Value Monte Carlo algorithms for estimating the solution to the coagulation equation

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1. Problem statement.

In spatially homogeneous case the Smoluchowski equation has the following form

$$\frac{\partial n_l(t)}{\partial t} = \frac{1}{2}\sum_{i+j=l} k_{ij} n_i(t)\, n_j(t) - \sum_{i \geqslant j} k_{il} n_i(t)\, n_l(t), \quad n_l(0) = n_l^{(0)}, \tag{1}$$

here $n_l(t)$ is the average number of l-sized particles at the instant t, ($l \in \mathbf{N}$); $k(i,j)$ are coagulation coefficients.

Solution of a kinetic equation can be estimated using simulation of a Markov chain which describes the evolution of the N-particles system. The weight modifications developed further are based on the technique suggested in [Mikhailov,Rogasinsky], which involves introduction of the number of the pair π responsible for a collision in the system to the number of phase coordinates. This allowed in [Mikhailov,Rogasinsky] to derive a special integral equation in the transformed phase space, which can be used to construct the standard weight modifications of the statistical simulation of the many-particle system due to multiplicative structure of the kernel K:

$$F(Z,t) = \int_0^t \int_{\mathbf{Z}} F(Z',t')\, K(Z',t' \to Z,t)\, dZ' dt' + F_0(Z)\delta(t), \tag{2}$$

here $Z = (X,\pi)$, $dZ = dX d\mu_0(\pi)$.

The kernel K in the equation (2) has the form:

$$K(Z', t' \to Z, t) = k(t' \to t|X')\frac{a(\pi)}{A(X')}K_1(X' \to X|\pi),$$

here

$$k(t' \to t|X') = A(X')\exp\{-(t-t')A(X')\},$$

$K_1(X' \to X|\pi)$ defines the transformation of the system after a collision of the pair $\pi = (i, j)$, which results in replacement of the interacting particles i and j by a particle of the size $l_i + l_j$.

$$N = N' - 1; X = (N, l_1, \cdots, l_N), \quad N \leqslant N_0, \quad l_i \in \overline{1, N_0}.$$

Usually, when kinetic equations are solved by direct simulation method the functionals $J_H(t)$ of the particle flux $\Phi(X, t)$ are estimated at given moments of time:

$$J_H(t) = \int H(X)\Phi(X, t)dX = \int_0^t \int_Z \tilde{H}(X, t-t')F(Z, t')dZdt',$$

here $H(X) \in L_\infty, \quad \widetilde{H}(X, t) = H(X)\exp\{-tA(X)\}.$

Let us denote a Markov chain $(Z_n, t_n), \quad n \in 0, 1, \ldots \nu$ (here ν is the index of the collision preceding the passage of the system beyond the time boundary T) with the normalized transition density

$$P(Z', t' \to Z, t) = p(t' \to t|X')P_1(\pi|X')P_2(X' \to X|\pi)$$

and normalized distribution density $P_0(Z, t) = P_0(Z)\delta(t)$ of the initial state.
Random weights are defined by the formulas

$$Q_0 = F_0(Z)/P_0(Z), \qquad Q_n = Q_{n-1}Q(Z_{n-1}, t_{n-1}; Z_n, t_n),$$

$$Q(Z_{n-1}, t_{n-1}; Z_n, t_n) = K(Z', t' \to Z, t)/P(Z', t' \to Z, t).$$

A "weight" collision estimator ξ can be used in order to estimate the functional $J_H(t)$:

$$\xi = \sum_{i=0}^{\nu} Q_n \tilde{H}(X_n, T - t_n) \quad \nu = \max\{n : \ t_n < T, \ n = 0, 1, \ldots, N_0 - 1\},$$

2. Simulation of the Markov chain.

1. $t_0 = 0$; the initial state is simulated $Z_0 \sim P_0(Z)$ and Q_0 is computed.

2. $t_n \sim P(Z_{n-1}, t_{n-1} \to Z_n, t_n)$ and Z_n is simulated, the random weights are modified after each transition in the system.

3. If $t_n < T$, than a summand $Q_n \tilde{H}(X_n, T - t_n)$ is computed, otherwise the chain terminates.

3. Test problem. As a test problem for application of the algorithm which will be described further, we take Cauchy problem (1) with

$$k_{ij} \equiv \frac{i+j}{2} \quad \text{and} \quad n_1(0) = 1,\ n_l(0) = 0, \quad l \geqslant 2.$$

This problem has an analytical solution:

$$n(l,t) = \mathrm{e}^{-0.5t} B\left(1 - \mathrm{e}^{-0.5t}, l\right), \ \ B\left(x, l\right) = \frac{(lx)^{l-1}\mathrm{e}^{-lx}}{l!}, \ \ l \geqslant 1. \quad (3)$$

For this problem the parameters of simulation are

$$a(\pi) \equiv a(i,j) = \frac{l_i + l_j}{2N_0}, \ \ A(X) = \frac{N-1}{2}. \quad (4)$$

4. Value simulation for Smoluchowski equation.

The value function $\varphi^*(X,t)$ is defined as a value of functional J_H calculated on a source function $\delta(X'-X)\delta(t'-t)$ which means that

$$\varphi^*(X,t) = \mathrm{E}\xi_{(X,t)}, \quad \text{here} \quad \xi_{(X,t)} = \tilde{H}(X,T-t)+\sum_{n=1}^{\nu} Q_n \tilde{H}(X_n,T-t_n).$$

We are going to estimate the following functionals at time instant T:

1. $J_H^{(1)}(T) \approx n_1(T)$ is the average number of monomers in the system
2. $J_H^{(12)}(T) = J_H^{(1)}(T) + J_H^{(2)}(T)$ is the sum of monomers and dimers

Theorem. *Let N_1' and N_1 be the number of monomers in ensemble before the next collision and after one, respectively.*
If the mean value of N_1 is proportional to N_1', then the value function is proportional to N_1.

The Theorem is valid for N_1+N_2 also, where N_2 stands for the number of dimers.

A Approximate value functions for time distribution to estimate $J_H^{(1)}(T)$:

$$\tilde{\varphi}_{1,I}^{*(m)}(t) = \mathrm{I}_\varepsilon(t),$$
$$\tilde{\varphi}_{1,A}^{*(m)}(t) = \left(\frac{2}{2+T_\varepsilon}\right)^2 \cdot \exp\left\{\frac{2}{2+T_\varepsilon}t\right\} \cdot \mathrm{I}_\varepsilon(t),$$

here $T_\varepsilon = T+\varepsilon$, $\mathrm{I}_\varepsilon(t)$ is the indicator function of the interval $[0, T_\varepsilon]$.

B Approximate value function for time distribution to estimate $J_H^{(12)}(T)$:

$$\tilde{\varphi}_{1,A}^{*(md)}(t) = \mathrm{I}_\varepsilon(t)\frac{8(1+T_\varepsilon)}{(2+T_\varepsilon)^3}\exp\left\{\left(\frac{3}{2+T_\varepsilon} - \frac{1}{1+T_\varepsilon}\right)t\right\}.$$

C Simulation of the interacting pair number to estimate $J_H^{(1)}(T)$.

Each of all possible interacting pairs falls into one of non-overlapping subsets: $\pi_1 \cup \pi_2 \cup \pi_0$.

$$1 \equiv \sum_{\pi} \frac{2}{N'(N'-1)} = p_1 \sum_{\pi_1} f_1(i,j) + p_2 \sum_{\pi_2} f_2(i,j) + p_0 \sum_{\pi_0} f_0(i,j)$$

In order to "preserve" the monomers we will simulate the interacting pair number using probabilities $q^{\pi}_{\mathfrak{m}}$, which are proportional to the number of monomers left in the system

$$q_1^{\pi} = \frac{p_1 (N_1' - 1)}{C}, \qquad q_2^{\pi} = \frac{p_2 (N_1' - 2)}{C}, \qquad q_0^{\pi} = \frac{p_0 N_1'}{C}, \qquad C = \mathbf{E}(N_1) = N_1' \frac{N'-2}{N'-1} \frac{N_0 - 1}{N_0}.$$

D Simulation of the interacting pair number to estimate $J_H^{(12)}(T)$.

$$q_{11}^{\pi} = (N_1' + N_2' - 1)\frac{p_{11}}{C}, \qquad q_{1k}^{\pi} = (N_1' + N_2' - 1)\frac{p_{1k}}{C}, \qquad q_{2k}^{\pi} = (N_1' + N_2' - 1)\frac{p_{2k}}{C};$$
$$q_{12}^{\pi} = (N_1' + N_2' - 2)\frac{p_{12}}{C}, \qquad q_{22}^{\pi} = (N_1' + N_2' - 2)\frac{p_{22}}{C}, \qquad q_{kk}^{\pi} = (N_1' + N_2' - 0)\frac{p_{kk}}{C},$$

here $C = \mathbf{E}(N_1 + N_2) = (N_1' + N_2')\frac{N'-2}{N'} + \frac{N_1'(N_1'-1)}{N'(N'-1)}$ is normalization factor.

These modifications are taken into consideration when the random weight is calculated: $Q = Q'p/q$.

Monomers and **Dimers** are uniformly chosen within the corresponding subsets.
Multimers are chosen within the subsets according to the following probabilities p_j:
for $J_H^{(1)}$: $j = N_1' + 1, \ldots, N'$:

Monomer-Multimer: $p_j = \dfrac{1 + l_j}{N' - 2N_1' + N_0}$.

Multimer-Multimer (j_0, i_0): $p_j = \dfrac{(N_0 - N_1') + l_j(N' - N_1' - 2)}{2(N_0 - N_1')(N' - N_1' - 1)} \Rightarrow \ j_0,$

for $i \neq j_0$ we use $\tilde{p}_i = \dfrac{p_i}{1 - p_{j_0}} \Rightarrow i_0.$

for $J_H^{(12)}$: $j = N_1' + N_2' + 1, \ldots, N'$:

Monomer-Multimer: $p_j = \dfrac{1 + l_j}{N' - 2N_1' - 3N_2' + N_0}$.

Dimer-Multimer: $p_j = \dfrac{2 + l_j}{2N' - 3N_1' - 4N_2' + N_0}$.

Multimer-Multimer (j_0, i_0): $p_j = \dfrac{(N_0 - N_1' - 2N_2') + l_j(N' - N_1' - N_2' - 2)}{2(N_0 - N_1' - 2N_2')(N' - N_1' - N_2' - 1)} \Rightarrow j_0.$

for $i \neq j_0$ we use $\tilde{p}_i = \dfrac{p_i}{1 - p_{j_0}} \Rightarrow i_0.$

Table 1: Estimation of $J_H^{(1)}(T)$ ($M = 10^3$; $N_0 = 10^3$).)

Simulation		$\tilde{J}_H^{(1)}(T)$	$\bar{\sigma}$	RE (%)	t_c	$\mathcal{S}_d/\mathcal{S}_v$
time	pair	$T = 1,\ \ n(1,1) = 4.09234 \cdot 10^{-1}$				
direct	direct	$4.09075 \cdot 10^{-1}$	$6.2 \cdot 10^{-4}$	0.04	1.5	1.00
$\tilde{\varphi}_{1,I}^{*(m)}$	direct	$4.09973 \cdot 10^{-1}$	$5.7 \cdot 10^{-4}$	0.18	1.6	1.08
$\tilde{\varphi}_{1,A}^{*(m)}$	direct	$4.09449 \cdot 10^{-1}$	$3.2 \cdot 10^{-4}$	0.05	1.7	3.45
direct	value	$4.08962 \cdot 10^{-1}$	$6.7 \cdot 10^{-4}$	0.06	1.5	0.87
$\tilde{\varphi}_{1,I}^{*(m)}$	value	$4.09867 \cdot 10^{-1}$	$5.3 \cdot 10^{-4}$	0.15	1.7	1.23
$\tilde{\varphi}_{1,A}^{*(m)}$	value	$4.09627 \cdot 10^{-1}$	$9.1 \cdot 10^{-5}$	0.10	1.7	**41.4**
		$T = 15,\ \ n(1,15) = 2.03581 \cdot 10^{-4}$				
direct	direct	$2.26000 \cdot 10^{-4}$	$1.5 \cdot 10^{-5}$	11.0	3.4	1.00
$\tilde{\varphi}_{1,I}^{*(m)}$	direct	$2.17486 \cdot 10^{-4}$	$9.8 \cdot 10^{-6}$	6.83	3.8	2.09
$\tilde{\varphi}_{1,A}^{*(m)}$	direct	$2.16655 \cdot 10^{-4}$	$8.7 \cdot 10^{-6}$	6.42	3.9	2.61
direct	value	$2.79535 \cdot 10^{-4}$	$1.2 \cdot 10^{-5}$	37.3	3.4	1.51
$\tilde{\varphi}_{1,I}^{*(m)}$	value	$2.09395 \cdot 10^{-4}$	$5.5 \cdot 10^{-6}$	2.86	3.7	6.76
$\tilde{\varphi}_{1,A}^{*(m)}$	value	$2.07266 \cdot 10^{-4}$	$3.9 \cdot 10^{-6}$	1.81	3.9	**12.7**

Table 2: Estimation of $J_H^{(12)}(T)$ ($M = 10^3$; $N_0 = 10^3$).

Simulation		$\tilde{J}_H^{(12)}(T)$	$\bar{\sigma}$	RE (%)	t_c	$\mathcal{S}_d/\mathcal{S}_v$
time	pair	$T = 1,\ \ n(1,1) + n(2,1) = 5.17876 \cdot 10^{-1}$				
direct	direct	$5.18496 \cdot 10^{-1}$	$6.1 \cdot 10^{-4}$	0.12	1.2	1.00
$\tilde{\varphi}_{1,A}^{*(md)}$	direct	$5.18629 \cdot 10^{-1}$	$2.4 \cdot 10^{-4}$	0.15	1.5	5.38
direct	value	$5.18331 \cdot 10^{-1}$	$5.9 \cdot 10^{-4}$	0.09	1.3	1.00
$\tilde{\varphi}_{1,A}^{*(md)}$	value	$5.18513 \cdot 10^{-1}$	$2.1 \cdot 10^{-4}$	0.12	1.6	**6.81**
		$T = 15,\ \ n(1,15) + n(2,15) = 2.78474 \cdot 10^{-4}$				
direct	direct	$2.55000 \cdot 10^{-4}$	$1.6 \cdot 10^{-5}$	8.43	2.4	1.00
$\tilde{\varphi}_{1,A}^{*(md)}$	direct	$2.66428 \cdot 10^{-4}$	$8.4 \cdot 10^{-6}$	4.33	3.0	2.81
direct	value	$3.65205 \cdot 10^{-4}$	$1.6 \cdot 10^{-5}$	31.2	2.5	0.99
$\tilde{\varphi}_{1,A}^{*(md)}$	value	$2.84914 \cdot 10^{-4}$	$5.3 \cdot 10^{-6}$	2.31	3.1	**7.01**

A considerable gain in computational costs is achieved via approximate value modeling of the time between collisions in the ensemble combined with the value modeling of the interacting pair number.

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