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STOCHASTIC PARTICLE APPROXIMATION TO THE GLOBAL MEASURE VALUED SOLUTIONS OF THE KELLER–SEGEL MODEL IN 2D

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Abstract. We construct an approximation to the measure valued, global in time solutions to the Keller-Segel model in 2D, based on systems of stochastic interacting particles. The advantage of our approach is that it reproduces the well-known dichtomy 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.

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, $\rho = \rho(t,x)$, and the concentration of the chemoattractant, $S = S(t,x)$. The famous Patlak-Keller-Segel model [11], which we consider in its parabolic-elliptic nondimensional setting, reads

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

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

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

$$\rho(x, t=0) = \rho_I(x) \qquad \text{for } x \in \mathbb{R}^2\,. \tag{3}$$

This system was extensively studied by many authors; [13] gives quite a complete survey of the results and an extensive bibliography. In the spatially two-dimensional case, the Poisson equation $\Delta S = -\rho$ is usually replaced by the Newtonian potential solution for S. Then the classical result

$$\frac{\mathrm{d}}{\mathrm{d}t}\int |x|^2 \rho(x)\,\mathrm{d}x = \frac{M}{2\pi}(8\pi - M)\,, \qquad \text{with } M := \int_{\mathbb{R}^2} \rho_I(x)\,\mathrm{d}x \tag{4}$$

indicates the well known dichotomy in the qualitative behavior of the system with the critical mass 8π [2, 3]. 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 the Poisson equation (2) is replaced by the regularized Newtonian potential solution

$$S_\varepsilon[\rho](x) = -\frac{1}{2\pi}\int_{\mathbb{R}^2} \log(|x-y| + \varepsilon)\rho(y)\,\mathrm{d}y\,. \tag{5}$$

This regularization is studied in [6], 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 [14], 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 ([14]) *For an interval $I \subset \mathbb{R}$, the set of time dependent measures with diagonal defects is defined as*

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

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

The limit of (1), (5) as $\varepsilon \to 0$ can be desribed as follows:

Theorem 1 ([6]) *For every $\varepsilon > 0$, the problem (1), (5) has a global weak solution $\rho_\varepsilon \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2)$. For every $T > 0$, as $\varepsilon \to 0$, a subsequence of solutions of (1), (5) converges tightly and uniformly in time to a time dependent measure $\rho(t)$. There exists $\nu(t)$ such that $(\rho, \nu) \in \mathscr{DM}^+((0,T);\mathbb{R}^2)$ is a generalized solution of*

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (j[\rho,\nu] - \nabla\rho) = 0 \tag{6}$$

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

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

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 (6), based on the following decomposition of the limiting measure valued solution $\rho(t) \in \mathscr{M}_1^+(\mathbb{R}^2)$:

$$\rho = \overline{\rho} + \hat{\rho}\,, \qquad \text{with } \hat{\rho}(t,x) = \sum_{n\in\mathscr{H}} M_n(t)\delta(x - x_n(t))\,,$$

for a finite set $\mathscr{H} \subset \mathbb{N}$, assuming $\overline{\rho}$ 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 $M_n(t) \geq 8\pi$. Then, the respective defect measure ν is of the form

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

where Id denotes the identity matrix in $\mathbb{R}^{2\times 2}$, and the following system of equations is obtained [6]:

$$\frac{\partial \overline{\rho}}{\partial t} + \nabla\cdot(\overline{\rho}\nabla S[\overline{\rho}] - \nabla\overline{\rho}) - \frac{1}{2\pi}\nabla\overline{\rho}\cdot\sum_{n\in\mathscr{H}} M_n(t)\frac{x - x_n}{|x-x_n|^2} = 0\,, \tag{7}$$

$$\dot{M}_n = M_n\overline{\rho}(x = x_n)\,, \tag{8}$$

$$\dot{x}_n = \nabla S[\overline{\rho}](x = x_n) - \frac{1}{2\pi}\sum_{n\neq m\in\mathscr{H}} M_m\frac{x_n - x_m}{|x_n - x_m|^2}\,. \tag{9}$$

A local-in-time existence result for initial value problems for this system can be found in [15]. In general, one has to expect blow-up events in the smooth part $\overline{\rho}$ 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 missing, however.

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 [1, 7, 12, 4]. 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 (7)–(9) with a system of interacting particles (Section 2). After a discretisation in time, this leads to a stochastic numerical method for computation of approximate solutions (Section 3). Finally, in Section 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 [9]; here we present its detailed description and some more numerical results, and the discussion in Section 4 is new.

2 Construction of the Stochastic Approximation and its Analysis

Formal derivation of the stochastic approximation

Let us start with the observation that for a given potential $S = S(x,t)$, equation (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 $\overline{\rho}$,

$$\overline{\rho}(x,t) \approx \sum_{n\in\mathscr{L}} M_n(t)\delta(x-x_n(t)) \tag{10}$$

for some finite index set $\mathscr{L} \subset \mathbb{N}$, 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,

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

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

Now the possible singularities of the density should come into the game. For this, we consider the strong formulation (7)–(9) with the finite set $\mathscr{H}$ of singular points $x_n(t)$, carrying masses $M_n(t)$, $n \in \mathscr{H}$. Inserting the ansatz (10) into (9), we obtain the system of ODEs describing the dynamics of the singular points,

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

where the first sum describes the interaction with the approximation of the smooth part of ρ, while the second sum stands for the interactions between the singular points.

Alltogether, we can summarize our considerations as

$$\mathrm{d}x_n = -\frac{1}{2\pi}\sum_{n\neq m\in(\mathscr{L}\cup\mathscr{H})} M_m \frac{x_n - x_m}{|x_n - x_m|^2} + \sqrt{2}\beta_n\,\mathrm{d}B_t^n\,, \tag{11}$$

for all $n \in (\mathscr{L}\cup\mathscr{H})$, where the "switch" β_n is equal one for $n \in \mathscr{L}$ and zero otherwise. As wee see, the only difference between the dynamics of the singular points and the dynamics of the particles approximating the smooth part of ρ 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 a stochastic processes.

As nice as the unified formulation (11) 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 discontinous 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 (11) 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 arbitrarily 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

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

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 $\mathscr{L}$, $\mathscr{H}$ 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 $n \in \mathscr{H}$. On the other hand, since we are interested in the situation when the number of particles approximating the smooth part of the solution tends to infinity, with their masses going uniformly to zero, we may assume that $M_n < 8\pi$ for $n \in \mathscr{L}$. This inspires the denomination of the $\mathscr{L}$-particles as *light particles* and of the $\mathscr{H}$-particles as *heavy particles*. Then, we can discriminate the following 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 (7)–(9). 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 $\overline{\rho}$ into the singular part $\hat{\rho}$, given by (8) (the singular particles "suck" the mass from their neighbourhood). The third type of collision is due to the dynamics of $\overline{\rho}$. 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 $\overline{\rho}$ is a formation of a multiple of Dirac delta, with initial mass 8π. Although this is known only for the radially symmetric case, see [10], 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 (7)–(9) if we use a large number of light particles with small enough masses.

Dynamical analysis - formal calculation of the critical mass

We will show that our method recovers the dynamical dichotomy of the Keller-Segel model, 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 start with a particle distribution comprising light particles only, with the total mass $M=\sum_{n\in\mathscr{L}} M_n(t=0)$. We denote by N the number of particles and by $x=x(t)$ the stochastic vector of the particle co-ordinates, $x=(x_{1_1},x_{1_2},\dots,x_{N_1},x_{N_2})$, 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

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

and the discrete second-order moment with respect to c

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

Then, the formal application of the Ito formula for the function u_c of the stochastic process x driven by the SDE (11) yields

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

and, again formally, taking expectation, we get

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

We observe that the qualitative dynamical behaviour of our system of particles is again determined by their total mass M, with the critical value 8π: Indeed, the sign of the time derivative of the expected second-order moment depends only on the total mass of the system, 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 (4) we got from the second-order moment calculation for the original system (1)–(2).

3 Time Discretization and Implementation

The stochastic particle approximation described in the previous section can be used as a basis for 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 (11) using the Euler-Maruyama method, arriving at the explicit scheme

$$x_n^{k+1}=x_n^k-\frac{\Delta t}{2\pi}\sum_{n\neq m\in(\mathscr{L}\cup\mathscr{H})} M_m\frac{x_n^k-x_m^k}{|x_n^k-x_m^k|^2}+\sqrt{2\Delta t}\beta_n\mathscr{N}_{(0,1)}\,, \tag{12}$$

subject to the initial condition

$$x_n^0=x_n^I\,,\quad M_n^0=M_n^I\qquad \text{for } n\in(\mathscr{L}\cup\mathscr{H})\,, \tag{13}$$

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

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

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, (8).

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 corsening, the details of the criterion for the detection of their collison 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 collision detection are important only in the case when at least one of the particles 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:

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

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

$$|d(0)|^2 \leq \frac{M_1 + M_2}{\pi}\Delta t\,. \tag{14}$$

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 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 indeed much stronger than the interaction with the rest of the system. Moreover, as already mentioned, we should check how (14) complies with the second equation of the strong formulation (8). 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 particles 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, those distance is d, during the time step Δt. According to (14), 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

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

we arrive at

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

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 $\overline{\rho}$ around x_1^k yields

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

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

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

Finally, concerning the collisions between light particles, we do not really need to care about the details of the collision mechanism, since the light particles merely approximate $\overline{\rho}$. An aggregation of two light particles into one can actually be seen 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 colliding, we are led to the idea of particle splitting as a mechanism of grid refinement. Before we discuss it in detail, let us conclude that the proposed criterion for detecting collisions, (14), is compliant with the strong formulation of the limiting problem (7)–(9).

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 great 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 (momentary) 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 collison 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 (12), 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):
$$x_n^{k+1/2} = x_n^k - \frac{\Delta t}{2\pi} \sum_{n \neq m \in (\mathscr{L} \cup \mathscr{H})} M_m \frac{x_n^k - x_m^k}{|x_n^k - x_m^k|^2} \qquad \text{for each } n \in (\mathscr{L} \cap \mathscr{H})\,.$$
2. Detection of collisions and (possible) redefinition of the sets $\mathscr{L}$ and $\mathscr{H}$.
3. Splitting of light particles, redefinition of the set $\mathscr{L}$.
4. Evaluation of the stochastic motions (diffusive step):
$$x_n^{k+1} = x_n^{k+1/2} + \sqrt{2\Delta t}\beta_n \mathscr{N}_{(0,1)} \qquad \text{for each } n \in (\mathscr{L} \cap \mathscr{H})\,.$$

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 the original one; the diffusive step then cares for their re-arrangement.

Acceleration strategies

Obviously, the one-to-one calculation of particle interactions in (12) makes our algorithm quadratic with respect to the number of particles. Consequently, in real 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 ([8] and references therein), which results in a $\mathscr{O}(N \log N)$ or even $\mathscr{O}(N)$ 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, performing just a small improvement. With this improvement we 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

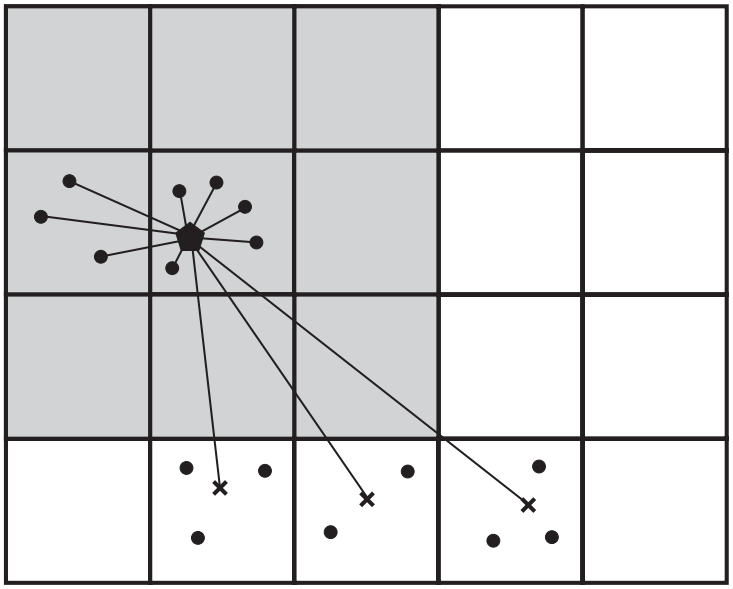


Figure 1: Accelerated algorithm. Interactions of a given particle (pentagon) with near particles (grey area) are evaluated one-to-one, while clusters of far particles (white area) are approximated by their centers of gravity (crosses).

$\{Q_1,\ldots,Q_K\}$, 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. 3). This significantly reduces the number of one-to-one interactions we must evaluate, although the algorithm retains its quadratic complexity.

Finally, let us remark that methods based on particle simulation are usually substantially less efficient then “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 calcuate the average of the particular outcomes (in other words, to 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 about any successful attempt to calculate global in time solutions to the Keller-Segel system including possible singularities. For instance, the finite volumes or finite element methods ([7], [12], [4]) become unstable close to the blow-up event and it is not possible to systematically detect the blow-up time. That’s why we think our algorithm has its justification.

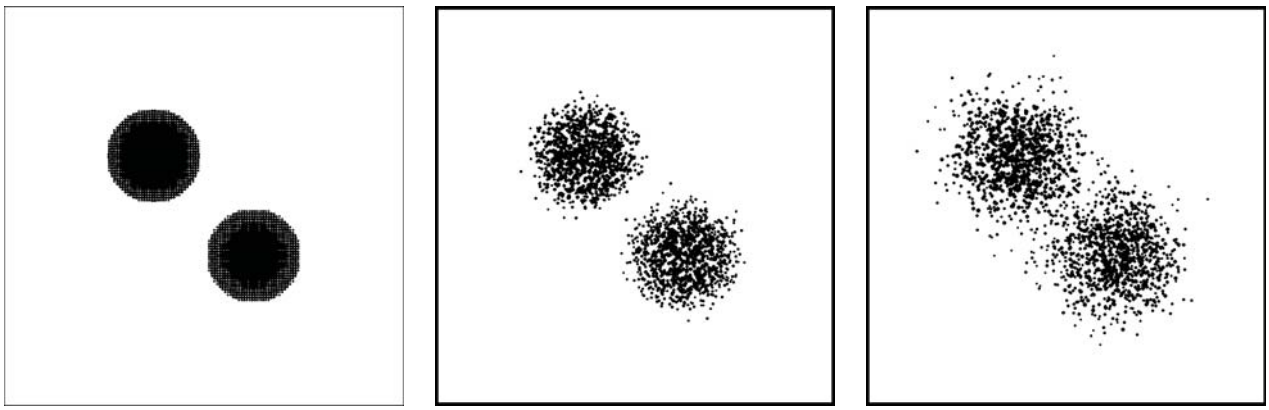
Numerical results

To illustrate the functionality of our method, we present two examples of numerical results. In both cases, we use 1500 particles with the same initial distribution in space - they are equidistantly spaced and their mass is chosen to approximate the smooth initial condition

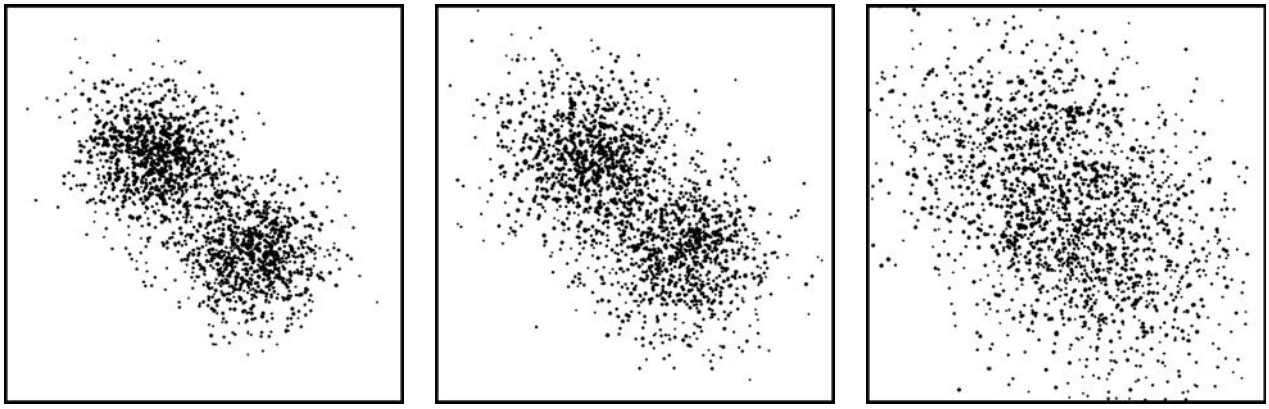
$$\rho_I(x) = \frac{14\lambda}{24}(1-|x-x_A|^2)^+ + \frac{10\lambda}{24}(1-|x-x_B|^2)^+,$$

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 mass is scaled to the total amount of 24π. In both cases the number of particles used in the simulation is 1500, the time step in the first case is 3×10^{-4}, in the second case 5×10^{-5}. In both cases the size of the displayed particles depends logarithmically on its 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), the diffusion is the stronger one of the two players in the game and the particles tend to be dispersed all around the computational domain:

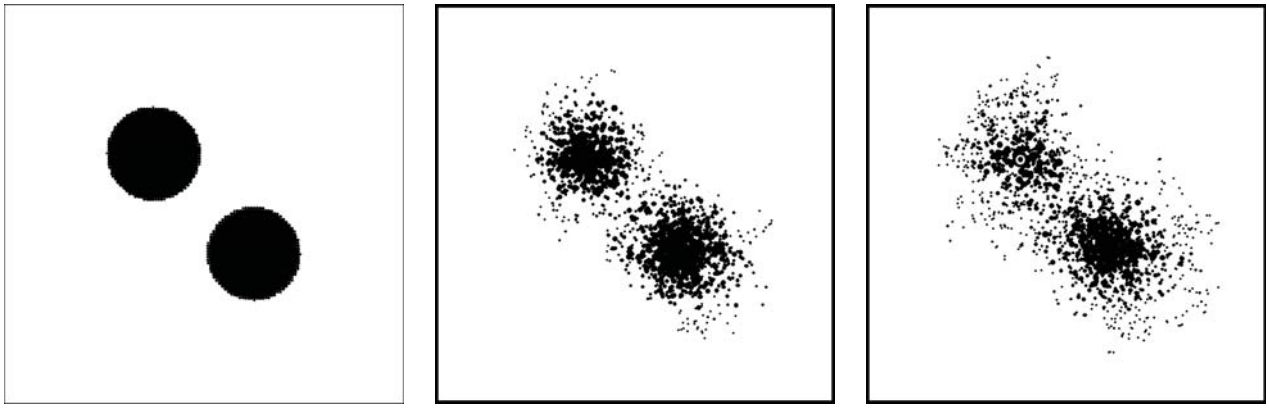


$t = 0.0$ $t = 0.001$ $t = 0.005$

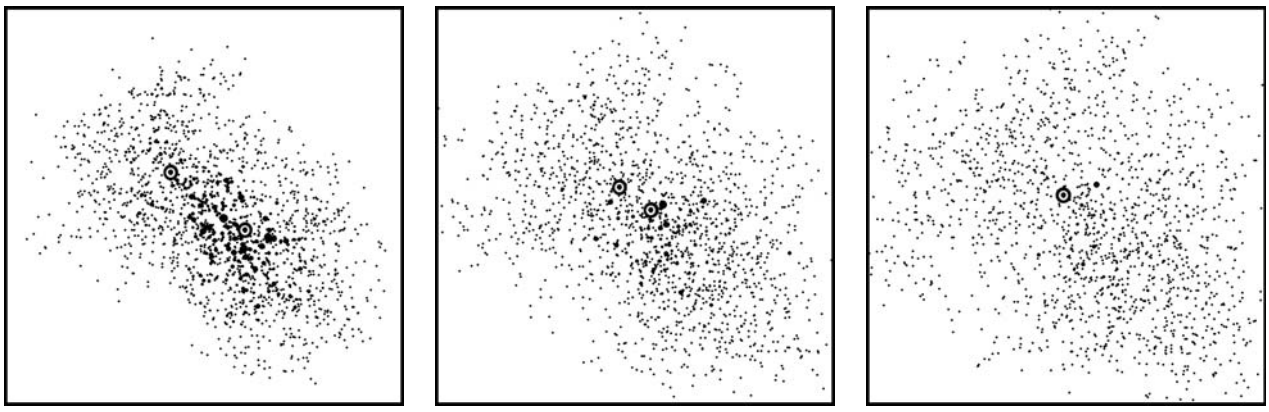


$t = 0.01$ $t = 0.017$ $t = 0.05$

To the contrary, in the supercritical case we observe formation of a first singularity in the region with the largest concentration of mass ($t = 0.0052$, displayed as a black-white-black target in the pictures below). After a while a second blow-up happens in the other densely populated region ($t = 0.012$). But still, there is a small fraction of mass which accounts to the smooth part of ρ. Incidentally, the two singularities collide to form one heavy particle ($t = 0.022$) carrying almost all the mass 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.



$t = 0.0$ $t = 0.003$ $t = 0.0052$



$t = 0.012$ $t = 0.02$ $t = 0.03$

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

$$\mathrm{d}x_n = -\frac{1}{2\pi}\frac{M}{N}\sum_{n\neq m\in\mathscr{L}} \mathscr{K}^\varepsilon(x_n - x_m) + \sqrt{2}\,\mathrm{d}B_t^n\,, \tag{15}$$

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

$$\mathscr{K}^\varepsilon(x) = \frac{x}{|x|(|x|+\varepsilon)} \qquad \text{for } x\in\mathbb{R}^2\,. \tag{16}$$

Our convergence proof is based on the (formally) equivalent formulation of the system of stochastic differential equations (15) in terms of the corresponding Kolmogorov forward equation

$$\frac{\partial p^N}{\partial t} + \sum_{n=1}^N \nabla_{x_n}\cdot\left[-\frac{1}{2\pi}\frac{M}{N}\sum_{m\neq n}\mathscr{K}^\varepsilon(x_n-x_m)p^N - \nabla_{x_n}p^N\right] = 0\,, \tag{17}$$

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

$$\begin{aligned} &p^N(t=0,x_1,\ldots,x_N) = p_I^N(x_1,\ldots,x_N)\,, \\ &p_I^N \geq 0 \text{ a.e. and } \int_{\mathbb{R}^{2N}} p_I^N\,\mathrm{d}x_1\ldots\mathrm{d}x_N = 1\,. \end{aligned} \tag{18}$$

Moreover, we make the important assumption about *indistinguishability* of the particles: The initial condition p_I^N is indifferent to permutations of its arguments. Observing that (17) is symmetric with respect to interchange of the x-variables, we may assume that the indistinguishability property 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 $\mathscr{K}^\varepsilon$ in L^∞ for each $\varepsilon > 0$, (17) has a unigue 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. We will prove that for N large enough, p^N is close to a product of N identical solutions of the regularized Keller-Segel model

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\nabla S^\varepsilon[\rho] - \nabla\rho) = 0\,, \tag{19}$$

where the regularized potential is given by

$$S_\varepsilon[\rho_\varepsilon](x) = -\frac{M}{2\pi}\int_{\mathbb{R}^2}\log(|x-y|+\varepsilon)\rho_\varepsilon(y)\,\mathrm{d}y\,. \tag{20}$$

Let us remark that the system (19)–(20) has a global weak solution $\rho(t)\in L^1(\mathbb{R}^2)\cap L^\infty(\mathbb{R}^2)$ for $t > 0$, see [6]. 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, [5]), we define for $k = 1,\dots,N$ the k-particle marginal

$$P_k^N(t,x_1,\dots,x_k) = \int_{\mathbb{R}^{2(N-k)}} p^N(t,x_1,\dots,x_N)\,\mathrm{d}x_{k+1}\dots\mathrm{d}x_N \tag{21}$$

and integrate (17) with respect to $x_{k+1},\dots,x_N$:

$$\frac{\partial P_k^N}{\partial t} + \sum_{n=1}^{k} \nabla_{x_n} \cdot \left[-\frac{M}{2\pi N} \sum_{n\neq m=1}^{N} \int_{\mathbb{R}^{2(N-k)}} \mathscr{K}^{\varepsilon}(x_n - x_m) p^N \,\mathrm{d}x_{k+1}\dots\mathrm{d}x_N - \nabla_{x_n} P_k^N \right] = 0\,. \tag{22}$$

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 (22) 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

$$\begin{aligned} &\sum_{m\neq n} \frac{M}{N} \int_{\mathbb{R}^{2(N-k)}} \mathscr{K}^{\varepsilon}(x_n - x_m) p \,\mathrm{d}x_{k+1}\dots\mathrm{d}x_N = \\ &(N-k)\frac{M}{N} \int_{\mathbb{R}^2} \mathscr{K}^{\varepsilon}(x_n - y) P_{k+1}(x_1,\dots,x_k,y)\,\mathrm{d}y + \\ &\frac{M}{N} \sum_{m\leq k, m\neq n} \mathscr{K}^{\varepsilon}(x_n - x_m) P_k(x_1,\dots,x_k)\,. \end{aligned} \tag{23}$$

This, inserted into (22), constitutes the so-called *BBGKY hierarchy* for our system of interacting particles.

Loosely speaking, the (formal) 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 $N \to \infty$, where

$$P_k(t,x_1,\dots,x_k) = \prod_{n=1}^{k} P_1(t,x_n) \qquad \forall t \geq 0\,, \tag{24}$$

and $\rho(t,x) := MP_1(t,x)$ is the solution to (19)–(20). The formal limit passage $N \to \infty$ in (22) yields the so-called *Boltzmann hierarchy* for $\{P_k\}_{k=1}^{\infty}$:

$$\partial_t P_k + \sum_{n=1}^{k} \nabla_{x_n} \cdot \left[-\frac{M}{2\pi} \int_{\mathbb{R}^2} \mathscr{K}^{\varepsilon}(x_n - y) P_{k+1}(x_1,\dots,x_k,y)\,\mathrm{d}y - \nabla_{x_n} P_k \right] = 0\,, \tag{25}$$

which is subject to the initial conditions

$$P_k(t=0,x_1,\dots,x_k) = \int_{\mathbb{R}^{2(N-k)}} p_I^N(t,x_1,\dots,x_N)\,\mathrm{d}x_{k+1}\dots\mathrm{d}x_N\,. \tag{26}$$

Now, if we assume that the *molecular chaos* (24) holds indeed for all $k \geq 1$ and insert into the last equation, we obtain

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

After dividing with $\prod_{m\neq n}^{k} P_1(x_m)$ and multiplying by M, we indeed arrive at (19)–(20) for $\rho(t,x) := MP_1(t,x)$. Thus, if we manage to prove uniqueness of solutions to the Boltzmann hierarchy (25), then this unique solution necessarily must be the factorizing solution given by (24). 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 (17)–(18) with the initial condition $p_I^N \in L^2(\mathbb{R}^{2N})$, satisfying the indistinguishability-of-particles property, 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 (21) 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 (25) subject to the initial condition (26). They satisfy the molecular chaos property*

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

with $\rho(t,x) := MP_1(t,x)$ being the weak solution of the regularized Keller-Segel model (19)–(20).

Proof: The existence and uniqueness of global weak solutions to the initial value problem (17)–(18) 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 (21) verify the weak formulation of the BBGKY hierarchy (22) for $k = 1,\dots,N-1$, subject to the initial conditions (26). The system is closed by setting $P_N^N := p^N$. For each $k = 1,\dots,N-1$ 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 (23) and are estimated as

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

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

$$\int_{\mathbb{R}^2}P_{k+1}^N(t,x_1,\dots,x_k,y)\,\mathrm{d}y = P_k^N(t,x_1,\dots,x_k)\,. \tag{27}$$

The B_n-terms correspond to the second part of the decomposition (23) and are treated simply as

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

Alltogether, using $\|\mathscr{K}^\varepsilon\|_{L^\infty} = 1/\varepsilon$, 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 (25) subject to the initial condition (26). Using a hierarchic procedure for selecting the subsequences (the index set for the $(k+1)$-subseqence 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:

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

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. ∎

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