Correlated Sampling

Perturbation calculations

- To determine the effect of small changes in the problem parameters on the solution to the problem.
- To examine the sensitivity of a solution to uncertainties in such factors as cross sections, material composition, geometry, source characteristics, etc.
- To identify the portions of a problem that must be specified to a high degree of accuracy and the portions that may be approximated without detriment to the solution.
- The accuracy, with which the changes are determined, depend on the calculational technique used, the fidelity to which the problem is modeled, and the convergence requirements placed on the calculation.

Perturbation calculations (cont.)

- All Monte Carlo results contain statistical errors independent of the inaccuracies that result from the usual factors related to the fidelity to which the problem is modeled.
- An attempt to compare answers obtained from two independent calculations that use nearly identical problem parameters is comparable to an attempt to compare the results of two nearly identical measurements.
- To have any validity, two independent Monte Carlo calculations that are used to analyze a perturbation in a system should have statistical uncertainties in the individual answers that are significantly smaller than the difference between those two results.

Perturbation calculations (cont.)

- *To estimate two quantities I_1 and I_2*

$$I_1 = \int g(x) f_1(x) dx \quad (1) \quad \text{and} \quad I_2 = \int g(x) f_2(x) dx \quad (2)$$

where $f_1(x)$ and $f_2(x)$ are probability density functions that reflect the baseline and perturbed cases, respectively.

- *With the corresponding estimates θ_1 and θ_2,*

$$\Delta\theta = \theta_1 - \theta_2 = \frac{1}{N}\sum_{i=1}^{N} g(X_i) - \frac{1}{N}\sum_{i=1}^{N} g(Y_i) = \frac{1}{N}\sum_{i=1}^{N} \Delta_i \,, \qquad (3)$$

where $\Delta_i = g(X_i) - g(Y_i)$. $\qquad (4)$

Perturbation calculations (cont.)

- The variances are

$$\sigma_1^2 = E\left[(\theta_1 - I_1)^2\right] \quad (5) \qquad \text{and} \qquad \sigma_2^2 = E\left[(\theta_2 - I_2)^2\right] \quad (6)$$

- Then the variance in difference b/w two estimates is

$$var(\theta_1 - \theta_2) = var(\theta_1) + var(\theta_2) - 2cov(\theta_1, \theta_2)$$

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 - 2cov(\theta_1, \theta_2) \qquad (7)$$

$$\text{where} \quad cov(\theta_1, \theta_2) = E\left[(\theta_1 - I_1)(\theta_2 - I_2)\right]. \qquad (8)$$

- The key to reduce the variance is to insure positive correlation between θ_1 and θ_2. This could be achieved by using the same sequence of random numbers for sampling both sets of random configurations X_i and Y_i.

Perturbation calculations (cont.)

- <u>If</u> the estimates θ_1 and θ_2 are statistically independent, then $cov(\theta_1, \theta_2) = 0$ and thus

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 , \qquad (9)$$

which is the best one can hope in estimating $I_1 - I_2$ using statistically independent Monte Carlo calculations for the baseline and perturbed results.

– This variance places a stringent limit on the reliability (or certainty) to which the change induced by the perturbation can be determined.

Perturbation calculations (cont.)

- *The result in (7) can be improved by using correlated calculations, instead of attempting to calculate two highly precise but statistically independent results, to reduce the uncertainty in the estimated difference. When the random variables X and Y in (3) are positively correlated, $\boxed{cov(\theta_1, \theta_2) > 0,}$ the variance in estimate for $\Delta\theta$ can be much less than that in (9).*

- *Positive correlation b/w the results can be obtained by correlated sampling i.e., by ensuring that every particle random walk, that does not involve an interaction in the perturbed portion of the problem, is the same in both of the calculations.*

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 - 2cov(\theta_1, \theta_2) \qquad (7)$$

$$\sigma^2 = \sigma_1^2 + \sigma_2^2 , \qquad (9)$$

Correlation Sampling

- To obtain the positive covariance or the correlation value of 1.
- By ensuring that every particle random walk, that does not involve an interaction in the perturbed portion of problem, is the same in both calculations.

  – As the effect of the perturbation goes to zero, those two calculations converge to the same result, independent of the statistical uncertainty in the individual answers, provided the same number of particles are tracked in both calculations.

  – Although the absolute uncertainty in the result remains as determined in the individual calculations, the uncertainty in the difference between those two calculations goes to zero as the calculation becomes identical.

  – The only difference between those two calculations is the changes produced by particle interactions or other events involving the perturbed region of the problem.

Correlation Sampling (cont.)

$$\sigma^2 = \sigma_1^{\,2} + \sigma_2^{\,2} - 2\,cov(\theta_1, \theta_2) \qquad (7)$$

- It is not essential that the individual uncertainties in the two answers be small, but only that the uncertainty in the difference between the two results be small.

- The key to correlated sampling in MC transport is to make sure that corresponding particle tracks in the baseline and the perturbed calculations use the same random number string.
  - Any particle that does not encounter the perturbed region of the problem scores the same in both calculations.
  - by using a second, separate, and independent random number generator.
  - There is always a risk that a portion of random number used in random walk of a particle be repeated.

Perturbation Calculation: example

- Sensitivity of the number of particles passing through a slab to the thickness of the slab?

  ---→ To examine the effect of an uncertainty in the thickness z [unit in the number of mean-free-path] of the slab on the number of particles passing through the slab.

- The probability of a normally incident particle passing through the baseline slab is

$$P_0 = e^{-z}$$

while the probability of a particle passing through the perturbed slab is

$$P_{pt} = e^{-z'}.$$

Perturbation Calculation: example (cont.)

- Assume a start particle weight of one, then the average of the weights of particles passing through the slab is

$$\langle x \rangle = \lim_{n\to\infty} \frac{1}{n} \sum_{n} x_i = e^{-z}$$

where x_i = 1 for particles that pass through the slab, and zero otherwise.

– Since $\langle x^2 \rangle = \langle x \rangle$ ($x_i = 1$ or 0), the standard deviation of <x> is

$$\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\langle x \rangle - \langle x \rangle^2} = \sqrt{e^{-z} - e^{-2z}}$$

which gives σ (z = 1) and σ' (z'=1.01).

Perturbation Calculation: example (cont.)

- For normally incident particles on a purely absorbing material, the change in the number of particles passing through the slab, with respect to the thickness of the slab, is

$$\frac{dP}{dz} = \frac{d}{dz}e^{-z} = -e^{-z},$$

where P is the probability of an incident particle passing through the slab.

– A linear approximation calculated analytically with the value z = 1 and z' = 1.01 gives

$$\left.\frac{dP}{dz}\right|_{z=1} \cong \frac{P_{pt} - P_0}{z' - z} = \frac{e^{-z'} - e^{-z}}{z' - z} = \frac{e^{-1.01} - e^{-1.00}}{0.01} = -0.3660.$$

Homework #5