Numerical studies of solutions for kinetic equations with many-particle collisions

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Abstract. In this work we present a method of low-rank tensor decompositions to accelerate evaluation of the right-hand side of systems of kinetic equations with many-particle collisional terms. These equations can be interpreted as a generalization of classical Smoluchowski aggregation equations allowing one to consider not only binary collisions of particles but also triple collisions. Straight-forward evaluation of the right-hand side for such system of \( N \) equations with \( k = 1, 2, \ldots, N \) requires \( O(N^3) \) numerical operations and we find such complexity too high for practical investigations. However, under assumptions that kinetic coefficients can be represented with either canonical polyadic (CP) or tensor train decomposition (TT) with the rank \( R \ll N \) we can propose algorithms evaluating the right-hand side with much lower complexities: \( O(NR\log N) \) and \( O(NR^2 \log N) \) for CP and TT respectively. We compare numerical solutions with different triple-collision rates and obtain a significant influence of accounting triple collisional effects.

1. Introduction
Smoluchowski-type kinetic equations can be considered as a traditional approach for description of the aggregation process in a complex spatially homogeneous physical system. Such ordinary differential equations correspond to a discrete model, where particles of the system collide inelastically in consequence of chaotic movement [1]. Each particle (cluster) consists of some minimal size particles (monomers). This model is applicable to various natural and industrial phenomena from the polymer growth and ultrafine metal clusters catalysts to formation of stars [2,3]. However in most studies only binary collisions of particles are taken into consideration [2,4]. That can be reasonably explained, because many-particle collisions lead to a growth of the computational cost of the solution and are often supposed to be rare events. Nevertheless some authors made a progress in studying such class of problems [5–7].

In this work we assume the presence of triple particle collisions along with binary ones including both the collisions between monomers as well as between clusters. Thus, the \( k \)-th kinetic equation defines the evolution of the concentration \( n_k(t) \) per volume unit of \( k \)-size
particles and can be written as \( \frac{dn_k}{dt} = S_k(n_1, n_2, \ldots) \) where
\[
S_k = \frac{1}{2} \sum_{i_1+i_2=k} C^{(2)}_{i_1,i_2} n_{i_1} n_{i_2} - n_k \sum_{i_1 \geq 1} C^{(2)}_{i_1,k} n_{i_1} + \frac{1}{6} \sum_{i_1+i_2+i_3=k} C^{(3)}_{i_1,i_2,i_3} n_{i_1} n_{i_2} n_{i_3} - \frac{n_k}{2} \sum_{i_1,i_2 \geq 1} C^{(3)}_{i_1,i_2,k} n_{i_1} n_{i_2}.
\]
Here, the first and the second terms correspond respectively to concentration increase and decrease rates of \( k \)-size particles due to binary collisions. The third and fourth terms analogously define effects consequent to ternary collisions. Kinetic coefficients \( C^{(2)}_{i_1,i_2} \) and \( C^{(3)}_{i_1,i_2,i_3} \) are binary and ternary collision rates of particles of the sizes \( i_1, i_2, i_3 \). Straight-forward evaluation of the right-hand side term \( S_k \) for all sizes \( k \) is too heavy for practical investigations, because it requires \( O(N^3) \) numerical operations for system of \( N \) equations with \( k = 1, 2, \ldots, N \).

A Cauchy problem for such system of considered above kinetic equations can be posed by defining initial condition \( n_k(0) = n_{k,0} \) for each size \( k \). The analytical solution for this problem is known only for kinetic coefficients of simple form (constant, additive and multiplicative) \([5,6,8]\). In the present work we provide a fast finite difference method for solving the Cauchy problem for mentioned kinetic equations. With the use of tensor decompositions and fast methods of numerical linear algebra we reach high level of accuracy of numerical solutions in really modest computational times. We also describe the obtained numerical results for a realistic model of aggregation process accounting for triple collision effects.

2. Model of many-particle aggregation
We consider the following kinetic coefficients for binary and ternary collisions
\[
C^{(2)}_{i_1,i_2} = \frac{\sqrt{2}}{4} \cdot (\sqrt{i_1} + \sqrt{i_2})^2 \cdot \sqrt{1/i_1 + 1/i_2},
\]
\[
C^{(3)}_{i_1,i_2,i_3} = \frac{\alpha_{3/2}}{324} \frac{\sqrt{6}}{\sqrt{i_1 i_2 i_3/(i_1 + i_2 + i_3)}} \left[ \frac{(\sqrt{i_1} + \sqrt{i_2} + \sqrt{i_3})^3}{\sqrt{1/i_1 + 1/i_2}} \cdot \frac{(\sqrt{i_1} + \sqrt{i_3})^3}{\sqrt{1/i_1 + 1/i_3}} + \frac{(\sqrt{i_2} + \sqrt{i_3})^3}{\sqrt{1/i_2 + 1/i_3}} \right].
\]
Here each particle is represented as a sphere. Model is based on the assumption, that any result of ternary collision is in fact the result of stabilization of intermediate nonstable formation of two particles by collision with the third one. We form the ternary collisional kinetic coefficients empirically by analogy with the classical binary ballistic coefficients. Moreover their symmetry and positiveness follow from the properties of studied aggregation process. The parameter \( \alpha_{3/2} \) defines the relative rate of ternary collisional events as compared to binary ones (i.e. the ratio of characteristic times of these processes). We use the monodisperse initial conditions \( n_{k,0} = \delta_{1,k} \) for all sizes \( k \) where \( \delta_{i,j} \) is the Kronecker symbol.

3. Numerical method
An approximate solution of the Cauchy problem for the system of Smoluchowski-type kinetic equations can be evaluated by means of finite-difference schemes. For example one can apply the second order Runge-Kutta scheme with a time step \( \Delta t \) for sizes \( k = 1, 2, \ldots, N \) of the form
\[
\frac{n_k^{s+1/2} - n_k^s}{\Delta t/2} = S_k(n_1^s, n_2^s, \ldots, n_N^s), \quad \frac{n_k^{s+1} - n_k^s}{\Delta t} = S_k(n_1^{s+1/2}, n_2^{s+1/2}, \ldots, n_N^{s+1/2}).
\]
Here the value \( n_k^s \) approximates \( n_k(s \cdot \Delta t) \). The scheme has an approximation error \( O((\Delta t)^2) \) of the analytical solution. However each step of the scheme requires \( O(N^3) \) numerical operations with the naive calculations as was said in the introduction. Yet it can be accelerated by the use
of tensor decompositions and fast methods of numerical linear algebra. This fact can be illustrated by ternary collision kinetic coefficients of the rank-one form \( C_{i_1,i_2,i_3}^{(3)} = u_{i_1} \cdot v_{i_2} \cdot w_{i_3} \) (the same holds for rank-one binary collision coefficients). Thus if we are to compute the following values of the third term in \( S_k \) for all sizes \( k \)

\[
P_k = \sum_{i_1+i_2+i_3=k} C_{i_1,i_2,i_3}^{(3)} n_{i_1} n_{i_2} n_{i_3} = \sum_{i_1+i_2+i_3=k} (u_{i_1} n_{i_1}) \cdot (v_{i_2} n_{i_2}) \cdot (w_{i_3} n_{i_3}), \quad k = 1, 2, \ldots, N,
\]

then we just have to succesively calculate the results of two shifted discrete convolutions

\[
P_k = \sum_{i=1}^{k-2} (u_i n_i) \cdot z_{k-i}, \quad z_k = \sum_{j=1}^{k-1} (v_j n_j) \cdot (w_{k-j} n_{k-j}), \quad k = 1, 2, \ldots, N.
\]

These calculations can be done via fast Fourier transform in \( O(N \log N) \) numerical operations [9]. One can generalize the mentioned procedure with kinetic coefficients of more complex form represented as a skeleton decomposition and the array \( C_{i_1,i_2,i_3}^{(3)} \) in order to evaluate the operators \( S_k \) for all \( k \). Suppose the array \( C^{(2)} = [C_{i_1,i_2}^{(2)}] \) is approximately represented as a skeleton decomposition and the array \( C^{(3)} = [C_{i_1,i_2,i_3}^{(3)}] \) has one of the following two forms

\[
C_{i_1,i_2,i_3}^{(3)} \approx \sum_{\rho=1}^{R} u_{i_1,\rho} \cdot v_{i_2,\rho} \cdot w_{i_3,\rho}; \quad C_{i_1,i_2,i_3}^{(3)} \approx \sum_{\rho_1,\rho_2=1}^{R} u_{i_1,\rho_1} \cdot v_{i_2,\rho_1,\rho_2} \cdot w_{i_3,\rho_2,i_3}.
\]

The first decomposition is a canonical polyadic (CP) and the second one is a tensor train (TT). Then the total computational cost of values \( S_k \) for all sizes \( k = 1, 2, \ldots, N \) together is \( O(N R \log N) \) and \( O(N R^2 \log N) \) for CP and TT-representations respectively. Note that there exists a robust method of tensor approximation by a TT-decomposition with complexity \( O(N R^3) \) numerical operations [10].

There is also a sequence of related results in terms of computational complexity and use of low-rank matrix and tensor decompositions. They are presented in recent studies of the physical systems allowing only binary collisions: in application to continuous coagulation models [11, 12], multicomponent coagulation processes [13, 14] and discrete equations of aggregation and fragmentation processes in both time-dependent [15,16] and stationary cases [17].

4. Numerical results

In the present section we decribe the numerical results concerning the influence of triple particle collisions. Here we do not show the results of tests concerning performance and accuracy of our method. For such results we refer the readers to our recent article [18]. Note, that in the mentioned work a good agreement was obtained between a numerical solution and the known analytical solution in special case of constant kinetic coefficients and monodisperse initial conditions.

In the numerical experiments we used the monodisperse initial conditions \( n_{k,0} = \delta_{i,k} \) and the kinetic coefficients of forms (1) and (2) for binary and ternary collisions respectively. From the results of the experiments we conclude that there is a significant influence of triple-particle collisions on the cluster distribution. One can see that on figure 1 illustrating the numerical solutions for Cauchy problem with and without accounting ternary collisional events. There the concentrations of large particles become nonzero two times faster with a quite small (twenty percent) relative rate of ternary collisions.

We also compared the behavior of the full cluster concentration \( n(t) \) and the relative geometric size \( R_1 \) and the volume size \( R_3 \) of clusters depending on the parameter \( \alpha_{3/2} \). These values are
defined as follows

\[ n(t) = \sum_{k=1}^{\infty} n_k(t), \quad R_\lambda(t) = \sum_{k=1}^{\infty} k^\lambda \cdot n_k(t)/n(t). \]

The values of the governing parameter were chosen as \( \alpha_{3/2} = 0.05, 0.1, 0.2 \). We also compared the obtained numerical results with ones in case of only binary collisions model (i.e. when \( C^{(3)} = 0 \)).

Figure 1. Cluster distribution with and without accounting ternary collisions. Logarithmic scale on both axes.

Figure 2. Evolution of the full cluster concentration \( n(t) \). Logarithmic scale on \( t \)-axis.

Figure 3. Evolution of the relative geometric size \( R_1 \) of clusters.

Figure 4. Evolution of the relative volume \( R_3 \) of clusters.

Figure 2 shows that with the growth of the ternary collision rate the full concentration of particles changes insignificantly. At the same time the mass of the system redistributes faster in particles of large sizes with the growth of the parameter \( \alpha_{3/2} \). The latter fact is shown on figures 3 and 4. It is clear, that the presence of ternary collisions has a great influence on the growth of relative moments \( R_\lambda \) of the solution of higher orders \( \lambda \). This also means that the total concentration of particles is dominated by small particles, but their size is defined by larger particles. The last result shows that only the ten percents of ternary collisions define approximately the double growth in the mean particle volume size.

5. Conclusions
In this work we recall a fast numerical method for solving the Cauchy problem for system of Smoluchowski-type kinetic equations of aggregation with triple-particle collisional terms.
The method is based on applications of low-rank tensor decompositions such as CP or TT. Such approach can be used with different physical models accounting ternary collisions.

With the use of the method we were able to compare numerical solutions corresponding to different relative ternary collision rates that manifest a significant influence of accounting triple collisional effects.

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