Accelerated local Monte Carlo estimate in calculation of laser radiation fields in tissue

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ABSTRACT

The Monte Carlo methods are widely used in biooptics to calculate different characteristics of the optical radiation fields. In the most cases the radiation characteristics including local ones (fluence, absorbed dose, etc.) are calculated with non-local Monte Carlo estimates [1-3], which give the values averaged over some region. These methods can lead to large systematical errors if the characteristics have fast space variation. At the same time there are local algorithms in the theory of the Monte Carlo methods. They are widely used in calculations of fields of ionizing radiation. In particular, the famous Kalos "local estimate" allows computations of radiation flux at a fixed point [4, 5]. This estimate solves the problem of the systematical error but because of infinite variance it has lower convergence and stability in comparison with non-local methods. Recently a method of acceleration of convergence of the Monte Carlo estimates possessing infinite variance was suggested [6,7]. In the present work this accelerated Monte Carlo algorithm is applied to the Kalos estimate under typical conditions of biooptics (rat liver irradiated by 1.064 mkm laser). It is shown that the algorithm gives the gain in computational time up to 100 times. Obtained results allow us to recommend this algorithm for calculation of local characteristics of laser radiation fields in biological tissues.

Keywords: Monte Carlo, local estimate, convergence, error reducing, laser radiation

1. INTRODUCTION

The Kalos local estimate for calculation of flux density $\Phi(\mathbf{r}^*)$ of scattered photons or neutrons (without multiplication) at a point $\mathbf{r}^*$ from a unit source (emitting 1 particle per second) is defined on analog particle trajectories $z_1, z_2, \ldots, z_\nu$ as following:

$$\xi = \sum_{i=1}^{\nu} h(z_i),\ h(\mathbf{r},\Omega) = \frac{\Sigma_S(\mathbf{r})}{\Sigma(\mathbf{r})}\,\frac{g(\Omega\Omega^*,\mathbf{r})\exp\{-\tau(\mathbf{r},\mathbf{r}^*)\}}{2\pi\,|\,\mathbf{r}^*-\mathbf{r}\,|^2},\ \Omega^* = \frac{\mathbf{r}^*-\mathbf{r}}{|\mathbf{r}^*-\mathbf{r}|}, \qquad (1)$$

where $z_n \equiv (\mathbf{r}_n, \Omega_n)$, $\mathbf{r}_n$ is the position of the n-th collision, Ω_n is the direction of the particle motion before this collision, ν is the number of particle collision on a trajectory, Σ, Σ_S are the total and scattering macroscopic cross-sections (coefficients of attenuation and scattering), g is the scattering function ($\int_{-1}^{1} g(\cos\theta,\mathbf{r})\,d\cos\theta = 1$); $\tau(\mathbf{r},\mathbf{r}^*) = \int_0^{|\mathbf{r}^*-\mathbf{r}|} \sigma(\mathbf{r}+\Omega^* l)\,dl$ is optical path length between $\mathbf{r}$ and $\mathbf{r}^*$. Expectation of the random variable (1), $\mathbf{M}\xi$, is equal to the flux $\Phi(\mathbf{r}^*)$ and therefore it can be calculated with the help of any estimate of the expectation. Usually the sample average is used:

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$$\Phi(\mathbf{r}^*) = \mathbf{M}\xi \approx \overline{\xi}_N \equiv (1/N)\sum_{i=1}^{N} \xi_i \,, \tag{2}$$

where $(\xi_1,..,\xi_N)$ is a sample of independent realizations of the local estimate ξ .

The local estimate allows us to avoid the systematical error of non-local estimates connected with approximation of the flux at a point by the flux averaged over some vicinity of this point. But it has one serious disadvantage: variance of (1) is infinite because of $|\mathbf{r}^* - \mathbf{r}|^2$ in denominator. As a result, the distribution of the sample average $\overline{\xi}_N$ converges not to normal law at $N \to \infty$, and statistical error decreases slower than in non-local methods where it decreases as $N^{-1/2}$. More exactly, the probability distribution function of $\overline{\xi}_N$, for $N \to \infty$, tends to so-called "stable" law with characteristic index α=3/2, location parameter $\mu = \mathbf{M}\xi$ and scale parameter $\sigma_N = c\, N^{-1/3}$ [8,9]:

$$P\{\overline{\xi}_N < x\} \sim G_{3/2}((x-\mu)/\sigma_N)\,,\ N \to \infty\,. \tag{3}$$

The constant c is defined by the distribution of ξ. The stable distribution $G_{3/2}$ and its density $g_{3/2}$ can not be expressed in terms of elementary or well-known special functions but its characteristic function can be done [11]. The characteristic function of the standard stable law $G_{3/2}(x)$ (location is 0, scale is 1) has the form:

$$f_{3/2}(t) = \exp\{-|t|^{3/2}\,[1 - i\,\mathrm{sign}(t)\,\mathrm{tg}(3\pi/4)]\}\,.$$

The probability distribution of the standard stable law is shown on fig. 1 [9]. In comparison with the normal law it is asymmetric and has the heavy right tail: $1 - G_{3/2}(x) \sim x^{-3/2}$, $x \to \infty$.

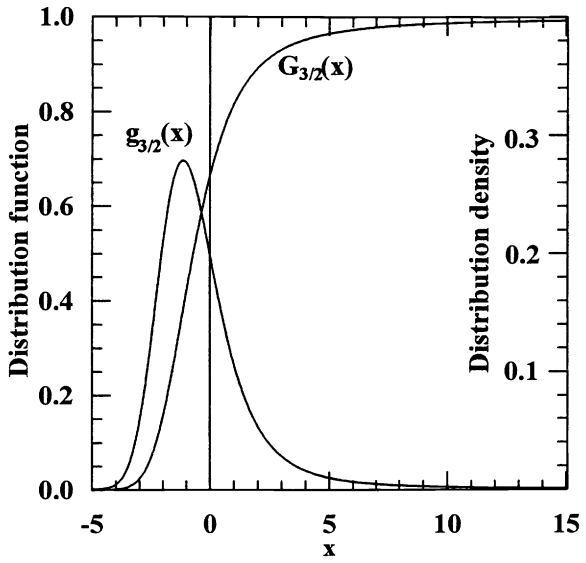

Figure 1. Probability distribution function, $G_{3/2}$, and probability density, $g_{3/2}$, of the standard stable law with characteristic index α=3/2. The vertical line corresponds to the expectation.

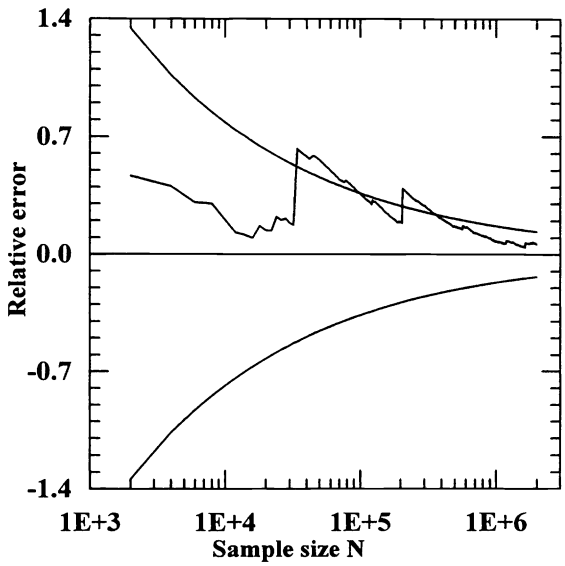

Figure 2. A typical example of behavior of relative error $(\overline{\xi}_N - \mathbf{M}\xi)/\mathbf{M}\xi$ at increasing of sample size N (broken line). Smooth lines show the confidence interval with level 0,9 in this example. The physical problem and details of calculations are described in section 3.

The law (3) leads to the law $N^{-1/3}$ for decreasing rate of the statistical error of the local estimate (2). In addition to the low rate the convergence has "bad quality". If in the case of non-local estimates the deviation of the sample average from expectation decreases more or less regularly at increasing of N then in the case of the local estimate the deviation $\overline{\xi}_N - \mathbf{M}\xi$ often has large "jumps" due to particle collisions near $\mathbf{r}^*$ (fig. 2). Such non-stable behavior of the local estimate poses significant problems in practical calculations.

The ordinary approach to improvement of the convergence is to replace the Monte Carlo estimate ξ by another one ξ' having the same expectation but finite variance. As a rule this substitution leads to substantial change and complication of computational code often with loss of their universality. Recently a new method of improvement of convergence of the estimates possessing the infinite variance was suggested [6, 7]. The essence of the method is to replace the sample average $\overline{\xi}_N$ by another estimate of $\mathbf{M}\xi$, which has faster convergence and other good properties due to using a priori information about distribution of $\overline{\xi}_N$: the distribution is close to the stable law. The Monte Carlo estimate ξ remains the same and one can use the codes simulating ξ without any changes.

2. IMPROVEMENT OF CONVERGENCE OF THE LOCAL ESTIMATE

Divide the initial sample $(\xi_1,..,\xi_N)$ of $N=n\cdot m$ realizations of ξ into m non-intersecting groups containing n realizations. Calculate the arithmetic average in each group and form a new sample:

$$(\overline{\xi}_{n,1},...,\overline{\xi}_{n,m}),\ \ \overline{\xi}_{n,j} \equiv (1/n) \sum_{i=(j-1)\cdot n+1}^{n\cdot j} \xi_i\ ,\ j=1,...,m \tag{4}$$

The random variables $\overline{\xi}_{nj}$ are independent and have the common distribution function, which approaches to the stable distribution $G_{3/2}((x-\mathbf{M}\xi)/\sigma_n)$ for $n \to \infty$. The idea of the accelerated method of estimating $\mathbf{M}\xi$, suggested in [6, 7], consists in application of some good estimate of the location parameter of this distribution to the sample (4). By using some estimate of the scale parameter authors [6, 7] suggest to estimate the statistical error of $\mathbf{M}\xi$ estimation on the same sample (4).

The accelerated method [6, 7] is based on two estimates:

$$\begin{aligned} \mu_{n,m} &\equiv \mu_{n,m}(\xi_1,...,\xi_{n\cdot m}) \equiv \sum_{i=1+a}^{m-b} l_i \overline{\xi}_{n(i)}, \\ \sigma_{n,m} &\equiv \sigma_{n,m}(\xi_1,...,\xi_{n\cdot m}) \equiv \sum_{i=1+a}^{m-b} s_i \overline{\xi}_{n(i)} \end{aligned} \tag{5}$$

The first estimate is intended to evaluate the mean $\mathbf{M}\xi$, the value to be calculated, the second one evaluates the standard deviation of $\mu_{n,m}$. In (5) $\overline{\xi}_{n(i)}$ is order statistics of the sample (4) (i.e. i-th element of the sample (4) after ordering by increasing of the elements of (4)); a, b are parameters of censoring ($a \geq 0$, $b \geq 1$, $a+b<m$); l_i, s_i are weights providing the minimal variances of estimates of location and scale parameters of the distribution $G_{3/2}$ among all unbiased linear (having the form (5)) estimates at fixed m, a, b. The weights do not depend on group size n, they are expressed through the expectations and covariances of order statistics of the sample from the standard stable law $G_{3/2}$ (see [12] for example).

We calculated tables of weights l_i and s_i for different parameters m, a, b. One of them is presented below.

Table 1. Weights l_i and s_i in estimates (5) at $m = 20$, $a = 2$, $b = 1$.

i	l_i	s_i
3	-0,2542	-0,1847
4	0,0191	0,0271
5	0,0463	0,0155
6	0,0663	0,0063
7	0,0859	0,0027
8	0,0953	0,0085

i	l_i	s_i
9	0,1038	0,0140
10	0,1100	0,0186
11	0,1138	0,0223
12	0,1155	0,0250
13	0,1151	0,0273
14	0,1116	0,0285

i	l_i	s_i
15	0,1041	0,0285
16	0,0882	0,0264
17	0,0604	0,0204
18	0,0222	0,0103
19	-0,0028	0,0009

There are three important advantages of the accelerated method in comparison with the conventional one (2):

- Variances of the estimates (5) are finite. As a result, the method has normal decreasing rate of the statistical error (as $N^{-1/2}$) at fixed n, and no large jumps appear at increasing of sample size.
- The method can be easily utilized on the base of existing codes realizing the conventional Monte Carlo method with keeping its merits: simplicity, possibility of simultaneous calculation of several quantities, and so on.
- The method contains in itself a simple parallel and highly efficient way of estimating the statistical error. To determine the error of the conventional method it is necessary to have an algorithm for calculation of the constant c of the scale parameter σ_N in (3). Such algorithm is supposed for the local estimate in [8, 9]. Its realization is much more difficult than in the case of the accelerated method.

- The cost of these advantages is some biasedness of the accelerated method, $\mathbf{M}\mu_{n,m} \neq \mathbf{M}\xi$, because of certain distinction of the distribution of $\overline{\xi}_{nj}$ in (4) from the stable law $G_{3/2}$ at finite group size n. To decrease the bias $\Delta_{n,m} \equiv \left|\mathbf{M}\mu_{n,m} - \mathbf{M}\xi\right|$ we can increase n. At fixed N such increasing will decrease the number of groups m and, therefore, increase the statistical error. We can also decrease the bias by increasing the censoring parameters a, b, but that will also increase the statistical error because the estimate efficiency will decrease. Our experience shows that in practice the acceptable values of parameters may be determined by a few trial calculations.

3. COMPUTATIONAL RESULTS

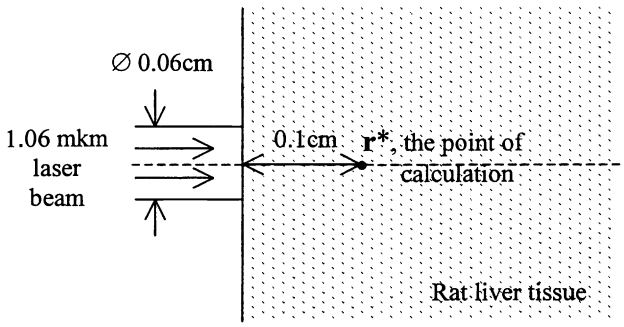

Figure 3. The test problem.

We realized the local estimate (1) for transport of photons of optical range in biological tissue and compared convergences of conventional (2) and accelerated (5) methods in a typical problem of experimental laser medicine. The photon flux density $\Phi(\mathbf{r}^*)$ from uniform unit ($1s^{-1}$) monodirectional cylindrical laser beam was calculated in the conditions shown on fig. 3. Optical parameters of the medium were taken from [9]: Σ_S $\Sigma_a = 1.29\ cm^{-1}$, $\Sigma_s = 63.4\ cm^{-1}$, g - Henyey-Greenstain function with anisotropy factor 0.87.

First, we compared the statistical errors at fixed sample size $N=10^5$ typical for calculations of such sort. The parameters $m=20$, $n=5000$, $a=2$, $b=1$ and the table 1 were used in the accelerated method. Empirical distribution functions of both the estimates $\mu_{n,m}$ and $\overline{\xi}_N$ evaluated on 10^4 their independent realizations are presented on fig. 4. One can see the heavy tail of the distribution of $\overline{\xi}_N$ and the bias of $\mu_{n,m}$.

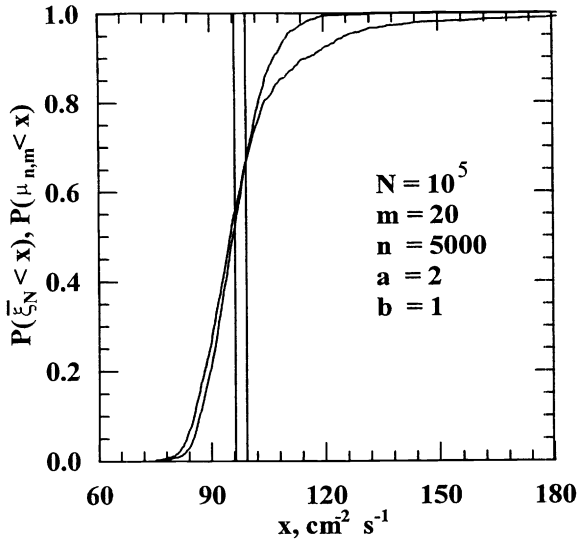

Figure 4. Probability distribution function of the conventional, $\bar{\xi}_N$, and accelerated, $\mu_{n,m}$, local estimates of the flux $\Phi(\mathbf{r}^*)$. The vertical lines show expectations. Solid lines relate to $\mu_{n,m}$.

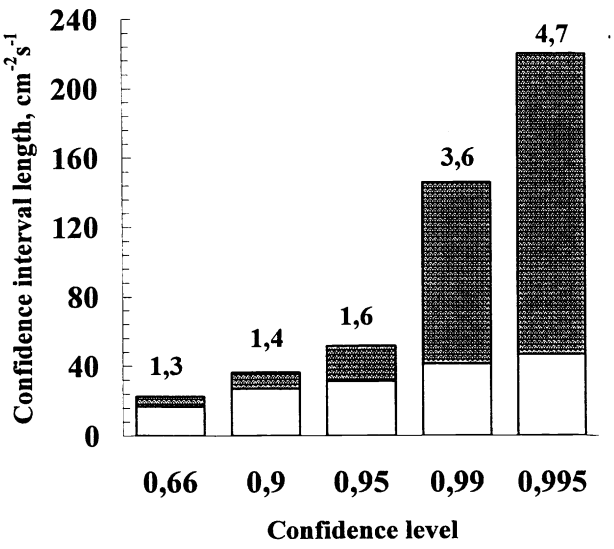

Figure 5. Confidence interval lengths determined from distributions of fig. 4. Whole bar: the conventional method; white bar: the accelerated method; numbers: the ratios of the lengths (the gain in accuracy).

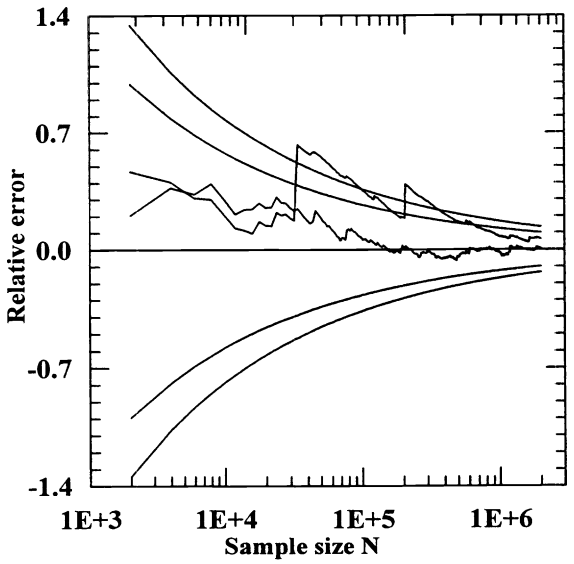

Figure 6. Relative error of the conventional and accelerated methods taken place in the calculation of $\Phi(\mathbf{r}^*)$ on the same samples as in the example of fig. 2 (broken lines). The smooth lines show level 0.9 confidence intervals. The solid lines relate to the accelerated method.

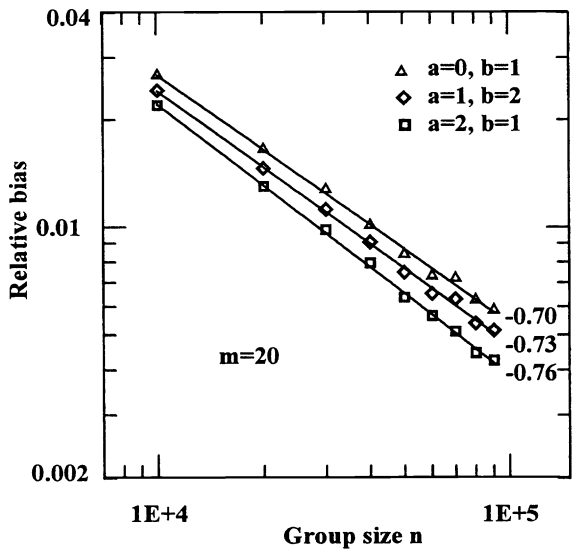

Figure 7. The relative bias of the accelerated local estimate at m= 20 and different censoring parameters a, b. The lines are the approximation by power law with least square techniques. The numbers near the lines are the powers.

With the help of these distributions we found symmetrical confidence intervals $\mu_{n,m} \pm \Delta$ and $\overline{\xi}_N \pm \overline{\Delta}$ for different confidence levels. The lengths 2Δ and $2\overline{\Delta}$ of these intervals are shown on fig. 5. It demonstrates that the statistical error of the conventional method exceeds the error of the accelerated one; the confidence intervals in the conventional method increases with increasing of the confidence level much faster than in accelerated method. As result, the gain in accuracy $\overline{\Delta}/\Delta$ rapidly increases with confidential level. The gain in the computational time due to replacement $\overline{\xi}_N$ by $\mu_{n,m}$ is $(\overline{\Delta}/\Delta)^3$, it exceeds 100 for the level 0.995.

The strong dependence of $\overline{\Delta}$ on confidence level reflects the above-mentioned "bad quality" of convergence of $\overline{\xi}_N$ (high probability of the large jumps). So, the replacement $\overline{\xi}_N$ by $\mu_{n,m}$ leads to significant improvement of the local estimate both in quantitative sense (decreasing of error) and qualitative sense (stabilization of convergence).

We studied numerically convergence of the accelerated estimate bias ($\Delta_{n,m} \to 0, n \to \infty$) of the flux density $\Phi(\mathbf{r}^*)$ in the test problem (fig.3) for different numbers of groups m and censoring parameters a, b. A typical result is presented on fig. 7. The studies showed the following:

- the convergence is well approximated by power law: $\Delta_{n,m} \sim n^{-k}$;
- dependence of the power k on the parameters m, a, b is not strong;
- the magnitude of $| k |$ (i.e. rate of the convergence) is rather large (0.7 – 1), these magnitudes significantly exceed the theoretical lower bound (0.457), established in [6] under rather general assumptions;

4. CONCLUSION

The accelerated local Monte Carlo method of calculation of radiation fields in problems of biooptics has essential advantage over the conventional one.

5. REFERENCES

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