Steady oscillations in kinetic model of aggregation process with collisional fragmentation

Sergey Matveev[1,*], , Aleksei Kalinov[1], Pavel Krapivsky[2] and Nikolai Brilliantov[1]

1. *Skolkovo Institute of Science and Technology*, Skolkovo Innovation Center, 3, Moscow, 143026, Russia
2. *Boston University*

* *matseralex@gmail.com*

Introduction

In this work, we study a kinetic model of aggregation process with collisional fragmentation

$$[i] + [j] \xrightarrow{K_{i,j}} [i+j], \qquad \texttt{aggregation}$$
$$[i] + [j] \xrightarrow{\lambda \cdot K_{i,j}} \underbrace{[1] + \ldots [1]}_{i+j} \qquad \texttt{shattering}$$

the governing equations can be read as

$$\begin{cases} \dfrac{dn_1}{dt} = -n_1 \sum\limits_{i=1}^{N} K_{1,i} n_i + \lambda \sum\limits_{i=2}^{N} \sum\limits_{j=2}^{N} (i+j) K_{i,j} n_i \, n_j + \lambda n_1 \sum\limits_{j=2}^{N} j K_{1,j} n_j \\ \dfrac{dn_k}{dt} = \ \frac{1}{2} \sum\limits_{i=1}^{k-1} K_{i,k-i} n_i n_{k-i} - (1+\lambda) n_k \sum\limits_{i=1}^{N} K_{k,i} n_i, \qquad k = \overline{2, N}. \end{cases}$$

We study them with use of two efficient implementations of numerical methods:

- direct simulation Monte Carlo
- finite-difference scheme exploiting the low-rank matrix representations [3]

Main Objectives

- Extension of DSMC methods to case of aggregation with collisional fragmentation,
- Validation of the steady oscillations in aggregation-shattering processes with stochastic modelling,
- Extension of the performed analysis for the case of time-dependent shattering parameter $\lambda(t)$.

DSMC simplest algorithm

The algorithm is

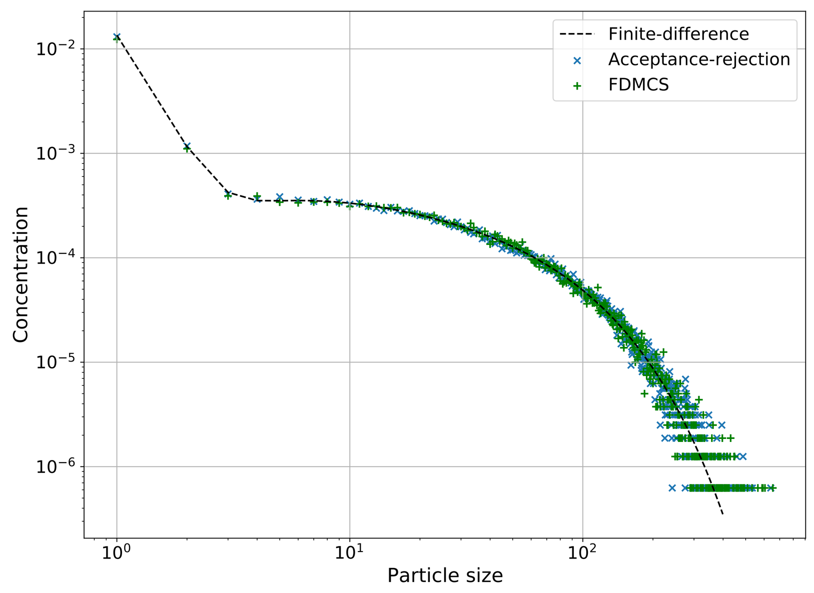
Algorithm 1 Acceptance-rejection method

1: Generate random number $r \in (0, 1)$
2: Choose random pair (i, j)
3: **If** $r < \frac{K_{s(i),s(j)}}{K_{\max}}$
4: add particle of size $s(i) + s(j)$ into array of particles (and delete two old),
5: $t = t + \tau$,
6: update τ, $K_{\max}$ and probabilities
7: Go to step 1
8: **Else**
9: $t = t + \tau$,
10: Go to step 1

One only needs to generate samples for the initial conditions. They are obvious for the mono-disperse case. We also tried the Fast DSMC approach [1].

Validation results

For the ballistic kenrnel we provided the numerical valiadation of our results



Particle size distribution at $t = 10$ for the ballistic kernel

$$K_{i,j} = (i^{1/3} + j^{1/3})^2 \sqrt{\frac{1}{i} + \frac{1}{j}}.$$

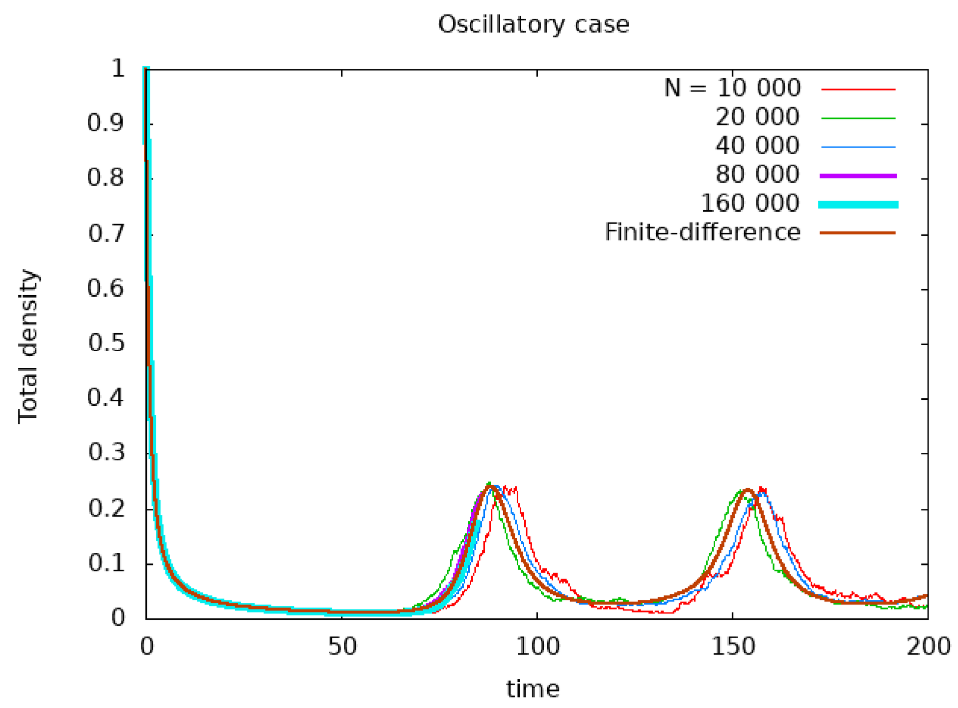
For Monte-Carlo algorithms initial number of particles is $N = 10^5$. Finite-difference scheme step size $\Delta t = 10^{-3}$. Results agree very-well

Oscillations

For the generalized Brownian coefficients

$$K_{i,j} = \left(\frac{i}{j}\right)^a + \left(\frac{j}{i}\right)^a$$

with $a > 0.5$ steady oscillations have been discovered recently with use of only the finite-difference methods [2]. Now we can present a cross validation of those oscillations with use of Acceptance-Rejection approach



Here we show the oscillations of the total density for $a = 0.95$, $\lambda = 0.005$. The results are very preliminary but qualitatively correct!

Conclusions

- We apply DSMC sccessfully for aggregation kinetics with collisional fragmentation.
- Demonstrate the cross-validation of numerical simulations for the ballistic kernel.
- Demonstrate the preliminary qualitative agreement of steady oscillatory solutions with finite-difference method.

References

[1] F Einar Kruis, Arkadi Maisels, and Heinz Fissan. Direct simulation monte carlo method for particle coagulation and aggregation. *AIChE Journal*, 46(9):1735–1742, 2000.

[2] S. A. Matveev, P. L. Krapivsky, A. P. Smirnov, E. E. Tyrtyshnikov, and N. V. Brilliantov. Oscillations in aggregation-shattering processes. *Phys. Rev. Lett.*, 119(26):260601, 2017.

[3] S A Matveev, A P Smirnov, and E E Tyrtyshnikov. A fast numerical method for the cauchy problem for the smoluchowski equation. *Journal of Computational Physics*, 282:23–32, 2015.

Acknowledgements

We acknowledge Alexander Osinsky for important discussions.