Generalized sensitivity analysis capability with the differential operator method in RMC Code

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ABSTRACT

Sensitivity analysis is an important way for us to know how the input parameters will affect the output of a system. Therefore, recently, there is an increased interest in developing sensitivity analysis methods in continuous-energy Monte Carlo Code due to the fact that Monte Carlo method can perform high-fidelity simulations of nuclear reactor. Previous studies mainly focused on developing sensitivity analysis method suitable for analyze eigenvalue. There are relatively few researches for performing sensitivity analysis of generalized response function by using continuous-energy Monte Carlo code. So, in this work, the differential operator method (DOM) has been investigated and implemented in continuous-energy Reactor Monte Carlo code (RMC) to perform sensitivity analysis of generalized response function in the form of ratios of reaction rate. The DOM implemented in RMC is based on the analog Monte Carlo transport mode and non-analog Monte Carlo transport mode. The correctness of the newly implemented method has been verified by comparing the results with those calculated by using the collision history-based method through the Jezeble and Flattop benchmark problems. In general, the results given by the DOM agree well with those obtained by the collision history-based method with an accuracy of 5%. Moreover, it is also shown that the non-analog Monte Carlo transport mode can obtain lower relative standard deviation of the sensitivity coefficients than the analog Monte Carlo transport mode.

KEYWORDS: Monte Carlo, sensitivity analysis, differential operator method, RMC

1. INTRODUCTION

With increased demand for economic and safety in nuclear reactor design, sensitivity and uncertainty analysis draw many research interests. In the past few years, a lot of research about eigenvalue sensitivity analysis have been conducted and several continuous-energy Monte Carlo codes such as SCALE[1], SERPENT2[2], MCNP6[3,4], Open MC[5], MONK[6], MORET5[7], McCARD[8] and the Reactor Monte Carlo (RMC) code[9–12] have been equipped with capability for performing sensitivity analysis of eigenvalue. Besides eigenvalue, some generalized responses such as reaction rate ratios, reaction rates and neutron fluxes are also important in the reactor design. So, methods suitable for performing sensitivity analysis of these different generalized response functions based on the continuous-energy Monte Carlo codes should be investigated. In the previous work, the collision history-based method is implemented in the continuous-energy Reactor Monte Carlo (RMC) code[13,14] to perform sensitivity analysis of reaction rate ratios and bilinear ratios. However, this method is based on analog Monte Carlo transport. Since most
Monte Carlo codes are based on nonanalog Monte Carlo transport, sensitivity analysis methods suitable for nonanalog Monte Carlo transport should be developed. The GEAR-MC method[15–17] was implemented in RMC[18] based on nonanalog Monte Carlo transport. However, this method is faced with huge memory consumption problem when performing sensitivity analysis. Therefore, the superhistory-based differential operator method (SH-DOM)[19] and the superhistory-based GEAR-MC method[20,21] were developed and implemented in RMC and both of them are based on the nonanalog Monte Carlo transport. In this work, the sensitivity coefficients produced by the differential operator method based on analog Monte Carlo transport and nonanalog Monte Carlo transport are compared.

Section 2 briefly reviews the differential operator method. Section 3 compares the sensitivity coefficients produced by the differential operator method with those produced by the collision history-based method for Jezebel and Flattop benchmark problems. Section 4 gives the conclusion.

2. METHODOLOGY

The DOM is first briefly reviewed here and the thorough description can be found in previous studies[22,23] for more thorough descriptions of DOM.

The sensitivity coefficient is defined as

\[ S_x^R = \frac{dR}{dx} / x \] (1)

where R is the response function, x is the input parameters such as nuclear data.

In this work, the following response function is investigated

\[ R = \langle x_1, \Psi \rangle / \langle x_2, \Psi \rangle \] (2)

where \( \langle \rangle \) means the response function is integrated over some phase space, \( x_1 \) and \( x_2 \) are the macroscopic cross sections for different reaction types and \( \Psi \) is the neutron flux.

Substituting Eq. (2) into Eq. (1) yields

\[ S_x^R = x \left( \frac{\partial}{\partial x} \frac{\langle x_1, \Psi \rangle}{\langle x_2, \Psi \rangle} - \frac{\partial}{\partial x} \frac{\langle x_1, \Psi \rangle}{\langle x_2, \Psi \rangle} \right) = \]

\[ = \frac{1}{Y} \sum_{j=1}^{L_n} \frac{1}{N_1 w_0} \sum_{n=1}^{N_1} \sum_{k=1}^{K_n} q_{0,n,k} d_{nj,k}[Y] \left( \frac{q_{0,n,k}}{q_{1,n,k}} + \frac{d_{nj,k}[Y]}{d_{n,k}[Y]} + \sum_{j=1}^{l-1} \left[ \frac{q_{0,n,f}}{q_{1,n,f}} + \frac{d_{nj,f}[k_{eff}]}{d_{n,f}[k_{eff}]} \right] \right) \] (3)

where \( Y = \langle x_1, \Psi \rangle \), \( Z = \langle x_2, \Psi \rangle \). \( L_n \) is the total number of active cycles. \( N_1 \) is the total number of neutrons in generation \( l \). \( w_0 \) is the initial weight of every particle in cycle \( l \). \( K_n \) is the total number of collisions in history \( n \) during generation \( l \). The quantity \( q_{0,n,k} / q_{1,n,k} \) represents the relative change in the probability of the random walk of neutron \( n \) entering collision \( k \) in the \( l \)th generation in which the source perturbation effect is not considered. \( q_{0,n,f} / q_{1,n,f} \) represents the relative change in the probability of the random walk of the ancestor neutron in the \( j \)th generation with source perturbation effect taken into account. \( d_{nj,k}[Y]/d_{n,k}[Y] \) is the perturbation in \( x \) of the contribution to reaction rate \( Y \) in the random walk...
of neutrons in the $l^{th}$ generation. The subscript $f$ represents the collision in generation $j$ that caused fission and produced the neutron. Furthermore, $d^0[k_{eff}]/d^1[k_{eff}]$ is the perturbation in $x$ of the contribution to the eigenvalue in the random walk of the $(l-\gamma)^{th}$ ancestor. The DOM flow chart is shown in Fig. 1. The sensitivity coefficients will be estimated until all the particles in a block have been simulated. In DOM, $w_{Sp}$ is estimated in the latent generation and $w_{NSP}$ is calculated in asymptotic generation as illustrated in Fig. 1.
Fig. 1. DOM flow chart.
3. RESULTS

In this work, the differential operator method for the analog Monte Carlo transport and the nonanalog Monte Carlo transport are implemented in continuous-energy Reactor Monte Carlo (RMC) code. The newly developed method was verified by comparing with results calculated by the collision history-based method in Jezebel and Flattop benchmark problems. All the calculations are performed on the Sunway TaihuLight supercomputer with 10 nodes. Each node has 24 CPUs (Intel Xeon E5-2680 v3 at 2.5 GHz) sharing 128 gigabytes of memory. The cross-section used in the calculation are produced from ENDF/B-VII nuclear data library. The following response function is selected

\[
R = \frac{\sum_{i}^{238\text{U}} (r, E) \Psi(r, E, \Omega) dE d\Omega}{\sum_{i}^{235\text{U}} (r, E) \Psi(r, E, \Omega) dE d\Omega}
\]

where \( \Psi(r, E, \Omega) \) is the neutron flux. \( \sum_{i}^{238\text{U}} \) and \( \sum_{i}^{235\text{U}} \) represents fission cross section for U-238 and U-235 respectively. The asymptotic generation is set to be ten to consider the fission source perturbation effect correctly\[2,3\].

3.1. Jezebel benchmark

The Jezebel benchmark[24] is a bare metallic sphere of plutonium. Sensitivity coefficients were evaluated for five isotopes. The response function is integrated over a small central sphere of 1-cm radius. The energy–integrated F28/F25 sensitivity coefficients for this benchmark are presented in Table I. As can be seen from the Table I, relative differences between differential operator method and collision history-based method are within 5%. This means differential operator method generally agrees with collision history-based method. Moreover, the sensitivity coefficients produced by the nonanalog Monte Carlo transport based differential operator method have lower relative standard deviation (RSD) than those produced by the analog Monte Carlo transport based differential operator method. This is because the variance reduction techniques used in the nonanalog Monte Carlo transport.

### Table I. Sensitivity coefficients for the Jezebel benchmark.

| Nuclide | Reaction type | Non-analog DOM | Analog DOM | RSD (%) | Collision-history | RSD (%) | Relative difference Non-analog DOM/Collision-history-based method (%) | Relative difference Analog DOM/Collision-history-based method (%) |
|---------|---------------|----------------|------------|---------|-------------------|---------|-----------------------------------------------|-----------------------------------------------|
| Pu-239  | nubar         | 1.95E-03       | 4.20       | 2.02E-03 | 4.49              | 1.99E-03 | 0.85                                           | -2.05                                         | 1.53                                           |
| Pu-239  | Inelastic     | -1.62E-01      | 0.14       | -1.62E-01 | 0.16              | -1.60E-01 | 0.04                                           | 1.28                                          | 1.01                                           |
| Pu-239  | n,2n          | -1.99E-03      | 0.84       | -2.00E-03 | 0.95              | -2.00E-03 | 0.23                                           | -0.35                                         | 0.17                                           |
| Pu-239  | Fission       | 4.97E-02       | 0.20       | 5.17E-02  | 0.28              | 5.18E-02  | 0.11                                           | -4.02                                         | -0.18                                          |
| Pu-239  | n,gamma       | 1.02E-02       | 0.11       | 1.02E-02  | 0.13              | 1.01E-02  | 0.09                                           | 1.11                                          | 0.91                                           |
| Pu-239  | Elastic       | -6.38E-02      | 0.59       | -6.34E-02 | 0.68              | -6.40E-02 | 0.18                                           | -0.27                                         | -0.90                                          |
| Pu-239  | Total         | -1.68E-01      | 0.26       | -1.65E-01 | 0.30              | -1.64E-01 | 0.08                                           | 2.34                                          | 0.64                                           |
| Pu-240  | nubar         | -1.85E-03      | 4.23       | -1.88E-03 | 4.64              | -1.84E-03 | 0.89                                           | 0.54                                          | 2.28                                           |
| Pu-240  | Elastic       | -4.01E-03      | 2.21       | -4.14E-03 | 2.41              | -4.06E-03 | 0.64                                           | -1.15                                         | 2.08                                           |
| Pu-240  | Inelastic     | -8.09E-03      | 0.62       | -8.04E-03 | 0.70              | -8.06E-03 | 0.18                                           | 0.46                                          | -0.19                                          |
| Pu-241  | n,gamma       | 3.96E-05       | 0.11       | 3.96E-05  | 0.13              | 4.07E-05  | 1.88                                           | -2.52                                         | -2.60                                          |
| Ga-69   | Total         | -3.93E-03      | 1.41       | -4.09E-03 | 1.53              | -3.95E-03 | 0.40                                           | -0.41                                         | 3.45                                           |
| Ga-69   | Inelastic     | -2.24E-03      | 1.06       | -2.26E-03 | 1.18              | -2.24E-03 | 0.30                                           | -0.05                                         | 1.01                                           |
3.2. Flattop benchmark

The Flattop benchmark[24] is a sphere of plutonium-gadolinium alloy that is reflected by a region of depleted uranium. The response function is also calculated in a small central sphere of 1-cm radius. Table II presents the energy –integrated sensitivity coefficients for seven different isotopes. Fairly good agreement between the differential operator method and the collision history-based method can be appreciated. The biggest difference between the differential operator method and the collision history predictions occurs in the Pu-239 elastic where the difference is 7.17%. This difference is caused by the large relative standard deviations of the sensitivity results produced by the analog based differential operator method and the collision history-based method. It can also be noted that the fission cross section sensitivity coefficients for U-235 and U-238 are larger than the other nuclear data. This is due to the fact that fission event of U-235 and U-238 contribute directly and dominantly to F28/F25.

Table II. Sensitivity coefficients for the Flattop benchmark.

| Nuclide | Reaction type | Non-analog | Analog | Collision-history | Relative difference Non-analog | Relative difference Analog |
|---------|---------------|------------|--------|-------------------|-------------------------------|---------------------------|
|         | Reaction type | RSD (%)    | RSD (%)| RSD (%)           | DOM/Collision-history-based method (%) | DOM/Collision-history-based method (%) |
| Pu-241  | Inelastic     | -4.76E-04  | 5.65   | -4.53E-04         | 1.54                          | -2.95E-03                 | 1.54                        |
| Pu-240  | Inelastic     | -6.14E-03  | 1.67   | -6.33E-03         | 1.28                          | -2.98E-03                 | 0.44                        |
| Pu-240  | n,gamma      | 1.25E-03   | 0.19   | 1.26E-03          | 0.33                          | -1.81E-03                 | 0.33                        |
| Pu-239  | Total         | 5.88E-02   | 1.78   | 5.94E-02          | 0.44                          | -1.28                      | 3.67                        |
| Pu-239  | Elastic       | -1.42E-02  | 6.20   | -1.54E-02         | 0.33                          | -1.81E-03                 | 0.33                        |
| Pu-239  | Inelastic     | -1.15E-01  | 0.39   | -1.15E-01         | 0.33                          | -1.81E-03                 | 0.33                        |
| Pu-239  | n,2n         | -1.42E-03  | 2.04   | -1.47E-03         | 0.33                          | -1.81E-03                 | 0.33                        |
| Pu-239  | Fission       | 1.71E-01   | 0.22   | 1.72E-01          | 0.26                          | -1.81E-03                 | 0.26                        |
| Pu-239  | n,gamma      | 1.88E-02   | 0.19   | 1.87E-02          | 0.22                          | -1.81E-03                 | 0.22                        |
| Pu-239  | nubar        | 5.70E-02   | 0.58   | 5.69E-02          | 0.66                          | -1.81E-03                 | 0.66                        |
| U-238   | Total         | 8.04E-01   | 0.20   | 8.04E-01          | 0.23                          | -1.81E-03                 | 0.23                        |
| U-238   | Elastic       | -1.23E-01  | 1.19   | -1.23E-01         | 1.40                          | -1.81E-03                 | 1.40                        |
| U-238   | Inelastic     | -8.14E-02  | 0.80   | -8.19E-02         | 0.91                          | -1.81E-03                 | 0.91                        |
| U-238   | n,2n         | -1.31E-03  | 3.75   | -1.24E-03         | 4.46                          | -1.81E-03                 | 4.46                        |
| U-238   | Fission       | 9.65E-01   | 0.02   | 9.65E-01          | 0.03                          | -1.81E-03                 | 0.03                        |
| U-238   | n,gamma      | 4.52E-02   | 0.35   | 4.51E-02          | 0.39                          | -1.81E-03                 | 0.39                        |
| U-238   | nubar        | -4.98E-02  | 0.55   | -4.97E-02         | 0.64                          | -1.81E-03                 | 0.64                        |
| U-235   | Total         | -1.01E+00  | 0.02   | -1.01E+00         | 0.02                          | -1.81E-03                 | 0.02                        |
| U-235   | Fission       | -1.00E+00  | 0.01   | -1.00E+00         | 0.01                          | -1.81E-03                 | 0.01                        |
| U-235   | n,gamma      | 6.15E-04   | 0.36   | 6.14E-04          | 0.40                          | -1.81E-03                 | 0.40                        |
| U-235   | nubar        | -7.61E-03  | 1.22   | -7.65E-03         | 1.37                          | -1.81E-03                 | 1.37                        |
| Ga-71   | Total         | -1.79E-03  | 5.86   | -1.81E-03         | 6.21                          | -1.81E-03                 | 6.21                        |
| Ga-71   | Inelastic     | -1.44E-03  | 2.75   | -1.48E-03         | 2.97                          | -1.81E-03                 | 2.97                        |
| Ga-71   | n,gamma      | 7.28E-05   | 0.28   | 7.31E-05          | 0.37                          | -1.81E-03                 | 0.37                        |
4. CONCLUSIONS

In this work, the differential operator method is implemented in the continuous-energy Monte Carlo code RMC to perform generalized sensitivity analysis for response function in the form of reaction rate ratios. The newly developed method is verified by comparing with the results obtained by using collision history-based method. The differential operator method produce response sensitivity coefficients that agreed well with those produced by the collision history-based method. Results also shown that the non-analog Monte Carlo transport mode can obtain lower relative standard deviation of the sensitivity coefficients than the analog Monte Carlo transport mode.

Future work will focus on extending the differential operator method to perform sensitivity analysis of reaction rates and applying the superhistory algorithm to solve the huge memory consumption problem encountered when using this method to perform sensitivity analysis of reaction rates.

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REFERENCES

1. C. M. PERFETTI, B. T. REARDEN, and W. R. MARTIN, “SCALE Continuous-Energy Eigenvalue Sensitivity Coefficient Calculations,” Nuclear Science and Engineering 182 (3), pp.332–353 (2016).
2. M. AUFIERO et al., “A collision history-based approach to sensitivity/perturbation calculations in the continuous energy Monte Carlo code SERPENT,” Annals of Nuclear Energy 85 June, pp.245–258 (2015).
3. B. C. KIEDROWSKI and F. B. BROWN, “Adjoint-Based k-Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo ,” Nuclear Science and Engineering 174 (3), pp.227–244 (2014).
4. B. C. KIEDROWSKI, F. B. BROWN, and P. P. H. WILSON, “Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo ,” Nuclear Science and Engineering 168 (3), pp.226–241 (2011).
5. X. PENG et al., “Development of continuous-energy sensitivity analysis capability in OpenMC,” Annals of Nuclear Energy 110, pp.362–383 (2017).
6. C. BAKER et al., CALCULATING UNCERTAINTY ON K-EFFECTIVE WITH MONK10, in: ICNC 2015, Charlotte, NC, September 13-17 (2015).
7. A. JINAPHANH, N. LECLAIRE, and B. COCHET, “Continuous-Energy Sensitivity Coefficients in the MORET Code,” Nuclear Science and Engineering 184 (1), pp.53–68 (2016).
8. H. J. Shim and C. H. Kim, “Adjoint Sensitivity and Uncertainty Analyses in Monte Carlo Forward Calculations,” Journal of Nuclear Science and Technology 48 (12), pp.1453–1461 (2011).
9. Y. QIU et al., “New strategies of sensitivity analysis capabilities in continuous-energy Monte Carlo code RMC,” Annals of Nuclear Energy 81, pp.50-61 (2015).
10. Y. QIU et al., “Computing eigenvalue sensitivity coefficients to nuclear data by adjoint superhistory method and adjoint Wielandt method implemented in RMC code,” Annals of Nuclear Energy 87, pp.228-241 (2016).
11. Y. QIU et al., “Computing eigenvalue sensitivity coefficients to nuclear data based on the CLUTCH method with RMC code,” Annals of Nuclear Energy 88, pp.237-251 (2016).
12. Y. QIU, K. WANG, and J. YU, “Development of Sensitivity Analysis Capability in RMC code,” Transactions of the American Nuclear Society, Vol. 111, Anaheim, CA, November 9–13 (2014).
13. Y. QIU et al., “Development of sensitivity analysis capabilities of generalized responses to nuclear data in Monte Carlo code RMC,” Annals of Nuclear Energy 97, pp.142-152 (2016).
14. Y. QIU et al., “Generalized Sensitivity Analysis With Continuous-Energy Monte Carlo Code RMC,” in ICONE24, Charlotte, North Carolina (2016).
15. C. M. PERFETTI and B. T. REARDEN, “A New Method for Calculating Generalized Response Sensitivities in Continuous-Energy Monte Carlo Applications in SCALE,” Transactions of the American Nuclear Society, Vol. 109, Washington, D.C., November 10–14 (2013).
16. C. M. PERFETTI and B. T. REARDEN, “Development of a Generalized Perturbation Theory Method for Sensitivity Analysis Using Continuous-Energy Monte Carlo Methods,” Nuclear Science and Engineering 182 (3), pp.354–368 (2016).
17. C. M. PERFETTI and B. T. REARDEN, “Performance Enhancements to the SCALE TSUNAMI-3D Generalized Response Sensitivity Capability,” Transactions of the American Nuclear Society, Vol. 111, Anaheim, California, November 9–13 (2014).
18. G. SHI et al., “Development of Generalized Response Sensitivity Analysis Capability in RMC Code,” in M&C 2019, Portland, Oregon, USA. August 25-29, (2019).
19. G. SHI et al., “Superhistory-based differential operator method for generalized responses sensitivity calculations,” Annals of Nuclear Energy 140, 107291, (2020).
20. G. SHI et al., “Development of Superhistory-based GEAR-MC method for Generalized Responses,” in ICAPP 2020 Abu Dhabi-UAE. 15–19 March, (2020).
21. G. SHI et al., “Improved Generalized Perturbation Theory Method for sensitivity analysis of generalized response function,” submitted to Progress in Nuclear Energy.
22. T. P. BURKE and B. C. KIEDROWSKI, “Monte Carlo Perturbation Theory Estimates of Sensitivities to System Dimensions,” Nuclear Science and Engineering 189 (3), pp.199–223 (2018).
23. K. F. RASKACH, “An Improvement of the Monte Carlo Generalized Differential Operator Method by Taking into Account First- and Second-Order Perturbations of Fission Source,” Nuclear Science and Engineering 162 (2), pp.158–166 (2009).
24. International Handbook of Evaluated Criticality Safety Benchmarks Experiments. OECD Nuclear Energy Agency Nuclear Science Committee of the Organization for Economic Co-operation and Development (2011).