The Effect of Small Perturbations in Multi-variant Calculations by PRIZMA-D code

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PRIZMA-D is a Monte Carlo code which solves eigenvalue problems for reactors and critical experiments. The code provides wide capabilities to define geometry, materials, tallies and variance reduction techniques. It is capable of tracking neutrons, photons, electrons, positrons and heavy charged particles with allowance for their mutual transformations.

The code solves a wide class of problems. It can be used, for example, to estimate:

1. the effective multiplication factor K_{eff}, neutron lifetime t_l from fission to fission, or the average number ν_{cp} of particles produced in fission;
2. some parameters (fluence, spectrum, dose) for the field of (n,γ)-radiation in reactor's vicinity;
3. the effect of (n,γ)-radiation on systems located in close proximity of a reactor;
4. penetration of neutrons and photons through a collimator and their effect on systems behind the collimator;
5. nuclear safety by predicting K_{eff} and the number of neutrons penetrating a container, with and without allowance for mirror reflection at its wall;

and other.

The tree of events is treated lexicographically. This approach suits the branching processes well but looses particle prehistory which often is needed if we want to calculate the scores of particles which underwent some specific events. In this case we use particle flagging which consists in applying special flags to particles, one flag for each particular event of interest. Then we define tally conditions – the list of flags which a particle must or must not carry. Using logical operations, we can define complex conditions combined of certain flags and some other particle parameters. The scores are tallied if only the condition is satisfied. The flags can be applied to or removed from a particle at the following phases of tracking:

- in the source after the particle has got its initial parameters;
- when the particle collides;
- after the type of particle interaction has been selected;
- after playing game with collision; and
- when the particle crosses a surface which separates one region from another.

In addition, there is a wide class of problems (for example, shielding applications) in which it is necessary to estimate the effect of small changes (perturbations) in some parameters on radiation characteristics. For these problems, it would be useful to correlate calculations of several variants where particle histories from the source to the perturbed region coincide. The problems are solved in the following setup.

A volume V is inserted in a system which consists of a source and a detector. The volume acts as a perturbation (in particular, it may contain a detector). It is necessary to estimate the effect of

1. Perturbed material: the variants differ in the material filling the volume V;
2. Increasing volume: V changes as
$V(1) = V_1$, $V(2) = V_1 + V2$,..., $V(k) = V_1 + V_2 + ... + V_k$.

3. Relocated volume: the volumes V(i), i= 1,…,k are defined in different locations of the system; they may differ in geometry and material;

4. Perturbed concentration: the variants differ in the concentration of materials in a region. The difference in concentration is defined using a complex material combined of several elementary substances; the weight concentration of one or several substances is changed (particularly, by changing only the density of material filling the region), the total weight concentration remaining equal to 1.

It is difficult to evaluate the effect of perturbations in independent runs because the expected differential effect is often several orders of magnitude smaller than the target quantity. A special method of correlated tracking was developed to obtain results in a single run.

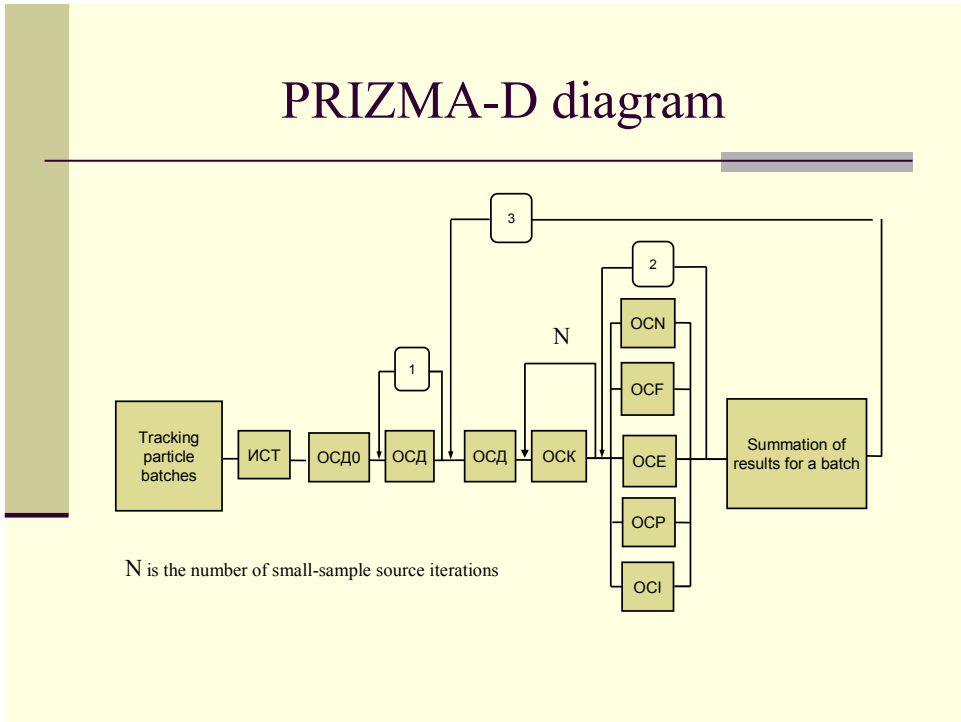
In problems corresponding to 1-3, one can consider two sorts of particles:

- the particles that do not enter the perturbed region; their scores are identical for all perturbations; and
- the particles that enter the perturbed region; their scores are identical until the perturbed region is entered.

Following from this feature, we developed a special technique of particle tracking. We define one flag for each perturbation, and apply all flags defined to source particles. When a source particle enters a perturbation region corresponding to one of the flags, it is split into two fragments: one wanders in the perturbed configuration (the other flags are removed), and the other wanders in the configuration without perturbations (it carries all flags except the one carried by the first fragment). In the case of perturbed concentrations, particles are tracked in the unperturbed configuration and their scores in perturbed configurations are changed using appropriate weight factors.

However, we have to resolve one more problem. The distribution of fission points in the source must correspond to the eigenfunction but each perturbation disturbs it. The problem can be solved in the following way.

Consider the block-diagram of the code PRIZMA-D.



- The ИСТ module defines the initial distribution of neutrons in a system.

- The ОСД_0 module defines the first fission points.
- In cycle 1 we get eigenvector (fission source distribution).
- In cycle 3 we track particles and tally their scores.

Cycle 3:

- The ОСД module gives the next generation of particles.
- The ОСК module tracks neutrons emitted from the fission points in the current generation (non-analog tracking is used if necessary).
- In cycle 2 we track secondary particles of other types.

When solving perturbation problems, we use a method of small source iterations which helps calculate the eigenvalue and the corresponding eigenvector in the OCK module.

Let M be the number of perturbations and N be the number of source iterations. At the first step, the fission source distribution obtained in the first part of cycle 3 for the unperturbed configuration is taken for all variants. In the OCK module, every neutron is tracked until it is absorbed, or escapes from the system, or reaches the N+1-th fission in the fission chain. The scores obtained for each variant at the i-th step ($1 \le i \le N$) are normalized to $n_{m,i}$ – the number of fission points at the previous (i-1) step. For example, if $n_{m,i+1}$ are fission points obtained at the i-th step, then $n_{m,i+1}/n_{m,i}$ is the unbiased estimate of K_{eff}. Thus, defining the number N of small iteration, we can take into account the effect of perturbations upon the fission source distribution for each variant. N is defined by users with respect to the degree of the perturbation effect.

The number of fission points $n_{m,i}$, obtained for each successive batch of source particles in the unperturbed variant, is random. That is why the scores for each particular configuration are normalized after the batch has been tracked. To estimate the perturbation effect, it is necessary to set a combined condition which defines the difference between the scores in perturbed and non-perturbed configurations. In this case we compare normalized quantities.

Consider test problems in which we do small source iterations. In each of them we calculated changes in K_{eff} in response to perturbations. We also evaluated the efficiency of single runs compared with independent ones. It was calculated using the formula:

The relative efficiency of correlated calculations

$$\sigma(\Delta K_i) = \sigma(K_0 - K_i)$$ - independent results

$$\sigma'(\Delta K_i) = \sigma'(K_0 - K_i)$$ - correlated results

$$\alpha_i = \frac{\sigma'(\Delta K_i)}{\sigma(\Delta K_i)}, i = \widehat{0,k}$$

$$V_i = \begin{cases} \alpha_i^2, \alpha_i > 1 \\ 0, \alpha_i = 1 \\ -1/\alpha_i^2, \alpha_i < 1 \end{cases}$$

Compared with independent (non-correlated) calculations, the correlated ones provide a gain

$$V = \frac{T_H}{T_M} * \sum V_i,$$

T_H is the total time of independent calculations
T_M is the time of a multi-variant run

The first test problem involved Godiva assembly.

A sphere of 8.741cm in radius is filled with uranium (U^{235} 94.73% and U^{238} 5.27%) 18.74g/cm^3 dense. Calculations were done for perturbed densities and perturbed concentrations. The number of independent calculations was 8.

Perturbed density

ΔKeff versus density

Ro, g/cm^3	$\Delta K_{eff}(\sigma)$			
	MCNP non-correlated	MCNP correlated	PRIZMA-D non-correlated	PRIZMA-D correlated
18.74	0.998063 (0.080)		0.99987 (0.0041)	0.99975 (0.020)
18.8			0.00261 (2.22)	0.002648 (0.081)
19.0			0.011500 (0.50)	0.01144 (0.082)
19.4			0.028910 (0.20)	0.02885 (0.084)
20.0	0.05499 (2.1)	0.05282 (0.28)	0.054580 (0.11)	0.05453 (0.087)
21.1	0.09467 (1.17)	0.09302 (0.3)	0.100370 (0.059)	0.10028 (0.095)
23.5	0.19389 (0.6)	0.18683 (0.34)	0.194380 (0.032)	0.1941 (0.12)
26.0	0.28256 (0.43)	0.27110 (0.38)	0.283790 (0.022)	0.2833 (0.18)

Gain

$$(744.4+37.2+5.7+1.6-2.6-14.1-67.0)*\frac{8}{1}\approx 5600$$

The table contains results of MCNP and PRIZMA-D calculations, independent and correlated. In the first line you see the values of K_{eff} for the unperturbed configuration. The rest lines contain ΔK_{eff} for each perturbation. The figures in brackets are standard deviations. The time of the single run by PRIZMA-D roughly equals the time of one independent calculation. If compare errors in correlated and independent calculations, it is seen that for small perturbations, the error in the correlated calculation is much better. The error increases as the perturbation does, and the last lines demonstrate that the error in independent calculations is better than in the correlated calculation. For this problem, we calculated the total efficiency of the correlated calculation compared with 8 independent runs. It made about $5*10^3$.

The next problem involves perturbed concentration.

Perturbed concentration

ΔKeff versus U^{238} concentration

Part U^{238},%	$\Delta K_{eff}(\sigma)$			
	MCNP non-correlated	MCNP correlated	PRIZMA-D non-correlated	PRIZMA-D correlated
5.27			0.999920 (0.0023)	0.999957 (0.0047)
6.0			-0.00381 (2.2)	-0.003772 (0.066)
7.5			-0.01164 (0.52)	-0.01159 (0.058)
10.0			-0.02481 (0.28)	-0.02482 (0.048)
13.0	-0.04233 (2.85)	-0.04251 (1.98)	-0.04102 (0.16)	-0.04105 (0.041)
26.0	-0.12292 (0.9)	-0.11749 (2.9)	-0.11620 (0.049)	-0.11613 (0.042)
38.0	-0.20778 (0.54)	-0.19346 (3.83)	-0.19338 (0.032)	-0.1927 (0.16)
50.0	-0.30269 (0.36)	-0.28273 (4.7)	-0.27988 (0.025)	-0.2810 (0.47)

Gain

$$(1111+80.4+34+15.2+1.4-25-353.4)*\frac{1}{14} \approx 61.6$$

Eight variants were considered. The weight concentration of U^{238} was varied between 5.27% and 50%. Obtained results are presented in Table 2. For the unperturbed variant where U^{238} concentration was 5.27%, the values of K_{eff} are given. For the rest variants, the table contains the values of $\Delta K_{eff}^{(i)} = K_{eff}^{(i)} - K_{eff}^{(1)}$, where i is the variant number. The time of the correlated calculation by PRIZMA-D is about 14 times greater than the total time of eight independent calculations.

The increasing volume problem was calculated for the critical assembly Godiva.

Increasing volume

Keff and ΔKeff versus radius

Radius, cm	PRIZMA-D non-correlated K_{eff}	PRIZMA-D non-correlated ΔK_{eff}	PRIZMA-D correlated K_{eff}	PRIZMA-D correlated ΔK_{eff}
8.741	0.99988 (0.0098)		1.0001 (0.080)	
9.0	1.0175 (0.0102)	-0.0176 (8.1)	1.0181 (0.072)	-0.01808 (0.90)
9.1	1.0238 (0.0099)	-0.0239 (5.9)	1.0246 (0.070)	-0.02454 (0.79)
9.2	1.0302 (0.0100)	-0.0303 (4.7)	1.0309 (0.068)	-0.03079 (0.72)
9.3	1.0362 (0.0100)	-0.0363 (3.9)	1.0368 (0.065)	-0.03676 (0.66)
9.4	1.0420 (0.0100)	-0.0421 (3.4)	1.0426 (0.064)	-0.04256 (0.62)
9.5	1.0476 (0.0100)	-0.0477 (3.0)	1.0483 (0.062)	-0.04820 (0.59)
9.6	1.0531 (0.0100)	-0.0540 (2.7)	1.0536 (0.060)	-0.05355 (0.56)

Gain

$$(80.8+55.6+42.6+34.9+30.0+25.8+23.2)*\frac{8}{1} \approx 2300$$

Eight variants were considered. The unperturbed variant is Godiva with the initial radius of 8.741cm. In the perturbed variants, the radius increases from 9.0 to 9.6 cm. The table contains K_{eff} for 8.741 cm, and K_{eff} and $\Delta K_{eff} = K_{eff}^{(i)} - K_{eff}^{(1)}$, where i is the variant number, for

the rest radii. The time of the correlated calculation by PRIZMA-D roughly equals the time of one independent calculation.

The last test problem exemplifies the relocated volume.

Consider a cylinder of radius R_c = 10 cm with a through hole of radius R_h = 4 cm along the center line. The cylinder is 20 cm long (boundaries: $z_l = -10$cm, $z_r = 10$cm). It is filled with U^{235} 0.99235%, U^{238} 0.00747%. A sphere of radius R=1.5cm, filled with a perfect absorber, moves along the hole. The following variants were calculated:

no sphere (unperturbed), and

the sphere is set at z = -10.0, -7.5, -5.0, -3.0, -2.0, -1.0, 0.0 (center).

Relocated volume

Keff and ΔKeff versus distance covered by the absorber in the channel

Distance from the left end, cm	PRIZMA-D non-correlated K_{eff}	PRIZMA-D non-correlated ΔK_{eff}	PRIZMA-D correlated K_{eff}	PRIZMA-D correlated ΔK_{eff}
∞	1.001311 (0.0034)		1.001199 (0.0077)	
-10.0	1.001088 (0.0034)	0.000223 (21.6)	1.001008 (0.0077)	0.000191 (1.5)
-7.5	0.998437 (0.0035)	0.002870 (1.7)	0.998319 (0.0078)	0.00288 (0.36)
-5.0	0.993444 (0.0034)	0.007867 (0.6)	0.993267 (0.0079)	0.00793 (0.21)
-3.0	0.989505 (0.0035)	0.011806 (0.4)	0.989411 (0.0079)	0.01179 (0.17)
-2.0	0.988041 (0.0035)	0.013260 (0.4)	0.987979 (0.0080)	0.01322 (0.16)
-1.0	0.987110 (0.0035)	0.014200 (0.3)	0.987092 (0.0080)	0.01411 (0.15)
0.0	0.98680 (0.0035)	0.014511 (0.3)	0.986772 (0.0080)	0.01443 (0.15)

Gain

$$(207.4+22.2+8.4+5.8+5.3+5.1+4.8)*\frac{8}{2} \approx 1036$$

Obtained results are presented in the table. For the unperturbed variant, he values of K_{eff} are provided, and the values of K_{eff} and $\Delta K_{eff} = K_{eff}^{(i)} - K_{eff}^{(1)}$, where i is the variant number, for unperturbed configurations. The time of the correlated calculation is twice as long as that of one independent calculation.

CONCLUSIONS

The implemented method of small source iterations works best if perturbations are small. If the perturbation effect is greater than 10% of the target quantity, the method may sometimes be found disadvantageous in comparison with independent calculations.

Its main shortcoming is the necessity to define the number of small iterations: if is large, the time of calculation significantly increases, and if it is very small, the fission source distribution cannot reach the eigenfunction distribution. Our experience suggests that 5 iterations are quite sufficient for most problems. Moreover, since results of each iteration are output, we can check convergence and correct iterations.