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Convergence of a Nanbu type method for the Smoluchowski equation

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Abstract. This paper studies a stochastic particle method for the numerical treatment of Smoluchowski's coagulation equation. Convergence in probability is established for the Monte Carlo estimators, when the number of particles tends to infinity. The deterministic limit is characterized as the solution of a discrete in time version of the Smoluchowski equation. The results are illustrated by numerical examples.

Contents

1. Introduction

The Smoluchowski equation first published in [5] describes the physical process of **coagulation**. This phenomenon is important in many fields of application, in particular in aerosol science (cf. [7]). We consider the **Smoluchowski equation** in its simplest form

$$\frac{\partial}{\partial t} n_l(t) = \frac{1}{2}\sum_{i=1}^{l-1} K_{i,l-i}\, n_i(t)\, n_{l-i}(t) - n_l(t)\sum_{i=1}^{\infty} K_{i,l}\, n_i(t)\,, \qquad l = 1,2,\ldots\,, \tag{1.1}$$

with the initial condition

$$n_l(0) = n_l^{(0)}\,, \qquad l = 1,2,\ldots\,. \tag{1.2}$$

Here $n_l(t)$ is the concentration of particles of size l (containing l structural units or monomers) at time $t \geq 0$.

Concerning the **initial value**, we assume that

$$n_l^{(0)} \geq 0\,, \qquad l = 1,2,\ldots\,, \tag{1.3}$$

$$n_l^{(0)} = 0\,, \qquad l > L_0 \tag{1.4}$$

and

$$\max_l n_l^{(0)} > 0\,. \tag{1.5}$$

Condition (1.4) assures, in particular, that the infinite sum on the right-hand side of (1.1) is finite at time zero, for arbitrary kernels K.

Concerning the **coagulation kernel** K, we assume that

$$\inf_{i,j\geq 1} K_{i,j} > 0 \tag{1.6}$$

and

$$K_{i,j} = K_{j,i}\,, \qquad i,j = 1,2,\dots\,. \tag{1.7}$$

Among numerical methods for solving Eq. (1.1) Monte Carlo algorithms based on interacting particle systems play an important role. We refer to the extensive reference list in [4]. The **purpose of this paper** is to give a rigorous convergence proof for a stochastic algorithm, which was proposed in [2] and was numerically investigated in [4]. We call this procedure a Nanbu type method because of its analogy with a corresponding numerical algorithm for the Boltzmann equation (cf. [3]). Convergence of the basic algorithms for the Boltzmann equation was established in [1], [6].

In Section 2 we describe the numerical algorithm in detail. Section 3 contains the main result showing convergence in probability of the Monte Carlo estimators to a deterministic limit as the number of simulation particles tends to infinity. The limit is determined as the solution of an equation, which is a discretized in time analogue of the Smoluchowski equation. In Section 4 we present the results of some numerical experiments illustrating the above mentioned convergence theorem as well as the convergence of the solution of the discretized equation to the solution of Eq. (1.1).

2. Description of the algorithm

Let us consider a stochastic particle system, where each particle is characterized by its size $l = 1,2,\dots$. The **state of the system** is determined by the sequence

$$N_1(t),\, N_2(t),\, \dots\,, \tag{2.1}$$

where $N_l(t)$ is the number of particles of size l at time $t \geq 0$. The system depends on a parameter $N = 1,2,\dots$, and its state is defined at discrete moments

$$t_k^{(N)}\,, \qquad k = 0,1,\dots\,, \qquad t_0^{(N)} = 0\,,$$

according to the rules following below. Between these points the system does not change.

Initial state: At time zero the system consists of N particles approximating the initial value in condition (1.2). More precisely, let

$$N = \sum_{l\geq 1} N_l(0) \tag{2.2}$$

and

$$\frac{N_l(0)}{c_0^{(N)}} \to n_l^{(0)} \quad \text{in probability as} \quad N \to \infty\,, \quad l = 1, 2, \ldots\,, \tag{2.3}$$

for some appropriate **normalizing sequence** $c_0^{(N)}$. In correspondence with (1.4), we assume that

$$N_l(0) = 0\,, \qquad l > L_0\,. \tag{2.4}$$

Remark 2.1 (Choice of the normalizing sequence) *From (2.2), (2.3), (2.4), (1.5) one obtains*

$$\frac{N}{c_0^{(N)}} = \sum_{l \geq 1} \frac{N_l(0)}{c_0^{(N)}} \to \sum_{l \geq 1} n_l^{(0)} > 0 \quad \textit{in probability as} \quad N \to \infty \tag{2.5}$$

so that

$$\lim_{N \to \infty} c_0^{(N)} = \infty\,. \tag{2.6}$$

An appropriate choice is

$$c_0^{(N)} = \frac{N}{\sum_{l \geq 1} n_l^{(0)}}\,. \tag{2.7}$$

Remark 2.2 *One may consider N as the number of monomers in the system at time zero, i.e.*

$$N = \sum_{l \geq 1} l\, N_l(0)\,, \tag{2.8}$$

instead of (2.2). Then (2.8), (2.3), (2.4) and (1.5) give

$$\frac{N}{c_0^{(N)}} = \sum_{l \geq 1} l\, \frac{N_l(0)}{c_0^{(N)}} \to \sum_{l \geq 1} l\, n_l^{(0)} > 0 \quad \textit{in probability as} \quad N \to \infty$$

so that in this case

$$c_0^{(N)} = \frac{N}{\sum_{l \geq 1} l\, n_l^{(0)}}$$

would be an appropriate choice of the normalizing sequence.

Time evolution: Given the state of the system (2.1) at time $t_k^{(N)}$, for some $k = 0, 1, \ldots$, and a normalizing sequence $c_k^{(N)}$, the state at time $t_{k+1}^{(N)}$ is constructed in several steps.

1. Choose the **time increment**

$$\Delta_k^{(N)} = \frac{\alpha}{\max\limits_i \{\sum_{j \geq 1} \frac{N_j(t_k^{(N)})}{c_k^{(N)}} K_{i,j}\}}\,, \tag{2.9}$$

where

$$0 < \alpha \leq 1 \tag{2.10}$$

is a **discretization parameter**, and define

$$t_{k+1}^{(N)} = t_k^{(N)} + \Delta_k^{(N)} . \tag{2.11}$$

2. Denote

$$N_1' = N_1(t_k^{(N)}) , \quad N_2' = N_2(t_k^{(N)}) , \quad \ldots .$$

3. For each particle of size l, $l = 1, 2, \ldots$, examine with the **reaction probability**

$$P_l^{(N)} := \frac{1}{2} \Delta_k^{(N)} \sum_{j \geq 1} \frac{N_j(t_k^{(N)})}{c_k^{(N)}} K_{l,j} , \qquad l = 1, 2, \ldots , \tag{2.12}$$

whether it interacts with any other particle.

3.1 If yes, then find the random size m of the reaction partner according to the **size distribution**

$$p_{l,m}^{(N)} := \frac{N_m(t_k^{(N)}) K_{l,m}}{\sum_{j \geq 1} N_j(t_k^{(N)}) K_{l,j}} , \qquad m \geq 1 , \tag{2.13}$$

and change

$$N_l' := N_l' - 1 , \quad N_m' := N_m' - 1 , \quad N_{l+m}' := N_{l+m}' + 1 . \tag{2.14}$$

3.2 If no, then do not change anything.

4. To keep all components non-negative **truncate** the system if necessary, i.e. define

$$\tilde{N}_l(t_{k+1}^{(N)}) := \max(0, N_l') , \qquad l = 1, 2, \ldots . \tag{2.15}$$

5. Check whether the number of particles satisfies

$$\sum_{l \geq 1} \tilde{N}_l(t_{k+1}^{(N)}) \leq \frac{N}{2} . \tag{2.16}$$

5.1 If yes, then **double** the system, i.e. define

$$N_l(t_{k+1}^{(N)}) := 2 \tilde{N}_l(t_{k+1}^{(N)}) , \qquad c_{k+1}^{(N)} := 2 c_k^{(N)} . \tag{2.17}$$

5.2 If no, then do not change anything, i.e. define

$$N_l(t_{k+1}^{(N)}) := \tilde{N}_l(t_{k+1}^{(N)}) , \qquad c_{k+1}^{(N)} := c_k^{(N)} . \tag{2.18}$$

Note that the probabilities (2.12), (2.13) are the same for all particles of the same size. The normalizing sequences, which are in fact random, satisfy $c_k^{(N)} = 2^\beta c_0^{(N)}$, where β is the number of those among the k time steps at which the doubling procedure (2.17) took place. Thus, one obtains

$$c_0^{(N)} \leq c_k^{(N)} \leq 2^k c_0^{(N)} , \qquad k = 0, 1, \ldots . \tag{2.19}$$

Remark 2.3 (Growth of the particle size) *During one time step, the largest non-zero component of the sequence (N_l) may increase at most by a factor 2 (cf. (2.14)). Thus, according to (2.4), one obtains*

$$N_l(t_k^{(N)}) = 0\,, \qquad l > 2^k\, L_0\,. \tag{2.20}$$

Consequently, the infinite sums in (2.9), (2.12) and (2.13) are actually finite.

Remark 2.4 (Number of monomers) *The mass conservation property of the Smoluchowski equation (1.1), i.e.*

$$\sum_{l\geq 1} l\, n_l(t) = \sum_{l\geq 1} l\, n_l(0)\,, \qquad t \geq 0\,,$$

(see (3.9), (3.10) below) is violated for the particle system due to the truncation (2.15). We have (cf. (2.14))

$$l\, N_l' + m\, N_m' + (l+m)\, N_{l+m}' = l\,(N_l' - 1) + m\,(N_m' - 1) + (l+m)\,(N_{l+m}' + 1)$$

and therefore

$$\sum_{l\geq 1} l\, N_l' = \sum_{l\geq 1} l\, N_l(t_k^{(N)})$$

but, according to (2.15), in general only

$$\sum_{l\geq 1} l\, N_l(t_{k+1}^{(N)}) \geq \sum_{l\geq 1} l\, N_l(t_k^{(N)})\,.$$

Remark 2.5 (Number of particles) *The number of particles in the system satisfies*

$$\frac{N}{2} \leq \sum_{l\geq 1} N_l(t_k^{(N)}) \leq N\,, \qquad k = 0, 1, \ldots\,, \tag{2.21}$$

which follows by induction from

$$\frac{1}{2} \sum_{l\geq 1} N_l(t_k^{(N)}) \leq \sum_{l\geq 1} \tilde{N}_l(t_{k+1}^{(N)}) \leq \sum_{l\geq 1} N_l(t_k^{(N)})\,.$$

From (2.21) and (2.19) one obtains

$$\frac{1}{c_k^{(N)}} \sum_{l\geq 1} N_l(t_k^{(N)}) \leq \frac{N}{c_0^{(N)}} \leq \sup_N \frac{N}{c_0^{(N)}} < \infty\,,$$

according to (2.5).

For the proof it will be sufficient to use the rough inequality

$$\sum_{l\geq 1} \tilde{N}_l(t_{k+1}^{(N)}) \leq 2 \sum_{l\geq 1} N_l(t_k^{(N)})\,,$$

which implies

$$\frac{1}{c_k^{(N)}} \sum_{l\geq 1} N_l(t_k^{(N)}) \leq 2^k\, \frac{N}{c_0^{(N)}} \leq 2^k\, \sup_N \frac{N}{c_0^{(N)}} < \infty\,, \tag{2.22}$$

according to (2.5).

3. Convergence theorem

We consider a **discrete approximation** to Eq. (1.1), namely

$$\hat{n}_l(t_{k+1}) = \hat{n}_l(t_k) + \Delta_k \left(\frac{1}{2} \sum_{i=1}^{l-1} K_{i,l-i}\, \hat{n}_i(t_k)\, \hat{n}_{l-i}(t_k) - \hat{n}_l(t_k) \sum_{i\geq 1} K_{i,l}\, \hat{n}_i(t_k) \right), \tag{3.1}$$
$$l = 1, 2, \ldots, \qquad k = 0, 1, \ldots,$$

with the initial condition

$$\hat{n}_l(0) = n_l^{(0)}, \qquad l = 1, 2, \ldots. \tag{3.2}$$

The time steps are defined as

$$\Delta_k = \frac{\alpha}{\max\limits_i \{\sum_{j\geq 1} \hat{n}_j(t_k)\, K_{i,j}\}}, \tag{3.3}$$

where α is the parameter from (2.9), (2.10), and

$$t_{k+1} = t_k + \Delta_k, \qquad k = 0, 1, \ldots, \qquad t_0 = 0.$$

The main result is the following.

Theorem 3.1 *Let the assumptions (2.3), (2.4) be fulfilled. Then*

$$\frac{N_l(t_k^{(N)})}{c_k^{(N)}} \to \hat{n}_l(t_k) \quad \text{in probability as} \quad N \to \infty, \qquad l = 1, 2, \ldots, \quad k = 0, 1, \ldots, \tag{3.4}$$

where $\hat{n}_l$ is the solution of Eq. (3.1) and $N_l(t_k^{(N)})$, $c_k^{(N)}$ were defined in Section 2.

We start with some preparations for the proof.

Lemma 3.2 *The solution of Eq. (3.1) satisfies*

$$\hat{n}_l(t_k) \geq 0, \qquad l = 1, 2, \ldots, \quad k = 0, 1, \ldots, \tag{3.5}$$

$$\hat{n}_l(t_k) = 0, \qquad l > 2^k L_0, \quad k = 0, 1, \ldots, \tag{3.6}$$

$$\sum_{l\geq 1} l\, \hat{n}_l(t_k) = \sum_{l\geq 1} l\, n_l^{(0)}, \qquad k = 0, 1, \ldots. \tag{3.7}$$

Proof. We prove the assertions by induction with respect to k. In the case $k = 0$ they are fulfilled because of (3.2), (1.3) and (1.4). Assuming that they are fulfilled for some k we prove them for $k+1$. Eq. (3.1) takes the form

$$\hat{n}_l(t_{k+1}) = \hat{n}_l(t_k) \left[1 - \Delta_k \sum_{i\geq 1} K_{i,l}\, \hat{n}_i(t_k) \right] + \frac{1}{2} \Delta_k \sum_{i=1}^{l-1} K_{i,l-i}\, \hat{n}_i(t_k)\, \hat{n}_{l-i}(t_k). \tag{3.8}$$

The term in brackets satisfies (cf. (3.3), (2.10), (1.7))

$$1-\Delta_k \sum_{i\geq 1} K_{i,l}\,\hat{n}_i(t_k) = 1-\alpha\frac{\sum_{i\geq 1} K_{i,l}\,\hat{n}_i(t_k)}{\max_i\{\sum_{j\geq 1}\hat{n}_j(t_k)\,K_{i,j}\}} \geq 1-\alpha \geq 0\,,$$

which implies (3.5). If $l > L_0\,2^{k+1}$, then either $\hat{n}_i(t_k)=0$ or $\hat{n}_{l-i}(t_k)=0$ so that the right-hand side of (3.8) vanishes and (3.6) follows. Finally, we note that

$$\begin{aligned}\sum_{l\geq 1} l\left[\frac{1}{2}\sum_{i=1}^{l-1} K_{i,l-i}\,b_i\,b_{l-i}\right] &= \frac{1}{2}\sum_{i\geq 1}\sum_{l>i} l\,K_{i,l-i}\,b_i\,b_{l-i} = \frac{1}{2}\sum_{i\geq 1}\sum_{l\geq 1}(l+i)\,K_{i,l}\,b_i\,b_l \\ &= \sum_{l\geq 1} l\,b_l \sum_{i\geq 1} K_{i,l}\,b_i\,, \end{aligned} \tag{3.9}$$

for any symmetric matrix K and any sequence (b_i). Now (3.1) and (3.9) imply

$$\sum_{l\geq 1} l\,\hat{n}_l(t_{k+1}) = \sum_{l\geq 1} l\,\hat{n}_l(t_k) \tag{3.10}$$

and (3.7) follows. □

Let the system $N_1(t_k^{(N)}), N_2(t_k^{(N)}), \ldots$ be fixed. For each **tested particle** (cf. step 3 in the description of the time evolution in Section 2)

$$(l,i)\,, \qquad l=1,2,\ldots\,, \qquad i=1,2,\ldots,N_l(t_k^{(N)})\,,$$

we introduce a random variable $\xi_{l,i}$ that determines whether the particle takes part in a reaction. These random variables are independent and distributed according to (cf. (2.12))

$$\mathrm{Prob}(\xi_{l,i}=1)=P_l^{(N)}\,, \qquad \mathrm{Prob}(\xi_{l,i}=0)=1-P_l^{(N)}\,. \tag{3.11}$$

We also introduce random variables $\eta_{l,i}$ for the size the **reaction partner**, which are independent of each other and of $(\xi_{l,i})$. Their distribution is (cf. (2.13))

$$\mathrm{Prob}(\eta_{l,i}=m)=p_{l,m}^{(N)}\,, \qquad m=1,2,\ldots\,. \tag{3.12}$$

We prove two lemmas related to these random variables.

Lemma 3.3 *Assume, for some $k=0,1,\ldots$,*

$$\frac{N_l(t_k^{(N)})}{c_k^{(N)}} \to \hat{n}_l(t_k) \quad \textit{in probability as} \quad N\to\infty\,, \quad l=1,2,\ldots\,. \tag{3.13}$$

Then

$$\frac{1}{c_k^{(N)}}\sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i} \to \frac{1}{2}\,\Delta_k\,\hat{n}_l(t_k)\sum_{j\geq 1} K_{l,j}\,\hat{n}_j(t_k)\,, \quad l=1,2,\ldots\,, \tag{3.14}$$

in probability as $N\to\infty$.

Proof. For the random variable on the left-hand side of (3.14),

$$\zeta_l^{(N)} := \frac{1}{c_k^{(N)}} \sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i}\,, \tag{3.15}$$

we prove that the expectation tends to the deterministic expression on the right-hand side, i.e.

$$\lim_{N\to\infty} E\,\zeta_l^{(N)} = \frac{1}{2}\,\Delta_k\,\hat{n}_l(t_k) \sum_{j\geq 1} K_{l,j}\,\hat{n}_j(t_k)\,, \tag{3.16}$$

and that the variance vanishes, i.e.

$$\lim_{N\to\infty} V\,\zeta_l^{(N)} = 0\,. \tag{3.17}$$

Let E_k denote the conditional expectation with respect to the σ-algebra generated by the sequence $N_1(t_k^{(N)}), N_2(t_k^{(N)}), \ldots$. Then (cf. (3.11), (2.12))

$$E_k\,\xi_{l,i} = P_l^{(N)} \tag{3.18}$$

and, consequently,

$$\begin{aligned} E\,\zeta_l^{(N)} &= E\,E_k\,\zeta_l^{(N)} = E\left[E_k\left[\frac{1}{c_k^{(N)}} \sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i}\right]\right] = E\left[\frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,P_l^{(N)}\right] \\ &= E\left[\frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,\frac{1}{2}\,\Delta_k^{(N)} \sum_{j\geq 1} \frac{N_j(t_k^{(N)})}{c_k^{(N)}}\,K_{l,j}\right]. \end{aligned} \tag{3.19}$$

Note that the random variable in brackets is bounded according to the definition (2.9) and the estimate (2.22). Thus, (3.16) follows from (3.13) and the fact that (cf. (2.9), (3.3))

$$\Delta_k^{(N)} = \frac{\alpha}{\max_i\{\sum_{l\geq 1} \frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,K_{i,l}\}} \to \frac{\alpha}{\max_i\{\sum_{l\geq 1} \hat{n}_l(t_k)\,K_{i,l}\}} = \Delta_k$$

in probability as $N \to \infty$. Note that

$$\sum_{l\geq 1} \frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,K_{i,l} \to \sum_{l\geq 1} \hat{n}_l(t_k)\,K_{i,l}\,, \qquad i = 1, 2, \ldots\,,$$

since the sums are over a finite set of indices, according to (2.20) and (3.6). Moreover,

$$\sum_{l\geq 1} \hat{n}_l(t_k)\,K_{i,l} \geq \inf_{i,j} K_{i,j}\,\max_l \hat{n}_l(t_k) > 0\,,$$

according to (3.7), (1.5) and (1.6).

In order to establish (3.17) we use the property

$$V\,\zeta_l^{(N)} = E\,V_k\,\zeta_l^{(N)} + E\,(E_k\,\zeta_l^{(N)})^2 - (E\zeta_l^{(N)})^2\,, \tag{3.20}$$

where

$$V_k\,\zeta_l^{(N)} = E_k(\zeta_l^{(N)})^2 - (E_k\,\zeta_l^{(N)})^2 .$$

From (3.16) we know that

$$\lim_{N\to\infty} (E\zeta_l^{(N)})^2 = \left[\frac{1}{2}\,\Delta_k\,\hat{n}_l(t_k)\sum_{j\geq 1} K_{l,j}\,\hat{n}_j(t_k)\right]^2 . \tag{3.21}$$

Using (3.18) we obtain

$$E\,(E_k\,\zeta_l^{(N)})^2 = E\left[E_k\left[\frac{1}{c_k^{(N)}}\sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i}\right]\right]^2 = E\left[\frac{N_l(t_k^{(N)})}{c_k^{(N)}}P_l^{(N)}\right]^2 .$$

This term is handled as the right-hand side of (3.19) giving

$$\lim_{N\to\infty} E\,(E_k\,\zeta_l^{(N)})^2 = \left[\frac{1}{2}\,\Delta_k\,\hat{n}_l(t_k)\sum_{j\geq 1} K_{l,j}\,\hat{n}_j(t_k)\right]^2 . \tag{3.22}$$

Finally we obtain from (3.15), (3.11)

$$V_k\,\zeta_l^{(N)} = \frac{1}{(c_k^{(N)})^2}\sum_{i=1}^{N_l(t_k^{(N)})} V_k\,\xi_{l,i} = \frac{N_l(t_k^{(N)})}{(c_k^{(N)})^2}\,P_l^{(N)}\,(1-P_l^{(N)}) . \tag{3.23}$$

This random variable is bounded according to the definitions (2.12), (2.9) and the estimate (2.22). Its expectation tends to zero according to (3.13), (2.19) and (2.6). Thus, (3.20), (3.21), (3.22), (3.23) imply (3.17). □

Lemma 3.4 *Assume, for some* $k = 0, 1, \dots$,

$$\frac{N_l(t_k^{(N)})}{c_k^{(N)}} \to \hat{n}_l(t_k) \quad \textit{in probability as} \quad N\to\infty , \qquad l = 1, 2, \dots .$$

Then

$$\frac{1}{c_k^{(N)}}\sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\,\delta_{\eta_{i,j}\,l} \to \frac{1}{2}\,\Delta_k\,\hat{n}_i(t_k)\,K_{i,l}\,\hat{n}_l(t_k) , \qquad i, l = 1, 2, \dots ,$$

in probability as $N\to\infty$ *, where* δ *denotes the Kronecker symbol.*

Proof. One obtains

$$E_k\,\xi_{i,j}\,\delta_{\eta_{i,j}\,l} = P_i^{(N)}\,p_{i,l}^{(N)} = \frac{1}{2}\,\Delta_k^{(N)}\,\frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,K_{i,l} ,$$

according to (3.11), (3.12), (2.12), (2.13). Thus,

$$E\left[\frac{1}{c_k^{(N)}}\sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\,\delta_{\eta_{i,j}\,l}\right] = E\left[\frac{N_i(t_k^{(N)})}{c_k^{(N)}}\,\frac{1}{2}\,\Delta_k^{(N)}\,\frac{N_l(t_k^{(N)})}{c_k^{(N)}}\,K_{i,l}\right] .$$

The rest of the argument is analogous to the proof of Lemma 3.3. □

Proof of Theorem 3.1. We prove the assertion by induction. In the case $k=0$ (3.4) is fulfilled because of (3.2) and assumption (2.3). We assume that (3.4) is fulfilled for some k and prove it for $k+1$.

Let $I_{l,1}^{(N)}$ be the number of particles of size l taking part in reactions as tested particles, $I_{l,2}^{(N)}$ – the number of particles of size l taking part in reactions as partners of tested particles, and $I_{l,3}^{(N)}$ – the number of new particles of size l. Then, according to (2.14),

$$N_l' = N_l(t_k^{(N)}) - I_{l,1}^{(N)} - I_{l,2}^{(N)} + I_{l,3}^{(N)}, \qquad l = 1,2,\dots . \tag{3.24}$$

Using the representations (cf. (3.11), (3.12))

$$\begin{aligned} I_{l,1}^{(N)} &= \sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i}, \\ I_{l,2}^{(N)} &= \sum_{i\geq 1} \sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\, \delta_{\eta_{i,j}\, l}, \\ I_{l,3}^{(N)} &= \sum_{i=1}^{l-1} \sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\, \delta_{\eta_{i,j}\, l-i}, \end{aligned}$$

we obtain from Lemmas 3.3 and 3.4

$$\frac{1}{c_k^{(N)}}\, I_{l,1}^{(N)} = \frac{1}{c_k^{(N)}} \sum_{i=1}^{N_l(t_k^{(N)})} \xi_{l,i} \to \frac{1}{2}\,\Delta_k\, \hat{n}_l(t_k) \sum_{j\geq 1} K_{l,j}\, \hat{n}_j(t_k),$$

$$\frac{1}{c_k^{(N)}}\, I_{l,2}^{(N)} = \sum_{i\geq 1} \frac{1}{c_k^{(N)}} \sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\, \delta_{\eta_{i,j}\, l} \to \frac{1}{2}\,\Delta_k \sum_{i\geq 1} \hat{n}_i(t_k)\, K_{i,l}\, \hat{n}_l(t_k),$$

and

$$\frac{1}{c_k^{(N)}}\, I_{l,3}^{(N)} = \sum_{i=1}^{l-1} \frac{1}{c_k^{(N)}} \sum_{j=1}^{N_i(t_k^{(N)})} \xi_{i,j}\, \delta_{\eta_{i,j}\, l-i} \to \frac{1}{2}\,\Delta_k \sum_{i=1}^{l-1} \hat{n}_i(t_k)\, K_{i,l-i}\, \hat{n}_{l-i}(t_k),$$

in probability as $N\to\infty$. Thus, according to (3.24), the induction hypothesis, (1.7) and (3.1),

$$\begin{aligned} \frac{1}{c_k^{(N)}}\, N_l' \;&\to\; \hat{n}_l(t_k) + \Delta_k \left(\frac{1}{2} \sum_{i=1}^{l-1} \hat{n}_i(t_k)\, K_{i,l-i}\, \hat{n}_{l-i}(t_k) - \hat{n}_l(t_k) \sum_{i\geq 1} \hat{n}_i(t_k)\, K_{i,l} \right) \\ &= \hat{n}_l(t_{k+1}) \end{aligned} \tag{3.25}$$

in probability as $N\to\infty$. Now (3.25), (2.15) and (3.5) imply

$$\frac{1}{c_k^{(N)}}\, \tilde{N}_l(t_{k+1}^{(N)}) = \frac{1}{c_k^{(N)}} \max(0, N_l') \to \hat{n}_l(t_{k+1}).$$

Finally we note that the doubling transformation does not change the limit, since

$$\frac{1}{c_{k+1}^{(N)}}\, N_l(t_{k+1}^{(N)}) = \frac{1}{c_k^{(N)}}\, \tilde{N}_l(t_{k+1}^{(N)})$$

in both cases (2.17) and (2.18). This completes the proof. □

4. Numerical experiments

In this section we illustrate two effects. The first is convergence for $N \to \infty$ of the numerical approximation to the solution of Eq. (3.1), i.e. the result of Theorem 3.1. This solution depends on the discretization parameter α (cf. (3.3)). The second effect to be shown is convergence for $\alpha \to 0$ of the solution of the discretized equation to the solution of the original equation (1.1).

We consider some special cases of Eq. (1.1), in which the analytical solution is known. Beside the solution n_l we calculate the **average particle size**

$$S(t) := \frac{\sum_{l\geq 1} l\, n_l(t)}{\sum_{l\geq 1} n_l(t)} = \frac{\sum_{l\geq 1} l\, n_l^{(0)}}{\sum_{l\geq 1} n_l(t)} \tag{4.1}$$

and the **particle size distribution**

$$s_l(t) := \frac{n_l(t)}{\sum_{l\geq 1} n_l(t)}\,, \qquad l = 1, 2, \ldots\,. \tag{4.2}$$

For the (normalized) initial value

$$n_1^{(0)} = 1\,, \qquad n_l^{(0)} = 0\,, \qquad l \geq 2\,, \tag{4.3}$$

and the coagulation kernel

$$K_{i,j} = 1\,, \qquad i, j = 1, 2, \ldots\,, \tag{4.4}$$

the exact solutions are

$$n_l(t) = \frac{\left(\frac{t}{2}\right)^{l-1}}{\left(1+\frac{t}{2}\right)^{l+1}}\,, \qquad s_l(t) = \frac{\left(\frac{t}{2}\right)^{l-1}}{\left(1+\frac{t}{2}\right)^{l}}\,, \qquad S(t) = 1 + \frac{t}{2}\,. \tag{4.5}$$

For the initial value (4.3) and the coagulation kernel

$$K_{i,j} = i + j\,, \qquad i, j = 1, 2, \ldots\,, \tag{4.6}$$

one has

$$n_l(t) = \frac{l^{l-1}}{l\,!}\, e^{-t}\, (1 - e^{-t})^{l-1}\, e^{-l\,(1-e^{-t})} \tag{4.7}$$

and

$$s_l(t) = \frac{l^{l-1}}{l\,!}\, (1 - e^{-t})^{l-1}\, e^{-l\,(1-e^{-t})}\,, \qquad S(t) = e^{t}\,. \tag{4.8}$$

The initial value of the system is

$$N_1(0) = N\,, \qquad N_l(0) = 0\,, \qquad l \geq 2\,, \tag{4.9}$$

so that (2.3) is fulfilled for the sequence (cf. (2.7), (4.3))

$$c_0^{(N)} = N\,. \tag{4.10}$$

Let the random functions

$$\frac{N_l(t)}{c^{(N)}(t)}\,, \qquad t \in [0,T]\,, \quad l = 1,2,\ldots\,,$$

be obtained by linear interpolation between the points $t_k^{(N)}$ (cf. (2.11)) and $c^{(N)}(t_k^{(N)}) := c_k^{(N)}$. Using averaging over M independent trajectories we construct the empirical mean values as well as confidence intervals in a standard way.

In order to investigate the convergence

$$\frac{N_l(t)}{c^{(N)}(t)} \to \hat{n}_l(t) \quad \text{as} \quad N \to \infty\,,$$

we consider the kernel (4.4), fix $\alpha = 0.8$ and calculate the random trajectories on a time interval of length $T = 10$. The results for two components $\hat{n}_3$ and $\hat{n}_5$ of the solution are given in **Table 1**. The columns "$\hat{n}_i$-err" and "$\hat{n}_i$-conf" ($i = 3,5$) show the supremum over the time interval of the systematic error and the length of the confidence interval, respectively, i.e.

$$\sup_{t\in[0,T]}\left|E\left[\frac{N_i(t)}{c^{(N)}(t)}\right] - \hat{n}_i(t)\right| \qquad \text{and} \qquad 3\sup_{t\in[0,T]}\sqrt{\frac{1}{M}V\left[\frac{N_i(t)}{c^{(N)}(t)}\right]}\,. \tag{4.11}$$

The truncation error related to (2.15), i.e.

$$\sup_{t\in[0,T]}\left|1 - \sum_{l\geq 1} l\,\frac{N_l(t)}{c^{(N)}(t)}\right|\,, \tag{4.12}$$

(cf. Remark 2.4, (4.9), (4.10)) is denoted by "trunc", while "steps" means the number of time steps on the interval. Both values are averaged over M trajectories.

Table 1

N	M	$\hat{n}_3$-err	$\hat{n}_3$-conf	$\hat{n}_5$-err	$\hat{n}_5$-conf	trunc	steps
16	640000	2.79e-2	2.97e-4	1.02e-2	1.26e-4	0.41	5.23
32	320000	2.01e-2	3.43e-4	7.92e-3	1.40e-4	0.22	5.05
64	160000	1.37e-2	3.84e-4	5.90e-3	1.55e-4	0.10	4.99
128	80000	8.26e-3	4.09e-4	4.18e-3	1.67e-4	0.04	4.99
256	40000	4.26e-3	4.20e-4	2.76e-3	1.76e-4	0.01	4.99
512	20000	1.95e-3	4.22e-4	1.60e-3	1.83e-4	0.00	5.00
1024	10000	1.21e-3	4.35e-4	9.72e-4	1.89e-4	0.00	5.00
2048	5000	3.87e-4	4.34e-4	4.90e-4	1.90e-4	0.00	5.00
4096	2500	1.78e-4	4.31e-4	2.71e-4	1.96e-4	0.00	5.00

The time dependent curves for the empirical means approximating the components $\hat{n}_3$ and $\hat{n}_5$ are shown in **Figures 1** and **2**. The lines correspond to $N = 32$ (dashed), $N = 128$ (dotted), $N = 512$ (dashed-dotted), and the exact limit (solid).

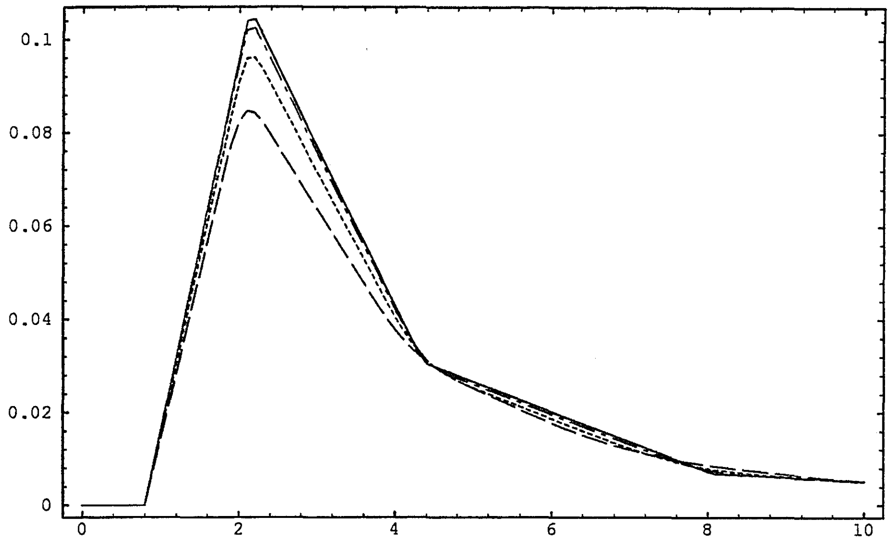

Figure 1: Convergence $\frac{N_3(t)}{c^{(N)}(t)} \to \hat{n}_3(t)$ as $N \to \infty$ (α fixed)

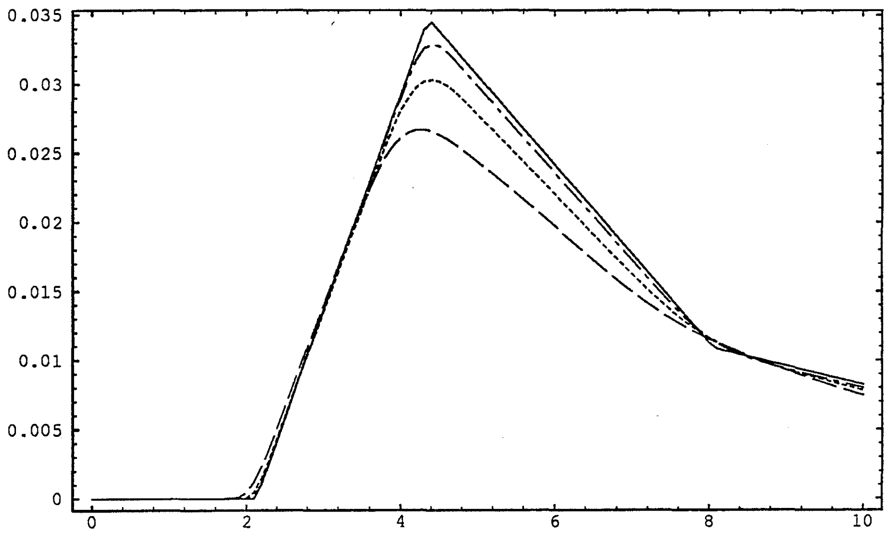

Figure 2: Convergence $\frac{N_5(t)}{c^{(N)}(t)} \to \hat{n}_5(t)$ as $N \to \infty$ (α fixed)

Next we numerically illustrate the convergence

$$\hat{n}_l(t) \to n_l(t) \quad \text{as} \quad \alpha \to 0 .$$

For this purpose, we fix $N = 10000$ and $M = 1000$ and again calculate the random trajectories of the system on the time interval of length $T = 10$. The results for the two components $\hat{n}_3$ and $\hat{n}_5$ are shown in **Table 2**. The meaning of the columns "n_i-err" and "n_i-conf" ($i = 3, 5$) is analogous to (4.11) taking now $n_i(t)$ (cf. (4.5)) as the exact reference value. The columns "t_1" and "t_2" show the first and second moment of time at which the system is doubled according to (2.16), (2.17).

Table 2

α	n_3-err	n_3-conf	n_5-err	n_5-conf	t_1	t_2
0.8	4.20e-2	4.58e-4	1.64e-2	2.03e-4	2.13	4.34
0.4	2.23e-2	2.55e-4	6.77e-3	1.38e-4	2.30	6.03
0.2	9.48e-3	2.34e-4	2.73e-3	1.13e-4	1.97	5.99
0.1	4.36e-3	2.37e-4	1.27e-3	1.09e-4	2.00	5.85
0.05	2.13e-3	2.22e-4	6.32e-4	1.10e-4	2.00	5.97
0.01	4.01e-4	2.12e-4	9.86e-5	1.12e-4	2.00	5.99

The time dependent curves for the empirical means approximating the components n_3 and n_5 are shown in **Figures 3** and **4**. The lines correspond to $\alpha = 0.8$ (dashed), $\alpha = 0.2$ (dotted), $\alpha = 0.05$ (dashed-dotted), and the exact limit (solid).

Numerical experiments with the kernel (4.6) (cf. (4.7), (4.8)) show a qualitatively similar behaviour, while the process of coagulation is going on much faster. Some results are shown in **Table 3**. Here the values $N = 10000$ and $M = 1000$ are fixed, and the meaning of "n_3-err" and "n_5-err" is as before. The truncation error (4.12) is denoted by "trunc", and "steps" means the number of time steps on the time interval of length $T = 1.75$. The column "S-err" shows the supremum over the time interval of the error for the average particle size (4.1). The column "s-err" shows the supremum over l of the error for the particle size distribution (4.2) at the end of the time interval.

Table 3

α	n_3-err	n_5-err	S-err	s-err	trunc	steps
0.2	1.13e-2	2.08e-3	1.17e-1	5.79e-3	0.04	302
0.1	4.88e-3	1.00e-3	7.93e-2	2.38e-3	0.02	627
0.05	3.15e-3	7.14e-4	3.85e-2	1.11e-3	0.00	1358

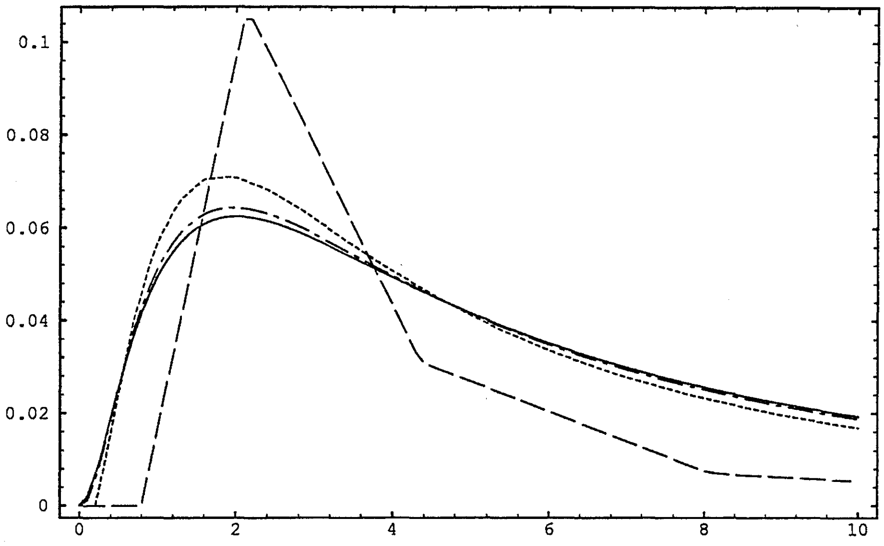

Figure 3: Convergence $\hat{n}_3(t) \to n_3(t)$ as $\alpha \to 0$ (N, M fixed)

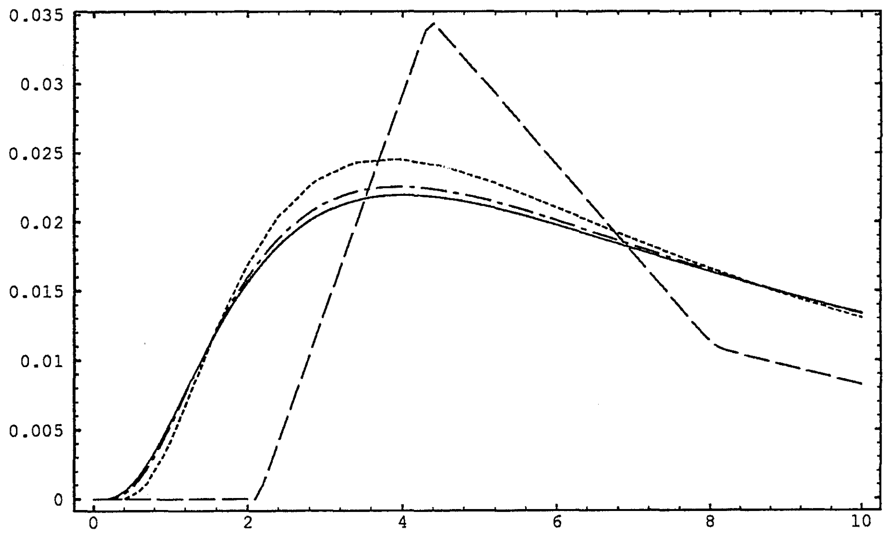

Figure 4: Convergence $\hat{n}_5(t) \to n_5(t)$ as $\alpha \to 0$ (N, M fixed)

References

[1] H. Babovsky and R. Illner. A convergence proof for Nanbu's simulation method for the full Boltzmann equation. *SIAM J. Numer. Anal.*, 26(1):45–65, 1989.

[2] K. Liffman. A direct simulation Monte Carlo method for cluster coagulation. *J. Comput. Phys.*, 100:116–127, 1992.

[3] K. Nanbu. Interrelations between various direct simulation methods for solving the Boltzmann equation. *J. Phys. Soc. Jpn.*, 52(10):3382–3388, 1983.

[4] K. K. Sabelfeld, S. V. Rogazinskii, A. A. Kolodko, and A. I. Levykin. Stochastic algorithms for solving Smoluchowski coagulation equation and applications to aerosol growth simulation. *Monte Carlo Methods Appl.*, 2(1):41–87, 1996.

[5] M. von Smoluchowski. Drei Vorträge über Diffusion, Brownsche Molukularbewegung und Koagulation von Kolloidteilchen. *Phys. Z.*, 17:557–585, 1916.

[6] W. Wagner. A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation. *J. Statist. Phys.*, 66(3/4):1011–1044, 1992.

[7] M. M. R. Williams and S. K. Loyalka. *Aerosol Science. Theory and Practice.* Pergamon, New York, 1991.

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