Monte Carlo
Perturbation Techniques

Shim, Hyung Jin

Nuclear Engineering Department,
Seoul National University

Background of MC Perturbation Techniques

- The two conventional MC perturbation techniques - the correlated sampling and differential operator sampling (DOS) methods - have been applied [1] to estimate the **temperature coefficient of the coolant in a D_2O test reactor**.

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

- Nagaya and Mori [2] strengthened the two conventional methods by taking into account the fission source perturbation (FSP).

  ([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).

- Recently, the MC perturbation techniques based on the adjoint flux estimated in the MC forward calculations have been developed and successfully applied for the density perturbation problems [3] and the nuclear data sensitivity and uncertainty (S/U) analyses [4].

  ([3] B. Kiedrowski, F. B. Brown, P. P. H. Wilson, "Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo," *Nucl. Sci. Eng.*, **168**, 226 (2011).)

  ([4] H. J. Shim, C. H. Kim, "Adjoint Sensitivity and Uncertainty Analyses in Monte Carlo Forward Calculations," *J. Nucl. Sci. Technol.*, **48**[12], 1453 (2011).)

- It is notable that the first-order DOS method with FSP (DOS/FSP method hereafter) is equivalent to the first-order adjoint weighted perturbation (AWP) method [4].

A. Steady-State Boltzmann Transport Equation

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

$$\mathbf{T}\phi = \frac{1}{k}\mathbf{F}\phi \qquad \text{(A.1)}$$

- The net loss operator **T** and the fission production operator **F** are defined by

$$\mathbf{T}\phi = \left[\mathbf{\Omega}\cdot\nabla + \Sigma_t(\mathbf{r},E)\right]\ \phi(\mathbf{r},E,\mathbf{\Omega}) - \int dE' \int d\mathbf{\Omega}'\Sigma_s(\mathbf{r};E',\mathbf{\Omega}' \to E,\mathbf{\Omega})\phi(\mathbf{r},E',\mathbf{\Omega}') \qquad \text{(A.2)}$$

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

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. *c* is the energy spectrum of fission neutrons.

A. Steady-State BTE (Contd.)

- By operating $\lambda \mathbf{F}\mathbf{T}^{-1}$ on its both sides of Eq. (A.1), it can be expressed as the following eigenvalue equation.

$$S = \frac{1}{k}\mathbf{H}S \qquad \text{(A.4)}$$

where the fission source density (FSD) S and the fission operator $\mathbf{H}$ are defined as

$$S \equiv \frac{1}{k}\mathbf{F}\phi \qquad \text{(A.5)}$$

$$\mathbf{H} = \mathbf{F}\mathbf{T}^{-1} \qquad \text{(A.6)}$$

Note that 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. (A.4) implies

$$\mathbf{H}S = \int d\mathbf{P}' H(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}') \qquad \text{(A.7)}$$

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

In order to derive an MC perturbation algorithm, we apply the solution of the collision density equation to the perturbation formulation.

B. Collision Density Equation

- The integral equation for the collision density $\psi(\mathbf{P})$ defined by $\Sigma_t(\mathbf{r},E)\phi(\mathbf{P})$ can be written as

$$\psi(\mathbf{P}) = \int d\mathbf{r}' T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) S(\mathbf{r}',E,\mathbf{\Omega}) + \int d\mathbf{P}' K_s(\mathbf{P}' \to \mathbf{P}) \psi(\mathbf{P}') \quad \cdots\cdots \quad \text{(B.1)}$$

K_s is defined by the product of the scattering collision kernel, C_s and the transition kernel [B.1] (or the free flight kernel), T:

$$K_s(\mathbf{P}' \to \mathbf{P}) = T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) \cdot C_s(\mathbf{r}';E',\mathbf{\Omega}' \to E,\mathbf{\Omega}); \quad \cdots\cdots \quad \text{(B.2)}$$

$$C_s(\mathbf{r}';E',\mathbf{\Omega}' \to E,\mathbf{\Omega}) = \sum_{r \neq fis.} \nu_r \frac{\Sigma_r(\mathbf{r}';E',\mathbf{\Omega}')}{\Sigma_t(\mathbf{r}',E')} f_r(E',\mathbf{\Omega}' \to E,\mathbf{\Omega}) \quad \cdots\cdots \quad \text{(B.3)}$$

$$T(E,\mathbf{\Omega};\mathbf{r}' \to \mathbf{r}) = \frac{\Sigma_t(\mathbf{r},E)}{|\mathbf{r}-\mathbf{r}'|^2} \exp\left[-\int_0^{|\mathbf{r}-\mathbf{r}'|} \Sigma_t\left(\mathbf{r} - s\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}, E\right) ds \right] \delta\left(\mathbf{\Omega} \cdot \frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} - 1 \right) \quad \cdots\cdots \quad \text{(B.4)}$$

ν_r is the average number of neutrons produced from a reaction type r and f_r is the probability that a collision of type r by a neutron of direction $\mathbf{\Omega}'$ and energy E' will produce a neutron in direction interval $d\Omega$ about $\mathbf{\Omega}$ with energy in dE about E.

([B.1] I. Lux, L. Koblinger, “Monte Carlo Particle Transport Methods: Neutron and Photon Calculations,” CRC Press (1991).)

B. Collision Density Equation (Contd.)

- For further derivations, we define the fission collision kernel by

$$C_f(\mathbf{r}; E', \mathbf{\Omega}' \to E, \mathbf{\Omega}) = \frac{\chi(E' \to E)}{4\pi} \cdot \frac{\nu(E')\Sigma_f(\mathbf{r}, E')}{\Sigma_t(\mathbf{r}, E')} \quad \text{(B.5)}$$

- From the Neumann series solution of Eq. (B.1) [B.1], the angular flux $\phi(\mathbf{P})$ can be expressed as

$$\phi(\mathbf{P}) = \frac{1}{\Sigma_t(\mathbf{r}, E)} \sum_{j=0}^{\infty} \psi_j(\mathbf{P}); \quad \text{(B.6)}$$

$$\psi_j(\mathbf{P}) = \int d\mathbf{P}_0 K_{s,j}(\mathbf{P}_0 \to \mathbf{P}) \int d\mathbf{r}' T(E', \mathbf{\Omega}'; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}', E', \mathbf{\Omega}'), \quad \text{(B.7)}$$

where the j-th scattering transport kernel, $K_{s,j}$ is defined by

$$\begin{aligned} K_{s,0}(\mathbf{P}_0 \to \mathbf{P}) &= \delta(\mathbf{P}_0 - \mathbf{P}), \\ K_{s,1}(\mathbf{P}_0 \to \mathbf{P}) &= K_s(\mathbf{P}_0 \to \mathbf{P}), \\ K_{s,j}(\mathbf{P}_0 \to \mathbf{P}) &= \int d\mathbf{P}_{j-1} \cdots \int d\mathbf{P}_1 K_s(\mathbf{P}_{j-1} \to \mathbf{P}) \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1);\ j = 2, 3, \cdots, \end{aligned} \quad \text{(B.8)}$$

and $E_0 = E'$, $\mathbf{\Omega}_0 = \mathbf{\Omega}'$.

B. Collision Density Equation (Contd.)

- By inserting Eq. (B.6) into Eq. (A.3), the definition of *S* of Eq. (A.5) can be written as

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

$$\phi(\mathbf{P}) = \frac{1}{\Sigma_t(\mathbf{r}, E)} \sum_{j=0}^{\infty} \psi_j(\mathbf{P});$$

$$S \equiv \frac{1}{k}\mathbf{F}\phi \quad \Rightarrow \quad S(\mathbf{P}) = \frac{1}{k}\int dE'' \int d\mathbf{\Omega}'' C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) \sum_{j=0}^{\infty} \psi_j(\mathbf{r}, E'', \mathbf{\Omega}'') \qquad \text{(B.9)}$$

- Insertion of Eq. (B.7) into Eq. (B.9) leads to

$$\mathbf{H}S = \int d\mathbf{P}' H(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}'); \qquad \text{(B.10)}$$

$$H(\mathbf{P}' \to \mathbf{P}) S(\mathbf{P}') =$$

$$\sum_{j=0}^{\infty} \int dE'' \int d\mathbf{\Omega}'' C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) \int d\mathbf{P}_0 K_{s,j}(\mathbf{P}_0 \to \mathbf{r}, E'', \mathbf{\Omega}'') \int d\mathbf{r}' T(E', \mathbf{\Omega}'; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{P}') \qquad \text{(B.11)}$$

Perturbation of a Tally Q

- By Taylor's series expansion, the variation of a tally Q due to a deviation of a input parameter α, denoted by $\Delta\alpha$, can be expressed as

$$Q(\alpha+\Delta\alpha)-Q(\alpha)\equiv\delta Q(\alpha)=\sum_{n=1}^{\infty}\frac{1}{n!}\frac{d^nQ}{d\alpha^n}(\Delta\alpha)^n=\sum_{n=1}^{\infty}\frac{1}{n!}U_n(\Delta\alpha)^n \quad \cdots\cdots (1)$$

where

$$U_n=\frac{d^nQ}{d\alpha^n} \quad \cdots\cdots (2)$$

- And the tally Q can be written using the corresponding detector response g and the collision density Ψ in the MC simulation as follows:

$$Q=\int g(\mathbf{P})\Psi(\mathbf{P})d\mathbf{P} \quad \cdots\cdots (3)$$

where $\mathbf{P}$ denotes the six-dimensional phase space vector ($\mathbf{r}$, E, $\mathbf{\Omega}$).

Perturbation of a Tally Q (Contd)

- Using the Neumann series solution of the collision density equation, the first order sensitivity U_1 can be expressed as

$$U_1 = \frac{dQ}{dx} = \sum_j U_{1,j}; \qquad \text{(4)}$$

$$\begin{aligned} U_{1,j} &= \frac{\partial}{\partial x}\left[\int d\mathbf{P} g(\mathbf{P}) \psi_j(\mathbf{P})\right] \\ &= \frac{\partial}{\partial x}\left[\int d\mathbf{P} g(\mathbf{P})\left(\int d\mathbf{P}_0 K_{s,j}(\mathbf{P}_0 \to \mathbf{P}) \int d\mathbf{r}' T(E',\mathbf{\Omega}';\mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}',E',\mathbf{\Omega}')\right)\right] \qquad \text{(5)} \end{aligned}$$

Differential Operator Sampling (DOS) + Perturbed Source Effect (PSE)

- In the differential operator sampling (DOS) method augmented by the fission source perturbation method, Eq. (5) can be written as

$$U_{1,j} = \int d\mathbf{P} \cdots \int d\mathbf{P}_0 \int d\mathbf{r}' \left\{ \begin{aligned} &\frac{1}{q(\mathbf{P})}\frac{\partial q(\mathbf{P})}{\partial x} + \sum_{k=1}^{j} \frac{1}{K_s(\mathbf{P}_{k-1} \to \mathbf{P}_k)} \frac{\partial K_s(\mathbf{P}_{k-1} \to \mathbf{P}_k)}{\partial x} \\ &+ \frac{1}{T(E',\mathbf{\Omega}';\mathbf{r}' \to \mathbf{r}_0)} \frac{\partial T(E',\mathbf{\Omega}';\mathbf{r}' \to \mathbf{r}_0)}{\partial x} + \frac{1}{S(\mathbf{P}')}\frac{\partial S(\mathbf{P}')}{\partial x} \end{aligned} \right\}$$

$$\cdot \left\{ q(\mathbf{P}) K_s(\mathbf{P}_{j-1} \to \mathbf{P}) \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1) T(E',\mathbf{\Omega}';\mathbf{r}' \to \mathbf{r}_0) S(\mathbf{P}') \right\}$$

$$= \int d\mathbf{P} \cdots \int d\mathbf{P}_0 \int d\mathbf{r}' \left\{ u^{1q}(\mathbf{P}) + \sum_{k=0}^{j} u^{1K}(\mathbf{P}_{k-1} \to \mathbf{P}_k) + u^{1S}(\mathbf{P}') \right\}$$

$$\cdot \left\{ q(\mathbf{P}) K_s(\mathbf{P}_{j-1} \to \mathbf{P}) \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1) T(E',\mathbf{\Omega}';\mathbf{r}' \to \mathbf{r}_0) S(\mathbf{P}') \right\} \quad \cdots\cdots (6)$$

First Order DOS + PSE (Contd.)

where

$$u^{1q}(\mathbf{P}) \equiv \frac{1}{q(\mathbf{P})}\frac{\partial q(\mathbf{P})}{\partial x} \quad \cdots\cdots \quad (7)$$

$= \text{first order sensitivity response of } Q$

$$u^{1K}(\mathbf{P}_{k-1} \to \mathbf{P}_k) \equiv \begin{cases} \dfrac{1}{K_s(\mathbf{P}_{k-1} \to \mathbf{P}_k)}\dfrac{\partial K_s(\mathbf{P}_{k-1} \to \mathbf{P}_k)}{\partial x} & (k = 1, 2, \cdots) \\ \dfrac{1}{T(E', \mathbf{\Omega}'; \mathbf{r}' \to \mathbf{r}_0)}\dfrac{\partial T(E', \mathbf{\Omega}'; \mathbf{r}' \to \mathbf{r}_0)}{\partial x} & (k = 0) \end{cases} \quad \cdots\cdots \quad (8)$$

$= \text{first order sensitivity response of transport kernel}$

$$u^{1S}(\mathbf{P}') \equiv \frac{1}{S(\mathbf{P}')}\frac{\partial S(\mathbf{P}')}{\partial x} \quad \cdots\cdots \quad (9)$$

$= \text{first order sensitivity response of fission source distribution}$

and $\mathbf{P}_j = \mathbf{P}$.

Cf. *k* Sensitivity Formulation

- In the MC adjoint-weighted perturbation method, the variation of k due to a change of parameter *x* is expressed by

$$\boxed{\frac{\Delta k_0}{k_0} \cong \frac{<\phi_0^\dagger, \Delta \mathbf{H} S_0>}{<\phi_0^\dagger, \mathbf{H} S_0>}} \quad \cdots\cdots \quad \text{(C.1)}$$

- Using the iterated fission probability concept for the adjoint flux, Eq. (C.1) is written as

$$\boxed{\Delta k_0 \cong \frac{1}{k_0{}^n} < \mathbf{H}^n, \Delta \mathbf{H} S_0 >} \quad \cdots\cdots \quad \text{(C.2)}$$

Cf. *k* Sensitivity Formulation (Contd)

- Now, consider an MC algorithm for how to calculate (Δk_0) in the course of the cycle-by-cycle FSD and eigenvalue estimates. To do so, note that, when expressed explicitly in terms of the transport kernels, **H***S* of Eq. (C.2) is given by

$$\mathbf{H}S = \sum_{j=0}^{\infty} \int dE'' \int d\mathbf{\Omega}'' C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) \int d\mathbf{P}_0 K_{s,j}(\mathbf{P}_0 \to \mathbf{r}, E'', \mathbf{\Omega}'') \int d\mathbf{r}' T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}', E_0, \mathbf{\Omega}_0)$$

(B.11)

- Then $\Delta\mathbf{H}S$ in Eq. (C.2) can be expressed as

$$\begin{aligned}
\Delta\mathbf{H}S &= \left(\Delta x \frac{\partial \mathbf{H}}{\partial x}\right) S \\
&= \Delta x \sum_{p=0}^{\infty} \int dE'' \int d\mathbf{\Omega}'' \int d\mathbf{P}_{p-1} \cdots \int d\mathbf{P}_0 \int d\mathbf{r}' \\
&\qquad \otimes \frac{\partial}{\partial x} \left\{ C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) K_s(\mathbf{P}_{p-1} \to \mathbf{r}, E'', \mathbf{\Omega}'') \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1) T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) \right\} S(\mathbf{r}', E_0, \mathbf{\Omega}_0) \\
&= \Delta x \sum_{p=0}^{\infty} \int dE'' \int d\mathbf{\Omega}'' \int d\mathbf{P}_{p-1} \cdots \int d\mathbf{P}_0 \int d\mathbf{r}' \, u^p(\mathbf{r}', E_0, \mathbf{\Omega}_0 \to \mathbf{P}) \\
&\qquad \otimes \left\{ C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) K_s(\mathbf{P}_{p-1} \to \mathbf{r}, E'', \mathbf{\Omega}'') \cdots K_s(\mathbf{P}_0 \to \mathbf{P}_1) T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) \right\} S(\mathbf{r}', E_0, \mathbf{\Omega}_0);
\end{aligned}$$

(C.3)

Cf. k Sensitivity Formulation (Contd)

$$u^p(\mathbf{r}', E_0, \mathbf{\Omega}_0 \to \mathbf{P}) = u_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega})$$
$$+ u_K(\mathbf{P}_{p-1} \to \mathbf{r}, E'', \mathbf{\Omega}'') + \sum_{k=0}^{p-2} u_K(\mathbf{P}_k \to \mathbf{P}_{k+1}) + u_T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0), \quad \text{(C.4)}$$

$$u_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega}) = \frac{1}{C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega})} \frac{\partial C_f(\mathbf{r}; E'', \mathbf{\Omega}'' \to E, \mathbf{\Omega})}{\partial x} \quad \text{(C.5)}$$

$$u_K(\mathbf{P}_k \to \mathbf{P}_{k+1}) = \frac{1}{K_s(\mathbf{P}_k \to \mathbf{P}_{k+1})} \frac{\partial K_s(\mathbf{P}_k \to \mathbf{P}_{k+1})}{\partial x} \quad \text{(C.6)}$$

$$u_T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) = \frac{1}{T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0)} \frac{\partial T(E_0, \mathbf{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0)}{\partial x} \quad \text{(C.7)}$$

Algorithm of the First Order DOS + PSE Method

- In Monte Carlo random walk process, when the *k*-th track starts with a neutron undergoing reaction type "*a*" with isotope *i'* at energy $E_{k\text{-}1}$ and $\mathbf{\Omega}_{k\text{-}1}$ is scattered to E_k and $\mathbf{\Omega}_{k,}$ and continues for a track length λ_k and collides, the sampled scattering collision kernel and the sampled free flight kernel can be written as

$$C_{s,k} \equiv C_s(\mathbf{r}_{k-1}; E_{k-1}, \mathbf{\Omega}_{k-1} \to E_k, \mathbf{\Omega}_k)$$

$$= \nu_a^{i'} \frac{N^{i'} \sigma_a^{i'}(E_{k-1})}{\Sigma_t(E_{k-1})} f_a^{i'}(E_{k-1}, \mathbf{\Omega}_{k-1} \to E_k, \mathbf{\Omega}_k) \qquad \cdots\cdots (10)$$

$$T_k \equiv T(E_k, \mathbf{\Omega}_k; \mathbf{r}_{k-1} \to \mathbf{r}_k) = \frac{\Sigma_t(E_k)}{\lambda_k^{\ 2}} \exp\left[-\Sigma_t(E_k)\lambda_k\right] \qquad \cdots\cdots (11)$$

- Using Eqs. (10) and (11), the first order sensitivity of the transport kernel of Eq. (8) for the *k*-th track can be calculated by

$$u_k^{1K} = \begin{cases} \dfrac{1}{C_{s,k}} \dfrac{\partial C_{s,k}}{\partial x} + \dfrac{1}{T_k} \dfrac{\partial T_k}{\partial x} & (k = 1, 2, \cdots) \\ \dfrac{1}{T_k} \dfrac{\partial T_k}{\partial x} & (k = 0) \end{cases} \qquad \cdots\cdots (12)$$

First Order DOS + PSE Algorithm (Contd.)

- For a deviation of a capture xs of nuclide i, Eq. (12) can be calculated using

$$\frac{1}{C_{s,k}}\frac{\partial C_{s,k}}{\partial \alpha}=\frac{1}{\nu_a^{i'}\dfrac{N^{i'}\sigma_a^{i'}(E_{k-1})}{\Sigma_t(E_{k-1})}f_a^{i'}(E_{k-1},\mathbf{\Omega}_{k-1}\rightarrow E_k,\mathbf{\Omega}_k)}\otimes\begin{pmatrix}\nu_a^{i'}\dfrac{N^{i'}\delta_{ii'}\delta_{a\gamma}}{\Sigma_t(E_{k-1})}f_a^{i'}(E_{k-1},\mathbf{\Omega}_{k-1}\rightarrow E_k,\mathbf{\Omega}_k)\\ -\nu_a^{i'}N^i\dfrac{N^{i'}\sigma_a^{i'}(E_{k-1})}{\Sigma_t(E_{k-1})^2}f_a^{i'}(E_{k-1},\mathbf{\Omega}_{k-1}\rightarrow E_k,\mathbf{\Omega}_k)\end{pmatrix}=\frac{1}{\sigma_a^i(E_{k-1})}\delta_{ii'}\delta_{a\gamma}-\frac{N^i}{\Sigma_t(E_{k-1})} \quad \text{.........} \quad (13)$$

$$\frac{1}{T_k}\frac{\partial T_k}{\partial \alpha}=\frac{1}{\dfrac{\Sigma_t(E_k)}{\lambda_k{}^2}\exp\left[-\Sigma_t(E_k)\lambda_k\right]}\begin{pmatrix}\dfrac{N^i}{\lambda_k{}^2}\exp\left[-\Sigma_t(E_k)\lambda_k\right]\\ -\lambda_k N^i\dfrac{\Sigma_t(E_k)}{\lambda_k{}^2}\exp\left[-\Sigma_t(E_k)\lambda_k\right]\end{pmatrix}=\frac{N^i}{\Sigma_t(E_k)}-\lambda_k N^i \quad \text{.........} \quad (14)$$

- For a deviation of ν_f of nuclide i in the MC eigenvalue calculations, u^{1K} becomes zero.

First Order DOS + PSE Algorithm (Contd.)

- For $q_f(P)$ $(=\nu\Sigma_f/\Sigma_t)$ which denotes a response function for the collision estimator of k_{eff}, the first order sensitivity u^{1qf} from the k-th track can be calculated by

$$u_k^{1q_f} = \frac{\Sigma_t(\mathbf{r}_k, E_k)}{\nu_f(\mathbf{r}_k, E_k)\Sigma_f(\mathbf{r}_k, E_k)} \frac{\partial}{\partial x}\left(\frac{\nu_f(\mathbf{r}_k, E_k)\Sigma_f(\mathbf{r}_k, E_k)}{\Sigma_t(\mathbf{r}_k, E_k)}\right) \qquad (15a)$$

- For a deviation of a capture xs of nuclide i, Eq. (15) can be written as

$$u_k^{1q_f} = -\frac{N^i}{\Sigma_t(\mathbf{r}_k, E_k)} \qquad (15b)$$

- And for a deviation of ν_f of nuclide i, u^{1qf} can be calculated by

$$u_k^{1q_f} = \frac{1}{\nu_f^i(\mathbf{r}_k, E_k)} \qquad (15c)$$

Source Perturbation Algorithm

- In the MC power method, S for the next cycle i, S_i is updated as

$$S_i = \frac{1}{k_{i-1}} \mathbf{H} S_{i-1}; \qquad \text{(16)}$$

$$k_{i-1} = < \mathbf{H} S_{i-1} > \qquad \text{(17)}$$

- From Eqs. (16) and (17), the sensitivity of S_i to the parameter x can be written as

$$\begin{aligned}\frac{\partial S_i}{\partial x} &= \frac{1}{k_{i-1}}\left(\frac{\partial \mathbf{H}}{\partial x} S_{i-1} + \mathbf{H}\frac{\partial S_{i-1}}{\partial x}\right) - \frac{\mathbf{H} S_{i-1}}{k_{i-1}{}^2}\left(< \frac{\partial \mathbf{H}}{\partial x} S_{i-1} > + < \mathbf{H}\frac{\partial S_{i-1}}{\partial x} > \right) \\ &= \frac{1}{k_{i-1}}\left\{\frac{\partial \mathbf{H}}{\partial x} S_{i-1} + \mathbf{H}\frac{\partial S_{i-1}}{\partial x} - S_i\left(< \frac{\partial \mathbf{H}}{\partial x} S_{i-1} > + < \mathbf{H}\frac{\partial S_{i-1}}{\partial x} > \right)\right\} \qquad \text{(18)}\end{aligned}$$

Source Perturbation Algorithm (Contd)

- Then u^{1S} in Eq. (9) can be written as

$$\frac{1}{S_i}\frac{\partial S_i}{\partial x} = \frac{1}{k_{i-1}\cdot S_i}\left(\frac{\partial \mathbf{H}}{\partial x}S_{i-1} + \mathbf{H}\frac{\partial S_{i-1}}{\partial x}\right) - \frac{1}{k_{i-1}}\left(<\frac{\partial \mathbf{H}}{\partial x}S_{i-1}> + <\mathbf{H}\frac{\partial S_{i-1}}{\partial x}>\right)$$

$$= \frac{1}{\cancel{k_{i-1}}\cdot\frac{1}{\cancel{k_{i-1}}}\mathbf{H}S_{i-1}}\left(\frac{\partial \mathbf{H}}{\partial x}S_{i-1} + \mathbf{H}\frac{\partial S_{i-1}}{\partial x}\right) - \frac{1}{k_{i-1}}\left(<\frac{\partial \mathbf{H}}{\partial x}S_{i-1}> + <\mathbf{H}\frac{\partial S_{i-1}}{\partial x}>\right)$$

$$= \left(\frac{1}{\mathbf{H}S_{i-1}}\frac{\partial \mathbf{H}}{\partial x}S_{i-1} - \frac{1}{<\mathbf{H}S_{i-1}>}<\frac{\partial \mathbf{H}}{\partial x}S_{i-1}>\right)$$

$$+ \left(\frac{1}{\mathbf{H}S_{i-1}}\mathbf{H}\frac{1}{S_{i-1}}\frac{\partial S_{i-1}}{\partial x}S_{i-1} - \frac{1}{<\mathbf{H}S_{i-1}>}<\mathbf{H}\frac{1}{S_{i-1}}\frac{\partial S_{i-1}}{\partial x}S_{i-1}>\right)$$

$$= \left(\frac{1}{\mathbf{H}S_{i-1}}\frac{\partial \mathbf{H}}{\partial x}S_{i-1} - \frac{1}{<\mathbf{H}S_{i-1}>}<\frac{\partial \mathbf{H}}{\partial x}S_{i-1}>\right)$$

$$+ \left(\frac{1}{\mathbf{H}S_{i-1}}\cdot\left(\frac{1}{S_{i-1}}\frac{\partial S_{i-1}}{\partial x}\right)\mathbf{H}S_{i-1} - \frac{1}{<\mathbf{H}S_{i-1}>}<\left(\frac{1}{S_{i-1}}\frac{\partial S_{i-1}}{\partial x}\right)\mathbf{H}S_{i-1}>\right) \quad \cdots\cdots (19)$$

Dr. Nagaya's Algorithm

Generation i-1 (Obtained in the previous cycle)

Generation i — Given initial weight factor for $\frac{1}{S_i}\frac{\partial S_i}{\partial a}$: $\overline{w}'_{0,i}$

Random walk process

- Score 1st-order weight factor $w'_{f,n}$ at each fission site.
- Score $\overline{w}'_{0,i} w_{f,n}$ at each collision.

Collision estimate for k_{eff}

$$\left(w'_{f,n} = \frac{1}{C_{f,\ell}}\frac{\partial C_{f,\ell}}{\partial a} + \frac{1}{T_\ell}\frac{\partial T_\ell}{\partial a} + \cdots \right)$$

After random walk process

- Estimate $\frac{\partial k_{PS,i}}{\partial a}$: $Est\left[\frac{\partial k_{PS,i}}{\partial a}\right] = \frac{1}{N}\sum_n \overline{w}'_{0,i} w_{f,n}$
- Normalize 1st-order weight factor : $w'_{f,n}$

$$\overline{w}'_{0,i+1} = w'_{f,n} - \frac{1}{M_i}\sum_n n_{f,n} w'_{f,n}$$

Number of fission neutrons at site n

Number of particles generated in generation i

Generation i+1 — Given initial weight factor for $\frac{1}{S_{i+1}}\frac{\partial S_{i+1}}{\partial a}$: $\overline{w}'_{0,i+1}$

Correlated Sampling Method

- Recall that $\mathbf{H}S$ is given by

$$\mathbf{H}S = \sum_{j=0}^{\infty} \int dE'' \int d\boldsymbol{\Omega}'' C_f(\mathbf{r}; E'', \boldsymbol{\Omega}'' \to E, \boldsymbol{\Omega}) \int d\mathbf{P}_0 K_{s,j}(\mathbf{P}_0 \to \mathbf{r}, E'', \boldsymbol{\Omega}'')$$
$$\otimes \int d\mathbf{r}' T(E_0, \boldsymbol{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}', E_0, \boldsymbol{\Omega}_0) \quad \text{(B.11)}$$

- Then $\mathbf{H}S$ for a perturbed system can be expressed as

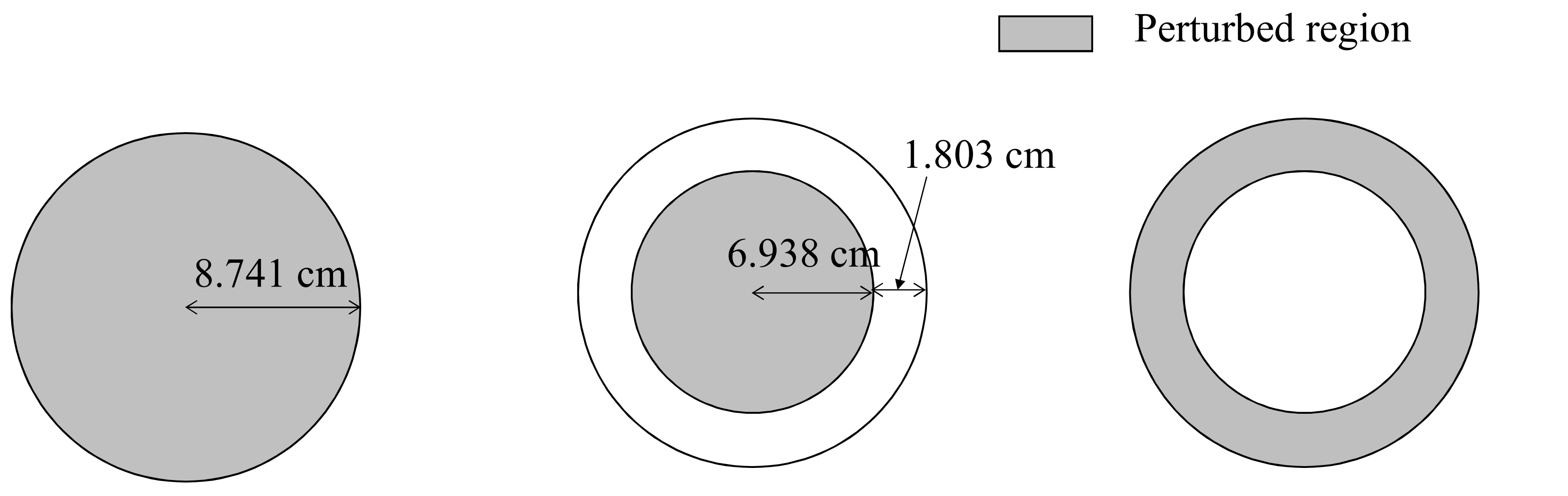
$$\mathbf{H}^* S = \sum_{j=0}^{\infty} \int dE'' \int d\boldsymbol{\Omega}'' C_f^*(\mathbf{r}; E'', \boldsymbol{\Omega}'' \to E, \boldsymbol{\Omega}) \int d\mathbf{P}_0 K_{s,j}^*(\mathbf{P}_0 \to \mathbf{r}, E'', \boldsymbol{\Omega}'')$$
$$\otimes \int d\mathbf{r}' T^*(E_0, \boldsymbol{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}', E_0, \boldsymbol{\Omega}_0) \quad (20)$$

- From Eqs. (B.11) and (20), $\Delta\mathbf{H}S$ can be calculated by

$$\Delta\mathbf{H}S = \mathbf{H}^* S - \mathbf{H}S$$
$$= \sum_{j=0}^{\infty} \int dE'' \int d\boldsymbol{\Omega}'' \int d\mathbf{P}_0 \int d\mathbf{r}' \left(\frac{C_f^*(\mathbf{r}; E'', \boldsymbol{\Omega}'' \to E, \boldsymbol{\Omega})}{C_f(\mathbf{r}; E'', \boldsymbol{\Omega}'' \to E, \boldsymbol{\Omega})} \cdot \prod_{p=0}^{j-1} \frac{K_s^*(\mathbf{P}_p \to \mathbf{P}_{p+1})}{K_s(\mathbf{P}_p \to \mathbf{P}_{p+1})} \cdot \frac{T^*(E_0, \boldsymbol{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0)}{T(E_0, \boldsymbol{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0)} - 1 \right)$$
$$\otimes C_f(\mathbf{r}; E'', \boldsymbol{\Omega}'' \to E, \boldsymbol{\Omega}) K_{s,j}(\mathbf{P}_0 \to \mathbf{r}, E'', \boldsymbol{\Omega}'') T\ (E_0, \boldsymbol{\Omega}_0; \mathbf{r}' \to \mathbf{r}_0) S(\mathbf{r}', E_0, \boldsymbol{\Omega}_0) \quad (21)$$

U^{235} Number Density Perturbation for Godiva Problems

- In order to investigate the accuracy of the new MC perturbation techniques, their results were compared with those calculated by direct subtractions for Godiva critical assembly problems.
- 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

(b) Central perturbation