

## Implementation of Generalized Adjoint Equation Solver for DeCART

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### 1. Introduction

Recently, MUSAD (Modules of Uncertainty and Sensitivity Analysis for DeCART) was developed for the uncertainty analysis of PMR200 core [1] and the fundamental adjoint solver was implemented into DeCART [2]. However, the application of the code was limited to the uncertainty to the multiplication factor, keff, because it was based on the classical perturbation theory. For the uncertainty analysis to the general response as like the power density, it is necessary to develop the analysis module based on the generalized perturbation theory and it needs the generalized adjoint solutions from DeCART.

In this paper, the generalized adjoint solver is implemented on DeCART and the calculation results are compared with the results by TSUNAMI of SCALE 6.1 [3].

### 2. Methods and Results

The general response is commonly expressed as the following.

$$R = \frac{\langle H_1(\alpha)\phi(\alpha) \rangle}{\langle H_2(\alpha)\phi(\alpha) \rangle} \quad (1)$$

Here,  $\alpha$  is an input parameter and  $H_1$  and  $H_2$  are response functions as like the cross sections. Eq.(1) can represent the various core parameters according to the response functions. Thus, the sensitivity of the response [1] to an input parameter can be presented as

$$S_{R,\alpha} = \frac{\delta R}{\delta \alpha} \quad (2)$$

The generalized perturbation theory can describe the sensitivity without directly obtaining the solutions of the perturbed state. It can be achieved using the solution of the generalized adjoint equation which must be obtained from DeCART.

In the next sections, the formulations for setting the generalized adjoint equation based on the generalized perturbation theory are described and then the scheme for the numerical solution of the equation in DeCART is presented in the section 2.3.

#### 2.1 Generalized Perturbation Theory

Neglecting over the second order term, the small perturbation of the general response, Eq.(1), can be approximated as the following

$$\delta R \cong \left\langle \left( \frac{\partial R}{\partial H_1} \frac{\partial H_1}{\partial \alpha} + \frac{\partial R}{\partial H_2} \frac{\partial H_2}{\partial \alpha} + \frac{\partial R}{\partial \phi} \frac{\partial \phi}{\partial \alpha} \right) \delta \alpha \right\rangle \quad (3)$$

Using the definition of the general response, Eq.(1), Eq.(3) can be rewritten as

$$\frac{\delta R}{R} \cong \frac{\langle \delta H_1 \phi \rangle}{\langle H_1 \phi \rangle} - \frac{\langle \delta H_2 \phi \rangle}{\langle H_2 \phi \rangle} + \frac{\langle H_1 \delta \phi \rangle}{\langle H_1 \phi \rangle} - \frac{\langle H_2 \delta \phi \rangle}{\langle H_2 \phi \rangle} \quad (5)$$

The first two terms are the direct components by the response functions which can be easily calculated from their definitions. However, the last two terms are the indirect components including the solution of the perturbation equation and they can't be simply calculated, because the each transport equation of the perturbed state must be solved for the solution. For the more simple form of the indirect term, the adjoint method can be used.

#### 2.2 Generalized Adjoint Equation

The first order perturbed equation for the eigenvalue problem can be expressed as the following

$$(A - \lambda B)\delta\phi = -(\delta A - \lambda\delta B)\phi + \delta\lambda B\phi \quad (6)$$

Thus, the generalized adjoint equation can be described as Eq.(7).

$$(A^* - \lambda B^*)\Gamma^* = S^* \equiv \frac{1}{R} \frac{\partial R}{\partial \phi} = \frac{H_1}{\langle H_1 \phi \rangle} - \frac{H_2}{\langle H_2 \phi \rangle} \quad (7)$$

Here,  $\Gamma^*$  is the generalized adjoint solution and the source term in the right side of Eq.(7) is set as the above form in order to simplify the indirect term of Eq.(5). Then, the generalized adjoint solution can be appropriately obtained according to the source term.

Taking the inner product with the weight of  $\Gamma^*$  in Eq.(6) and the weight of  $\delta\phi$  in Eq.(7), respectively, and using the definition of the adjoint operator, one can readily obtain the relation as the following

$$\left( \frac{\delta R}{R} \right)_{indirect} \cong \frac{\langle H_1 \delta \phi \rangle}{\langle H_1 \phi \rangle} - \frac{\langle H_2 \delta \phi \rangle}{\langle H_2 \phi \rangle} = -\langle \Gamma^* (\delta A - \lambda \delta B) \phi \rangle + \delta \lambda \langle \Gamma^* B \phi \rangle \quad (8)$$

However, the second term of the right side in Eq.(8) still includes the perturbed eigenvalue,  $\delta\lambda$ , which must be obtained from the perturbed equation. For eliminating the second term, an auxiliary condition must be introduced as

$$\langle \Gamma^* B \phi \rangle = 0 \quad (9)$$

This means that the generalized adjoint solution,  $\Gamma^*$ , satisfying the above condition can be calculated from Eq.(7). Using the definition of the adjoint operator, one can easily obtain the general solution as Eq.(10) which consists of the particular solution,  $\Gamma_p^*$ , and the homogeneous solution,  $\phi^*$ , of Eq.(7) and satisfies the condition, Eq.(9).

$$\Gamma^* = \Gamma_p^* - \frac{\langle \phi B^* \Gamma_p^* \rangle}{\langle \phi B^* \phi^* \rangle} \phi^* \quad (10)$$

Therefore, the general adjoint equation and its condition can be established as Eq.(7) and Eq.(10), respectively, and the solution can be obtained using the iterative scheme described in next section.

### 2.3 Scheme for Numerical Solution

For obtaining the solution of the generalized adjoint equation, the fixed source problem, Eq.(7), must be solved using a iterative method as the following.

$$A^* \Gamma_{n+1}^* = \lambda B^* \Gamma_n^* + \frac{H_1}{\langle H_1 \phi \rangle} - \frac{H_2}{\langle H_2 \phi \rangle} \quad (11)$$

If considering the additional condition, Eq.(10), Eq.(11) becomes

$$A^* \Gamma_{n+1}^* = \lambda B^* \left( \Gamma_n^* - \frac{\langle \phi B^* \Gamma_n^* \rangle}{\langle \phi B^* \phi^* \rangle} \phi^* \right) + \frac{H_1}{\langle H_1 \phi \rangle} - \frac{H_2}{\langle H_2 \phi \rangle} \quad (12)$$

Here,  $\lambda$  is the fundamental eigenvalue,  $\phi$  is the solution of the forward equation, and  $\phi^*$  is the solution of the fundamental adjoint equation.

First, DeCART solves the forward equation and the fundamental eigenvalue and the solution should be obtained. Then, the fundamental adjoint equation must be calculated and the generalized adjoint solution can be produced from Eq.(12).

### 2.4 Numerical Results

For the verification of this code, the results of the code on PMR200 pin cell were compared to them of TSUNAMI of SCALE package.

Fig. 1 shows the comparison of the generalized adjoint flux for the response of  $\nu \Sigma_f$  in the fuel region between SCALE and DeCART. Here,  $R = \frac{\langle \nu \Sigma_{fg} \phi_g \rangle}{\langle \phi_g \rangle}$

and  $S_g^* = \frac{\nu \Sigma_{fg}}{\langle \nu \Sigma_{fg} \phi_g \rangle} - \frac{1}{\langle \phi_g \rangle}$ . The plot presents that two results are in a good agreement and the trend is similar to the fission cross section of U235, because the generalized adjoint flux represents the average importance of the neutron at the energy group  $g$  to the response,  $\nu \Sigma_f$ . On the other hand, the slightly increased adjoint flux around 10MeV is attributable to the fission cross section of U238. The adjoint flux drop between 5eV and 10eV corresponds to the peak of the importance to the capture cross section as shown in Fig. 2.

Fig. 2 presents the generalized adjoint solutions for the response of the capture cross section in the fuel region. It can be seen from the plot that the trend of the importance is similar to the capture cross section of U238 and the two codes product the similar results except the resonance region. The discrepancy is attributable to the difference methods and codes of the resonance treatment between two codes.

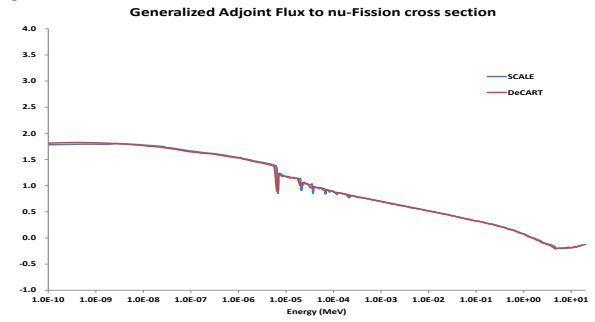


Fig. 1. Generalized Adjoint Flux for Response,  $\nu \Sigma_f$

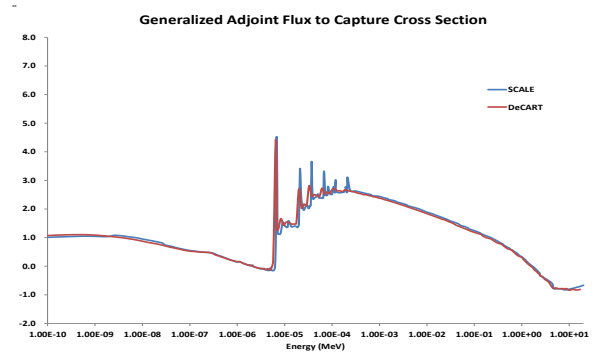


Fig. 2. Generalized Adjoint Flux for Response,  $\Sigma_c$

## 3. Conclusions

In this paper, the generalized adjoint solver based on the generalized perturbation theory is implemented on DeCART and the verification calculations were carried out. As the results, the adjoint flux for the general response coincides with the reference solution and it is expected that the solver could produce the parameters for the sensitivity and uncertainty analysis.

## REFERENCES

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