Bull. Nov. Comp. Center, Num. Anal., 4 (1993), 27–34

Calculation of time constant of particle breeding by Monte Carlo method using parametric derivatives

G.Z. Lotova

The paper contains the results of time constant calculations for the process of particle breeding. The calculations are based on the estimates of parametric derivatives of the particle flux. The transfer process of radiation is assumed to be stationary.

1. Connection between parametric derivatives and time constant

The following integral-differential equation is used as a standard mathematical model of the stationary transfer process (see, e.g., [1], [2]):

$$L\Phi + \Sigma\Phi = S\Phi + S_f\Phi + f_0, \tag{1.1}$$

where

$$f_0 \equiv f_0(\vec{r},\vec{v}), \quad \Sigma \equiv \Sigma(\vec{r},\vec{v}), \quad L\Phi \equiv \vec{\omega}\nabla\Phi(\vec{r},\vec{v}),$$

$$S\Phi \equiv \int_V \Sigma_s(\vec{r},\vec{v}_1)W_s(\vec{v},\vec{v}_1,\vec{r})\Phi(\vec{r},\vec{v}_1)\,d\vec{v}_1,$$

$$S_f\Phi \equiv \int_V \nu(\vec{r},\vec{v}_1)\Sigma_f(\vec{r},\vec{v}_1)W_f(\vec{v},\vec{v}_1,\vec{r})\Phi(\vec{r},\vec{v}_1)\,d\vec{v}_1, \quad \vec{r} \in \boldsymbol{D} \subset \boldsymbol{R}_3.$$

Here

$\Phi(\vec{r},\vec{v})$ is a particle flux (usually flux of neutrons);

$\boldsymbol{V}$ is a velocity space; $\vec{v} = v\vec{\omega}$, $v = |\vec{v}|$;

$\Sigma_s(\vec{r},\vec{v})$, $\Sigma_f(\vec{r},\vec{v})$ **and** $\Sigma_c(\vec{r},\vec{v})$ are the macroscopic cross sections of scattering, fission and absorption respectively;

$\Sigma = \Sigma_s + \Sigma_f + \Sigma_c$;

$W_s(\vec{v}, \vec{v}_1, \vec{r})$ is an indicatrix of scattering;

$W_f(\vec{v}, \vec{v}_1, \vec{r})$ is an indicatrix of fission;

$\nu(\vec{r}, \vec{v}_1)$ is an average number of secondary particles per fission act caused by the particle of velocity $\vec{v}_1$ at the point $\vec{r}$;

$f_0(\vec{r}, \vec{v})$ is a distribution density of the particle source.

The medium is proposed to be bounded by a convex surface. Assume that $\Sigma = \Sigma_c \neq 0$ is on the outside.

Denote by τ^* the time constant of particle breeding. This constant determines (see, e.g., [6]) the exponential time asymptotics of the function Φ. It is known ([6]) that addition of quantity τ^*/v to the absorption cross section makes the system critical, and that τ^* is an eigenvalue of the equation

$$L\Phi + \left(\Sigma + \frac{\tau}{v}\right)\Phi = S\Phi + S_f\Phi + f_0. \tag{1.2}$$

From here on Φ means the depending on τ solution of this equation.

G. A. Mikhailov [3] showed that for derivatives of Φ with respect to parameter τ for any $\vec{r}$ and $\vec{v}$ holds

$$\lim_{m\to\infty} \frac{m\Phi^{(m-1)}(\tau_0)}{\Phi^{(m)}(\tau_0)} = \tau^* - \tau_0,$$

where τ_0 is an initial value of τ. Similar convergence may be obtained (see [3]) for the linear functionals

$$J_1 = \int_{\mathbf{D}}\int_{\mathbf{V}} \Phi(\vec{r}, \vec{v})\, d\vec{r}d\vec{v}, \quad J_2 = \int_{\mathbf{D}}\int_{\mathbf{V}} \Sigma(\vec{r}, \vec{v})\Phi(\vec{r}, \vec{v})\, d\vec{r}d\vec{v},$$

namely,

$$\lim_{m\to\infty} \frac{mJ_i^{(m-1)}(\tau_0)}{J_i^{(m)}(\tau_0)} = \tau^* - \tau_0, \quad i = 1, 2.$$

Therefore, to approximate τ^* it is sufficient to choose τ_0 and find the values of the derivatives $J_i^{(m)}(\tau_0)$.

It was shown [3] that estimates of quantities $J^{(m)}$ can be found by differentiation of the weighted collision estimate. This method will be applied in the sequel. The variances of the estimates are finite if the inequality

$$\sup\left(\frac{\Sigma_s}{\Sigma} + \nu^2\frac{\Sigma_f}{\Sigma}\right) = q < 1 \tag{1.3}$$

holds. This condition will be used to determinate τ_0.

2. Results of τ^* calculations based on diffusion approximation

Let us consider transfer process with constants

$$\Sigma = 1, \quad \Sigma_f = 0.03, \quad \Sigma_s = 0.97, \quad \Sigma_c = 0, \quad \nu = 2.5, \quad v = 1 \qquad (2.1)$$

in a ball of radius R. Assume that all the particles are of equal energy and the process of scattering is isotropic. We will use the diffusion approximation with extrapolated boundary as a mathematical model of the process (see [2])

$$\triangle\Phi(r) + c\Phi(r) = -g(r), \qquad \Phi\big|_{R+\alpha/\Sigma} \equiv 0. \qquad (2.2)$$

Here $g(r)$ is a three-dimensional distribution density of the isotropic particle source, $r = |\vec{r}|$, $c = 3(\nu-1)\Sigma_f\Sigma_s = 0.13095$, $\alpha = 0.71044$. The critical value of R in the context of approximation (2.2) is expressed by formula ([4])

$$R_{\text{cr}} = \frac{\pi}{\sqrt{3(\nu-1)\Sigma_f\Sigma_s}} - \frac{\alpha}{\Sigma} = 7.971107.$$

The system with constants (2.1) and $R = R_{\text{cr}}$ is evidently critical. As noticed above (see Section 1) the system remains critical if one add the quantity τ^*/v to the absorption cross section. Thus, $\tau^* = 0$ in our case. Let us replace Σ by $(\Sigma+\tau/v)$. Then the value $\tau^* = 0$ will be the eigenvalue of problem (1.2).

Let us take as an initial one the value of τ which guarantees finiteness of the variances of weighted estimates. The parametric derivatives will be calculated at this point. Criterian (1.3) implies

$$\frac{\Sigma_s}{\Sigma+\tau/v} + \nu^2\frac{\Sigma_f}{\Sigma+\tau/v} < 1, \qquad \frac{\tau}{v} > \Sigma_s + \nu^2\Sigma_f - \Sigma = 0.1575.$$

Therefore, the numerical experiment was carried out for $\tau_0 = 0.16$ and the ball radius equal to R_{cr}.

With the Green function $G(r,r')$ for the equation (2.2) we obtain for $g(r) = \delta(r'-r)$

$$\tilde{\Phi}(r) = G(r,0) = \frac{\sin(a+b-r\sqrt{c})}{4\pi r\sin(a+b)},$$

where

$$a = R\sqrt{c} = 2.8845, \qquad b = \frac{\alpha}{\Sigma+\tau/v}\sqrt{c}.$$

The quantity $\tilde{\Phi}$ means the total particle flux measured at the centre of a ball which is induced by the "unit pover" source placed at the distance of r from the centre.

Put

$$g(r) = \begin{cases} 1/r, & R_0 < r < R, \\ 0, & \text{otherwise}, \end{cases} \tag{2.3}$$

where R_0 is a constant small as compared to R. Then the solution of problem (2.2) for $r = 0$ takes the form

$$\Phi(0) = \int_D \tilde{\Phi}(r) g(r)\, dr.$$

Consider the following integral as an initial functional (taking into account the Jacobian r^2) :

$$J(\tau) = \left(\Sigma + \frac{\tau}{v}\right) \Phi(0) = \left(\Sigma + \frac{\tau}{v}\right) \int_0^R \tilde{\Phi}(r) r^2 g(r)\, dr$$

$$= P\left(f_1 - \cos(R_0\sqrt{c}) f_2 - \rho \sin(R_0\sqrt{c})\right),$$

where P is a constant, $H = \alpha\sqrt{c} = 0.257097$,

$$\rho = \Sigma + \frac{\tau}{v}, \quad f_1 = \frac{\rho \cos(H/\rho)}{\sin(a + H/\rho)}, \quad f_2 = \rho \operatorname{ctg}(a + H/\rho).$$

The derivatives of the functions f_1 and f_2 with respect to τ are equal to

$$f_1' = \frac{1}{\rho} f_1 + \frac{H}{\rho^3} f_1 f_2 + \frac{H \sin H/\rho}{\rho \sin(a + H/\rho)}, \qquad f_2' = \frac{1}{\rho} f_2 + \frac{H}{\rho}\left(1 + \frac{f_2^2}{\rho^2}\right),$$

$$f_1'' = \frac{2H f_2}{\rho^3}\left(f_1' - \frac{f_1}{\rho}\right), \qquad f_2'' = \frac{2H^2 f_2}{\rho^4}\left(1 + \frac{f_2^2}{\rho^2}\right),$$

$$f_1^{(3)} = \frac{2H}{\rho^4}\left(f_1' - \frac{f_1}{\rho}\right)\left(H - 3f_2 + \frac{3H f_2^2}{\rho^2}\right),$$

$$f_2^{(3)} = \frac{2H^2}{\rho^5}\left(1 + \frac{f_2^2}{\rho^2}\right)\left(H - 3f_2 + \frac{3H f_2^2}{\rho^2}\right),$$

$$f_1^{(4)} = \frac{8H}{\rho^5}\left(f_1' - \frac{f_1}{\rho}\right)\left(\frac{H f_2}{\rho^2} - 1\right)\left(2H - 3f_2 + \frac{3H f_2^2}{\rho^2}\right),$$

$$f_2^{(4)} = \frac{8H^2}{\rho^6}\left(1 + \frac{f_2^2}{\rho^2}\right)\left(\frac{H f_2}{\rho^2} - 1\right)\left(2H - 3f_2 + \frac{3H f_2^2}{\rho^2}\right).$$

The results of computations for $R_0 = R/5$ and $R_0 = R/3$ (see Table 1) confirm the convergence

$$\tau_m^* = \frac{mJ^{(m-1)}}{J^{(m)}} + \tau_0 \longrightarrow \tau^* = 0 \quad \text{as} \quad m \to \infty.$$

Table 1. The results of τ^* computations based on the diffusion approximation

m	$R_0 = R/5$		$R_0 = R/3$	
	$J^{(m)}/P$	τ_m^*	$J^{(m)}/P$	τ_m^*
1	−267.725	−0.0592	−228.614	−0.0573
2	3428.76	0.0038	2923.80	0.0036
3	−64289.3	0.0000	−54821.3	0.0000
4	1607232	0.0000	1370532	0.0000

3. Calculations of τ^* based on the simulation of trajectories

We study here the transfer process examined in Section 2, which is characterized by the same constants (2.1) and R ($R = 7.971107$) and the same distribution density of the particle source (2.3).

Consider as an initial functional the following inner product:

$$J = \Phi(0) = (\Phi(r), \delta(r)).$$

It is convenient for this problem to use the adjoint transfer equation (see [1]). By the theorem of optical mutuality (see [1]) we find

$$J = (\Phi(r), \delta(r)) = (\Phi^*(r), g(r)),$$

where $\Phi^*(r)$ is the solution of the adjoint equation

$$-L\Phi^* + \left(\Sigma + \frac{\tau}{v}\right)\Phi^* = S\Phi^* + S_f\Phi^* + \delta(r).$$

Thus, to find the functional J one can simulate the transfer process from the source with density $\delta(r)$ and determine the reading of detector with the weight function $g(r)$.

It was remarked in Section 1 that to estimate $J^{(m)}$ one can differentiate the collision estimate. For the nonphysical collision chain with the initial density

$$\pi(x_0) = \frac{(\Sigma + \tau_0)\exp(-(\Sigma + \tau_0)r_0)}{r_0^2}$$

and transition density

$$p(\vec{x}_1, \vec{x}) = \frac{\Sigma_{k_1}}{\Sigma + \tau_0} W_{k_1}(\vec{v}, \vec{v}_1, \vec{r}) \frac{(\Sigma + \tau_0)\exp(-\tau_0|\vec{r} - \vec{r}_1|)}{|\vec{r} - \vec{r}_1|^2} \delta\left(\vec{\omega} - \frac{\vec{r} - \vec{r}_1}{|\vec{r} - \vec{r}_1|}\right)$$

the estimate of the functional J equals

$$\xi = \sum_{n=0}^{N} Q_n\, g(x_n).$$

Here $x = (\vec{r}, \vec{v}, k)$, k is the number of the collision type ([3]), Q_n are auxiliary random weights calculated by the formulas

$$Q_0(\tau) = \frac{f(x_0)}{(\Sigma + \tau)\pi(x_0)}, \qquad Q_n(\tau) = \frac{1}{\Sigma + \tau} Q_{n-1}(\tau) \frac{k(x_{n-1}, x_n)}{p(x_{n-1}, x_n)},$$

$f(x)$ is the density of first collisions,

$$f(x_0) = \frac{(\Sigma + \tau_0)\exp(-(\Sigma + \tau_0)r_0)}{r_0^2},$$

$k(x_1, x)$ is the distribution density of the average number of secondary collisions followed the collision of the particle having the velocity $\vec{v}_1$ at the point $\vec{r}_1$ (see [3])

$$k(x_1, x) = \frac{\Sigma_k}{\Sigma} \tilde{\nu}_1\, W_{k_1}(\vec{v}, \vec{v}_1, \vec{r}) \frac{\Sigma \exp(-\tau(\vec{r}_1, \vec{r}, \vec{v}))}{|\vec{r} - \vec{r}_1|^2} \delta\left(\vec{\omega} - \frac{\vec{r} - \vec{r}_1}{|\vec{r} - \vec{r}_1|}\right).$$

The quantity $\tilde{\nu}_1$ takes value 2.5, when the fission occurs, otherwise $\tilde{\nu}_1 = 1$.

The following representations for the weights can be obtained by simple transformation:

$$Q_0(\tau) = \frac{\exp(-(\tau - \tau_0)r_0)}{\Sigma + \tau_0}, \qquad Q_n(\tau) = \tilde{\nu}_n \frac{\exp(-(\tau - \tau_0)t_n)}{\Sigma + \tau_0},$$

where $\tilde{\nu}_n = \nu^{m_n}$, m_n is the number of fissions up to the n-th collision of particle, t_n is total path time of the particle up to the n-th collision.

Differentiation of the weights m times yields

$$Q_0^{(m)}(\tau_0) = \frac{r_0^m (-1)^m}{\Sigma + \tau_0}, \qquad Q_n^{(m)}(\tau_0) = \tilde{\nu}_n \frac{(-1)^m t_n^m}{\Sigma + \tau_0}.$$

It was pointed out in [3] that the variance of the weight estimate can be decreased by simulating the process without absorption, but with the replacements

$$\Sigma_f \to \Sigma_f + \Sigma_c\,, \qquad \nu \to \frac{\nu\Sigma_f}{\Sigma_f + \Sigma_c}. \tag{3.1}$$

As the result of this replacement the trajectories (and computation time) grow about 7 times longer. The data presented in Table 2 show that the approximation errors of $\tilde{\tau}_m^*$ and $\hat{\tau}_m^*$ (20 000 trajectories being used) are in order of magnitude less than those of τ_m^* (100 000 trajectories), which were calculated on the trajectories without the replacement (3.1). The quantities σ_m, $\tilde{\sigma}_m$, $\hat{\sigma}_m$ are the majorants of the mean square errors.

Table 2. The results of computations based on the Monte Carlo method

m	$R_0 = R/5$		$R_0 = R/3$
	$\tau_m^* \pm \sigma_m$	$\tilde{\tau}_m^* \pm \tilde{\sigma}_m$	$\hat{\tau}_m^* \pm \hat{\sigma}_m$
1	0.043 ± 0.003	0.044 ± 0.001	0.070 ± 0.001
2	0.011 ± 0.006	0.012 ± 0.002	0.031 ± 0.002
3	0.003 ± 0.011	0.005 ± 0.003	0.015 ± 0.002
4	0.001 ± 0.017	0.003 ± 0.004	0.007 ± 0.004
5	-0.006 ± 0.025	0.001 ± 0.005	0.004 ± 0.005
6	-0.010 ± 0.036	-0.0003 ± 0.006	0.001 ± 0.006
7	-0.015 ± 0.050	-0.002 ± 0.008	-0.001 ± 0.008
8	-0.019 ± 0.068	-0.004 ± 0.010	-0.003 ± 0.010
9	-0.024 ± 0.086	-0.006 ± 0.012	-0.005 ± 0.012
10	-0.030 ± 0.107	-0.007 ± 0.015	-0.006 ± 0.015

As noted in [3], the convergence τ^* to 0 is better, when $g(r)$ is a more exact approximation for Φ^* (see Table 2, where value $R_0 = R/5$ corresponds to the better approximation).

Notice that we observe some negative drift of the estimate τ_m^* for sufficiently large m. Similar phenomenon appeared also in [5]. This effect could be explained by the tendency of understating (in modulus) of high derivatives by the Monte Carlo method.

The author is grateful to Professor G.A. Mikhailov for the formulation of the problem and permanent attention to the work.

References

[1] G.A. Mikhailov, Minimization of Computational Costs of Non-analogue Monte Carlo Methods, World Sientific, Singapore, New Jersey, London, Hong Kong, 1991.

[2] V.V. Smelov, Lectures on the Neutron Transfer Theory, Atomizdat, Moscow, 1978 (in Russian).

[3] G.A. Mikhailov, New Monte Carlo methods for calculations of critical values of the parameters for particle transfer equation, Dokl. RAN, 332, No. 1, 1993 (in Russian).

[4] N.S. Koshlyakov, E.B. Gleener, M.M. Smirnov, Differential Equations of Mathematical Physics, GIFML, Moscow, 1962 (in Russian).

[5] G.A. Mikhailov, Monte Carlo method with calculations of parametric derivatives for solutions of metaharmonic equations, Preprint, No. 990, Computer Center, Siberian Div. of Russ. Ac. Sci., Novosibirsk, 1993 (in Russian).

[6] R. Meghreblian, D. Holmes, Reactor Analysis, McGraw-Hill Book Company, New York, Toronto, London, 1960.