³⁸U are very important uncertainty contributors for most responses and become more important in the HFP case. Although the inelastic scattering reaction is a threshold energy reaction in fast-group, the uncertainty contributions are considerable to most responses. This is one of the reasons why the fast-group homogenized cross-sectional uncertainties are usually larger.

As an example, Figure 12 gives the sensitivitycoefficients of Σ_{s1-2} to σ_{γ} and σ_{inel} of ²³⁸U and the



Figure 11. The relative covariance matrix and relative standard deviation of responses of PB-2 HFP case.

PB-2 HFP cases. PB-2 HZP PB-2 HFP Contribution to $\Delta R/R(\%)$ Cross-sectional pair Contribution to $\Delta R/R(\%)$ Cross-sectional pair $^{238}U(\sigma_{\gamma}-\sigma_{\gamma})$ 238 U(σ_{γ} - σ_{γ}) 0.343 0.421 ${}^{235}U(\sigma_{\gamma}^{\gamma}-\sigma_{\gamma}^{\prime})$ ${}^{1}H(\sigma_{\gamma}-\sigma_{\gamma})$ $\frac{^{238}\mathsf{U}(\sigma_{\text{inel}}^{\gamma}-\sigma_{\text{inel}}^{r})}{^{235}\mathsf{U}(\sigma_{\gamma}-\sigma_{\gamma})}$ 0.178 0.269 0.147 0.185 0.121 0.136

Table 1. The five most significant uncertainty contributors for $k_{\rm eff}$ in the PB-2 HZP and





Figure 12. The relative standard derivation and sensitivitycoefficients of σ_{γ} and σ_{inel} .

relative standard deviations of these cross sections. It can be seen that the uncertainties and the sensitivitycoefficients of inelastic scattering reaction are considerable, causing a significant uncertainty contribution.

The sensitivity-coefficients in HFP case are larger than these in HZP case within the fast energy range. The main reason is the temperature effect. HFP leads to

a 40% coolant void in BWR, causing a hardening of the neutron-flux spectrum relative to HZP. The sensitivitycoefficients of fast energy groups will increase consequently as shown in Figure 12, causing a larger uncertainty contribution concomitantly. This phenomenon is especially reflected in the behaviors of σ_{inel} of 238 U for all responses. It should be pointed out that the inelastic scattering reaction is a threshold reaction, so the sensitivity-coefficients and standard deviation value are zero below the threshold energy $(4.085 \times 10^4 \text{ eV})$. Consequently, the relative standard deviation of σ_{inel} is cutoff in the logarithmic coordinate in Figure 12.

5. Summaries and conclusions

A new hybrid method is proposed to perform the S&U analysis of the lattice-physics calculation based on continuous-energy cross sections for eigenvalue and few-group homogenized cross sections. The sensitivity analysis can be performed for responses with respect to continuous-energy cross sections to take the implicit effect into account with the subgroup resonance calculation method.

Table 2. The five most significant uncertainty contributors Σ_{c1} in the PB-2 HZP and PB-2 HFP cases.

PB-2 HZP		PB-2 HFP	
Cross-sectional pair	Contribution to $\Delta R/R(\%)$	Cross-sectional pair	Contribution to $\Delta R/R(\%)$
238 U($\sigma_{\text{inel}} - \sigma_{\text{inel}}$)	1.000	238 U($\sigma_{\text{inel}} - \sigma_{\text{inel}}$)	1.210
$^{238}U(\sigma_{v}-\sigma_{v})$	0.693	$^{238}U(\sigma_{\nu}-\sigma_{\nu})$	0.672
$^{1}H(\sigma_{elas} - \sigma_{elas})$	0.293	$^{1}H(\sigma_{elas} - \sigma_{elas})$	0.265
$^{235}U(\sigma_{y}-\sigma_{y})$	0.237	$^{235}U(\sigma_{1} - \sigma_{1})$	0.246
$^{16}O(\sigma_{elas}^{r}-\sigma_{elas}^{r})$	0.104	$^{16}O(\sigma_{elas}^{r}-\sigma_{elas}^{r})$	0.121

Table 3. The five most significant uncertainty contributors $\upsilon \Sigma_{\mathrm{fl}}$ in the PB-2 HZP and PB-2 HFP cases.

PB-2 HZP		PB-2 HFP		
Cross-sectional pair	Contribution to $\Delta R/R(\%)$	Cross-sectional pair	Contribution to $\Delta R/R(\%)$	
238 U(σ_{inel} - σ_{inel})	0.469	238 U(σ_{inel} - σ_{inel})	0.596	
$^{238}U(\nu - \nu)$	0.395	$^{238}U(\nu - \nu)$	0.374	
235 U(σ_{f} - σ_{f})	0.225	235 U(σ_{f} - σ_{f})	0.227	
238 U(σ_{f} - σ_{f})	0.172	238 U(σ_{f} - σ_{f})	0.162	
$^{235}U(\nu-\nu)$	0.954	238 U(σ_{γ} - σ_{γ})	0.113	

PB-2 HZP		PB-2 HFP		
Cross-sectional pair	Contribution to $\Delta R/R(\%)$	Cross-sectional pair	Contribution to $\Delta R/R(\%)$	
$\begin{array}{c} ^{238} \mathrm{U}(\sigma_{\mathrm{inel}} - \sigma_{\mathrm{inel}}) \\ ^{1}\mathrm{H}(\sigma_{\mathrm{elas}} - \sigma_{\mathrm{elas}}) \\ ^{238} \mathrm{U}(\sigma_{\gamma} - \sigma_{\gamma}) \\ ^{16}\mathrm{O}(\sigma_{\mathrm{elas}} - \sigma_{\mathrm{elas}}) \\ ^{235} \mathrm{U}(\sigma_{\gamma} - \sigma_{\gamma}) \end{array}$	1.080 0.629 0.177 0.062 0.045	$\begin{array}{c} ^{238} \mathrm{U}(\sigma_{\mathrm{inel}}-\sigma_{\mathrm{inel}}) \\ ^{1}\mathrm{H}(\sigma_{\mathrm{elas}}-\sigma_{\mathrm{elas}}) \\ ^{238} \mathrm{U}(\sigma_{\gamma}-\sigma_{\gamma}) \\ ^{16}\mathrm{O}(\sigma_{\mathrm{elas}}-\sigma_{\mathrm{elas}}) \\ ^{235} \mathrm{U}(\sigma_{\gamma}-\sigma_{\gamma}) \end{array}$	1.310 0.614 0.277 0.078 0.072	

Table 4. The five most significant uncertainty contributors Σ_{s1-2} in the PB-2 HZP and PB-2 HFP cases.

The total sensitivity-coefficients of eigenvalue and few-group homogenized cross section calculated by the proposed method have good agreements with those given by the DP method, which is considered as the reference method. The errors introduced by linear approximation and NR approximation for the calculations of the resonance cross-sectional sensitivity-coefficients were investigated. The sensitivity-coefficients can be considerably improved especially in the low-energy resonance groups and at low background cross sections. Response sensitivity analysis shows that sensitivitycoefficients will be overestimated in most cases if the resonance self-shielding effects are not taken into account except for some special cases.

The uncertainties of eigenvalue and few-group homogenized cross sections are quantified based on the covariance data from ENDF/B-VII.1. The uncertainties of some few-group homogenized cross sections are more than 1.0%, such as the capture cross sections and the scattering cross sections of the fast group, etc. The uncertainties of the fast-group homogenized cross sections are larger than those of the thermal group as a whole. Moreover, the fast-group cross-sectional uncertainty contributions become larger with the increase of temperature, which is caused by the hardening neutronflux spectrum at the HFP condition for the BWR pincell problem.

In summary, this paper assesses the S&U of lattice parameters based on continuous-energy cross sections for both accuracy and consistency with the subgroup resonance calculation method. Future work should perform core calculation S&U analysis based on the improved S&U results of few-group homogenized cross sections. The GPT-based method can be used for sensitivity calculation of the core responses, such as k_{eff} , power distribution, assembly reaction rate, reactivity worth, and then the covariance data can be used by the first-order uncertainty propagation formula to perform uncertainty calculation. The statistical sampling method [20] can be also used for uncertainty calculation through sampling the few-group homogenized cross sections according to the covariance data. When burnup is considered, the two-step calculation procedure may be difficult to treat the effects [22,23]. Appropriate algorithm or approximation may be developed in the future work.

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