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Equivalence of the Adjoint-Weighted Monte Carlo Perturbation Method and the First Order Differential Operator Sampling Method with Fission Source Perturbation

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Contents

Background

- The Monte Carlo perturbation methods have become a powerful means not only to estimate the change of the reactivity in response to a small change of a nuclear design parameter but also to perform the sensitivity and uncertainty (S/U) calculations of nuclear design parameters with regard to the uncertain nuclear data.

- The traditional MC perturbation methods [1] such as the differential operator sampling (DOS) and the correlated sampling have been widely applied for the sensitivity calculations. However these methods do not utilize the adjoint flux so that the perturbed fission source effect should be taken into account by the fission source perturbation (FSP) method [2].

  [1] H. Rief, "Generalized Monte Carlo Perturbation Algorithms for Correlated Sampling and a Second-Order Taylor Series Approach," *Ann. Nucl. Energy*, **11**, 455 (1984).

  [2] Y. Nagaya, T. Mori, "Impact of Perturbed Fission Source on the Effective Multiplication Factor in Monte Carlo Perturbation Calculations," *J. Nucl. Sci. Technol.*, **42**[5], 428 (2005).

- Though Ueki and Hoogenboom [3] have ever investigated an MC perturbation analysis with the forward and adjoint solutions, it requires adjoint history simulations.

  [3] T. Ueki, J. E. Hoogenboom, "Exact Monte Carlo Perturbation Analysis by Forward-Adjoint Coupling in Radiation Transport Calculations," *J. Comput. Phys.*, **171**, 509 (2001).

Objectives

- Recently, there have been significant advances to estimate the adjoint-weighted kinetics parameter in the MC forward calculations by utilizing a physical meaning of the adjoint flux which can be estimated in the MC forward calculations.
- The MC adjoint flux estimation method using the iterated fission probability (IFP) was readily applied for the adjoint-weighted perturbation (AWP) methods [4,5].

  [4] B. C. Kiedrowski, F. B. Brown, "Adjoint-weighting for critical systems with continuous energy Monte Carlo," *Nuclear Criticality Safety Division Topical Meeting on Realism, Robustness and the Nuclear Renassance 2009*, Richland, WA, Sep. 13 (2009).

  [5] H.J. Shim, C.S. Gil, C.H. Kim, "Nuclear Data Sensitivity and Uncertainty Analysis Using Adjoint Flux Estimated in Monte Carlo Forward Calculations," *International Conference on Nuclear Data for Science and Technology* 2010, Jeju Island, Korea, April 26-30 (2010).

- The objectives of this presentation are
  - to prove that the first-order DOS method with FSP effect taken into account (DOS/FSP method hereafter) is equivalent to the first-order AWP method
  - and to demonstrate numerically the equivalence of the first-order DOS/FSP and AWP methods through S/U analyses of the Godiva criticality problems.

Perturbation Formulation for MC Eigenvalue Cal. (1/3)

- To start with, the MC eigenvalue equation for the fission source density (FSD), S, is given by

$$S = \lambda \mathbf{H} S; \qquad (1)$$

$$\lambda = \frac{1}{k}$$

where S satisfies $\int S(\mathbf{P}) d\mathbf{P} = 1$ where $\mathbf{P}$ denotes the state vector of a neutron in the six-dimensional phase space, ($\mathbf{r}$, E, $\mathbf{\Omega}$).

- $\mathbf{H}S$ in Eq. (1) implies

$$\mathbf{H}S = \int d\mathbf{P}' H(\mathbf{P}' \rightarrow \mathbf{P}) S(\mathbf{P}') \qquad (2)$$

where $H(\mathbf{P}' \rightarrow \mathbf{P})$ means the number of first-generation fission neutrons born per unit phase space volume about $\mathbf{P}$, due to a parent neutron born at $\mathbf{P}'$.

Perturbation Formulation for MC Eigenvalue Cal. (2/3)

- The perturbed system equation by a change of the input parameter x can be written as

$$S + \Delta S = (\lambda + \Delta\lambda)\ (\mathbf{H} + \Delta\mathbf{H})\ (S + \Delta S); \qquad (3)$$

$$\Delta\mathbf{H} = \frac{\partial \mathbf{H}}{\partial x}\Delta x \qquad (4)$$

- Taking the inner product of both sides of Eq. (3) with a weight function $w(\mathbf{r}, E, \mathbf{\Omega})$ and solving for the change in the eigenvalue, one can obtain

$$\Delta\lambda = \frac{< w, \left(\mathbf{I} - \lambda(\mathbf{H} + \Delta\mathbf{H})\right)\Delta S > - < w, \lambda\Delta\mathbf{H}S >}{< w, (\mathbf{H} + \Delta\mathbf{H})(S + \Delta S) >} \qquad (5)$$

where the angle bracket notation indicates the integration over the domain of a product of two functions and $\mathbf{I}$ denotes the identity operator.

- By neglecting products of perturbations in Eq. (6), a first-order estimate for the eigenvalue perturbation can be written as

$$\Delta\lambda \cong \frac{< w, (\mathbf{I} - \lambda\mathbf{H})\Delta S > - < w, \lambda\Delta\mathbf{H}S >}{< w, \mathbf{H}S >} \qquad (6)$$

Perturbation Formulation for MC Eigenvalue Cal. (3/3)

- Suppose that w is chosen to be the λ-mode adjoint function ϕ^* that obeys

$$\mathbf{M}^*\phi^* = \lambda \mathbf{F}^*\phi^* \qquad \text{(7)}$$

where the adjoint operators are defined by

$$\mathbf{M}^*\phi^* = \left[-\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\phi^*(\mathbf{r},E,\mathbf{\Omega}) - \int dE' \int d\mathbf{\Omega}' \Sigma_s(\mathbf{r};E,\mathbf{\Omega}\to E',\mathbf{\Omega}')\phi^*(\mathbf{r},E',\mathbf{\Omega}'), \qquad \text{(8)}$$

$$\mathbf{F}^*\phi^* = \int dE' \int d\mathbf{\Omega}' \frac{\chi(E')}{4\pi} \nu(E)\Sigma_f(\mathbf{r},E)\phi^*(\mathbf{r},E',\mathbf{\Omega}') \qquad \text{(9)}$$

- By inverting $\mathbf{M}^*$ in Eq. (10) and introducing the operator $\mathbf{H}$ defined by Eq. (2), one can obtain

$$\phi^* = \lambda\left(\mathbf{M}^*\right)^{-1}\mathbf{F}^*\phi^* = \lambda\left(\mathbf{F}\mathbf{M}^{-1}\right)^*\phi^* = \lambda\mathbf{H}^*\phi^* \qquad \text{(10)}$$

- Because $<\phi^*,(\mathbf{I}-\lambda\mathbf{H})\Delta S>=<\Delta S,(\mathbf{I}-\lambda\mathbf{H}^*)\phi^*>=0$ by Eq. (10), Eq. (6) becomes

$$\frac{\Delta\lambda}{\lambda} \cong \frac{-<\phi^*,\Delta\mathbf{H}S>}{<\phi^*,\mathbf{H}S>} \qquad \text{(11)}$$

- Because λ=1/k, Eq. (11) can be rewritten as

$$\boxed{\frac{\Delta k}{k} \cong \frac{<\phi^*,\Delta\mathbf{H}S>}{<\phi^*,\mathbf{H}S>}} \qquad \text{(12)}$$

Physical Meaning of ϕ_0^* (1/2)

$$\boxed{\phi^* = \frac{1}{k}\mathbf{H}^*\phi^*} \quad \cdots\cdots\cdots (10)$$

- The fundamental mode adjoint flux ϕ_0^* can be obtained by applying the power method to Eq. (10).

$$\phi_0^* = \lim_{n\to\infty} \phi_{0,n}^*;$$

$$\phi_{0,n}^* = \left(\frac{1}{k_0}\mathbf{H}^*\right)^n \phi_{0,init.}^* = \frac{1}{k_0^{\,n}}\left(\mathbf{H}^n\right)^* \phi_{0,init.}^* \quad \cdots\cdots\cdots (13)$$

n is the iteration or generation index and k_0 is the fundamental mode eigenvalue. $\phi_{0,n}^*$ is the n-th iterative solution to be obtained with an arbitrary non-zero starting distribution function $\phi_{0,init.}^*$.

Physical Meaning of ϕ_0^* (2/2)

- Because of the definition for **H** in Eq. (13), the integral notation for Eq. (13) can be written as

$$\phi_{0,n}^*(\mathbf{P}) = \frac{1}{k_0^{\,n}} \int d\mathbf{P}' H^n(\mathbf{P} \rightarrow \mathbf{P}') \phi_{0,init.}^*(\mathbf{P}) \qquad \text{(14)}$$

where $H^n(\mathbf{P} \rightarrow \mathbf{P}')$ denotes the number of n-th generation fission neutrons born per unit phase space volume about $\mathbf{P}'$, due to a parent neutron born at **P.**

- Then when $\phi_{0,init.}^*(\mathbf{P}) = 1$, $\phi_{0,\mathrm{n}}{}^*(\mathbf{P})$ of Eq. (14) can be interpreted as the number of fission neutrons produced in the n-th generation due to a unit source neutron located at **P** and normalized to satisfying $\int \phi_0^*(\mathbf{P}) S_0(\mathbf{P}) d\mathbf{P} = 1$.

$$\phi_{0,n}^*(\mathbf{P}) = \frac{1}{k_0^{\,n}} \int d\mathbf{P}' H^n(\mathbf{P} \rightarrow \mathbf{P}') \qquad \text{(15)}$$

- When n is large enough for the iterative solution to converge, $\phi_0{}^*$ can be approximated by $\phi_{0,n}{}^*$.

$$\phi_0^* \cong \phi_{0,n}^*; \; n >> 1 \qquad \text{(16)}$$

Application of ϕ_0^* to AWP Formulation

- Insertion of Eq. (15) into the k_0 uncertainty equation of Eq. (12) yields

$$\frac{\Delta k_0}{k_0} \cong \frac{< \phi_{0,n}^*, \Delta \mathbf{H} S_0 >}{< \phi_{0,n}^*, \mathbf{H} S_0 >}$$

$$= \frac{\frac{1}{k_0^{\,n}} \int d\mathbf{P} \int d\mathbf{P}' H^n(\mathbf{P} \to \mathbf{P}') \int d\mathbf{P}'' \Delta H(\mathbf{P}'' \to \mathbf{P}) S_0(\mathbf{P}'')}{\frac{1}{k_0^{\,n}} \int d\mathbf{P} \int d\mathbf{P}' H^n(\mathbf{P} \to \mathbf{P}') \int d\mathbf{P}'' H(\mathbf{P}'' \to \mathbf{P}) S_0(\mathbf{P}'')}. \quad \text{(17)}$$

where S_0 denotes the fundamental mode fission source distribution.

- Because $\mathbf{H}S_0 = k_0 S_0$ and $\int S(\mathbf{P}) d\mathbf{P} = 1$, the denominator of Eq. (17) becomes k_0.
- Therefore from Eq. (17), Δk can be written as

$$\Delta k_0 \cong < \phi_{0,n}^*, \Delta \mathbf{H} S_0 >$$

$$= \frac{1}{k_0^{\,n}} \int d\mathbf{P} \int d\mathbf{P}' H^n(\mathbf{P} \to \mathbf{P}') \int d\mathbf{P}'' \Delta H(\mathbf{P}'' \to \mathbf{P}) S_0(\mathbf{P}'')$$

$$= \frac{1}{k_0^{\,n}} < \mathbf{H}^n \Delta \mathbf{H} S_0 > . \quad \text{(18)}$$

Formulation of First Order DOS/FSP Method (1/4)

- In the MC power method, S for the next cycle $i+1$, S_{i+1} is updated as

$$S_{i+1} = \frac{1}{k_i}\mathbf{H}S_i; \qquad \text{(19)}$$

$$k_i = < \mathbf{H}S_i > \qquad \text{(20)}$$

- By the first order DOS method augmented by FSP, the sensitivity of eigenvalue at cycle i, k_i to the parameter x is calculated by

$$\frac{\partial k_i}{\partial x} = < \frac{\partial \mathbf{H}}{\partial x} S_i > + < \mathbf{H} \frac{\partial S_i}{\partial x} > \qquad \text{(21)}$$

- And from Eq. (19), the sensitivity of S_i to x can be written as

$$\begin{aligned} \frac{\partial S_i}{\partial x} &= \frac{1}{k_{i-1}} \left(\frac{\partial \mathbf{H}}{\partial x} S_{i-1} + \mathbf{H} \frac{\partial S_{i-1}}{\partial x} \right) - \frac{\mathbf{H}S_{i-1}}{k_{i-1}^{\,2}} \left(< \frac{\partial \mathbf{H}}{\partial x} S_{i-1} > + < \mathbf{H} \frac{\partial S_{i-1}}{\partial x} > \right) \\ &= \frac{1}{k_{i-1}} \left\{ \frac{\partial \mathbf{H}}{\partial x} S_{i-1} + \mathbf{H} \frac{\partial S_{i-1}}{\partial x} - S_i \left(< \frac{\partial \mathbf{H}}{\partial x} S_{i-1} > + < \mathbf{H} \frac{\partial S_{i-1}}{\partial x} > \right) \right\} \end{aligned} \qquad \text{(22)}$$

Formulation of First Order DOS/FSP Method (2/4)

- Using Eq. (22), the successive updates from cycle *i*-*n*, where $\partial S_{i-n}/\partial x$ is assumed to be zero, yields

$$\frac{\partial S_i}{\partial x} = \frac{1}{k_{i-1}}\left(\frac{\partial \mathbf{H}}{\partial x} S_{i-1} - S_i < \frac{\partial \mathbf{H}}{\partial x} S_{i-1} > \right) + \frac{1}{k_{i-1}k_{i-2}}\left(\mathbf{H}\frac{\partial \mathbf{H}}{\partial x} S_{i-2} - S_i < \mathbf{H}\frac{\partial \mathbf{H}}{\partial x} S_{i-2} > \right)$$
$$+ \cdots + \frac{1}{k_{i-1}k_{i-2}\cdots k_{i-n}}\left(\mathbf{H}^{n-1}\frac{\partial \mathbf{H}}{\partial x} S_{i-n} - S_i < \mathbf{H}^{n-1}\frac{\partial \mathbf{H}}{\partial x} S_{i-n} > \right)$$
$$= \sum_{j=0}^{n-1} \frac{1}{\prod_{j'=i-j-1}^{i-1} k_{j'}} \left(\mathbf{H}^{j}\frac{\partial \mathbf{H}}{\partial x} S_{i-j-1} - S_i < \mathbf{H}^{j}\frac{\partial \mathbf{H}}{\partial x} S_{i-j-1} > \right). \qquad (23)$$

- Suppose that the sensitivity calculation is performed after the FSD converges to the fundamental mode. In other words, let's assume that the following conditions are met for the active cycle index, *i*;

$$k_i = k_0, S_i = S_0 \ (i = 1, 2, \ldots) \qquad (24)$$

k_0 and S_0 are the fundamental mode eigenvalue and eigenvector of Eq. (1).

Formulation of First Order DOS/FSP Method (3/4)

- Using the conditions of Eq. (24), Eq. (23) can be expressed as

$$\frac{\partial S_i}{\partial x} = \frac{1}{k_0}\left\{\sum_{j=0}^{n-1}\left(\frac{\mathbf{H}}{k_0}\right)^j \frac{\partial \mathbf{H}}{\partial x} S_0 - S_0 < \sum_{j=0}^{n-1}\left(\frac{\mathbf{H}}{k_0}\right)^j \frac{\partial \mathbf{H}}{\partial x} S_0 >\right\}$$

$$= \frac{1}{k_0}\left\{\frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 - S_0 < \frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 >\right\}. \qquad \text{(25)}$$

- Insertion of Eq. (25) into Eq. (21) yields

$$\frac{\partial k_i}{\partial x} =< \frac{\partial \mathbf{H}}{\partial x} S_0 > + < \frac{\mathbf{H}}{k_0}\left\{\frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 - S_0 < \frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 >\right\} >$$

$$=< \frac{\partial \mathbf{H}}{\partial x} S_0 > - < \cancel{(1-\mathbf{H}/k_0)}\frac{1-\left(\mathbf{H}/k_0\right)^n}{\cancel{1-\mathbf{H}/k_0}}\frac{\partial \mathbf{H}}{\partial x} S_0 > + < \frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 >$$

$$- < \cancel{\frac{\mathbf{H}}{k_0} S_0} > < \frac{1-\left(\mathbf{H}/k_0\right)^n}{1-\mathbf{H}/k_0}\frac{\partial \mathbf{H}}{\partial x} S_0 >$$

$$=< \left(\mathbf{H}/k_0\right)^n \frac{\partial \mathbf{H}}{\partial x} S_0 >= \frac{1}{k_0{}^n} < \mathbf{H}^n \frac{\partial \mathbf{H}}{\partial x} S_0 > \qquad \text{(26)}$$

Formulation of First Order DOS/FSP Method (4/4)

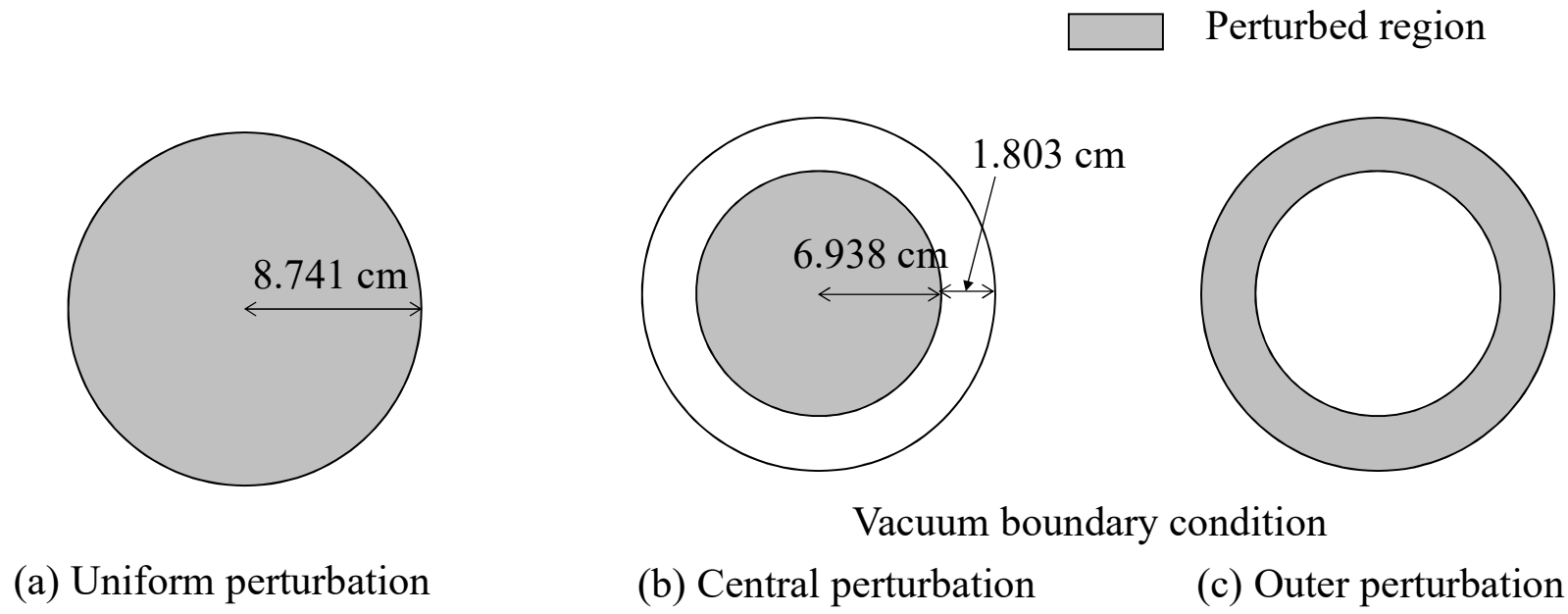
- Eq. (26) indicates that $\partial k_i/\partial x$ is independent of the cycle index i when the FSD is converged to S_0 and ignore its statistical fluctuations.
- Noting $\Delta k=\Delta x(\partial k_i/\partial x)$ and $\Delta\mathbf{H}=\Delta x(\partial\mathbf{H}/\partial x)$, Eq. (26) can be transformed to

$$(\Delta k_0)_i = \frac{1}{{k_0}^n} < \mathbf{H}^n \Delta\mathbf{H} S_0 > . \qquad (27)$$

- From the comparison of Eq. (27) with Eq. (18), one can clearly observe that the $(\Delta k_0)_i$ estimated by the first-order DOS/FSP method is the same as that by the first-order AWP method.

U^{235} Number Density Perturbation for Godiva Problems

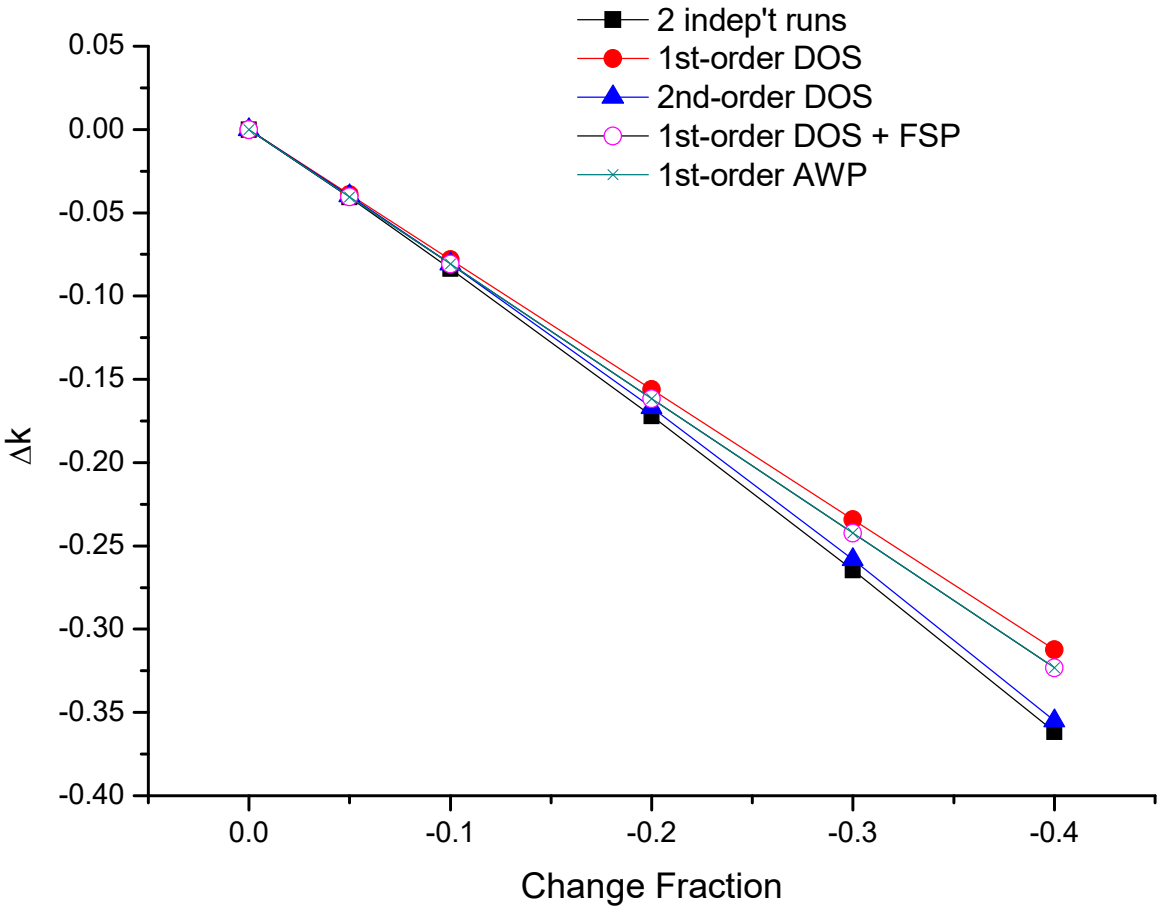
- In order to confirm numerically the equivalence of the two first-order MC perturbation methods, we have calculated the changes in *k* due to globally or locally induced U-235 density changes in Godiva.
- The Godiva geometry is a bare uranium sphere with a radius of 8.741 cm. The original density is 18.74 g/cm^3 and the composition is 94.73 wt% U^{235} and 5.27 wt% U^{238}.



(a) Uniform perturbation (b) Central perturbation (c) Outer perturbation

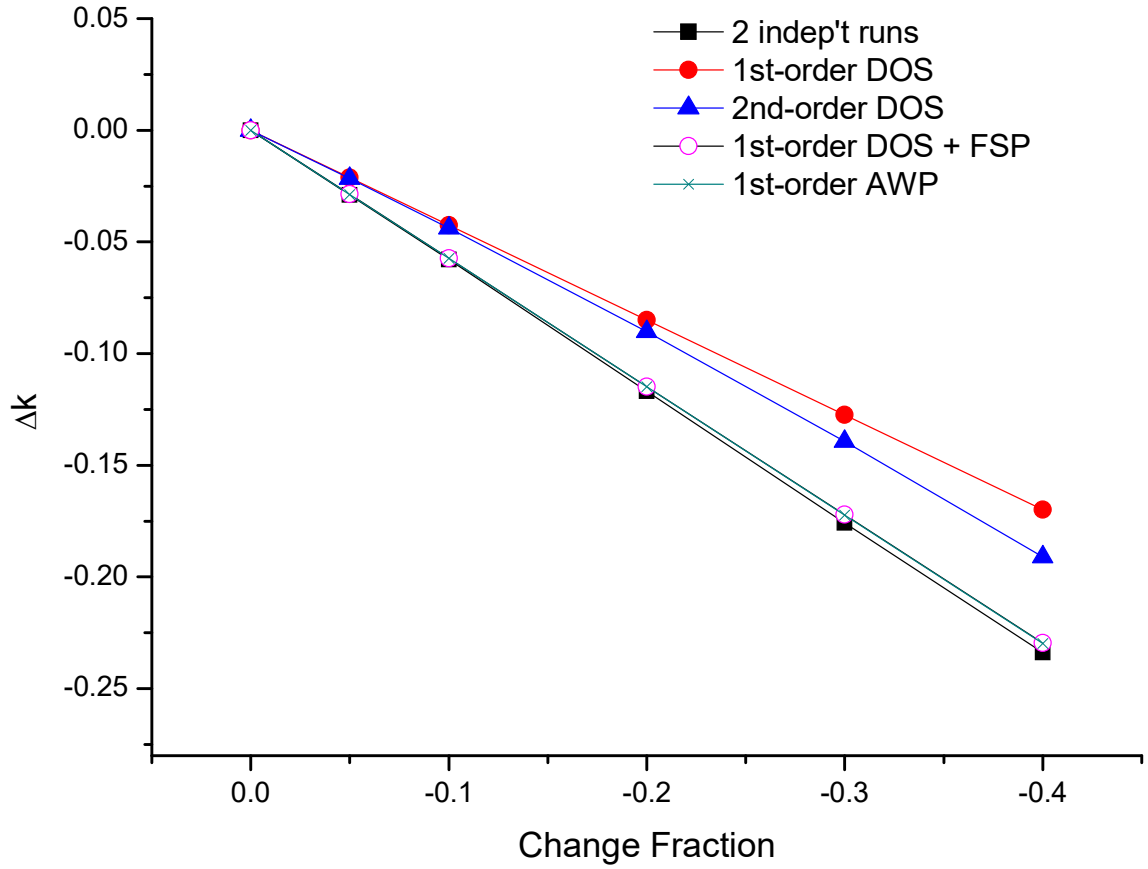
Number Density Perturbation of Godiva

(a) Uniform perturbation



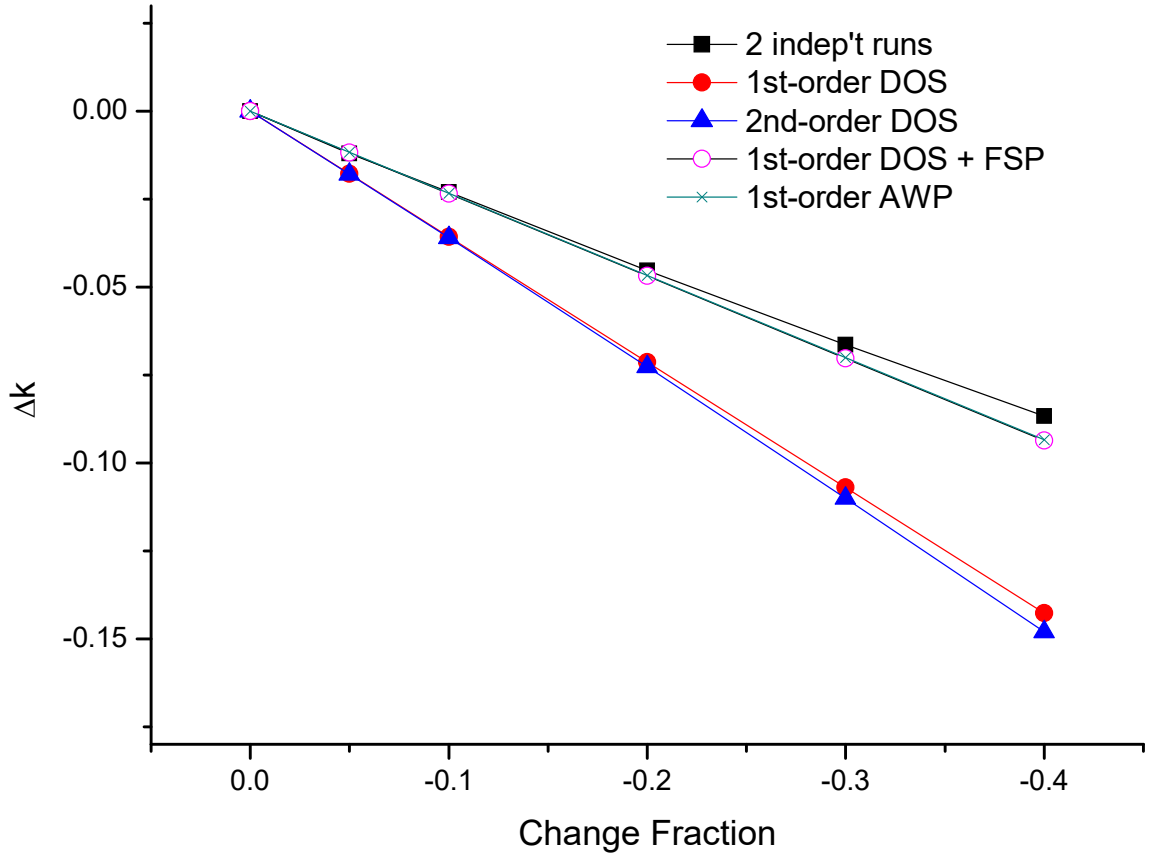
Number Density Perturbation of Godiva

(b) Central perturbation



Number Density Perturbation of Godiva

(c) Outer perturbation



Comparison of k_{eff} and uncertainties due to the cov. in U235 JENDL-3.3 for the GODIVA problem

Code	Neutronics	KENO-V.a	ANISN	McCARD[b]	
	S/U	TSUNAMI[a]	SUSD3D[a]	1st-order DOS/FSP	AWP
Energy Group		238	44	Cont.	
Covariance Data		238 grp	44 grp	30 grp	
Unc. due to U-235 (%)	ν, ν	0.15	0.15	0.15	0.15
	(n,γ), (n,γ)	0.15	0.17	0.16	0.16
	(n,γ), (n,n)	0.07	0.05	0.05	0.05
	(n,2n), (n,2n)	0.02	0.01	0.01	0.01
	(n,fis), (n,fis)	0.17	0.17	0.17	0.17
	(n,fis), (n,n)	-0.05	-0.03	-0.04	-0.04
	(n,n), (n,n)	0.33	0.32	0.38	0.38
	total	0.43	0.43	0.47	0.48

a) The results by TSUNAMI and SUSD3D were excerpt from the paper of KNS 2008 Spring Mtg. entitled by "Uncertainty Analysis of k_{eff} on the GODIVA Core Using Recently Developed Covariance Data".

b) The calculations were performed for 1000 active cycles with 10,000 histories per cycle.

Conclusions

- We have shown that the first-order AWP method is identical to the first-order DOS method with the FSP taken into account by comparing the derived formulations for the two methods.

- In order to confirm numerically the equivalence of the two first-order MC perturbation methods, we have calculated the changes in k due to globally or locally induced U-235 density changes in Godiva and also analyzed contributions of U-235 cross section uncertainties to the uncertainty of k, $\sigma_{XX}(k)$, of the Godiva by nuclear data types.
- We have demonstrated that Δk's and $\sigma_{XX}(k)$'s from the first-order AWP method are the same as those from the first-order DOS/FSP method and that $\sigma_{XX}(k)$'s from by the AWP method agree remarkably well with those from the deterministic S/U codes.
- This then leads us to conclude that the first-order AWP method is a useful alternative to the same order DOS/FSP method.

Uncertainty Quantification (1/3)

- A nuclear parameter Q can be viewed as a function of input parameters such as system geometry, material composition, cross section data, etc. Then Q can be expressed as

$$Q \equiv Q(\cdots, \underbrace{\cdots, x_{r,g}^{n}, \cdots}_{x_{r,g}^{n}\,(n \in I,\ r \in \Gamma,\ g \in G)}, \cdots) \qquad \text{(A.1)}$$

  $x_{r,g}^{n}$ is the g-th group microscopic cross section of reaction type r of isotope n. I, Γ , and G represent the total number of isotopes, reaction types, and energy groups, respectively.

- Because of the data uncertainties, there can be an infinitely different set of cross section inputs to Q. This may result in different Q's as many as the number of input sets. Let's designate the k-th cross section input set which may be sampled from the cross section distribution.

$$Q_k \equiv Q(\cdots, \underbrace{\cdots, \left(x_{r,g}^{n}\right)_k, \cdots}_{\left(x_{r,g}^{n}\right)_k\,(n \in I, r \in \Gamma, g \in G)}, \cdots) \qquad \text{(A.2)}$$

Uncertainty Quantification (2/3)

- The mean of Q, $\overline{Q}$, and its variance $\sigma^2[Q]$ can be given by

$$\overline{Q} = \lim_{N\to\infty} \frac{1}{N} \sum_{k=1}^{N} Q_k \qquad \text{(A.3)}$$

$$\sigma^2[Q] = \lim_{N\to\infty} \frac{1}{N-1} \sum_{k=1}^{N} \left(Q_k - \overline{Q}\right)^2 \qquad \text{(A.4)}$$

- Let's assume that $\overline{Q}$ is determined by

$$\overline{Q} \equiv Q(\cdots, \underbrace{\cdots, \overline{x_{r,g}^n}, \cdots}_{\overline{x_{r,g}^n}(n\in I, r\in\Gamma, g\in G)}, \cdots) \qquad \text{(A.5)}$$

with $\overline{x_{r,g}^n}$ denoting the mean of the cross section which is defined in the same way as $\overline{Q}$ in Eq. (A.3).

- From the Taylor series expansion of Eq. (A.2) to the first order of the cross section variations about their mean values, $(Q_k - \overline{Q})$ in Eq. (A.4) leads to

$$Q_k - \overline{Q} \cong \sum_{n,r,g} \left(\left(x_{r,g}^n\right)_k - \overline{x_{r,g}^n} \right) \frac{\partial Q}{\partial x_{r,g}^n} \qquad \text{(A.6)}$$

Uncertainty Quantification (3/3)

- The substitution of Eq. (A.6) into Eq. (A.4) results in

$$\sigma^2[Q] \cong \sum_{n,r,g} \sum_{n',r',g'} \mathrm{cov}[x^n_{r,g}, x^{n'}_{r',g'}] \left(\frac{\partial Q}{\partial x^n_{r,g}} \right) \left(\frac{\partial Q}{\partial x^{n'}_{r',g'}} \right); \qquad \text{(A.7)}$$

$$\mathrm{cov}[x^n_{r,g}, x^{n'}_{r',g'}] = \lim_{N\to\infty} \frac{1}{N-1} \sum_{k=1}^{N} \left(\left(x^n_{r,g} \right)_k - \overline{x^n_{r,g}} \right) \left(\left(x^{n'}_{r',g'} \right)_k - \overline{x^{n'}_{r',g'}} \right) \qquad \text{(A.8)}$$

- Introducing the sensitivity coefficient of Q to $x^n_{r,g}$, $S_Q[x^n_{r,g}]$ defined by

$$S_Q[x^n_{r,g}] \equiv \frac{\overline{x^n_{r,g}}}{\overline{Q}} \cdot \frac{\partial Q}{\partial x^n_{r,g}} \qquad \text{(A.9)}$$

the relative variance from Eq. (A.7) can be expressed as

$$\boxed{\left(\frac{\sigma[Q]}{\overline{Q}} \right)^2 \cong \sum_{i,r,g} \sum_{i',r',g'} \frac{\mathrm{cov}[x^n_{r,g}, x^{n'}_{r',g'}]}{\overline{x^n_{r,g}} \cdot \overline{x^{n'}_{r',g'}}} S_Q[x^n_{r,g}] S_Q[x^{n'}_{r',g'}]} \qquad \text{(A.10)}$$

where $\mathrm{cov}[x^n_{r,g}, x^{n'}_{r',g'}] \Big/ (\overline{x^n_{r,g}} \cdot \overline{x^{n'}_{r',g'}})$ means the relative covariance between $x^n_{r,g}$ and $x^{n'}_{r',g'}$.

Benefit of Adjoint Weight Function (1/4)

- This conventional perturbation theory for the critical eigenvalue is excerpted from Ref. [7].

  [7] M. L. Williams, "CRC Handbook of Nuclear Reactors Calculations Volume III, Perturbation Theory for Nuclear Reactor Analysis," Y. Ronen, Ed., CRC Press, Boca Raton, FL, 1986.

- The steady-state Boltzmann transport equation can be written in an operator notation as

$$\boxed{\mathbf{M}\phi = \lambda \mathbf{F}\phi} \qquad (1)$$

ϕ is the angular flux and λ is the lambda mode eigenvalue defined by $1/k$. The net loss operator **M** and the fission production operator **F** are defined by

$$\mathbf{M}\phi = \left[\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\ \phi(\mathbf{r},E,\mathbf{\Omega}) - \int dE' \int d\mathbf{\Omega}' \Sigma_s(\mathbf{r};E',\mathbf{\Omega}' \rightarrow E,\mathbf{\Omega})\phi(\mathbf{r},E',\mathbf{\Omega}'), \qquad (2)$$

$$\mathbf{F}\phi = \frac{\chi(E)}{4\pi} \int dE' \int d\mathbf{\Omega}' \nu(E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E',\mathbf{\Omega}') \qquad (3)$$

Σ_t, Σ_s, and Σ_f are the total, scattering and fission cross-sections, respectively. ν is the mean number of fission neutrons produced from a fission reaction. χ is the energy spectrum of fission neutrons.

Benefit of Adjoint Weight Function(2/4)

- If we take the inner product of both sides of Eq. (1) with some arbitrary, nonzero weight function w, and solve for λ, the following expression is obtained

$$\lambda = \frac{< w, \mathbf{M}\phi >}{< w, \mathbf{F}\phi >} \qquad \text{(B.1)}$$

where the angle bracket notation indicates the integration over the domain of a product of two functions.

- The equation for a perturbed system by a change of the cross-section x can be written as

$$(\mathbf{M}+\Delta\mathbf{M})(\phi+\Delta\phi) = (\lambda+\Delta\lambda)(\mathbf{F}+\Delta\mathbf{F})(\phi+\Delta\phi) \qquad \text{(B.2)}$$

$$\Delta\mathbf{M} = \frac{\partial\mathbf{M}}{\partial x}\Delta x \qquad \text{(B.3)}$$

$$\Delta\mathbf{F} = \frac{\partial\mathbf{F}}{\partial x}\Delta x \qquad \text{(B.4)}$$

Benefit of Adjoint Weight Function(3/4)

- Taking the inner product of both sides of Eq. (B.2) with a weight function $w(\mathbf{r}, E, \mathbf{\Omega})$ and solving for the change in the eigenvalue, one can obtain

$$\Delta\lambda = \frac{< w, \left(\Delta\mathbf{M} - \lambda\Delta\mathbf{F}\right)\left(\phi + \Delta\phi\right) > + < w, \left(\mathbf{M} - \lambda\mathbf{F}\right)\Delta\phi >}{< w, \left(\mathbf{F} + \Delta\mathbf{F}\right)\left(\phi + \Delta\phi\right) >} \qquad \text{(B.5)}$$

- By neglecting products of perturbations in Eq. (B.5), a first-order estimate for the eigenvalue perturbation can be written as

$$\boxed{\Delta\lambda \cong \frac{< w, \left(\Delta\mathbf{M} - \lambda\Delta\mathbf{F}\right)\phi > + < w, \left(\mathbf{M} - \lambda\mathbf{F}\right)\Delta\phi >}{< w, \mathbf{F}\phi >}} \qquad \text{(B.6)}$$

Benefit of Adjoint Weight Function (4/4)

- Suppose that w is chosen to be the λ-mode adjoint function ϕ^* that obeys

$$\mathbf{M}^*\phi^* = \lambda \mathbf{F}^*\phi^* \qquad \text{(B.7)}$$

where the adjoint operators are defined by

$$\mathbf{M}^*\phi^* = \left[-\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\phi^*(\mathbf{r},E,\mathbf{\Omega}) - \int dE' \int d\mathbf{\Omega}' \Sigma_s(\mathbf{r};E,\mathbf{\Omega}\to E',\mathbf{\Omega}')\phi^*(\mathbf{r},E',\mathbf{\Omega}'), \qquad \text{(B.8)}$$

$$\mathbf{F}^*\phi^* = \int dE' \int d\mathbf{\Omega}' \frac{\chi(E')}{4\pi} \nu(E)\Sigma_f(\mathbf{r},E)\phi^*(\mathbf{r},E',\mathbf{\Omega}') \qquad \text{(B.9)}$$

- Because $<\phi^*,(\mathbf{M}-\lambda\mathbf{F})\Delta\phi> = <\Delta\phi,(\mathbf{M}^*-\lambda\mathbf{F}^*)\phi^*> = 0$ by Eq. (B.7), Eq. (B.6) can be reduced to

$$\boxed{\frac{\Delta\lambda}{\lambda} \cong \frac{<\phi^*,(\Delta\mathbf{M}-\lambda\Delta\mathbf{F})\phi>}{\lambda<\phi^*,\mathbf{F}\phi>}} \qquad \text{(B.10)}$$

- From the definition of k, Eq. (B.10) can be rewritten as

$$\frac{\Delta k}{k} \cong \frac{<\phi^*,\left(\frac{1}{k}\Delta\mathbf{F}-\Delta\mathbf{M}\right)\phi>}{<\phi^*,\frac{\mathbf{F}}{k}\phi>} \qquad \text{(B.11)}$$