J Stat Phys (2009) 135: 133–151
DOI 10.1007/s10955-009-9717-1

Stochastic Particle Approximation for Measure Valued Solutions of the 2D Keller-Segel System

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Received: 21 July 2008 / Accepted: 28 February 2009 / Published online: 14 March 2009

Abstract We construct an approximation to the measure valued, global in time solutions to the (Patlak-)Keller-Segel model in 2D, based on systems of stochastic interacting particles. The advantage of our approach is that it reproduces the well-known dichotomy in the qualitative behavior of the system and, moreover, captures the solution even after the (possible) blow-up events. We present a numerical method based on this approach and show some numerical results. Moreover, we make a first step toward the convergence analysis of our scheme by proving the convergence of the stochastic particle approximation for the Keller-Segel model with a regularized interaction potential. The proof is based on a BBGKY-like approach for the corresponding particle distribution function.

Keywords Chemotaxis · (Patlak-)Keller-Segel model · Blow-up · Stochastic interacting particles · BBGKY hierarchy

1 Introduction

This paper is concerned with the mathematical modelling of chemotaxis, a biological phenomenon in which living organisms direct their movements according to certain chemicals in their environment. At the macroscopic level, the biological system is described by the number density of cells, $\varrho = \varrho(t, x)$, and the concentration of the chemoattractant,

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$S = S(t,x)$. The famous Patlak-Keller-Segel model [12], which we consider in its parabolic-elliptic nondimensional setting, reads

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \nabla S - \nabla \varrho) = 0\,, \tag{1}$$

$$-\Delta S = \varrho\,, \tag{2}$$

for $t > 0$ and $x \in \mathbb{R}^2$, subject to the initial condition

$$\varrho(x, t = 0) = \varrho_I(x) \quad \text{for } x \in \mathbb{R}^2\,. \tag{3}$$

This system was extensively studied by many authors; [15] gives quite a complete survey of the results and an extensive bibliography. In the spatially two-dimensional case, the Poisson equation $\Delta S = -\varrho$ is usually replaced by the Newtonian potential solution,

$$S[\varrho](x) = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \log(|x-y|)\varrho(y)\,\mathrm{d}y\,. \tag{4}$$

Then the classical result

$$\frac{\mathrm{d}}{\mathrm{d}t}\int |x|^2\varrho(x)\,\mathrm{d}x = \frac{M}{2\pi}(8\pi - M)\,, \quad \text{with } M := \int_{\mathbb{R}^2} \varrho_I(x)\,\mathrm{d}x \tag{5}$$

indicates the well known dichotomy in the qualitative behavior of the system with the critical mass 8π:

a) If $M < 8\pi$, the system (1), (4) has a global smooth solution, [2].
b) If $M = 8\pi$, the system has a global smooth solution, which blow up for $t \to \infty$, [4].
c) If $M > 8\pi$, the system has no global smooth solutions.

The proof of existence of global solutions is based on the boundedness of the free energy,

$$F[\varrho] = \int_{\mathbb{R}^2} \varrho \log \varrho - \frac{1}{2}\varrho S[\varrho]\,\mathrm{d}x\,,$$

which is obtained by using the logarithmic Hardy-Littlewood-Sobolev inequality in its sharp form.

Biologically, the possible concentration of the cell density in the supercritical case $M > 8\pi$ represents aggregation of cells, and the description of the dynamics of these aggregates and of their interaction with the non-aggregated cells is of natural interest. This led to the study of various regularizations of (1)–(2); we are interested in the particular case when (4) is replaced by the regularized Newtonian potential solution

$$S_\varepsilon[\varrho](x) = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \log(|x-y|+\varepsilon)\varrho(y)\,\mathrm{d}y\,. \tag{6}$$

This regularization is studied in [7], the main result being a rigorous characterization of the limiting solutions as $\varepsilon \to 0$ globally in time and for arbitrary initial mass. It is based on the framework developed by Poupaud in [16], which he applied to the two-dimensional incompressible Euler equations as well as to the Keller-Segel system without diffusion of the cells. The basic structure is the set of time dependent measures with diagonal defects:

Definition 1 ([16]) For an interval $I \subset \mathbb{R}$, the set of time dependent measures with diagonal defects is defined as

$$\mathcal{DM}^+(I,\mathbb{R}^2) = \Big\{ (\varrho,\nu) : \varrho(t) \in \mathcal{M}_1^+(\mathbb{R}^2)\ \forall t \in I,\ \nu(t) \in \mathcal{M}(I\times\mathbb{R}^2)^{2\times 2},$$
$$\varrho \text{ is tightly continuous with respect to } t\,,$$
$$\nu \text{ is a nonnegative, symmetric, matrix valued measure}\,,$$
$$\operatorname{tr}(\nu(t,x)) \le \sum_{a\in S_{at}(\varrho(t))} \varrho(t)(\{a\})^2\delta(x-a)\Big\}\,,$$

where $\mathcal{M}$ denotes spaces of Radon measures, $\mathcal{M}_1^+$ the subspace of nonnegative bounded measures and $S_{at}(\varrho(t))$ stands for the atomic support of the measure $\varrho(t)$.

The limit of (1), (6) as $\varepsilon \to 0$ can be described as follows:

Theorem 1 [7] *For every $\varepsilon > 0$, the problem (1), (6) has a global weak solution $\varrho_\varepsilon \in L^1(\mathbb{R}^2)\cap L^\infty(\mathbb{R}^2)$. For every $T > 0$, as $\varepsilon \to 0$, a subsequence of solutions of (1), (6) converges tightly and uniformly in time to a time dependent measure $\varrho(t)$. There exists $\nu(t)$ such that $(\varrho,\nu) \in \mathcal{DM}^+((0,T);\mathbb{R}^2)$ is a generalized solution of*

$$\frac{\partial\varrho}{\partial t} + \nabla\cdot(j[\varrho,\nu] - \nabla\varrho) = 0 \tag{7}$$

in the sense of distributions, where the distributional definition of the convective flux $j[\varrho,\nu]$ with a test function $\varphi \in C_c^\infty((0,T),\mathbb{R}^2)$ is given by

$$\int_0^T\int_{\mathbb{R}^2} j[\varrho,\nu](t,x)\varphi(t,x)\,\mathrm{d}x\,\mathrm{d}t$$
$$= -\frac{1}{4\pi}\int_0^T\int_{\mathbb{R}^4} K(x-y)\varrho(t,x)\varrho(t,y)(\varphi(t,x)-\varphi(t,y))\,\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}t$$
$$-\frac{1}{4\pi}\int_0^T\int_{\mathbb{R}^2} \nu(t,x)\nabla\varphi(t,x)\,\mathrm{d}x\,\mathrm{d}t\,,$$

with $K(x) = \frac{x}{|x|^2}$ for $x \neq 0$ and $K(0) = 0$. The initial condition (3) is satisfied in the sense of tight continuity.

Relevant for our study is the strong formulation of the limiting system (7), based on the following decomposition of the limiting measure valued solution $\varrho(t) \in \mathcal{M}_1^+(\mathbb{R}^2)$:

$$\varrho = \overline{\varrho} + \hat{\varrho}\,, \quad \text{with } \hat{\varrho}(t,x) = \sum_{n\in\mathcal{H}} M_n(t)\delta(x - x_n(t))\,,$$

for a finite set $\mathcal{H} \subset \mathbb{N}$, assuming $\overline{\varrho}$ is smooth and t varies in a time interval where the atomic support of ϱ consists of smooth paths $x_n(t)$ carrying smooth weights $M_n(t) \ge 8\pi$. Then, the respective defect measure ν is of the form

$$\nu(x,t) = \sum_{n\in\mathcal{H}} 4\pi M_n(t)\delta(x - x_n(t))\mathrm{Id}\,,$$

where Id denotes the identity matrix in $\mathbb{R}^{2\times 2}$, and the following system of equations is obtained [7]:

$$\frac{\partial \overline{\varrho}}{\partial t} + \nabla \cdot (\overline{\varrho} \nabla S[\overline{\varrho}] - \nabla \overline{\varrho}) - \frac{1}{2\pi} \nabla \overline{\varrho} \cdot \sum_{n \in \mathcal{H}} M_n(t) \frac{x - x_n}{|x - x_n|^2} = 0\,, \tag{8}$$

$$\dot{M}_n = M_n \overline{\varrho}(x = x_n)\,, \tag{9}$$

$$\dot{x}_n = \nabla S[\overline{\varrho}](x = x_n) - \frac{1}{2\pi} \sum_{n \neq m \in \mathcal{H}} M_m \frac{x_n - x_m}{|x_n - x_m|^2}\,. \tag{10}$$

This system was derived for the first time by Velázquez [19, 20] and a local-in-time existence result for initial value problems was given in [21]. In general, one has to expect blow-up events in the smooth part $\overline{\varrho}$ and/or collisions of point aggregates in finite time. At such instants, a restart is required with either an additional point aggregate after a blow-up event or with a smaller number of point aggregates after a collision. A rigorous theory producing global solutions by such a procedure is still missing, however. Nevertheless, one can formally derive a formula for the time derivative of the second order moment [7], which in our notation reads

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^2} |x|^2 \varrho \,\mathrm{d}x = 4\overline{M} - \frac{1}{2\pi} \left(M^2 - \sum_{n \in \mathcal{H}} M_n^2 \right), \tag{11}$$

where $M = \int_{\mathbb{R}^2} \varrho \,\mathrm{d}x$ is the total mass of the system and $\overline{M} = \int_{\mathbb{R}^2} \overline{\varrho} \,\mathrm{d}x$ is the total mass of its smooth part.

Contrary to the large amount of literature dedicated to the analysis of the Keller-Segel system, we are aware of only a few publications dealing with its numerical treatment [3, 5, 8, 13, 17, 18]. However, these are only capable to produce an approximation of the solution up to the blow-up event. Since our interest is to develop a method for computation of the global in time, measure valued solution, we propose a discrete approximation of (8)–(10) with a system of interacting particles (Sect. 2). After a discretization in time, this leads to a stochastic numerical method for computation of approximate solutions (Sect. 3). Finally, in Sect. 4, we make a first step toward the convergence analysis of our scheme by proving the convergence of the stochastic particle approximation for the model with a regularized interaction potential. The proof is based on a BBGKY-like approach for the corresponding particle distribution function. Our particle discretization method has already been shortly announced in [10]; here we present its detailed description and some more numerical results, and the discussion in Sect. 4 is new.

2 Construction of the Stochastic Approximation and its Analysis

2.1 Formal Derivation of the Stochastic Approximation

Let us start with the observation that for a given potential $S = S(x, t)$, (1) is the Kolmogorov forward (or Fokker-Planck) equation corresponding to the stochastic differential equation

$$\mathrm{d}X_t = \nabla_x S(X_t, t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}B_t\,,$$

where B_t is a two-dimensional Brownian motion. To describe the nonlinearity of the model, we propose the following particle approximation of (the smooth part of) the density $\overline{\varrho}$,

$$\overline{\varrho}(x,t) \approx \sum_{n\in\mathcal{L}} M_n(t)\delta(x - x_n(t)) \tag{12}$$

for some finite index set $\mathcal{L} \subset \mathbb{N}$, with smooth point masses $M_n(t) > 0$ and smooth particle paths $x_n(t)$. With this ansatz, we formally obtain the (finite dimensional) system of SDEs for the particle paths,

$$\mathrm{d}x_n = -\frac{1}{2\pi} \sum_{n\neq m\in\mathcal{L}} M_m \frac{x_n - x_m}{|x_n - x_m|^2} + \sqrt{2}\,\mathrm{d}B_t^n \quad \text{for } n \in \mathcal{L}\,,$$

where B_t^n are mutually independent two-dimensional Brownian motions and the sum runs over all $m \in \mathcal{L}$ such that $m \neq n$.

Now the possible singularities of the density should come into the game. For this, we consider the strong formulation (8)–(10) with the finite set $\mathcal{H}$ of singular points $x_n(t)$, carrying masses $M_n(t)$, $n \in \mathcal{H}$. Inserting the ansatz (12) into (10), we obtain the system of ODEs describing the dynamics of the singular points,

$$\mathrm{d}x_n = -\frac{1}{2\pi} \sum_{m\in\mathcal{L}} M_m \frac{x_n - x_m}{|x_n - x_m|^2} - \frac{1}{2\pi} \sum_{n\neq m\in\mathcal{H}} M_m \frac{x_n - x_m}{|x_n - x_m|^2}\,, \quad \text{for } n \in \mathcal{H}\,,$$

where the first sum describes the interaction with the approximation of $\overline{\varrho}$, while the second sum stands for the interactions between the singular points.

Alltogether, we can summarize our considerations as

$$\mathrm{d}x_n = -\frac{1}{2\pi} \sum_{n\neq m\in(\mathcal{L}\cup\mathcal{H})} M_m \frac{x_n - x_m}{|x_n - x_m|^2} + \sqrt{2}\beta_n\,\mathrm{d}B_t^n\,, \tag{13}$$

for all $n \in (\mathcal{L} \cup \mathcal{H})$, where the "switch" β_n is equal 1 for $n \in \mathcal{L}$ and zero otherwise. As we see, the only difference between the dynamics of the singular points and the dynamics of the particles approximating $\overline{\varrho}$ is that the latter are, in addition to the interaction with all other particles, driven by the Brownian motion. However, the paths of the singular points must of course as well be considered as stochastic processes.

As nice as the unified formulation (13) might seem, we quickly come to difficulties when the question of existence of solutions is imposed. Of course, due to possible collisions, we cannot expect solutions to exist globally in time. But also the question of local in time existence is a delicate one. Since the interaction kernel is discontinuous and even unbounded, the classical theory does not apply here. Moreover, we can get into trouble immediately, if we impose an initial condition with $x_n(t = 0) = x_m(t = 0)$ for some $n \neq m$. Obviously, this is a pathologic situation and we will exclude it from our further considerations. But even with a well-behaved initial condition, it is not clear whether a finite time interval exists, on which a solution to (13) can be defined almost surely (in other words, the probability of a collision of any two particles within the time interval is zero). In fact, some considerations, which are out of scope of this paper and will be treated in a future work, indicate that the contrary is true, i.e., that the probability of a collision is positive for arbitrary short time intervals.

However, due to the simple structure of the equation, we can define the solution pathwise: For each path ω of the Wiener process B_t, we define

$$x_n(t;\omega) = x_n^0 - \frac{1}{2\pi} \sum_{n \neq m \in (\mathcal{L} \cup \mathcal{H})} \int_0^t M_m \frac{x_n(s;\omega) - x_m(s;\omega)}{|x_n(s;\omega) - x_m(s;\omega)|^2} \, \mathrm{d}s + \sqrt{2}\beta_n B_t^n(\omega) \,,$$

$$x_n(0;\omega) = x_n^0 \,,$$

for t from the maximal time interval $[0, T_\omega)$ during which no collision happens (and the above formula makes sense). At the collision instant T_ω we restart and perform the procedure with one or more particles less, depending on the number of particles that collided. So, for example, if the first and second particle of the set $\{(x_1, M_1), (x_2, M_2), \ldots, (x_N, M_N)\}$ collided, then we restart with the set of $N - 1$ particles in the configuration $\{(x_1, M_1 + M_2), (x_3, M_3), \ldots, (x_N, M_N)\}$. However, it is not clear to which of the two sets $\mathcal{L}$, $\mathcal{H}$ the newly created particle should belong to. This question is intimately connected with the problem of blow-up detection. First of all, let us recall that each of the singular points of ϱ must be at least 8π in mass, i.e., $M_n \geq 8\pi$ for each $n \in \mathcal{H}$. On the other hand, since we are interested in the situation when the number of particles approximating the smooth part of the solution is large, and their masses are uniformly small, we may assume that $M_n < 8\pi$ for $n \in \mathcal{L}$. This inspires the denomination of the $\mathcal{L}$-particles as *light particles* and of the $\mathcal{H}$-particles as *heavy particles*. Then, we can discriminate four possible collision scenarios:

i) Collision of two heavy particles; the resulting aggregated particle will be heavy, too.
ii) Collision of one heavy and one light particle; the resulting aggregated particle will be heavy.
iii) Collision of two light particles with joint mass lower then 8π. In this case, the aggregated particle will be light, too.
iv) Collision of two light particles with joint mass bigger then 8π. The aggregated particle gets heavy.

These four scenarios are easy to identify with the effects that can be recognized in the strong formulation of the limiting system (8)–(10). The first scenario describes the aggregation of two singular points of ϱ. The second one stands for the transport of mass from the smooth part $\overline{\varrho}$ into the singular part $\hat{\varrho}$, given by (9) (the singular particles "suck" the mass from their neighbourhood). The third type of collision is due to the dynamics of $\overline{\varrho}$. Finally, the last scenario is the most interesting one - namely, it defines the criterion for detecting blow-up of the smooth solution. First of all, we must admit that such a definition only makes sense if the only possible blow-up mechanism of $\overline{\varrho}$ is a formation of a multiple of Dirac delta, with initial mass 8π. Although this is known only for the radially symmetric case, see [1, 11, 14], there are strong reasons to believe that it is also the case in general situations. Moreover, this mechanism can only produce good approximation of the true solution to (8)–(10) if we use a large number of light particles with small enough masses.

2.2 Dynamical Analysis—Formal Calculation of the Critical Mass

We will show that our method recovers the dynamical dichotomy of the Keller-Segel model with the critical mass 8π, i.e., that for a subcritical total mass the solution tends to spread out over the whole $\mathbb{R}^2$, while for a supercritical one concentration is to be expected. However, the calculation will be purely formal and, even worse, based on the assumption that there exists a time interval $[0, T^\star]$ during which no collision happens almost surely. As already noted, such an assumption is likely to be false.

Anyway, let us assume we have a system of heavy and light particles with the total mass $M = \sum_{n\in(\mathcal{L}\cup\mathcal{H})} M_n$; the total mass of the light particles will be denoted by $\overline{M}(t) = \sum_{n\in\mathcal{L}} M_n(t)$. We denote by N the total number of particles and by $x = x(t)$ the stochastic vector of the particle co-ordinates, $x = (x_{1_1}, x_{1_2}, \ldots, x_{N_1}, x_{N_2})$, where (x_{n_1}, x_{n_2}) denotes the co-ordinates of the n-th particle. Then, for $t \in [0, T^\star]$, we define the centre of gravity of the system

$$c(t,x) = \frac{1}{N}\sum_{n\in\mathcal{L}\cup\mathcal{H}} M_n x_n(t)\,,$$

and the discrete second-order moment with respect to c

$$u_c(t,x) = \sum_{n\in\mathcal{L}\cup\mathcal{H}} M_n |x_n(t) - c(t,x)|^2\,.$$

Then, the formal application of the Itô formula for the function u_c of the stochastic process $x(t)$ driven by the SDE (13) yields

$$\begin{aligned}\mathrm{d}u_c(x) = &-\frac{1}{2\pi}\left(M^2 - \sum_{n\in\mathcal{L}\cup\mathcal{H}} M_n^2\right)\mathrm{d}t - 2\sqrt{2}\sum_{n\in\mathcal{L}} M_n(x_n - c)\cdot \mathrm{d}B_t^n\\ &+4\sum_{n\in\mathcal{L}} M_n\left(1 - \frac{M_n}{M}\right)\mathrm{d}t\,,\end{aligned}$$

and, again formally, taking expectation, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}u_c(x) = -\frac{1}{2\pi}\left(M^2 - \sum_{n\in\mathcal{L}\cup\mathcal{H}} M_n^2\right)\mathrm{d}t + 4\sum_{n\in\mathcal{L}} M_n\left(1 - \frac{M_n}{M}\right)\mathrm{d}t\,. \tag{14}$$

With this formula, we can make two important observations:

- First, we consider the case when the system consists of light particles only ($\mathcal{H} = \emptyset$); then, (14) can be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}u_c(x) = \left(-\frac{1}{2\pi} + \frac{4}{M}\right)\left(M^2 - \sum_{n\in\mathcal{L}} M_n^2\right) \tag{15}$$

  and we see that the sign of the time derivative of the expected second-order moment depends only on the total mass of the system, with the critical value 8π, and not on the number of particles or the distribution of their masses. Moreover, when the number of particles tends to infinity, while their masses uniformly tend to zero, the right hand side converges to $\frac{M}{2\pi}(8\pi - M)$, which is the result (5) we got from the second-order moment calculation for the original system (1)–(2).
- Second, if the system has a supercritical total mass $M > 8\pi$ and $\mathcal{H} \neq \emptyset$, performing again the limit when the number of light particles tends to infinity with masses uniformly tending to zero, (14) becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{E}u_c(x) = 4\overline{M} - \frac{1}{2\pi}\left(M^2 - \sum_{n\in\mathcal{H}} M_n^2\right), \tag{16}$$

  which is nothing but the formula (11) for the strong formulation of the Keller-Segel system after blow-up, (8)–(10).

3 Time Discretization and Implementation

The stochastic particle approximation described in the previous section can be used as a basis for constructing a numerical method. For this sake, we introduce the equidistant time grid $t^k = k\Delta t$, $k \in \mathbb{N}$, with the time step Δt. By x_n^k we denote the value of x_n at time t^k. We perform the time discretization of the SDE (13) using the Euler-Maruyama method, arriving at the explicit scheme

$$x_n^{k+1} = x_n^k - \frac{\Delta t}{2\pi} \sum_{n \neq m \in (\mathcal{L} \cup \mathcal{H})} M_m \frac{x_n^k - x_m^k}{|x_n^k - x_m^k|^2} + \sqrt{2\Delta t}\beta_n \mathcal{N}_{(0,1)}\,, \tag{17}$$

subject to the initial condition

$$x_n^0 = x_n^I\,, \qquad M_n^0 = M_n^I \quad \text{for } n \in (\mathcal{L} \cup \mathcal{H})\,, \tag{18}$$

where $\mathcal{N}_{(0,1)}$ is a normalized, normally distributed random 2D vector, and the initial condition satisfies

$$x_n^I \neq x_m^I \quad \text{for } n \neq m\,, \qquad 0 < M_n^I < 8\pi \quad \text{for } n \in \mathcal{L}\,, \qquad 8\pi \leq M_n^I \quad \text{for } n \in \mathcal{H}\,.$$

Of course, the question immediately comes out, how do we detect collisions of particles at the time-discretized level. Let us note that this is not just a technical question; to the contrary, since collisions are the only mechanism how mass is transfered between particles, the details of the collision mechanism influence the performance of the method. In particular, we should check that our scheme approximates well the flow of the mass from the smooth part of ϱ into the singular points, which is described by the second equation of the strong formulation, (9).

Intuitively, as collisions we should treat such situations, when two particles got so close to each other, such that the probability that they indeed collide during the next time step is high enough. Moreover, since collisions of light particles can be seen merely as grid coarsening, the details of the collision criterion in this case are not so relevant; we just should not let the grid get too coarse, which is achieved by particle splitting (see below). Therefore, the details of the mechanism of collision detection are critical only in the case when at least one of the particles involved is heavy. Let us consider the simplest possible situation with two heavy particles with masses M_1 and M_2 and initial positions $x_1(0)$ and $x_2(0)$. Their movement is governed by the following system of ODEs:

$$\dot{x}_1(t) = -\frac{M_2}{2\pi} \frac{x_1 - x_2}{|x_1 - x_2|^2}\,,$$
$$\dot{x}_2(t) = -\frac{M_1}{2\pi} \frac{x_2 - x_1}{|x_2 - x_1|^2}\,.$$

Defining the distance $d(t) = x_1(t) - x_2(t)$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}|d(t)|^2 = -\frac{M_1 + M_2}{\pi}\,,$$

and the two particles collide during the time interval $[0, \Delta t]$ if and only if

$$|d(0)|^2 \leq \frac{M_1 + M_2}{\pi}\Delta t\,. \tag{19}$$

Can we accept this formula as a reasonable criterion for detection of collisions in our numerical method? First of all, let us note that this is obviously the best we can do for detecting collisions of two heavy particles, at least if we do not take into account the influence of the surrounding particles. Choosing a reasonably short time step, two particles may collide only if they are very close to each other; in this case their mutual interaction will be much stronger than the interaction with the rest of the system. Secondly, as already mentioned, we should check how (19) complies with the second equation of the strong formulation (9). To this end, let us consider one heavy particle located at x_1^k with mass $M_1 \geq 8\pi$, surrounded by a large number of light particles. During the timestep $[t^k, t^{k+1}]$, the mass of the heavy particle increases due to collisions with the light particles as

$$M_1^{k+1} = M_1^k + \int_{\mathbb{R}^2} \int_0^{8\pi} p(x, m, t^k) P(M_1^k, m, |x_1^k - x|, \Delta t) m \, \mathrm{d}m \, \mathrm{d}x \,,$$

where $p(x, m, t)$ is the probability density that a (light) particle with mass m is located at x in time t and $P(M, m, d, \Delta t)$ is the probability of a collision of a particle with mass M and a particle with mass m, whose distance is d, during the time step Δt. According to (19), it is

$$P(M, m, d, \Delta t) = \chi\left(\left\{d^2 \leq \frac{M+m}{\pi} \Delta t\right\}\right),$$

where χ is the characteristic function. Since we assume that the masses of the light particles are much smaller than 8π, we may approximate $P(M_1^k, m, |x_1^k - x|, \Delta t)$ with $P(M_1^k, 0, |x_1^k - x|, \Delta t)$. Therefore, realizing that

$$\int_0^{8\pi} p(x, m, t) m \, \mathrm{d}m = \overline{\varrho}(x, t) \,,$$

we arrive at

$$M_1^{k+1} = M_1^k + \int_{B_R(x_1^k)} \overline{\varrho}(x) \, \mathrm{d}x \,,$$

where $B_R(x_1^k)$ is the ball centered at x_1^k with the diameter $R = \sqrt{\frac{M_1^k \Delta t}{\pi}}$. Taylor expansion of $\overline{\varrho}$ around x_1^k yields

$$\int_{B_R(x_1)} \overline{\varrho}(x) \, \mathrm{d}x = \overline{\varrho}(x_1^k) M_1^k \Delta t + \mathcal{O}(|\Delta t|^2) \,,$$

and, finally, in the limit $\Delta t \to 0$ we recover the relation we sought after

$$\dot{M}_1(t) = M_1 \overline{\varrho}(x_1) \,.$$

Therefore, we may conclude that the proposed criterion for detecting collisions, (19), is compliant with the strong formulation of the limiting problem (8)–(10).

3.1 Particle Splitting

As already mentioned, collisions between light particles can be seen just as coarsening of the discrete grid. However, to retain the quality of the approximation, we must not allow

the grid to get too coarse; in other words, we should keep the number of light particles above some given level. Since we cannot prevent the particles from aggregating (this would apparently lead to an instability of the algorithm), we are led to the idea of particle splitting as a mechanism of grid refinement. The basic idea when looking for a suitable strategy of particle splitting is that we want to keep the number of light particles constant, in hope to retain the "quality" of the approximation at the initial level during the whole computation. In other words, the gain of particles due to splitting should exactly balance the loss due to collisions. Then we still have a lot of freedom in how to choose the particles which are about to be split and how to distribute their masses. Usually, the aim of grid refinement is to create finer grid structures in areas with large gradients of the solution. In our case this approach seems to be quite problematic, not only due to possible difficulties with evaluation of gradients, but mainly due to the fact that it would lead to intensive splitting of particles in regions where a singularity is about to develop - an undesirable effect, with regard to the way how we detect blow-up on the discrete level. Our aim is rather to equalize the average spatial number density of particles in the computational domain. We could look for areas with (momentarily) lower particle density, but, as our numerical experiments have shown, the simple method of choosing the particles to be split after each time step just at random works well enough. Of course, only light particles are subject to splitting.

Finally, we must define how the mass of the original particle is distributed between the two descendants. The performance of the algorithm will be only negligibly influenced by the particular choice of the distribution strategy, therefore, we employ the simplest idea of dividing the particle mass into two halves. One might argue that halving massive (but still regular) particles, which represent an emerging blow-up, could inhibit the formation of singularities. However, our numerical experiments show that, on average, this effect does not influence the blow-up instant at all, since "almost always" the original massive particle is re-created by collision of its descendants in the next time step.

After we discussed the basic building blocks of our algorithm, we may specify how these are combined together. As we see from (17), the interactions of the particles can be evaluated independently from their stochastic motions. This leads us to some kind of operator-splitting strategy; for each time step, the following procedures are executed:

1. Evaluation of the interactions (convective step):

$$x_n^{k+1/2} = x_n^k - \frac{\Delta t}{2\pi} \sum_{n \neq m \in (\mathcal{L} \cup \mathcal{H})} M_m \frac{x_n^k - x_m^k}{|x_n^k - x_m^k|^2} \quad \text{for each } n \in (\mathcal{L} \cup \mathcal{H}) .$$

2. Detection of collisions and (possible) redefinition of the sets $\mathcal{L}$ and $\mathcal{H}$.
3. Splitting of light particles, redefinition of the set $\mathcal{L}$.
4. Evaluation of the stochastic motions (diffusive step):

$$x_n^{k+1} = x_n^{k+1/2} + \sqrt{2\Delta t}\,\beta_n \mathcal{N}_{(0,1)} \quad \text{for each } n \in (\mathcal{L} \cup \mathcal{H}) .$$

Finally, let us remark that performing the splitting procedure before the diffusive step allows to leave the pairs of particles that were created by splitting just at the place of their ancestor; the diffusive step then cares for their re-arrangement.

3.2 Choice of the Time Step Length

The length of the time step, Δt, should be small enough to ensure stability of the system of particles (such that not too many collisions take place); on the other hand, a too short time

step is not optimal from the point of view of computational cost. For simplicity, let us assume that we start with an initial configuration of N particles, distributed over a computational domain of diameter L. Then the typical distance between neighboring particles is $|\widetilde{\Delta x}| \equiv L/\sqrt{N}$, and the typical mass of a particle is M/N. The typical length of the path a particle would travel during one time step due to interaction (convection) is of the order $\frac{\Delta t M}{2\pi\sqrt{N}L}$, while the typical path of its random motion due to diffusion is of the order $\sqrt{2\Delta t}$. Therefore, to ensure the stability of the system, we need that both of these quantities are small compared to $|\widetilde{\Delta x}|$, i.e., that

$$\Delta t \ll \min\left\{2\pi\frac{L^2}{M}, \frac{L^2}{2N}\right\}.$$

Since for a large number of particles the second requirement will be more severe, we can conclude that the time step should be smaller than $L^2/2N$.

3.3 Acceleration Strategies

Obviously, the one-to-one calculation of particle interactions in (17) makes our algorithm quadratic with respect to the number of particles. Consequently, in practical calculations one is limited to use at most a few thousands of particles. A well known strategy to circumvent the quadratic complexity of the N-body algorithms is the fast multipole method ([9] and references therein), which results in an $\mathcal{O}(N \log N)$ or even $\mathcal{O}(N)$ scheme. This would be definitely the method of our choice if we desired to run our calculations with large particle sets. However, since the fast multipole method is relatively costly from the implementational point of view, and since we can get reasonable results using only thousands of particles, we stick to our original algorithm, implementing just a small improvement. With this modification, the algorithm will still have quadratic complexity, but we'll be able to considerably reduce the constant staying in front of N^2.

The idea behind is that when we compute the interactions of a given particle, say P, with several particles, say $\{Q_1, \ldots, Q_K\}$, which are far enough from P, but close to each other, we can approximate the influence of these particles on P by considering the interaction of P with a "virtual" particle, located in the centre of gravity of the set $\{Q_1, \ldots, Q_K\}$, carrying their total mass. Again, there exist elaborate algorithms for detecting such particle clusters; we will simply impose a grid of rectangles over the computational domain and consider all particles belonging to a particular rectangle as a cluster. This facilitates quick localization of the particles. Then, for near particles, we evaluate the interactions one-to-one, while for far particles we approximate the interaction by using the centre of gravity of the far cluster (see Fig. 1). This significantly reduces the number of one-to-one interactions to be evaluated, although the algorithm retains its quadratic complexity.

Finally, let us remark that, at least in the 2D case, methods based on particle simulation are usually substantially less efficient than "traditional" methods for solving convection-diffusion equations, like finite volumes or finite elements. Moreover, to obtain good approximation of the smooth part of the solution, one should execute the simulation many times and calculate the average of the particular outcomes (in other words, estimate the expected value of the stochastic process). We are aware of this limitation of our approach; on the other hand, we do not know any other successful attempt to calculate global in time solutions to the Keller-Segel system including possible singularities. For instance, the finite volumes or

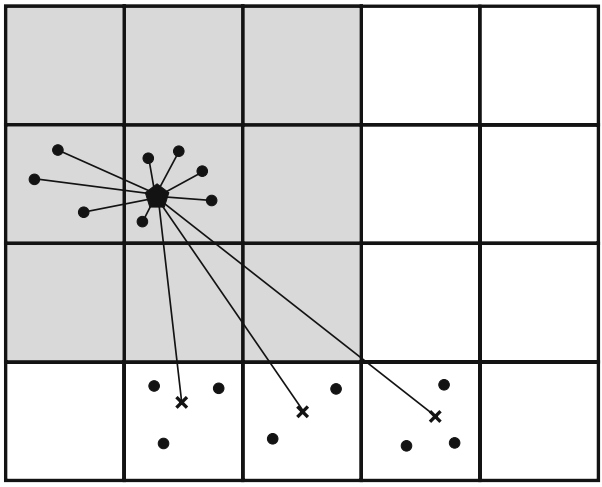


Fig. 1 Accelerated algorithm. Interactions of a given particle (*pentagon*) with near particles (*grey area*) are evaluated one-to-one, while clusters of far particles (*white area*) are approximated by their centers of gravity (*crosses*)

finite element methods ([5, 8, 13]) become unstable close to the blow-up event and it is not possible to systematically detect the blow-up time. That is why we do think our algorithm has its justification. Moreover, our method is technically easily portable to the 3D case, where it already could compete with the above mentioned "traditional" schemes. Nevertheless, since the mathematical description of aggregation in 3D is much less developed, we do not make any attempts in this direction.

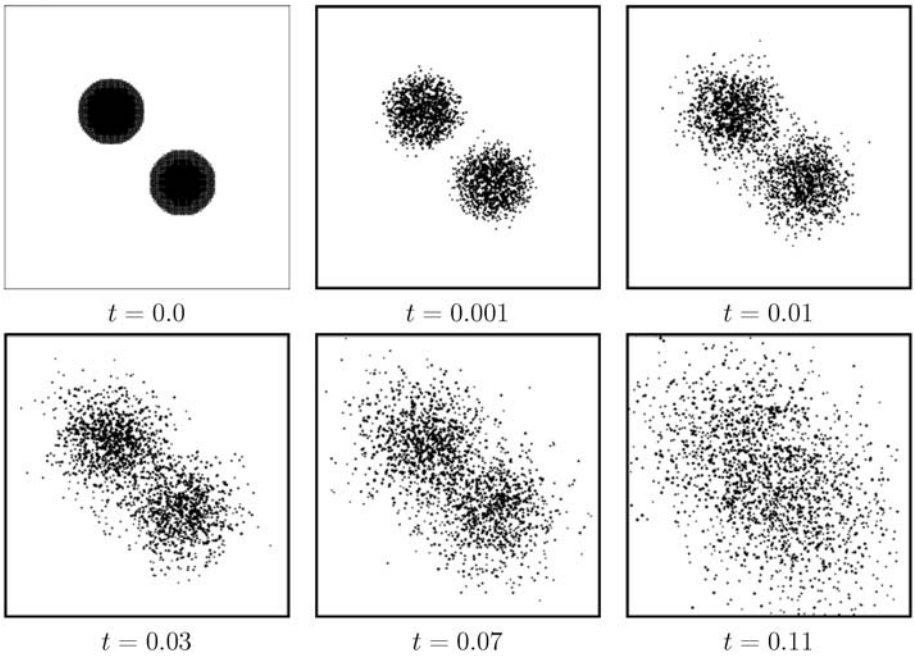
3.4 Numerical Results

To illustrate the functionality of our method, we present two examples of numerical results. In both cases, we use 2000 particles with the same initial distribution in space—they are equidistantly spaced and their mass is chosen to approximate the smooth initial condition

$$\varrho_I(x) = \frac{14\lambda}{24}(1 - |x - x_A|^2)^+ + \frac{10\lambda}{24}(1 - |x - x_B|^2)^+,$$

where x_A and x_B are fixed points with $|x_A - x_B| = 3$ and λ is a scaling parameter; x^+ denotes the positive part of x. For the first example, λ is chosen such that the total mass of the system is 4π, while for the second simulation the total mass is scaled to 24π. In both cases the number of particles used in the simulation is 2000, the time step is $\Delta t = 10^{-3}$. The size of the displayed particles depends logarithmically on their mass.

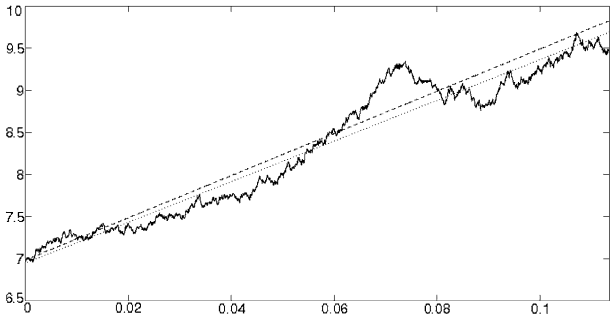
In the following pictures we see the very different behavior of the system in the two cases. In the first case (subcritical total mass), diffusion is stronger than the effect of interaction and the particles tend to be dispersed all around the computational domain:



In Fig. 2, we plotted the evolution of the second order moment in this case. With the total mass of 4π, formula (5) gives $\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{R}^2}\varrho|x|^2\,\mathrm{d}x = 8\pi$, which is displayed by the dashed line. The actual evolution of the discrete second order moment, $\sum_{n\in\mathcal{L}} M_n|x_n|^2$, is plotted with the continuous line and we can clearly see the stochastic nature of the scheme. We used regression analysis (linear interpolation with the least squares method) to reveal the trend of the data (dotted line). We see that the slope of the interpolating line is slightly less than 8π, which is a consequence of the discretization, as explained by formula (15). Our numerical experiments confirm that using more particles in the simulation leads to better agreement between the predicted (dashed line) and interpolated (dotted line) second order moment.

To the contrary, in the supercritical case we observe formation of a first singularity in the middle of the upper left region ($t = 0.0052$, displayed as a black-white-black target in the pictures below). After a while a second blow-up develops in the other region ($t = 0.011$). But still, there persists a small fraction of mass in the smooth part of ϱ. Incidentally, the two singularities collide to form one heavy particle ($t = 0.022$) carrying almost all of the mass

Fig. 2 Second order moment, subcritical case



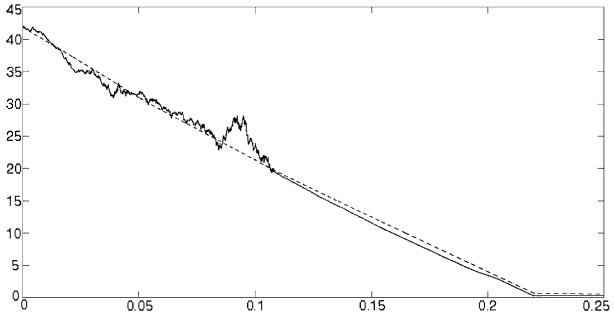
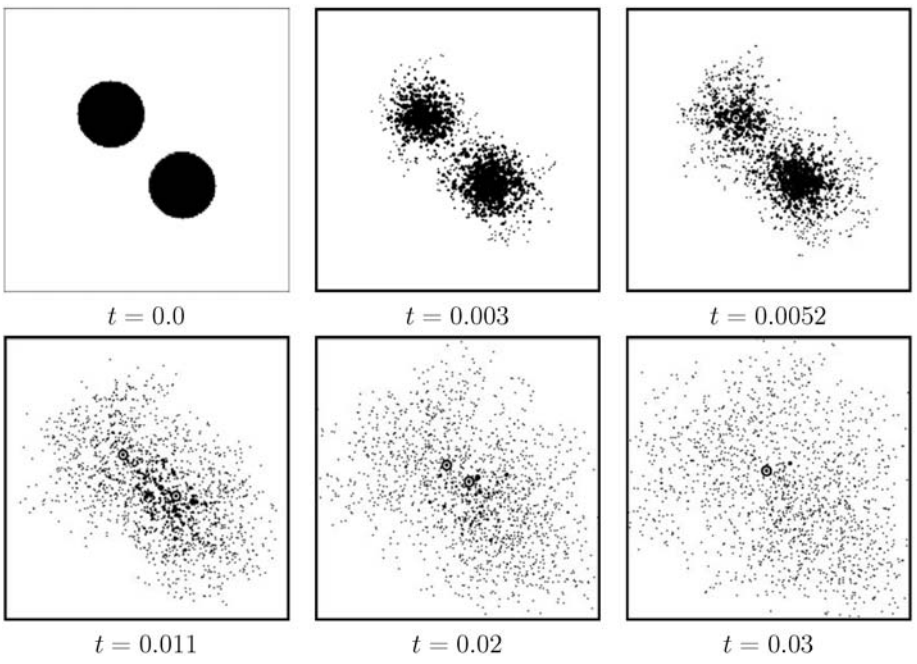


Fig. 3 Second order moment, supercritical case

of the system. A small smooth rest is then subject to diffusion on one hand, and subject to interaction with the singularity on the other hand.

The evolution of the second order moment is plotted in Fig. 3. The prediction, given by formula (16), is plotted by the dashed curve; until the time $t = 0.022$ (collision of the two singular particles), it is a straight line with slope -192π (an inspection of formula (16) shows that formation of a new singularity does not alter the value of the time derivative). At the time instant $t = 0.022$, the slope switches to a very small negative number, since almost all of the mass is concentrated in the single heavy particle and only a very small rest $\overline{M}$ remains in the smooth part. The evolution of the actual discrete second order moment is plotted with the continuous curve; first, it is very irregular, but at $t = 0.11$ it becomes quite smooth. This is explained by the fact that at this instant, the second heavy particle is created, which largely reduces the stochasticity of the system (most of the mass is located in the two heavy particles, which are not subject to the Brownian motion). After this point, the evolution of the second order moment is mostly determined by the motion of the two heavy particles and agrees very well with the prediction.



4 Convergence Proof for the Regularized Model

Since the question of convergence of the above described approximation scheme when the number of light particles tends to infinity is a rather difficult one, we postpone it to our future work. Here we make only a quite simple first step, which consists in considering, for a fixed parameter $\varepsilon > 0$, the scheme

$$\mathrm{d}x_n = -\frac{1}{2\pi}\frac{M}{N}\sum_{n\neq m,m=1}^{n} \mathcal{K}^\varepsilon(x_n - x_m) + \sqrt{2}\,\mathrm{d}B_t^n\,, \qquad n = 1,\dots,N\,, \tag{20}$$

for a (fixed) set of light particles, numbered by $1,\dots,N$. For simplicity, we assume that each particle carries the same mass M/N. $\mathcal{K}^\varepsilon$ denotes the regularized interaction potential

$$\mathcal{K}^\varepsilon(x) = \frac{x}{|x|(|x|+\varepsilon)} \qquad \text{for } x \in \mathbb{R}^2\,. \tag{21}$$

Our convergence proof is based on the (formally) equivalent formulation of the system of stochastic differential equations (20) in terms of the corresponding Kolmogorov forward equation,

$$\frac{\partial p^N}{\partial t} + \sum_{n=1}^{N} \nabla_{x_n} \cdot \left[-\frac{1}{2\pi}\frac{M}{N}\sum_{m\neq n} \mathcal{K}^\varepsilon(x_n - x_m)\,p^N - \nabla_{x_n} p^N \right] = 0\,, \tag{22}$$

where $p^N = p^N(t, x_1, \dots, x_N)$ is the N-particle distribution function, subject to the initial condition

$$\begin{aligned} p^N(t=0, x_1, \dots, x_N) &= p_I^N(x_1, \dots, x_N)\,, \\ p_I^N \geq 0 \text{ a.e. and } &\int_{\mathbb{R}^{2N}} p_I^N \,\mathrm{d}x_1 \dots \mathrm{d}x_N = 1\,. \end{aligned} \tag{23}$$

Moreover, we make the important assumption about the *indistinguishability-of-particles*: The initial condition p_I^N is indifferent to permutations of its arguments, i.e., for any permutation π of the N arguments, we have

$$p_I^N(x_1, \dots, x_N) = p_I^N(\pi(x_1, \dots, x_N))\,. \tag{24}$$

Observing that (22) is symmetric with respect to interchange of the x-variables, we may assume that the indistinguishability property of p_I^N is propagated in time, such that $p^N(t)$ is indifferent to permutations of its x-arguments too, for all $t > 0$.

We will show that, due to the boundedness of $\mathcal{K}^\varepsilon$ in L^∞ for each $\varepsilon > 0$, (22) has a unique global weak solution p^N in $L^2_{loc}([0,\infty); W^{1,2}(\mathbb{R}^{2N})) \cap C([0,\infty); L^2(\mathbb{R}^{2N}))$; in other words, there is no chemotactic collapse (in finite time). We will prove that for N large enough, p^N is close to a product of N identical scaled solutions of the regularized Keller-Segel model

$$\frac{\partial \varrho}{\partial t} + \nabla \cdot (\varrho \nabla S^\varepsilon[\varrho] - \nabla \varrho) = 0\,, \tag{25}$$

with the regularized potential

$$S_\varepsilon[\varrho_\varepsilon](x) = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \log(|x-y|+\varepsilon)\varrho_\varepsilon(y)\,\mathrm{d}y\,. \tag{26}$$

The existence and uniqueness of global solutions to the system (25)–(26) has been proven in [7]. One could say that the relative simplicity of the forthcoming proof is a consequence of the fact that the regularized problem does not exhibit blow-up behavior.

To derive an analogue of what is called the BBGKY hierarchy in the classical kinetic theory (see, for instance, [6]), we define for $k = 1, \dots, N$ the k-particle marginal

$$P_k^N(t, x_1, \dots, x_k) = \int_{\mathbb{R}^{2(N-k)}} p^N(t, x_1, \dots, x_N)\, \mathrm{d}x_{k+1} \dots \mathrm{d}x_N \tag{27}$$

and integrate (22) with respect to $x_{k+1}, \dots, x_N$:

$$\frac{\partial P_k^N}{\partial t} + \sum_{n=1}^{k} \nabla_{x_n} \cdot \left[-\frac{M}{2\pi N} \sum_{n \neq m = 1}^{N} \int_{\mathbb{R}^{2(N-k)}} \mathcal{K}^\varepsilon(x_n - x_m)\, p^N \, \mathrm{d}x_{k+1} \dots \mathrm{d}x_N - \nabla_{x_n} P_k^N \right] = 0\,. \tag{28}$$

Obviously, due to the indistinguishability assumption, P_k^N is independent of the particular choice of the set of its x-arguments; moreover, $P_N^N \equiv p^N$. We split the inner sum in (28) into the part with $m > k$ (interaction of the first k particles with all others) and $m \leq k$ (interaction among the first k particles) to obtain

$$\begin{aligned} &\sum_{m \neq n} \frac{M}{N} \int_{\mathbb{R}^{2(N-k)}} \mathcal{K}^\varepsilon(x_n - x_m)\, p \, \mathrm{d}x_{k+1} \dots \mathrm{d}x_N \\ &\quad = (N-k) \frac{M}{N} \int_{\mathbb{R}^2} \mathcal{K}^\varepsilon(x_n - y)\, P_{k+1}^N(x_1, \dots, x_k, y)\, \mathrm{d}y \\ &\qquad + \frac{M}{N} \sum_{m \leq k, m \neq n} \mathcal{K}^\varepsilon(x_n - x_m)\, P_k^N(x_1, \dots, x_k)\,. \end{aligned} \tag{29}$$

This, inserted into (28), constitutes the so-called *BBGKY hierarchy* for our system of interacting particles.

Loosely speaking, the convergence proof amounts to the statement that, as $N \to \infty$, the properly scaled N-particle distribution function tends to a product of solutions of the regularized Keller-Segel model. In a more exact formulation: For each $k \geq 1$, P_k^N converges to P_k as $N \to \infty$, such that for all $t \geq 0$ holds

$$P_k(t, x_1, \dots, x_k) = \prod_{n=1}^{k} P_1(t, x_n) \quad \text{for a.e. } x \in \mathbb{R}^{2k}\,, \tag{30}$$

and $\varrho(t, x) := M P_1(t, x)$ is the solution to (25)–(26). The formal limit passage $N \to \infty$ in (28) yields the so-called *Boltzmann hierarchy* for $\{P_k\}_{k=1}^\infty$:

$$\partial_t P_k + \sum_{n=1}^{k} \nabla_{x_n} \cdot \left[-\frac{M}{2\pi} \int_{\mathbb{R}^2} \mathcal{K}^\varepsilon(x_n - y)\, P_{k+1}(x_1, \dots, x_k, y)\, \mathrm{d}y - \nabla_{x_n} P_k \right] = 0\,, \tag{31}$$

which is subject to the initial conditions

$$P_k(t = 0, x_1, \dots, x_k) = \int_{\mathbb{R}^{2(N-k)}} p_I^N(t, x_1, \dots, x_N)\, \mathrm{d}x_{k+1} \dots \mathrm{d}x_N\,. \tag{32}$$

Now, if we assume that the *molecular chaos property* (30) holds indeed for all $k \geq 1$ and insert into the last equation, we obtain

$$\sum_{n=1}^{k} \partial_t P_1(x_n) \prod_{m\neq n}^{k} P_1(x_m) + \sum_{n=1}^{k} \nabla_{x_n} \cdot \left[-\frac{M}{2\pi} \prod_{m\neq n}^{k} P_1(x_m) \int_{\mathbb{R}^2} \mathcal{K}^{\varepsilon}(x_n - y) P_1(y) P_1(x_n) \, \mathrm{d}y \right.$$
$$\left. - \prod_{m\neq n}^{k} P_1(x_m) \nabla_{x_n} P_1(x_n) \right] = 0 .$$

After dividing with $\prod_{m\neq n}^{k} P_1(x_m)$ and multiplying by M, we indeed arrive at (25)–(26) for $\varrho(t,x) := M P_1(t,x)$. Thus, if we manage to prove uniqueness of solutions to the Boltzmann hierarchy (31), then this unique solution necessarily must be the factorizing solution given by (30). This in turn means that if we verify the convergence of P_k^N as $N \to \infty$, the limit factorizes and we conclude. These two statements are established in the following theorem:

Theorem 2 *For each $\varepsilon > 0$ and $N \geq 2$, the regularized Kolmogorov forward equation (22)–(23) with the initial condition $p_I^N \in L^2(\mathbb{R}^{2N})$, satisfying the molecular chaos property (30), has a unique global weak solution $p^N \in L^2_{loc}([0,\infty); W^{1,2}(\mathbb{R}^{2N})) \cap C([0,\infty); L^2(\mathbb{R}^{2N}))$. This solution verifies the indistinguishability-of-particles property and conserves mass. The k-particle marginals P_k^N given by (27) have weakly converging subsequences in $L^2_{loc}([0,\infty); W^{1,2}(\mathbb{R}^{2N}))$ as $N \to \infty$ for each $k \geq 1$ and the respective limits P_k are the unique weak solutions in $L^2([0,\infty); W^{1,2}(\mathbb{R}^{2k}))$ to the Boltzmann hierarchy (31) subject to the initial condition (32). They satisfy the molecular chaos property*

$$P_k(t, x_1, \ldots, x_k) = \prod_{n=1}^{k} P_1(t, x_n) \quad \text{for a.e. } x \in \mathbb{R}^{2k}, \forall t \geq 0 ,$$

with $\varrho(t,x) := M P_1(t,x)$ being the weak solution of the regularized Keller-Segel model (25)–(26).

Proof The existence and uniqueness of global weak solutions to the initial value problem (22)–(23) is a classical result of the theory of linear parabolic PDEs. Due to the symmetry of the equation with respect to interchange of variables, the unique solution must propagate the indistinguishability-of-particles property of the initial condition. Conservation of mass is a consequence of the divergence form of the equation.

Using appropriate test functions, it is easy to check that the k-particle marginals (27) verify the weak formulation of the BBGKY hierarchy (28) for $k = 1, \ldots, N-1$, subject to the initial conditions (32). The system is closed by setting $P_N^N := p^N$. For each $k = 1, \ldots, N-1$ we derive an a-priori estimate by multiplying the equation by P_k^N and integrating by parts with respect to the x-variables:

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{1}{2} \left\| P_k^N \right\|_{L^2}^2 + \left\| \nabla_x P_k^N \right\|_{L^2}^2 \leq \sum_{n=1}^{k} (A_n + B_n) ,$$

where the A_n-terms correspond to the first part of the decomposition (29) and are estimated as

$$A_n = \left| (N-k) \frac{M}{2\pi N} \int_{\mathbb{R}^{2k}} \left(\int_{\mathbb{R}^2} \mathcal{K}^{\varepsilon}(x_n - y) P_{k+1}^N(t, x_1, \ldots, x_k, y) \, \mathrm{d}y \right) \cdot \nabla_{x_n} P_k^N \, \mathrm{d}x \right|$$

$$\leq (N-k)\frac{M}{2\pi N}\|\mathcal{K}^\varepsilon\|_{L^\infty}\int_{\mathbb{R}^{2k}}\left|\int_{\mathbb{R}^2}P_{k+1}^N(t,x_1,\ldots,x_k,y)\,\mathrm{d}y\right|\left|\nabla_{x_n}P_k^N\right|\,\mathrm{d}x$$
$$= (N-k)\frac{M}{2\pi N}\|\mathcal{K}^\varepsilon\|_{L^\infty}\int_{\mathbb{R}^{2k}}\left|P_k^N\right|\left|\nabla_{x_n}P_k^N\right|\,\mathrm{d}x\,.$$

For the last step, which is in fact essential for the derivation of the a-priori estimate, we used the chain property of the marginals,

$$\int_{\mathbb{R}^2}P_{k+1}^N(t,x_1,\ldots,x_k,y)\,\mathrm{d}y = P_k^N(t,x_1,\ldots,x_k)\,. \tag{33}$$

The B_n-terms correspond to the second part of the decomposition (29) and are treated simply as

$$B_n = \left|\frac{M}{2\pi N}\int_{\mathbb{R}^{2k}}\sum_{m\leq k,m\neq n}\mathcal{K}^\varepsilon(x_n-x_m)\,P_k^N\cdot\nabla_{x_n}P_k^N\,\mathrm{d}x\right|$$
$$\leq \frac{1}{2\pi}\frac{M}{N}(k-1)\,\|\mathcal{K}^\varepsilon\|_{L^\infty}\int_{\mathbb{R}^{2k}}|P_k^N||\nabla_{x_n}P_k^N|\,\mathrm{d}x\,.$$

Alltogether, using $\|\mathcal{K}^\varepsilon\|_{L^\infty}=1/\varepsilon$, we arrive at

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\left\|P_k^N\right\|_{L^2}^2+\left\|\nabla_x P_k^N\right\|_{L^2}^2\leq\frac{M}{2\pi\varepsilon}\frac{N-1}{N}\sum_{n=1}^k\int_{\mathbb{R}^{2k}}|P_k^N||\nabla_{x_n}P_k^N|\,\mathrm{d}x\,.$$

Young inequality with some $0<\delta<\varepsilon$ gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\left\|P_k^N\right\|_{L^2}^2+\left(1-\frac{\delta}{\varepsilon}\right)\left\|\nabla P_k^N\right\|_{L^2}^2\leq\frac{M^2}{4\pi^2}\frac{k}{\delta\varepsilon}\left\|P_k^N\right\|_{L^2}^2\,,$$

and an application of Gronwall lemma yields, for each fixed $k\geq 1$, an a-priori estimate for the sequence $\{P_k^N\}_{N=k}^\infty$ in $L^2_{loc}([0,\infty);W^{1,2}(\mathbb{R}^{2k}))$ uniformly with respect to N. Thus, we have weakly converging subsequences as $N\to\infty$ and we can easily pass to the weak formulation of the Boltzmann hierarchy (31) subject to the initial condition (32). Using a hierarchic procedure for selecting the subsequences (the index set for the $(k+1)$-subsequence is a subset of the index set for the k-subsequence), it is easy to check that the chain property of marginals is preserved in the limit, and we can repeat the above steps to show the a-priori estimate for the solutions of the Boltzmann hierarchy of the form:

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{2}\|P_k\|_{L^2}^2+\left(1-\frac{\delta}{\varepsilon}\right)\|\nabla_x P_k\|_{L^2}^2\leq\frac{M^2}{4\pi^2}\frac{k}{\delta\varepsilon}\|P_k\|_{L^2}^2\,,\quad 0<\delta<\varepsilon\,.$$

An application of the Gronwall inequality gives the uniqueness of weak solutions: For each hierarchy of initial conditions there exists a unique hierarchy of solutions $\{P_k\}_{k=1}^\infty$. In particular, the limit P_k is independent of the choice of the particular subsequence of $\{P_k^N\}_{N=k}^\infty$. Consequently, the hierarchy must be generated by the molecular chaos property. □

Acknowledgements This work has been supported by the Austrian Science Foundation (grants no. W008 and P18367), by the EU-funded DEASE network (contract no. DEASE: MEST-CT-2005-021122), and by the Vienna Science and Technology Fund.

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