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Adaptive time-stepping for aggregation-shattering kinetics

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Abstract: We propose an experimental study of adaptive time-stepping methods for efficient modeling of the aggregation-fragmentation kinetics. Precise modeling of this phenomena usually requires utilization of the large systems of nonlinear ordinary differential equations and intensive computations. We study the performance of three explicit Runge–Kutta time-integration methods and provide simulations for two types of problems: finding of equilibrium solutions and simulations for kinetics with periodic solutions. The first class of problems may be analyzed through the relaxation of the solution to the stationary state at large time. In this case, the adaptive time-stepping may help to reach this state using big steps reducing cost of the calculations without loss of accuracy. In the second case, the problem becomes numerically unstable at certain points of the phase space and may require tiny steps making the simulations very time-consuming. Adaptive criteria allows to increase the steps for most of the remaining points and speedup simulations significantly.

Keywords: adaptive Runge–Kutta methods, aggregation, fragmentation, kinetic equations, nonlinear differential equations.

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Адаптивные шаги по времени для агрегационно-фрагментационной кинетики

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Аннотация: Мы предлагаем экспериментальное исследование методов интегрирования по времени с адаптивными шагами по времени для эффективного моделирования кинетики агрегации-фрагментации. Точное моделирование этого явления обычно требует использования больших систем нелинейных обыкновенных дифференциальных уравнений и интенсивных вычислений. Мы исследуем производительность трех явных методов Рунге–Кутты и проводим моделирование для двух типов задач: нахождение равновесных решений и моделирование для кинетики с периодическими решениями. Первый класс задач может быть проанализирован посредством релаксации решения к стационарному состоянию на больших временах. В этом случае адаптивные временные шаги могут помочь достичь этого состояния с использованием больших шагов, снижая стоимость вычислений без потери точности. Во втором случае задача оказывается численно неустойчивой в определенных точках фазового пространства и может потребовать крошечных шагов, что делает моделирование с постоянными шагами очень трудоемким. Адаптивные критерии позволяют увеличить шаги для большинства оставшихся точек и значительно ускорить моделирование.

Ключевые слова: методы Рунге–Кутты с адаптивными шагами, агрегация, фрагментация, кинетические уравнения, нелинейные дифференциальные уравнения.

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1. Introduction. Kinetic processes of aggregation and fragmentation often can be described with the use of nonlinear ordinary differential equations. These processes are widespread in nature and important for many industrial applications [1, 2]. The smallest possible aggregates are usually called monomers. They may coalesce due to the collisions and generate larger aggregates. Further, these particles can also collide with

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each other and grow up to larger particles consisting of thousands or even millions of monomers. If one knows or fixes the kinetic rates $K_{i,j}$ (kernel) for the reactions $[i] + [j] \to [i + j]$ with some formal expression (e.g. $K_{i,j} = (i/j)^{1/3} + (j/i)^{1/3} + 2$), then the basic equations are well-known as Smoluchowski equations [3]:

$$\frac{dn_s}{dt} = \underbrace{\frac{1}{2}\sum_{i+j=s} K_{i,j} n_i n_j}_{\text{“birth” of particle of size } s} - \underbrace{n_s \sum_{i=1}^{\infty} K_{s,i} n_i}_{\text{“death” of particles of size } s}, \qquad s = 1, 2, \ldots, \infty. \tag{1}$$

These equations describe evolution of the concentrations $n_s(t)$ of the particles of size s due to their “birth” after the coalescence of smaller aggregates and due to their “death” after merging events. All interactions in such system are assumed to be pairwise, mass-conserving and spatially homogeneous.

Fixing some initial conditions as $n_s(t = 0)$, one gets the Cauchy problem for this formally infinite system of nonlinear ODEs. This problem can be solved analytically only in the very rare special cases (e.g. constant kinetic rates with monodisperse or exponential initial conditions [4]). Hence, there is a certain need in efficient numerical algorithms for their investigation. Asymptotic and scaling features of the solutions $n_s(t)$ for $s \gg 1$, $t \gg 1$ are important for physicists [5, 6]. However, their justification often may require utilization of enormous finite sub-systems

$$\frac{dn_s}{dt} = \underbrace{\frac{1}{2}\sum_{i+j=s} K_{i,j} n_i n_j}_{\text{“birth” of particle of size } s} - \underbrace{n_s \sum_{i=1}^{M} K_{s,i} n_i}_{\text{“death” of particles of size } s}, \qquad s = 1, 2, \ldots, M. \tag{2}$$

These systems of ODEs with $M \gg 1$ allow to approximate the solution of initial equations (2) rather well for the large time intervals [6–8]. Straight-forward computations with the classical Runge–Kutta methods for these large systems require too much computing resources that should be likely reduced (each computation of the right-hand side takes $O(M^2)$ operations). A family of efficient methods allowing to evaluate the right-hand side for $O(MR \log M)$ operations was proposed for the case of the low-rank kernels

$$K_{i,j} = \sum_{\alpha=1}^{R} U_{i,\alpha} V_{\alpha,j}, \quad R \ll M.$$

These methods allow to do computations with hundreds of thousands kinetic equations on basic laptops [9]. Coupling of the low-rank decompositions with the time-integration methods has already been utilized for a broad class of problems. They include the irreversible aggregation with sources and sinks of particles [10]

$$\frac{dn_s}{dt} = \frac{1}{2}\sum_{i+j=s} K_{i,j} n_i n_j - n_s \sum_{i=1}^{M} K_{s,i} n_i + \underbrace{P_k}_{\text{sources}}, \quad s = 1, 2, \ldots, M, \tag{3}$$

and aggregation-shattering kinetics [11, 12]

$$\frac{dn_1}{dt} = \underbrace{-n_1 \sum_{i=1}^{M} K_{1,i} n_i}_{\text{collisional aggregation}} + \underbrace{\frac{\lambda}{2}\sum_{i\geqslant 2}\sum_{j\geqslant 2}(i+j) K_{i,j} n_i n_j + \lambda \sum_{j\geqslant 2} j K_{1,j} n_j}_{\text{new monomers after collisional shattering events}},$$

$$\frac{dn_s}{dt} = \underbrace{\frac{1}{2}\sum_{i+j=s} K_{i,j} n_i n_j - n_s \sum_{i=1}^{M} K_{s,i} n_i}_{\text{collisional aggregation terms}} - \underbrace{\lambda n_s \sum_{i=1}^{M} K_{s,i} n_i}_{\text{shattering into monomers}}, \qquad s = 2, 3, \ldots, M. \tag{4}$$

The parameter $0 < \lambda \ll 1$ in (4) corresponds to intensity of binary collisional shattering events. Other studies also include temperature-dependent Smoluchoswki equations [13, 14] and spatially inhomogeneous problems [15].

Despite application of the low-rank decompositions leads to the drastic speedup of computations, most of interesting experiments were done with the simplest constant time-steps that often might be a bottleneck for research.

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In case of the irreversible aggregation problem (3) with multiple sources of particles [10], there exist complex stationary particle size distributions that seem to be extremely difficult to construct accurately using alternative approaches such as miscellaneous Monte Carlo methods [16–19] or coarse-graining approaches [20, 21]. Unfortunately, these stationary and quasi-stationary solutions may require to produce simulations for extremely large final times and number equations [10, 22].

At the same time, the dynamic oscillations are possible in aggregation models [11, 23]. For instance, the simulations for the periodic solutions arising in the aggregation-shattering kinetics (4) require very tiny time-steps [11]. Otherwise, the simulations with constant larger time-steps become numerically unstable and crash.

Adaptive schemes for the numerical integration of differential equations allow to automatically select the time-step depending on the characteristics of the system. These schemes are especially useful when the system has a variable sensitivity to changes over time or when an accurate solution is needed in certain time domains. One example of adaptive integration schemes is the Runge–Kutta method with automatic step selection (adaptive Runge–Kutta method see e.g. [24, 25]). In this method, the integration step is varied in such a way as to control the approximation error. For small time changes in the system, the integration step can be increased to save the computing resources, and for the fast dynamics the integration step can be reduced to ensure the accuracy of the solution.

Adaptive time integration schemes are widely used in various fields, such as modeling of dynamic systems, numerical solution of differential equations in physics, biology, economics and other sciences. They allow to effectively and accurately simulate the behavior of systems with variable conditions.

There exists an old empirical criteria for stable calculations with Euler scheme for the choice of time-step

$$\tau(t) \leqslant a \cdot \left[\max \sum_{j=1}^{M} K_{i,j} n_j(t) \right]^{-1}$$

with $a \lesssim 1$. In practice, one may set $1/10 < a < 1/4$, but reaching the peak performance might require additional fine-tuning [6, 13]. Such a criteria is rather often used, but it cannot be generalized for the higher order methods as well as was elaborated only for the irreversible aggregation models.

We conduct a numerical investigation showing that adaptive time-steps can be successfully applied to these problems. In this work we

1. implement the adaptive time-steps for the second, fourth order Runge–Kutta and for the Runge–Kutta–Fehlberg methods in application to aggregation kinetics;

2. show that there is a computational speedup with adaptive-time steps for the problems with stationary and oscillating solutions by dozens of times;

3. present that the relaxation dynamics of the solutions to the stationary state for the large $T \gg 1$ can be tracked with adaptive-time steps.

2. Methods. In order to solve any of the listed problems (1)–(4) by any time-integration method, we firstly re-write them in a compact operator form:

$$\begin{cases} \dfrac{d\boldsymbol{n}}{dt} = \boldsymbol{S}(\boldsymbol{n}), \\ \\ \boldsymbol{n}(t=0) = \boldsymbol{n}_0, \end{cases} \tag{5}$$

where $\boldsymbol{n}(t)$ corresponds to the vector of concentrations $[n_1(t), \ldots, n_M(t)]^{\mathsf{T}}$ and $\boldsymbol{S}(\boldsymbol{n})$ denotes the right-hand side for the system of target ODEs. In this work, we do not discuss the complexity of evaluation of $\boldsymbol{S}(\boldsymbol{n})$ but only refer to the original work [9], where we have shown that its calculation process requires $O(MR \log M)$ operations for the low-rank kernels with rank $R \ll M$. We utilize this approach and concentrate on investigation of performance of the time-integration methods. Namely, we use the following explicit schemes:

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- the second-order Runge–Kutta method (RK2)

$$\begin{aligned}
\boldsymbol{k}_1 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k),\\
\boldsymbol{k}_2 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k + \boldsymbol{k}_1),\\
\boldsymbol{n}^{k+1} &= \boldsymbol{n}^k + \frac{\boldsymbol{k}_1 + \boldsymbol{k}_2}{2}.
\end{aligned}$$

- the fourth-order Runge–Kutta method (RK4)

$$\begin{aligned}
\boldsymbol{k}_1 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k),\\
\boldsymbol{k}_2 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k + \frac{1}{2}\boldsymbol{k}_1),\\
\boldsymbol{k}_3 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k + \frac{1}{2}\boldsymbol{k}_2),\\
\boldsymbol{k}_4 &= \tau \cdot \boldsymbol{S}(\boldsymbol{n}^k + \boldsymbol{k}_3),\\
\boldsymbol{n}^{k+1} &= \boldsymbol{n}^k + \frac{\boldsymbol{k}_1 + 2\boldsymbol{k}_2 + 2\boldsymbol{k}_3 + \boldsymbol{k}_4}{6}.
\end{aligned}$$

- the Runge–Kutta–Fehlberg method (RKF45) [26]

$$\begin{aligned}
\boldsymbol{k}_1 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k\right),\\
\boldsymbol{k}_2 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k + \frac{1}{4}\boldsymbol{k}_1\right),\\
\boldsymbol{k}_3 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k + \frac{3\boldsymbol{k}_1 + 9\boldsymbol{k}_2}{32}\right),\\
\boldsymbol{k}_4 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k + \frac{1932\boldsymbol{k}_1 - 7200\boldsymbol{k}_2 + 7296\boldsymbol{k}_3}{2197}\right),\\
\boldsymbol{k}_5 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k + \frac{439}{216}\boldsymbol{k}_1 - 8\boldsymbol{k}_2 + \frac{3680}{513}\boldsymbol{k}_3 - \frac{845}{4104}\boldsymbol{k}_4\right),\\
\boldsymbol{k}_6 &= \tau \cdot \boldsymbol{S}\left(\boldsymbol{n}^k - \frac{8}{27}\boldsymbol{k}_1 + 2\boldsymbol{k}_2 - \frac{3544}{2565}\boldsymbol{k}_3 + \frac{1859}{4104}\boldsymbol{k}_4 - \frac{11}{40}\boldsymbol{k}_5\right),\\
\boldsymbol{n}_{RK5} &= \underbrace{\boldsymbol{n}^k + \frac{16}{135}\boldsymbol{k}_1 + \frac{6656}{12825}\boldsymbol{k}_3 + \frac{28561}{56430}\boldsymbol{k}_4 - \frac{9}{50}\boldsymbol{k}_5 + \frac{2}{55}\boldsymbol{k}_6}_{\text{step with the fifth order of accuracy for adaptive criteria.}},\\
\boldsymbol{n}^{k+1} &= \underbrace{\boldsymbol{n}^k + \frac{25}{216}\boldsymbol{k}_1 + \frac{1408}{2565}\boldsymbol{k}_3 + \frac{2197}{4104}\boldsymbol{k}_4 - \frac{1}{5}\boldsymbol{k}_5}_{\text{final step with the fouth order of accuracy, if criteria is fulfilled}}.
\end{aligned}$$

Thus, we seek to apply the adaptive criteria for choosing the time-integration step τ in order to reduce number of calls of $\boldsymbol{S}(\boldsymbol{n})$ during the simulations.

In case of the RK2 and the RK4 methods we utilize the general trick for automatic selection of the step-size (see e.g. Ch. 8, Par. 3 of [24] or [25]) doing a pair of steps with $\tau/2$, obtaining a vector $\widehat{\boldsymbol{n}}^{k+1}$ and a single step τ getting $\boldsymbol{n}^{k+1}$. After it, the relative convergence error should be investigated according to basic theory and the time step is updated according to simple equation [27]

$$\tau_{new} = s \cdot \tau_{old} \cdot \left(\frac{tol}{||\widehat{\boldsymbol{n}}^{\boldsymbol{k+1}} - \boldsymbol{n}^{\boldsymbol{k+1}}||_2}\right)^{1/p}, \tag{6}$$

where tol is the tolerance specified by the user, p is the order of the method ($p = 2$ for the RK2 and $p = 4$ for the RK4), $||\cdot||_2$ is Euclidian norm and $0 < s < 1$ is a safety factor (we use $s = 1/4$).

Finally, if the error exceeds the pre-selected tolerance, the time-step should be halved and the refinement test will have to be repeated. If the error is less than the tolerance criteria, then the next step can be done with twice larger τ and the refinement criteria should be checked again.

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For the RKF45 we follow the original criterion from paper by Fehlberg [26]: the current iteration of the method has to be repeated until the estimate of the error becomes less than the maximum permissible one as we set *tol* parameter. In this case, for each attempt the step decreases in proportion to the fifth root of the ratio of the maximal permissible error to the current one. For example, if the error exceeds the permissible level by two times, then the step is reduced by approximately 20%. If the error becomes smaller than the target level, then we increase the step size according to the rule. For instance, if the error is two times less than the permissible one, then the step increases by about 3%. If the errors are equal, then the step is reduced by 10%.

3. Numerical experiments.

3.1. Complex steady-state for irreversible aggregation with multiple sources. At first, we study the performance of the adaptive time-integration methods in application to irreversible aggregation equations with multiple sources (3). These equations can be probed with various kernels including the constant one

$$K_{i,j} \equiv 1,$$

the ballistic one

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

or with the family of the generalized Brownian kernels

$$K_{i,j} = \left(\frac{i}{j}\right)^{\alpha} + \left(\frac{j}{i}\right)^{\alpha}, \quad 0 \leqslant \alpha < 1/2, \quad c \geqslant 0.$$

In recent work [10], we have found complex stationary solutions for these equations for all types of these kernels for a case of two constant sources of particles

$$P_k = \begin{cases} 1, & k = 1, \\ p, & k = 100, \\ 0, & k \neq 1, 100. \end{cases}$$

Such complex stationary particle size distributions (see Figure 1) correspond to the equilibrium state between the injection and sink processes for $t \to \infty$ leading to a system of nonlinear equations

$$0 = \frac{1}{2} \sum_{i+j=s} K_{i,j} n_i n_j - n_s \sum_{i=1}^{M} K_{s,i} n_i + P_k, \quad s = 1, 2, \ldots, M. \qquad (7)$$

The solutions of this system do not depend on the initial conditions for ODEs (hence, we consider them as monosdisperse one, namely $n_k(t = 0) = \delta_{k,1}$, where $\delta_{i,j}$ is a Kronecker symbol). Finding such particle size distributions is an extremely tough problem via Monte Carlo simulations. This is primarily caused by their highly oscillating form and long relaxation times. They were found with use of the deterministic iterative methods in application to (7): one can apply Anderson acceleration [10] or Newton method [22]. The iterative approach is very efficient and can be easily coupled with

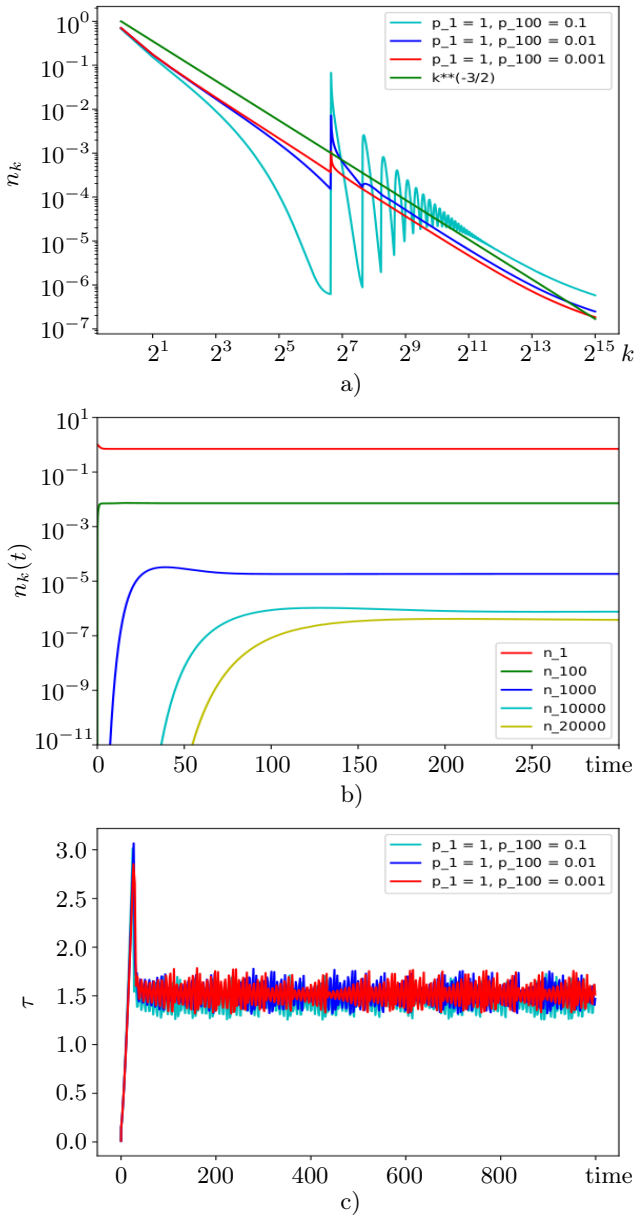

Figure 1. The problem with monodisperse conditions $M = 32768$ and a constant power of the source of monomers $P_1 = 1$ and several values of P_{100} from 10^{-3} to 10^{-1}: a) the numerical stationary solutions oscillate for a wide range of the particle sizes in agreement with [10] and relax to the scaling $n_k \simeq k^{-3/2}$, $k \gg 1$; b) dynamics of the concentrations $n_k(t)$ for multiple masses; c) the adaptive time-step increases quite rapidly and oscillates around 1.5 units of dimensionless t for a long interval of model time

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Table 1. Computational times in seconds and numbers of requests to the right-hand side with the constant kernel $K_{i,j} = 1$, $M = 32768$, and $T \in [0, 1000]$

Scheme	Const. $\tau = 0.01$	$tol = 10^{-4}$	$tol = 10^{-6}$	$tol = 10^{-8}$
RK2	131.5 / 40000	2.737 / 784	17.66 / 4888	135.1 / 46882
RK4	255.4 / 80000	3.633 / 1056	19.18 / 5780	177.5 / 54180
RKF45	397.6 / 120000	3.223 / 876	3.557 / 972	4.579 / 1260

Table 2. Computational times in seconds and number of requests to the right-hand side for the Brownian kernel with $K_{i,j} = (i/j)^{1/3} + (j/i)^{1/3}$, $M = 32768$, and $T \in [0, 1000]$

Scheme	Const. $\tau = 0.01$	$tol = 10^{-4}$	$tol = 10^{-6}$	$tol = 10^{-8}$
RK2	279.33 / 40000	35.52 / 5036	51.61 / 8784	305.94 / 49862
RK4	482.12 / 80000	46.95 / 7508	70.60 / 11792	340.5 / 58788
RKF45	690.5 / 120000	58.23 / 9966	57.25 / 9924	58.29 / 10056

low-rank methods for evaluation of the right-hand size $\boldsymbol{S}(\boldsymbol{n})$. It allows to obtain the numerical solutions for the large systems even with million of equations.

However, the relaxation dynamics (see panel in the center of the Figure 1) cannot be tracked with older methodology at all. At the same time, stationary solutions are reachable only for the large times and adaptive time-stepping methods become a necessary tool allowing to obtain the results in reasonable computing times. We sum up the results of our benchmarks in Table 1 and Table 2. Both computational times in seconds and number of evaluations of the right-hand side decrease significantly.

3.2. Aggregation-shattering with dynamic oscillations. The second example of a complex model for application of the adaptive time-stepping rules are the kinetic equations for aggregation-shattering processes (4). Dynamic oscillations are possible for this model [11] with non-local kernels

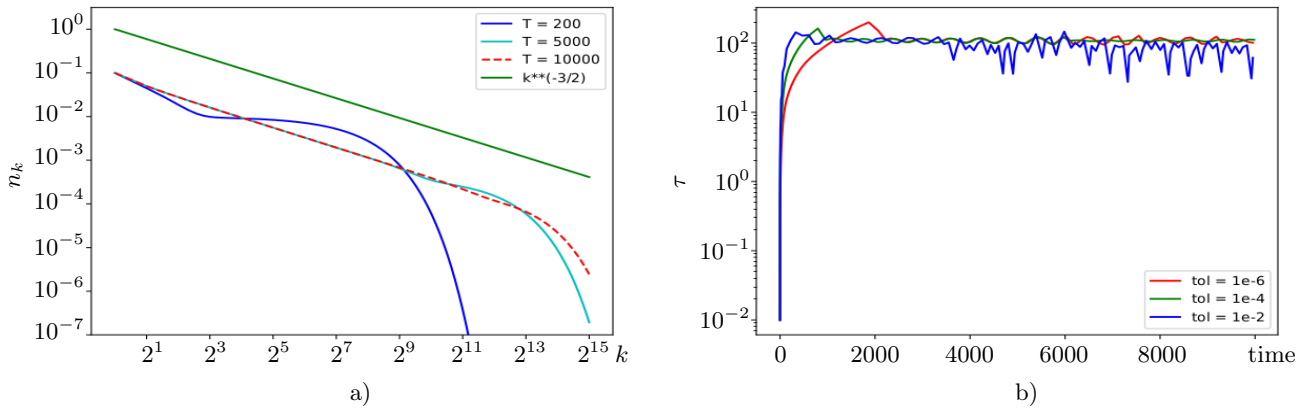
$$K_{i,j} = \left(\frac{i}{j}\right)^{\alpha} + \left(\frac{j}{i}\right)^{\alpha}, \quad \alpha > 1/2,$$

with small shattering rates $0 < \lambda \leqslant \lambda^* \ll 1$ and various initial conditions (in this work we study the monodisperse case $n_k(t = 0) = \delta_{k,1}$, where $\delta_{i,j}$ is a Kronecker symbol).

In Figure 2 we demonstrate the slow relaxation of the solution of the aggregation-shattering equations to the stationary state

$$n_k \simeq k^{-\beta} \cdot e^{-\lambda^2 k}, \quad k \gg 1.$$

This observation is in agreement with previously elaborated theory [12] for the constant kernel ($\beta = 3/2$ for $\alpha = 0$ and $\lambda = 0.01$). We see that this relaxation is slow and takes a lot of time. Utilization of the adaptive



a) b)

Figure 2. Numerical experiments for the constant kernel with $\alpha = 0$, $M = 32768$ and $\lambda = 0.01$ and monodisperse initial conditions: a) very slow relaxation of n_k for $k \gg 1$ to the stationary distribution $n_k \propto k^{-3/2}$, the scaling becomes stable only for $T = 10^4$ and the solutions become close to the basic asymptotic form only for very large T; b) the time steps grow up to very large values if the adaptive time-stepping rule is applied

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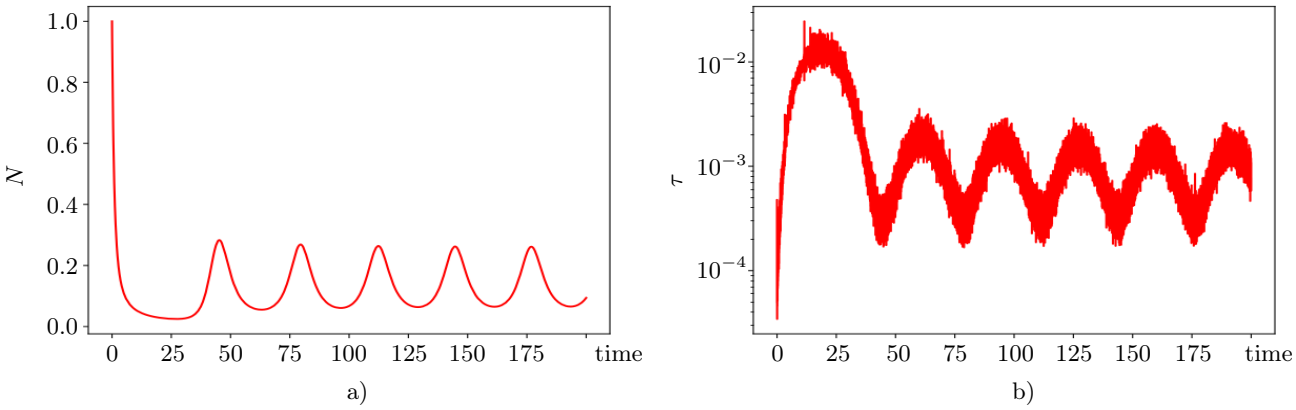

Figure 3. Numerical experiments for the generalized Brownian kernel with $\alpha = 0.95$, $M = 32768$ and $\lambda = 0.01$ and monodisperse initial conditions: a) dynamic oscillations of the total density $N(t)$ are in agreement with baseline paper [11]; b) the adaptive time steps also oscillate with time and lead to speedup the computations

time-steps allows to track this transition dynamics with good accuracy within modest computing time. The previously elaborated iterative methods (see e.g. [21, 22]) allow to obtain only the numerical approximations of the final stationary particle size distributions in contrast with our approach.

The small non-monotonicity in the numerical solution for $T = 5000$ (see Figure 2) qualitatively agrees with the experimental data of the Voyager Radio Science Subsystem [28] for the Saturn's A ring, that can be seen in the related plot for this model from [12]. Thus, we may infer that the real particle size distribution is close to the dynamic equilibrium predicted by theory, but it takes a long time to reach it.

In Figure 3 we demonstrate the results of our experiments for the kernel with $\alpha = 0.98$ and $\lambda = 0.01$. In this case, the equations (4) lead to the dynamic oscillations. These oscillations were observed only numerically [11] and seem to arise via Hopf bifurcation. The dynamic oscillations are also possible for the open irreversible aggregation model with the sources and sinks [23], but the aggregation-shattering kinetics is mass-conserving and such cyclic solutions even more interesting.

The corresponding simulations based on the second order Runge–Kutta method require tremendously small constant time-steps for stable calculations. Thus, even experiments for oscillations with twenty or forty thousand kinetic equations may take dozens of hours of computations.

On the right panel of Figure 3 we see that the adaptive steps also oscillate with time and change almost by two orders of magnitude during each cycle. Application of the adaptive criteria allows to speedup these tough calculations by 10–15 times as we show in the Table 3. Based on this observation, we see that computations can be significantly accelerated without loss of their accuracy.

4. Conclusion. In this work we have studied the performance of several explicit time-integration methods with adaptive time-stepping criteria in application to problems of aggregation-fragmentation kinetics. Based on our numerical experiments, we conclude that complicated calculations for different models can be accelerated by dozens of times.

We also demonstrate that application of the time-integration methods with adaptive time-steps allows to obtain the dynamics of relaxation process for the problems with stationary solutions using modest computing resources. Utilization of chosen dynamic time-stepping criteria allows us to exploit the higher-order Runge–Kutta methods instead of the well-known classical criteria for the simplest Euler scheme.

Table 3. Timings in seconds of numerical computations for the aggregation-shattering problem with dynamic oscillations ($\alpha = 0.95$, $M = 32768$, $\lambda = 0.01$). The same calculations with constant time-steps $\tau = 5 \cdot 10^{-5}$ (the numerical integration becomes instable for the larger time-steps) require approximately 23 hours

Scheme	$tol = 10^{-4}$	$tol = 10^{-6}$	$tol = 10^{-8}$
RK2	4160	4217	5250
RK4	6399	6084	6520
RKF45	9924	9700	9869

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Robust implementation of any implicit time-integration is an interesting direction for future research. It might be useful for the spatially inhomogeneous coagulation equations [2] playing important role in ecological modeling [29]. This task seems to be challenging due to a certain need in efficient and highly accurate methods solving the systems of non-linear equations generated by Smoluchowski operator [22]. The cost of internal iterations within implicit time-steps has to be smaller than straight-forward sequence of explicit time-steps.

References

1. P. L. Krapivsky, S. Redner, and E. Ben-Naim, *A Kinetic View of Statistical Physics* (Cambridge Univ. Press, Cambridge, 2010). doi 10.1017/CBO9780511780516.
2. A. E. Aloyan, V. O. Arutyunyan, and A. N. Yermakov, "Dynamics of Gas Admixtures and Aerosols in Forest and Peat Fires," Rus. J. Num. Anal. Math. Model. **29** (2), 79–92 (2014). doi 10.1515/rnam-2014-0007.
3. M. V. Smoluchowski, "Versuch einer Mathematischen Theorie der Koagulationskinetik Kolloider Lösungen," Zeit. Physikalische Chemie **92U** (1), 129–168 (1918). doi 10.1515/zpch-1918-9209.
4. A. A. Lushnikov, "Evolution of Coagulating Systems: III. Coagulating mixtures," J. Colloid Interface Sci. **54** (1), 94–101 (1976). doi 10.1016/0021-9797(76)90288-5.
5. F. Leyvraz, "Scaling Theory and Exactly Solved Models in the Kinetics of Irreversible Aggregation," Phys. Rep. **383** (2–3), 95–212 (2003). doi 10.1016/S0370-1573(03)00241-2.
6. K. Kang, S. Redner, P. Meakin, and F. Leyvraz, "Long-Time Crossover Phenomena in Coagulation Kinetics," Phys. Rev. A **33** (2), 1171–1182 (1986). doi 10.1103/PhysRevA.33.1171.
7. J. B. McLeod, "On an Infinite Set of Non-Linear Differential Equations," Q. J. Math. **13** (1), 119–128 (1962). doi 10.1093/qmath/13.1.119.
8. S. Kaushik and R. Kumar, "Steady-State Solution for Discrete Oort–Hulst–Safronov Coagulation Equation," Int. J. Dyn. Syst. Differ. Equ. **13** (2), 144–163 (2023). doi 10.1504/IJDSDE.2023.130311.
9. S. A. Matveev, A. P. Smirnov, and E. E. Tyrtyshnikov, "A Fast Numerical Method for the Cauchy Problem for the Smoluchowski Equation," J. Comput. Phys. **282**, 23–32 (2015). doi 10.1016/j.jcp.2014.11.003.
10. S. A. Matveev, A. A. Sorokin, A. P. Smirnov, and E. E. Tyrtyshnikov, "Oscillating Stationary Distributions of Nanoclusters in an Open System," Math. Comput. Model. Dyn. Syst. **26** (6), 562–575 (2020). doi 10.1080/13873954.2020.1793786.
11. S. A. Matveev, P. L. Krapivsky, A. P. Smirnov, et al., "Oscillations in Aggregation-Shattering Processes," Phys. Rev. Lett. **119** (26), Article Number 260601 (2017). doi 10.1103/PhysRevLett.119.260601.
12. N. V. Brilliantov, P. L. Krapivsky, A. Bodrova, et al., "Size Distribution of Particles in Saturn's Rings from Aggregation and Fragmentation," Proc. National Academy of Sci. **112** (31), 9536–9541 (2015). doi 10.1073/pnas.1503957112.
13. A. I. Osinsky, "Low-Rank Method for Fast Solution of Generalized Smoluchowski Equations," J. Comput. Phys. **422**, Article Number 109764 (2020). doi 10.1016/j.jcp.2020.109764.
14. A. I. Osinsky and N. V. Brilliantov, "Exact Solutions of Temperature-Dependent Smoluchowski Equations," J. Phys. A: Math. Theor. **55** (42), Article Number 425003 (2022). doi 10.1088/1751-8121/ac971b.
15. M. A. Larchenko, R. R. Zagidullin, V. V. Palyulin, and N. V. Brilliantov, "Application of Machine Learning Technique for a Fast Forecast of Aggregation Kinetics in Space-Inhomogeneous Systems," https://arxiv.org/pdf/2312.04660. Cited September 10, 2024.
16. M. Smith and T. Matsoukas, "Constant-Number Monte Carlo Simulation of Population Balances," Chem. Eng. Sci. **53** (9), 1777–1786 (1998). doi 10.1016/S0009-2509(98)00045-1.
17. F. E. Kruis, A. Maisels, and H. Fissan, "Direct Simulation Monte Carlo Method for Particle Coagulation and Aggregation," AIChE J. **46** (9), 1735–1742 (2000). doi 10.1002/aic.690460905.
18. E. Debry, B. Sportisse, and B. Jourdain, "A Stochastic Approach for the Numerical Simulation of the General Dynamics Equation for Aerosols," J. Comput. Phys. **184** (2), 649–669 (2003). doi 10.1016/S0021-9991(02)00041-4.
19. K. K. Sabelfeld, S. V. Rogasinsky, A. A. Kolodko, and A. I. Levykin, "Stochastic Algorithms for Solving Smoluchovsky Coagulation Equation and Applications to Aerosol Growth Simulation," Monte Carlo Methods Appl. **2** (1), 41–88 (1996). doi 10.1515/mcma.1996.2.1.41.
20. M. H. Lee, "On the Validity of the Coagulation Equation and the Nature of Runaway Growth," Icarus **143** (1), 74–86 (2000). doi 10.1006/icar.1999.6239.

2024, **25** (3), 347–356. doi 10.26089/NumMet.v25r327

21. V. Stadnichuk, A. Bodrova, and N. Brilliantov, "Smoluchowski Aggregation–Fragmentation Equations: Fast Numerical Method to Find Steady-State Solutions," Int. J. Mod. Phys. B **29** (29), Article Number 1550208 (2015). doi 10.1142/S0217979215502082.
22. I. V. Timokhin, S. A. Matveev, N. Siddharth, et al., "Newton Method for Stationary and Quasi-Stationary Problems for Smoluchowski-Type Equations," J. Comput. Phys. **382**, 124–137 (2019). doi 10.1016/j.jcp.2019.01.013.
23. R. C. Ball, C. Connaughton, P. P. Jones, et al., "Collective Oscillations in Irreversible Coagulation Driven by Monomer Inputs and Large-Cluster Outputs," Phys. Rev. Lett. **109** (16), Article Number 168304 (2012). doi 10.1103/PhysRevLett.109.168304.
24. N. S. Bakhvalov, G. M. Kobel'kov, and N. P. Zhidkov, *Numerical Methods* [in Russian]. (Fizmatlit, Moscow, 2000).
25. T. A. Driscoll and R. J. Braun, *Fundamentals of Numerical Computation* (SIAM Press, Philadelphia, 2018). doi 10.1137/1.9781611975086.fm.
26. E. Fehlberg, "Classical Fourth and Lower Order Runge–Kutta Formulas with Stepsize Control and Their Application to Heat Transfer Problems," Computing **6**, 61–71 (1970). doi 10.1007/BF02241732.
27. M. Saleh, E. Kovács, and N. Kallur, "Adaptive Step Size Controllers Based on Runge–Kutta and Linear-Neighbor Methods for Solving the Non-Stationary Heat Conduction Equation," Netw. Heterog. Media **18** (3), 1059–1082 (2023). doi 10.3934/nhm.2023046.
28. H. A. Zebker, E. A. Marouf, and G. L. Tyler, "Saturn's Rings: Particle Size Distributions for Thin Layer Models," Icarus **64** (3), 531–548 (1985). doi 10.1016/0019-1035(85)90074-0.
29. T. V. Khodzher, V. A. Zagaynov, A. A. Lushnikov, et al., "Study of Aerosol Nano-and Submicron Particle Compositions in the Atmosphere of Lake Baikal during Natural Fire Events and Their Interaction with Water Surface," Water, Air and Soil Pollut. **232** (7), Article Number 266 (2021). doi 10.1007/s11270-021-05237-6.

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