Bull. Nov. Comp. Center, Num. Anal., 10 (2001), 19–24

Bias of the Bird type estimator*

A.A. Kolodko

1. Introduction

Let us consider a system of spatially homogeneous Smoluchowski equations in the following form:

$$\frac{\partial u_l(t)}{\partial t} = \frac{1}{2} \sum_{i+j=l} K_{ij} u_i u_j - \sum_{i\geq 1} K_{li} u_l u_i, \quad l \geq 1, \tag{1}$$

with monodisperse initial conditions

$$u_1(0) = 1, \quad u_l(0) = 0, \quad l \geq 2. \tag{2}$$

We will suggest that the coagulation coefficients are finite, i.e., there exists such $k_{\max} < \infty$ that $\max_{i,j} K_{ij} \leq k_{\max}$. Then, we will consider the time interval $[0, T]$, where there exists the unique solution to problem (1), (2) conserving its mass in such a way, that $\sum_{l\geq 1} l u_l(t) = 1$, $t \in [0, T]$. The questions of the uniqueness, existence and mass conservation are discussed in particular in [1].

Among numerical methods for solving this problem, Monte Carlo algorithms, based on the direct simulation of the coagulation process in a model particle system, play an important role. Note, that the Smoluchowski equations have nearly the same structure, as the Boltzmann equation; so, it is quite natural to use for them the well-developed stochastic algorithms for solving the latter. The present work develops the algorithm constructed by Bird [2] for solving the Boltzmann equation and applied for the Smoluchowski equations in [4, 5].

The Bird type method is based on the statistical simulation of the coagulation process in a model particle system. Its parameter is the number of particles N in the model system. The state of the system at moment t is defined by the vector $(l_1, \ldots, l_N; t)$. Here l_i defines the size of the i-th particle of the system. The evolution of this system is described in detail in [3, 4] and the estimator of the solution to (1), (2) can be presented as follows:

*Supported by INTAS under Grant 99-1501.

$$U_i(t) = \frac{1}{N}\sum_{j=1}^{N} \delta_{il_j(t)}, \quad i \geq 1.$$

The initial state of the system for problem (1), (2) is defined as follows: $l_i = 1$, $i = 1, \dots, N$, i.e., $U_i(t) = u_i(t)$, $i \geq 1$.

In [4, 5], the asymptotical unbiasedness of this estimator as $N \to \infty$ has been proved, assuming that the "molecular chaos" hypothesis is true for the pdf of the states of the system. The present work is devoted to the investigation of the bias of $U(t)$ in the dependence on the value of parameter N. The results are presented of both analytical (Section 2) and numerical (Section 3) investigation.

2. Analytical estimation of the bias

We denote by $u(t) = (u_l(t))_{l\geq 1}$ the solution to (1), (2) and by $U(t) = (U_l(t))_{l\geq 1}$ the estimator, constructed by the Bird type method.

Let us define the space of sequences

$$X_q = \left\{ x = (x_l)_{l\geq 1} \,\middle|\, \sum_{l\geq 1} l|x_l| \leq C \right\}, \quad q \in [0, 1],$$

where C is a constant, endowed with the norm $\|x\|_q = \sum_{l\geq 1} l^q |x_l|$. Note, that the nonnegativity of the components of $u(t)$ and $U(t)$ and mass conservation property (see, e.g. [6] and the description of the Bird type method in [3, 4]) yield $u(t) \in X_q$ and $U(t) \in X_q$.

Finally, let us denote $\mathrm{cov}(t)$ the following covariance vector, related to the estimator, constructed by the Bird type method:

$$\mathrm{cov}(t) = \left(\sum_{j\geq 1} \mathrm{Cov}[U_i(t), U_j(t)] \right)_{i\geq 1}.$$

sThe following theorem provides the estimation of the bias of the Bird type method for $q = 0$.

Theorem. *For each N and $t \in [0, T]$ the following inequality is valid:*

$$\|\mathbb{E}[U(t)] - u(t)\|_0 \leq \left(\frac{3}{4N} + \sup_{\tau\leq t} \|\,\mathrm{cov}(\tau)\|_0 \right) \frac{\exp(4k_{\max}t) - 1}{2}.$$

Before proving the theorem, we will formulate without proof the following lemmas.

Lemma 1. *Let us denote by $\mathcal{K}(x) = (\mathcal{K}_l(x))_{l\geq 1}$ the following operator on X_q:*

$$\mathcal{K}_l(x) = \frac{1}{2}\sum_{i+j=l} K_{ij}x_ix_j - x_l\sum_{i\geq 1} K_{li}x_i.$$

The following inequalities are valid:

$$\|\mathcal{K}(x) - \mathcal{K}(y)\|_q \leq 4k_{\max}\|x-y\|_q \quad \text{for each } x,y\in X_q, \tag{3}$$

$$\|\mathbb{E}[\mathcal{K}(U(t))] - \mathcal{K}(\mathbb{E}[U(t)])\|_0 \leq 2k_{\max}\|\operatorname{cov}(t)\|_0. \tag{4}$$

Lemma 2. *Let $\theta(t)$ be a function continuous on $[0,T]$ and suppose that $\theta(t) \leq \int_0^t(\alpha\theta(\tau)+\beta)\,d\tau$ for each $t\in[0,T]$, where α and β are constants.*
Then, for each $t\in[0,T]$

$$\theta(t) \leq \frac{\beta}{\alpha}(\exp(\alpha t)-1). \tag{5}$$

Proof of the theorem. Let us denote $p_N(l_1,\ldots,l_N;\,t)$ the pdf of the states of the model system in the Bird method. Then, we denote

$$p_N^{(2)}(l_i,l_j;\,t) = \sum_{l_1\geq 1}\cdots\sum_{l_{i-1}\geq 1}\sum_{l_{i+1}\geq 1}\cdots\sum_{l_{j-1}\geq 1}\sum_{l_{j+1}\geq 1}\cdots\sum_{l_N\geq 1} p_N(l_1,\ldots,l_N;\,t),$$

$$p_N^{(1)}(l_i;\,t) = \sum_{l_1\geq 1}\cdots\sum_{l_{i-1}\geq 1}\sum_{l_{i+1}\geq 1}\cdots\sum_{l_N\geq 1} p_N(l_1,\ldots,l_N;\,t).$$

It was shown in [3, 5] that the following equation is valid for $p_N^{(1)}(l;\,t)$, $l\geq 1$:

$$\frac{\partial}{\partial t}p_N^{(1)}(l;\,t) = \frac{N-1}{N}\left(\frac{1}{2}\sum_{i+j=l}K_{ij}p_N^{(2)}(i,j;\,t) - \sum_{i\geq 1}K_{il}p_N^{(2)}(l,i;\,t)\right). \tag{6}$$

Note, that

$$\begin{aligned}
&\mathbb{E}\left[U_m(t)U_n(t)\right]\\
&\quad= \frac{1}{N^2}\sum_{l_1\geq 1}\cdots\sum_{l_N\geq 1}\left(\sum_{i=1}^N\sum_{j=1}^N \delta_{ml_i}\delta_{nl_j}p_N(l_1,\ldots,l_N;\,t)\right)\\
&\quad= \frac{1}{N^2}\sum_{l_1\geq 1}\cdots\sum_{l_N\geq 1}\left(\left(\sum_{i=1}^N\sum_{\substack{j=1,\\ j\neq i}}^N + \sum_{i=1}^N\sum_{j=i}\right)\delta_{ml_i}\delta_{nl_j}p_N(l_1,\ldots,l_N;\,t)\right)\\
&\quad= \frac{1}{N^2}(S_1+S_2),
\end{aligned}$$

where

$$S_2 = \sum_{i=1}^{N} \sum_{l_i \geq 1} \delta_{ml_i} \delta_{nl_i} p_N^{(1)}(l_i;\, t) = N \delta_{mn} p_N^{(1)}(m;\, t),$$

$$S_1 = \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \sum_{l_i \geq 1} \sum_{l_j \geq 1} \delta_{ml_i} \delta_{nl_j} p_N^{(2)}(l_i, l_j;\, t) = N(N-1) p_N^{(2)}(m, n;\, t).$$

Finally,

$$\mathbb{E}\left[U_m(t) U_n(t)\right] = \frac{N-1}{N} p_N^{(2)}(m, n;\, t) + \frac{1}{N} \delta_{mn} p_N^{(1)}(m;\, t). \tag{7}$$

Analogously, $\mathbb{E}\left[U_l(t))\right] = p_N^{(1)}(l;\, t)$. Then, (7) yields

$$\frac{N-1}{N} p_N^{(2)}(i, j;\, t) = \mathbb{E}\left[U_i(t) U_j(t)\right] - \frac{1}{N} \delta_{mn} p_N^{(1)}(m;\, t)$$

and equations (6) can be written as follows:

$$\begin{aligned} \frac{\partial}{\partial t} \mathbb{E}[U_l(t)] &= \frac{1}{2} \sum_{i+j=l} K_{ij} \mathbb{E}[U_i] \mathbb{E}[U_j] - \mathbb{E}[U_l] \sum_{i \geq 1} K_{il} \mathbb{E}[U_i] + \\ &\quad \frac{1}{2} \sum_{i+j=l} K_{ij} \operatorname{Cov}[U_i, U_j] - \sum_{i \geq 1} K_{il} \operatorname{Cov}[U_i, U_l] - \frac{1}{N} R_l(t), \end{aligned} \tag{8}$$

where

$$\begin{aligned} R_l(t) &= \frac{1}{2} \sum_{i+j=l} K_{ij} \delta_{ij} p_N^{(1)}(i;\, t) - \sum_{i \geq 1} K_{il} \delta_{il} p_N^{(1)}(i;\, t) \\ &= \frac{1}{2} I(\operatorname{odd}(l)) K_{\frac{l}{2}\frac{l}{2}} p_N^{(1)}(l/2;\, t) - K_{ll} p_N^{(1)}(l;\, t). \end{aligned}$$

Note, that

$$\|R(t)\|_0 \leq \frac{1}{2} k_{\max} \sum_{l \geq 1} I(\operatorname{odd}(l)) p_N^{(1)}(l/2;\, t) + k_{\max} \sum_{l \geq 1} p_N^{(1)}(l;\, t) \leq \frac{3k_{\max}}{2}. \tag{9}$$

Using (1), (8), (9), and inequalities from Lemma 1, we can obtain that

$$\frac{\partial}{\partial t} \|\mathbb{E}[U(t)] - u(t)\|_0 \leq 4k_{\max} \|\mathbb{E}[U(t)] - u(t)\|_0 + 2k_{\max} \|\operatorname{cov}(t)\|_0 + \frac{3k_{\max}}{2N},$$

and according to the choice of $U(0)$,

$$\begin{aligned} &\|\mathbb{E}[U(t)] - u(t)\|_0 \\ &\quad \leq \int_0^t \left(4k_{\max} \|\mathbb{E}[U(\tau)] - u(\tau)\|_0 + 2k_{\max} \|\operatorname{cov}(\tau)\|_0 + \frac{3k_{\max}}{2N} \right) d\tau. \end{aligned}$$

Then, Lemma 2 yields the inequality, stated in the theorem. □

3. Numerical investigation of the bias

Theorem formulated in Section 2 shows that the information about the vector

$$\mathrm{cov}(t) = \Big(\sum_{j\geq 1} \mathrm{Cov}[U_i(t), U_j(t)]\Big)_{i\geq 1}$$

allows to estimate the value of the bias of the Bird type method. Though this value still cannot be estimated analytically, the numerical investigations show that it is inverse to the number of particles in the model system N.

In Table 1, we show the values of several components of vector $\mathrm{cov}(t)$ (their maximum values with respect to $t \in [0, T]$) for different values of N for $K_{ij} = 1$ and $T = 20$.

Table 1. The value of $\sup_{t\in[0;T]} \mathrm{cov}_l(t)$ for $K_{ij} = 1$ and $T = 20$

N	$l=1$	$l=2$	$l=4$	$l=8$	N Traj
128	1.62e−3	2.58e−4	1.21e−4	2.25e−5	240000
256	8.11e−4	1.32e−4	6.05e−5	1.12e−5	120000
512	4.06e−4	6.80e−5	3.09e−5	5.47e−6	60000
1024	2.06e−4	3.45e−5	1.52e−5	2.89e−6	30000

Table 2. The value of $\sup_{t\in[0,T]} \|\mathbb{E}[U(t)] - u(t)\|_q$ for $K_{ij} = 1$ and $T = 20$

N	$q=0.1$	$q=0.2$	$q=0.4$	N Traj
128	7.68e−3 ± 0.12e−3	7.22e−3 ± 0.11e−3	6.07e−3 ± 0.09e−3	240000
256	3.87e−3 ± 0.12e−3	3.64e−3 ± 0.11e−3	3.00e−3 ± 0.09e−3	120000
512	1.90e−3 ± 0.12e−3	1.78e−3 ± 0.11e−3	1.50e−3 ± 0.10e−3	60000
1024	1.01e−3 ± 0.12e−3	9.50e−4 ± 1.11e−4	7.96e−4 ± 0.97e−4	30000

The numerical investigation of the value of

$$\sup_{t\in[0,T]} \|\mathbb{E}[U(t)] - u(t)\|_q$$

for different values of q shows that it vanishes inverse to N with its growth. In Table 2, the results of these investigations are shown for $q = 0.1$, $q = 0.2$, and $q = 0.4$ for different values of N for $K_{ij} = 1$ and $T = 20$.

References

[1] Ball J.M., Carr J. The discrete coagulation-fragmentation equations: existence, uniqueness, and density conservation // Journal of Statistical Physics. – 1990. – Vol. 61, № 1–2. – P. 203–234.

[2] Bird G. Molecular Gas Dynamics. – Moscow: Mir, 1981.

[3] Kolodko A.A. Direct statistical simulation of the coagulation process. – Novosibirsk, 1996. – (Preprint / RAN. Sib. Branch of Computing Center; 1072) (in Russian).

[4] Rogasinsky S.V. Algorithms of statistical simulation for solving some kinetic equations: Thesis PhD ... Comp. Science. – Novosibirsk, 1989.

[5] Sabelfeld K.K., Rogasinsky S.V., Kolodko A.A., Levykin A.I. Stochastic algorithms for solving Smolouchovsky coagulation equation and applications to aerosol growth simulation // Monte Carlo Methods and Appl. – 1996. – Vol. 2, № 1. – P. 41–87.

[6] Voloshtchuk V.M., Sedunov Ju.S. The Coagulation Processes in Dispersed Systems. – Leningrad: Gidrometeoizdat, 1975.