BLOW-UP OF SOLUTIONS TO SEMI-DISCRETE PARABOLIC-ELLIPTIC KELLER-SEGEL MODELS

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ABSTRACT. The existence of weak solutions and upper bounds for the blow-up time for time-discrete parabolic-elliptic Keller-Segel models for chemotaxis in the two-dimensional whole space are proved. For various time discretizations, including the implicit Euler, BDF, and Runge-Kutta methods, the same bounds for the blow-up time as in the continuous case are derived by discrete versions of the virial argument. The theoretical results are illustrated by numerical simulations using an upwind finite-element method combined with second-order time discretizations.

1. INTRODUCTION

This paper is concerned with the derivation of upper bounds for the blow-up time in semi-discrete Keller-Segel systems in \mathbb{R}^2 . The (Patlak-) Keller-Segel model describes the evolution of the cell density of bacteria or amoebae that are attracted by a chemical substance [24, 35]. Under simplifying assumptions, the cell density n(x, t) and the density of the chemo-attractant c(x, t) satisfy the parabolic-elliptic equations

(1)
$$\partial_t n = \operatorname{div}(\nabla n - n\nabla c), \quad -\Delta c + \alpha c = n \quad \text{in } \mathbb{R}^2,$$

where $\alpha \geq 0$ measures the degradation rate of the chemical substance. Denoting by B_{α} the Bessel potential if $\alpha > 0$ and the Newton potential if $\alpha = 0$ (see the appendix for the definitions), this system can be formulated more compactly as a single equation,

(2)
$$\partial_t n = \operatorname{div} \left(\nabla n - n (\nabla B_\alpha * n) \right)$$
 in \mathbb{R}^2

with the initial condition

 $n(\cdot, 0) = n_0 \quad \text{in } \mathbb{R}^2.$

1.1. Blow-up properties. The coupling in equations (1) is a positive feedback: The cells produce a signal that attracts other cells. The cell aggregation is counterbalanced by diffusion, but if the cell density is sufficiently large, the chemical interaction dominates diffusion and may lead to finite-time blow-up of the cell density.

System (1) exhibits a dichotomy. Consider first the case without degradation, $\alpha = 0$. If the initial mass satisfies $M := \int_{\mathbb{R}^2} n_0 dx < 8\pi$, no aggregation takes place and the cells

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just diffuse for all times [6]. On the other hand, if the mass is supercritical, $M > 8\pi$, and the second moment $I_0 := \int_{\mathbb{R}^2} n_0 |x|^2 dx$ is finite, the solutions blow up in finite time. In the limit case $M = 8\pi$, there is blow-up in infinite time with constant second moment [5]. We remark that the critical space is $L^{d/2}(\mathbb{R}^d)$ in space dimensions $d \ge 2$ [16]. When the signal degradates, $\alpha > 0$, a similar criterium holds: The solutions exist for all time for subcritical initial masses $M < 8\pi$, and they blow up in finite time for supercritical masses $M > 8\pi$ and sufficiently small second moment I_0 [10]. The blow-up time T_{max} can be estimated from above by

(3)
$$T_{\max} \le T^* := \frac{2\pi I_0}{M(M - 8\pi - 2\sqrt{\alpha M I_0})}$$

The upper bound for the system with degradation becomes larger than that one without degradation, indicating that blow-up happens later than without degradation, which is biologically reasonable. The idea of the proof is a virial argument: The second moment $I(t) = \int_{\mathbb{R}^2} n(\cdot, t) dx$ solves the differential inequality

(4)
$$\frac{dI}{dt} \le -\frac{M}{2\pi}(M - 8\pi) + \frac{\sqrt{\alpha}}{\pi}M^{3/2}\sqrt{I}.$$

If $\alpha = 0$, this expression becomes an identity. Now, if $t > T^*$, we infer that I(t) < 0, contradicting $n(\cdot, t) \ge 0$.

Very detailed numerical simulations of the collapse phenomenon in the parabolic-parabolic system have been performed in, e.g., [9]. The asymptotic profile of blow-up solutions in the parabolic-elliptic model was studied in [17]. Numerical blow-up times were computed, for instance, in [19] using a kind of H^2 norm indicator; in [9] using the moving-mesh method; and in [18] using discontinuous Galerkin approximations.

The aim of this paper is to prove the existence of weak solutions to various versions of time-discrete equations and to derive discrete versions of inequality (4). We analyze the implicit Euler and higher-order schemes, including BDF (Backward Differentiation Formula) and Runge-Kutta schemes. Our goal is not to design efficient numerical schemes but to continue our program to "translate" mathematical techniques from continuous to discrete situations [28, 29, 30].

The proof of inequality (4) is based on three properties: nonnegativity of n(x,t), mass conservation, and a symmetry argument in the nonlocal term in (2). The implicit Euler scheme satisfies all these properties, while the nonnegativity cannot be proved for higherorder schemes, although it seems to hold numerically (see Section 4). We discuss this issue below.

1.2. State of the art. The literature on the analysis and numerical approximation of Keller-Segel models is enormous. Therefore, we review only papers concerned with the analysis of numerical schemes and the blow-up behavior of the discrete solutions, in particular possessing structure-preserving features. We do not claim completeness and refer to the introduction of [1] for more references.

Most of the numerical schemes for the Keller-Segel model utilize the implicit Euler method for the time discretization and aim to preserve some properties of the continuous equations, like (local) mass conservation, positivity (more precisely, nonnegativity) preservation, or energy dissipation. These schemes use (semi-implicit) finite-difference methods [13, 32, 40]; an upwind finite-element discretization [37]; an Eulerian-Lagrangian scheme based on the characteristics method [42]; a Galerkin method with a diminishing flux limiter [45]; and finite-volume methods [20, 49]. A finite-volume scheme was also studied in [1] but with a first-order semi-exponentially fitted time discretization. Finally, a mass-transport steepest descent scheme was analyzed in [4]. All these schemes are based on first-order discretizations.

Only few results are concerned with higher-order time integrators. Strongly $A(\theta)$ -stable Runge-Kutta finite-element discretizations were analyzed in [34], and the convergence of the discrete solution was shown. However, mass conservation or positivity preservation was not verified. As A-stable time integrators are computationally very costly, often splitting methods are used. A third-order strong stability preserving (SSP) Runge-Kutta time discretization for the advection term and the second-order Krylov IIF (implicit integration factor) method for the reaction-diffusion term, together with a positivity-preserving discontinuous Galerkin approximation in space, was suggested in [48], but without any analysis.

A number of papers are concerned with the preservation of the nonnegativity of the cell density. An example is [14], where a semi-discrete central-upwind scheme was proposed. Moreover, in [15], a hybrid finite-volume finite-difference method was combined with SSP explicit Runge-Kutta schemes (for the parabolic-parabolic case) or the explicit Euler scheme (for the parabolic-elliptic case). Clearly, a CFL condition is needed to ensure the stability of the explicit schemes. Another approach was used in [47] for a related tumor-angiogenesis model, where a Taylor series method in time allows for higher-order but still explicit schemes.

We remark that there do not exist SSP implicit Runge-Kutta or multistep methods of higher order [22, Section 6]. Moreover, SSP for such methods is guaranteed only under some finite time step condition [7, 43] (also see the recent work [25]). In view of these results, positivity preservation of our higher-order schemes cannot be expected.

We do not aim to preserve the free energy of the Keller-Segel system since such schemes usually destroy the symmetry property needed for the blow-up argument; see Remark 3 for details. An exception is the work [4], where the virial blow-up argument could be used for an implicit Euler steepest descent scheme, which also provides the decay of the gradientflow energy. Some estimates on the discrete free energy in an implicit Euler finite-volume approximation were shown in [49]. A numerical scheme that dissipates the free energy numerically was suggested in [12] using a gradient-flow formulation of the energy functional with respect to a quadratic transportation distance. It is shown in [40] that the dissipation of the discrete free energy may fail in an upwind finite-difference scheme. The dissipation of the discrete entropy in a finite-volume modified Keller-Segel system was proved in [3].

The novelty of this paper is the derivation of the critical initial mass and an upper bound for the blow-up time for various time discretizations, where the values are the same as in the continuous case. This shows that the "continuous" methods carry over to the semi-discrete case. Because of the virial argument, the extension to spatial discretizations is more delicate. A possible direction is to extend the virial argument to a discrete Bessel potential, but we leave details to a future work.

1.3. Main results. Our main results can be sketched as follows (details will be given in sections 2 and 3). Let n_k be an approximation of $n(\cdot, k\tau)$, where $\tau > 0$ is the time step and $k \in \mathbb{N}$. We recall the definitions $M = \int_{\mathbb{R}^2} n_0 dx$ of the initial mass and $I_0 = \int_{\mathbb{R}^2} n_0 |x|^2 dx$ of the initial second moment.

- Existence of solutions to the implicit Euler scheme (Theorem 1): For given $n_{k-1} \ge 0$ and sufficiently small time step τ , there exists a unique weak solutions n_k to the semi-discrete equations. Moreover, the scheme preserves the positivity, conserves the mass, and has finite second moment.
- Finite-time blow-up for the implicit Euler scheme (Theorem 2): Let $M > 8\pi$ and let I_0 be finite (if $\alpha = 0$) or I_0 and τ be sufficiently small (if $\alpha > 0$). Then the semi-discrete solution exists only up to discrete times $k\tau \leq T^*$, where T^* is defined in (3).
- BDF schemes: For sufficiently small $\tau > 0$, there exists a unique weak solution to the BDF-2 and BDF-3 scheme, conserving the mass and having finite second moment. Moreover, under the same assumptions as for the implicit Euler scheme, the solution blows up and $k\tau \leq T^*$ (Theorem 5 for BDF-2 and $\alpha \geq 0$, Theorem 7 for BDF-3 and $\alpha = 0$).
- Runge-Kutta schemes (Theorem 9): If $\alpha = 0$ and under the same assumptions as for the implicit Euler scheme, the solution blows up and $k\tau \leq T^*$. The same result holds for the implicit midpoint and trapezoidal rule if $\alpha > 0$.

The interesting fact is that the upper bound T^* is the same for both the continuous and semi-discrete equations. Observe that the existence results do not require the condition $M < 8\pi$, since they are local. In particular, the smallness condition on τ is natural, and the time step needs to be chosen smaller and smaller when the blow-up time is approached.

The paper is organized as follows. Section 2 is concerned with the analysis of the implicit Euler scheme, while some higher-order schemes (BDF, Runge-Kutta) are investigated in section 3. In section 4 we provide some numerical examples to illustrate our theoretical statements. Finally, the appendix collects some auxiliary results.

2. Implicit Euler scheme

We show the existence of weak solutions to the implicit Euler approximation of the Keller-Segel system (2) and their finite-time blow-up, where

(5)
$$\frac{1}{\tau}(n_k - n_{k-1}) = \operatorname{div}\left(\nabla n_k - n_k \nabla B_\alpha * n_k\right) \quad \text{in } \mathbb{R}^2.$$

Here, $\tau > 0$ is the time step and B_{α} is the Bessel potential if $\alpha > 0$ and the Newton potential if $\alpha = 0$ (see the appendix). First, we study the existence of solutions. For this, let $X := L^1(\mathbb{R}^2) \cap L^{\infty}(\mathbb{R}^2)$ with norm $\|u\|_X = \max\{\|u\|_{L^1(\mathbb{R}^2)}, \|u\|_{L^{\infty}(\mathbb{R}^2)}\}$ for $u \in X$.

Theorem 1 (Existence for the implicit Euler scheme). Let $n_{k-1} \in X$ and

$$\tau < \frac{1}{(\pi + 1/2)^2} \frac{1}{(\|n_{k-1}\|_X + 1)^4}$$

Then there exists a unique weak solution $n_k \in X \cap H^1(\mathbb{R}^2)$ to (5) such that

- nonnegativity: if $n_{k-1} \ge 0$ then $n_k \ge 0$ in \mathbb{R}^2 ,
- conservation of mass: ∫_{ℝ²} n_kdx = ∫_{ℝ²} n_{k-1}dx,
 control of second moment: if ∫_{ℝ²} n_{k-1}|x|²dx < ∞ then ∫_{ℝ²} n_k|x|²dx < ∞.

Proof. The strategy is to prove first the existence of a unique very weak solution $n_k \in X$ to the truncated problem

(6)
$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1})\phi dx = \int_{\mathbb{R}^2} n_k \Delta \phi dx + \int_{\mathbb{R}^2} n_k^+ (\nabla B_\alpha * n_k) \cdot \nabla \phi dx$$

for all $\phi \in H^1(\mathbb{R}^2)$, where $n_k^+ = \max\{0, n_k\}$. The second step is to show that $n_k \in H^1(\mathbb{R}^2)$. Then we can use $n_k^- = \min\{0, n_k\}$ as a test function in the weak formulation and prove that $n_k \geq 0$.

Step 1: Solution to (6). To simplify the notation, we write $n := n_k$ and $n_0 := n_{k-1}$. We introduce the operator $\nabla c: X \to L^{\infty}(\mathbb{R}^2)^2, \nabla c[n] = \nabla B_{\alpha} * n$. We claim that this operator is well-defined and continuous. Indeed, set for $\alpha \geq 0$,

(7)
$$g_{\alpha}(r) := \int_{0}^{\infty} e^{-s - \alpha r^{2}/(4s)} dx \le 1 \quad \text{for } r > 0.$$

Then, after the substitution $s = |x|^2/(4t)$, we can write

(8)
$$\nabla B_{\alpha}(z) = -\frac{1}{2\pi} \frac{z}{|z|^2} g_{\alpha}(|z|), \quad z \in \mathbb{R}^2,$$

and it follows that

(9)
$$\begin{aligned} |\nabla c[n](x)| &= \left| \frac{1}{2\pi} \int_{\mathbb{R}^2} \frac{x-y}{|x-y|^2} g_\alpha(|x-y|) n(y) dy \right| \\ &\leq \frac{1}{2\pi} \int_{|x-y| \leq 1} \frac{|n(y)|}{|x-y|} dy + \frac{1}{2\pi} \int_{|x-y| > 1} \frac{|n(y)|}{|x-y|} dy \\ &\leq \|n\|_{L^{\infty}(\mathbb{R}^2)} + \frac{1}{2\pi} \|n\|_{L^1(\mathbb{R}^2)} \leq b \|n\|_X. \end{aligned}$$

where $b := 1 + 1/(2\pi)$. This shows the continuity of ∇c .

Next, for given $\widetilde{n} \in X$, the linear problem

$$-\Delta n + \tau^{-1}(n - n_0) = -\operatorname{div}(\widetilde{n}^+ \nabla c[\widetilde{n}])$$

has a unique solution in $H^1(\mathbb{R}^2)$. Indeed, since we have $\widetilde{n}^+ \in L^2(\mathbb{R}^2), \, \nabla c[\widetilde{n}] \in L^\infty(\mathbb{R}^2)^2$, and therefore $f := \tilde{n}^+ \nabla c[\tilde{n}] \in L^2(\mathbb{R}^2)^2$, we can apply Lemma 16 in the appendix yielding the unique solvability of the linear problem. The solution is given by

(10)
$$n = \frac{1}{\tau} B_{1/\tau} * n_0 - \nabla B_{1/\tau} * (\tilde{n}^+ \nabla c[\tilde{n}]).$$

Hence, we can define the fixed-point operator $T: X \to X$ by $T[\tilde{n}] := n$, and n is given by (10). Clearly, any fixed point of T is a solution to (6). We apply the Banach fixed-point theorem to T on the set $S := \{n \in X : ||n||_X \le ||n_0||_X + 1\}$. For this, we need to show that $T: S \to S$ is a contraction.

For the proof of $T(S) \subset S$, we use Lemma 14, the Young inequality with p = q = r = 1 (see the appendix), and (9):

$$\begin{aligned} \|T[n]\|_{L^{1}(\mathbb{R}^{2})} &\leq \frac{1}{\tau} \|B_{1/\tau} * n_{0}\|_{L^{1}(\mathbb{R}^{2})} + \|\nabla B_{1/\tau} * (n^{+}\nabla c[n])\|_{L^{1}(\mathbb{R}^{2})} \\ &\leq \frac{1}{\tau} \|B_{1/\tau}\|_{L^{1}(\mathbb{R}^{2})} \|n_{0}\|_{L^{1}(\mathbb{R}^{2})} + \|\nabla B_{1/\tau}\|_{L^{1}(\mathbb{R}^{2})} \|\nabla c[n]\|_{L^{\infty}(\mathbb{R}^{2})} \|n\|_{L^{1}(\mathbb{R}^{2})} \\ &\leq \|n_{0}\|_{L^{1}(\mathbb{R}^{2})} + \frac{\pi}{2} \tau^{1/2} b \|n\|_{X}^{2}. \end{aligned}$$

Similarly, we obtain

$$||T[n]||_{L^{\infty}(\mathbb{R}^2)} \le ||n_0||_{L^{\infty}(\mathbb{R}^2)} + \frac{\pi}{2}\tau^{1/2}b||n||_X^2$$

Combining the previous two estimates, we conclude that

$$||T[n]||_X \le ||n_0||_X + \frac{\pi}{2}\tau^{1/2}b||n||_X^2$$

Then choosing $\tau < (\pi b)^{-2} (||n_0||_X + 1)^{-4}$, we see that $||T[n]||_X \le ||n_0||_X + 1/2$, which shows that $T[n] \in S$.

To show the contraction property, let $n, m \in S$. Then, estimating as above,

$$\begin{aligned} \|T[n] - T[m]\|_{X} &\leq \left\|\nabla B_{1/\tau} * \left(n^{+}\nabla c[n] - m^{+}\nabla c[m]\right)\right\|_{X} \\ &\leq \left\|\nabla B_{1/\tau}\right\|_{L^{1}(\mathbb{R}^{2})} \left\| (n^{+} - m^{+})\nabla c[n] + m^{+}(\nabla c[n] - \nabla c[m])\right\|_{X} \\ &\leq \frac{\pi}{2}\tau^{1/2} \left(\|n^{+} - m^{+}\|_{X}\|\nabla c[n]\|_{L^{\infty}(\mathbb{R}^{2})} + \|m\|_{X}\|\nabla c[n - m]\|_{L^{\infty}(\mathbb{R}^{2})} \right) \\ &\leq \pi\tau^{1/2} b \left(\|n_{0}\|_{X} + 1 \right) \|n - m\|_{X}. \end{aligned}$$

Since $\pi \tau^{1/2} b(||n_0||_X + 1) < 1$, T is a contraction. By the Banach fixed-point theorem, T has a fixed point $n_k \in X$, which is a solution to (6).

Step 2: Regularity of the solution to (6). We prove that for any $\alpha \geq 0$, $n_k \in H^1(\mathbb{R}^2)$ solves

(11)
$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1})\phi dx = -\int_{\mathbb{R}^2} \nabla n_k \cdot \nabla \phi dx + \int_{\mathbb{R}^2} n_k^+ (\nabla B_\alpha * n_k) \cdot \nabla \phi dx$$

for all $\phi \in H^1(\mathbb{R}^2)$ and satisfies

(12)
$$\|n_k\|_{H^1(\mathbb{R}^2)} \le C_0 \|n_{k-1}\|_{L^2(\mathbb{R}^2)}$$

for some positive constant C_0 which depends on τ and $||n_{k-1}||_X$.

Again, we set $n := n_k$ and $n_0 := n_{k-1}$. Since $n \in X \subset L^2(\mathbb{R}^2)$, we have $n^+ \nabla c[n] \in L^2(\mathbb{R}^2)^2$. Therefore, by Lemma 16, $n \in H^1(\mathbb{R}^2)$ is the unique solution to (11). We take n

as a test function in that equation and use the Young inequality:

$$\frac{1}{2\tau} \int_{\mathbb{R}^2} (n^2 - n_0^2) dx \le \frac{1}{\tau} \int_{\mathbb{R}^2} (n - n_0) n dx = -\|\nabla n\|_{L^2(\mathbb{R}^2)}^2 + \int_{\mathbb{R}^2} n^+ \nabla c[n] \cdot \nabla n dx$$
$$\le -\frac{1}{2} \|\nabla n\|_{L^2(\mathbb{R}^2)}^2 + \frac{1}{2} \|n\|_{L^2(\mathbb{R}^2)}^2 \|\nabla c[n]\|_{L^\infty(\mathbb{R}^2)}^2.$$

By (9) and $||n||_X \le ||n_0||_X + 1$, we find that

$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n^2 - n_0^2) dx + \|\nabla n\|_{L^2(\mathbb{R}^2)}^2 \le b^2 \|n\|_X^2 \|n\|_{L^2(\mathbb{R}^2)}^2 \le b^2 (\|n_0\|_X + 1)^2 \|n\|_{L^2(\mathbb{R}^2)}^2.$$

Then, since $\beta := 1 - b^2 (||n_0||_X + 1)^2 \tau > 0$, we infer that

$$||n||_{L^{2}(\mathbb{R}^{2})}^{2} \leq \frac{1}{\beta} ||n_{0}||_{L^{2}(\mathbb{R}^{2})}^{2},$$

and the claim follows with $C_0 = 1/\sqrt{\beta}$.

Step 3: Nonnegativity of n_k . Let $n_{k-1} \ge 0$ in \mathbb{R}^2 . We use $n_k^- = \min\{0, n_k\} \in H^1(\mathbb{R}^2)$ as a test function in (11):

$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k^-)^2 dx \le \frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1}) n_k^- dx = -\int_{\mathbb{R}^2} |\nabla n_k^-|^2 dx + \int_{\mathbb{R}^2} n_k^+ \nabla c[n_k] \cdot \nabla n_k^- dx \le 0,$$

since $n_{k-1}n_k^- \leq 0$ and the last integral on the right-hand side vanishes. This shows that $n_k \geq 0$ in \mathbb{R}^2 , and $n_k^+ = n_k$ in (11).

Step 4: Mass conservation. The statement follows immediately if we could use $\phi(x) = 1$ as a test function in (6). Since this function is not integrable, we need to approximate. As in [26], we introduce the radially symmetric cut-off function $\phi_R(x) = \phi(|x|/R)$, where $R \ge 1$ and

(13)
$$\phi(r) = \begin{cases} 1 & \text{for } 0 \le r \le 1, \\ 1 - 2(r-1)^2 & \text{for } 1 < r \le 3/2, \\ 2(2-r)^2 & \text{for } 3/2 < r \le 2, \\ 0 & \text{for } r \ge 2. \end{cases}$$

The following properties hold:

(14)

$$\begin{aligned}
\phi_R \in H^2(\mathbb{R}^2), \quad \lim_{R \to \infty} \phi_R(x) &= 1 & \text{for all } x \in \mathbb{R}^2, \\
|\nabla \phi_R(x) - \nabla \phi_R(y)| &\leq \frac{C_1}{R^2} |x - y|, \quad |\Delta \phi_R(x)| \leq \frac{C_2}{R^2} & \text{for all } x, y \in \mathbb{R}^2
\end{aligned}$$

for some constants C_1 , $C_2 > 0$. Let $0 \leq \rho^{\varepsilon} \in C_0^{\infty}(\mathbb{R}^2)$ be a standard mollifier and set $\phi_R^{\varepsilon} = \phi_R * \rho^{\varepsilon}$. Then $\phi_R^{\varepsilon} \to \phi_R$ in $H^2(\mathbb{R}^2)$ as $\varepsilon \to 0$ [27, Lemma 1.8.2]. Consequently, up to

a subsequence, which is not relabeled, $\phi_R^{\varepsilon} \to \phi_R$, $\nabla \phi_R^{\varepsilon} \to \nabla \phi_R$, and $\Delta \phi_R^{\varepsilon} \to \Delta \phi_R$ a.e. in \mathbb{R}^2 . We use ϕ_R^{ε} as a test function in (6) and insert (8):

$$\left|\frac{1}{\tau}\int_{\mathbb{R}^2} (n_k - n_{k-1})\phi_R^{\varepsilon} dx\right| = \left|\int_{\mathbb{R}^2} n_k \Delta \phi_R^{\varepsilon} dx + \int_{\mathbb{R}^2} n_k (\nabla B_\alpha * n_k) \cdot \nabla \phi_R^{\varepsilon} dx\right|$$
$$\leq \frac{C_2}{R^2} \|n_k\|_{L^1(\mathbb{R}^2)} + \frac{1}{2\pi} \left|\int_{\mathbb{R}^2} \int_{\mathbb{R}^2} n_k(x) n_k(y) g_\alpha(|x-y|) \frac{x-y}{|x-y|^2} \cdot \nabla \phi_R^{\varepsilon}(x) dx dy\right|.$$

By symmetry and (14), the second integral can be estimated as

$$\frac{1}{2\pi} \left| \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} n_k(x) n_k(y) g_\alpha(|x-y|) \frac{x-y}{|x-y|^2} \cdot \nabla \phi_R^{\varepsilon}(x) dx dy \right| \\
= \frac{1}{4\pi} \left| \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} n_k(x) n_k(y) g_\alpha(|x-y|) \frac{x-y}{|x-y|^2} \cdot \left(\nabla \phi_R^{\varepsilon}(x) - \nabla \phi_R^{\varepsilon}(y) \right) dy dx \right| \\
\leq \frac{C_1}{4\pi R^2} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} n_k(x) n_k(y) dy dx = \frac{C_1}{4\pi R^2} \|n_k\|_{L^1(\mathbb{R}^2)}^2.$$

These estimates allow us to apply the dominated convergence theorem, which leads, in the limit $\varepsilon \to 0$, to

$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1}) \phi_R dx = \int_{\mathbb{R}^2} n_k \Delta \phi_R dx + \int_{\mathbb{R}^2} n_k (\nabla B_\alpha * n_k) \cdot \nabla \phi_R dx.$$

The same estimates as before show that both integrals on the right-hand side can be estimated by a multiple of $1/R^2$ such that the limit $R \to \infty$ leads to

$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1}) dx = 0,$$

which gives mass conservation.

Step 5: Control of the second moment. Similarly as in step 4, we approximate $|x|^2$ by setting $\psi_R(x) = |x|^2 \phi_R(x)$, where ϕ_R is defined in (13). Then $\psi_R \in H^2(\mathbb{R}^2)$, $\nabla \psi_R$ is Lipschitz continuous on \mathbb{R}^2 , and $\Delta \psi_R$ is bounded. Taking a standard mollifier $\rho^{\varepsilon} \geq 0$, we set $\psi_R^{\varepsilon} = \psi_R * \rho^{\varepsilon} \in C_0^{\infty}(\mathbb{R}^2)$. Using ψ_R^{ε} as a test function in (6) and passing to the limit $\varepsilon \to 0$ and then $R \to \infty$, it follows that

(15)
$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1}) |x|^2 dx = 4 \int_{\mathbb{R}^2} n_k dx + 2 \int_{\mathbb{R}^2} n_k (\nabla B_\alpha * n_k) \cdot x dx.$$

Young's inequality and estimate (9) for $\nabla c[n_k] = \nabla B_{\alpha} * n_k$ show that

$$2\left|\int_{\mathbb{R}^2} n_k (\nabla B_\alpha * n_k) \cdot x dx\right| \le 2b \|n_k\|_X \int_{\mathbb{R}^2} n_k |x| dx$$
$$\le b \|n_k\|_X \int_{\mathbb{R}^2} n_k dx + b \|n_k\|_X \int_{\mathbb{R}^2} n_k |x|^2 dx.$$

Therefore, with $||n_k||_X \le ||n_{k-1}||_X + 1$, (15) gives

$$\left(1 - \tau b(\|n_{k-1}\|_X + 1)\right) \int_{\mathbb{R}^2} n_k |x|^2 dx \le \int_{\mathbb{R}^2} n_{k-1} |x|^2 dx + \tau (4 + b\|n_k\|_X) \int_{\mathbb{R}^2} n_0 dx.$$

Since $1 - \tau b(||n_{k-1}||_X + 1) > 0$, we infer that the second moment of n_k is bounded if the second moment of n_{k-1} does so.

Next, we turn to the finite-time blow up of semi-discrete solutions. Set, for $\alpha > 0$,

(16)
$$I^* := \frac{(M - 8\pi)^2}{4\alpha M}, \quad \tau^* := \frac{\pi (M - 8\pi)}{2\alpha M^2}$$

Theorem 2 (Blow-up for the implicit Euler scheme). Assume that

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi$$

Let $(n_k) \subset L^1(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ be a sequence of nonnegative weak solutions to (5). Then this sequence is finite with maximal index k_{\max} , where, if $\alpha = 0$,

(17)
$$k_{\max} \le \frac{2\pi I_0}{\tau M(M - 8\pi)}$$

In case $\alpha > 0$, if additionally $I_0 \leq I^*$ and $\tau < \tau^*$ then

(18)
$$k_{\max} \le \frac{2\pi I_0}{\tau M(M - 8\pi - 2\sqrt{\alpha M I_0})}.$$

Proof. Let first $\alpha = 0$ and let n_k be a weak solution to (5) with $k > 2\pi I_0/(\tau M(M - 8\pi))$, i.e., we assume that (17) does not hold. We set $I_k = \int_{\mathbb{R}^2} n_k |x|^2 dx$. Then, by (15), for any $j \leq k$,

$$I_{j} - I_{j-1} = 4\tau \int_{\mathbb{R}^{2}} n_{j} dx + 2\tau \int_{\mathbb{R}^{2}} n_{j} (\nabla B_{0} * n_{j}) \cdot x dx$$

= $4\tau M - \frac{\tau}{\pi} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} n_{j} (x) \frac{x \cdot (x - y)}{|x - y|^{2}} n_{j} (y) dy dx,$

where we used the conservation of mass and the definition of $\nabla B_0 * n_k$. A symmetry argument leads to

$$I_{j} - I_{j-1} = 4\tau M - \frac{\tau}{2\pi} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} \frac{(x-y) \cdot (x-y)}{|x-y|^{2}} n_{j}(x) n_{j}(y) dy dx$$
$$= 4\tau M - \frac{\tau}{2\pi} M^{2} = \frac{\tau M}{2\pi} (8\pi - M).$$

Summing this identity over j = 1, ..., k and taking into account the choice of k gives

$$I_k = I_0 - \frac{k\tau M}{2\pi} (M - 8\pi) < 0,$$

which is a contradiction to $n_k \ge 0$.

Next, let $\alpha > 0$. For the proof, we follow the lines of [10, Section 6] but the end of the proof is different. Let $n_k \ge 0$ be a weak solution to (5) such that (18) is not true. Similarly as above, we find that

$$I_k - I_{k-1} = 4\tau \int_{\mathbb{R}^2} n_k dx + 2\tau \int_{\mathbb{R}^2} n_k (\nabla B_\alpha * n_k) \cdot x dx$$

(19)
$$= 4\tau M - \frac{\tau}{2\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} g_\alpha(|x-y|) n_k(x) n_k(y) dy dx$$
$$= \frac{\tau M}{2\pi} (8\pi - M) + \frac{\tau}{2\pi} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} \left(1 - g_\alpha(|x-y|)\right) n_k(x) n_k(y) dy dx,$$

where we recall definition (7) of g_{α} .

We need to estimate $1 - g_{\alpha}(r)$. For this, let $z \in \mathbb{R}^2$, $r = |z| \in (0, 1/\sqrt{\alpha})$. We compute

$$\frac{d}{dr}(1-g_{\alpha}(r)) = \frac{\alpha r}{2} \int_0^\infty \frac{1}{s} e^{-s-\alpha r^2/(4s)} ds = 2\pi \alpha |z| B_1(\sqrt{\alpha}z) \le \sqrt{\alpha}K,$$

where $K = 2\pi \sup_{|x|<1} |x| B_1(|x|)$. It is known that $B_1(x)$ behaves asymptotically as $-\log |x|$ as $|x| \to 0$, so K is finite. A numerical computation shows that $\sup_{|x|<1} |x| B_1(|x|) \approx 0.0742$ and $K \approx 0.4662$. We conclude that

$$0 \le 1 - g_{\alpha}(|z|) \le \sqrt{\alpha}K|z| \quad \text{for } 0 < \sqrt{\alpha}|z| < 1.$$

This bound, together with $1 - g_{\alpha}(|z|) \leq 1$, shows that the last integral in (19) can be estimated as follows:

(20)

$$\frac{\tau}{2\pi} \int \int_{\{\sqrt{\alpha}|x-y|<1\}} \left(1 - g_{\alpha}(|x-y|)\right) n_{k}(x) n_{k}(y) dy dx \\
+ \frac{\tau}{2\pi} \int \int_{\{\sqrt{\alpha}|x-y|\geq1\}} \left(1 - g_{\alpha}(|x-y|)\right) n_{k}(x) n_{k}(y) dy dx \\
\leq \tau \frac{\sqrt{\alpha}}{2\pi} \max\{1, K\} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} |x-y| n_{k}(x) n_{k}(y) dy dx \\
\leq \tau \frac{\sqrt{\alpha}}{\pi} M \int_{\mathbb{R}^{2}} |y| n_{k}(y) dy \leq \tau \frac{\sqrt{\alpha}}{\pi} M^{3/2} I_{k}^{1/2},$$

where we have applied the Cauchy-Schwarz inequality in the last step. We infer from (19) that

$$I_k - I_{k-1} \le \frac{\tau}{2\pi} M(8\pi - M) + \tau \frac{\sqrt{\alpha}}{\pi} M^{3/2} I_k^{1/2}.$$

Now, the argument differs from that one used in [10]. Set $\beta = \sqrt{\alpha} M^{3/2} / \pi$ and $\gamma = M(M - 8\pi)/(2\pi)$. Then we need to solve the recursive inequality

(21)
$$I_k - I_{k-1} \le \tau f(I_k) := \tau \left(\beta I_k^{1/2} - \gamma\right).$$

By definition of I^* , we have $f(I^*) = 0$. Since f is increasing and $I_0 \leq I^*$, it holds that $f(I_0) \leq 0$. We proceed by induction. Let $f(I_{k-1}) \leq 0$. We suppose that $f(I_k) > 0$ and show that this leads to a contradiction. Inequality (21) is equivalent to

$$\frac{I_k^{1/2} - I_{k-1}^{1/2}}{I_k^{1/2} - \gamma/\beta} \frac{I_k^{1/2} + I_{k-1}^{1/2}}{\beta} \le \tau,$$

Since $f(I_{k-1}) \leq 0$, the first factor is larger than or equal to one, and taking into account $f(I_k) > 0$ or $I_k^{1/2} > \gamma/\beta$, we deduce that

$$\frac{\gamma}{\beta^2} < \frac{I_k^{1/2}}{\beta} \le \frac{I_k^{1/2} + I_{k-1}^{1/2}}{\beta} \le \tau,$$

which contradicts the smallness condition $\tau < \tau^* = \gamma/\beta^2$. We infer that $f(I_k) \leq 0$.

Then, summing (21) from $k = 1, \ldots, j$,

$$I_j \le I_0 + \tau \sum_{k=1}^j f(I_k) \le I_0 + \tau j f(I_0)$$

We deduce that I_j becomes negative for $j > -I_0/(\tau f(I_0))$ which contradicts $n_k \ge 0$. This completes the proof.

Remark 3 (Semi-discrete energy dissipation). It is possible to design semi-discrete schemes that dissipate the discrete free energy

$$E_k = \int_{\mathbb{R}^2} \left(n_k (\log n_k - 1) - \frac{1}{2} c_k n_k \right) dx$$

(and conserve the mass and preserve the positivity). An example, taken from [40], is the semi-implicit scheme

(22)
$$\tau^{-1}(n_k - n_{k-1}) = \operatorname{div}(n_k - n_k \nabla c_{k-1}), \quad -\Delta c_{k-1} + \alpha c_{k-1} = n_{k-1} \quad \text{in } \mathbb{R}^2.$$

Indeed, by the convexity of $s \mapsto s \log s$, we obtain

$$\int_{\mathbb{R}^2} \left(n_k (\log n_k - 1) - n_{k-1} (\log n_{k-1} - 1) \right) dx$$

$$\leq \int_{\mathbb{R}^2} (n_k - n_{k-1}) \log n_k dx = \tau \int_{\mathbb{R}^2} \left(-\frac{|\nabla n_k|^2}{n_k} + \nabla c_{k-1} \cdot \nabla n_k \right) dx.$$

Furthermore, translating the computation in [36, Section 5.2.1] to the semi-discrete case,

$$\frac{1}{2} \int_{\mathbb{R}^2} (n_k c_k - n_{k-1} c_{k-1}) dx = \frac{1}{2} \int_{\mathbb{R}^2} \left((n_k - n_{k-1}) c_k + n_{k-1} (c_k - c_{k-1}) \right) dx$$
$$= \frac{1}{2} \int_{\mathbb{R}^2} \left((n_k - n_{k-1}) c_k + \left(-\Delta (c_k - c_{k-1}) + \alpha (c_k - c_{k-1}) \right) c_{k-1} \right) dx$$
$$= \int_{\mathbb{R}^2} (n_k - n_{k-1}) c_{k-1} dx = -\tau \int_{\mathbb{R}^2} \left(\nabla n_k \cdot \nabla c_{k-1} + n_k |\nabla c_{k-1}|^2 \right) dx.$$

Subtracting the latter from the former expression, we conclude that

$$E_k - E_{k-1} \le -\tau \int_{\mathbb{R}^2} n_k |\nabla(\log n_k - c_{k-1})|^2 dx \le 0.$$

Unfortunately, scheme (22) does not allow us to apply the symmetrization argument used in the proof of Theorem 2, since the drift part depends on two different time steps. The question whether (22) admits solutions that blow up in finite time remains open. \Box

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3. Higher-order schemes

We investigate BDF and general Runge-Kutta schemes.

3.1. **BDF-2 scheme.** The scheme reads as

(23)
$$\frac{1}{\tau} \left(\frac{3}{2} n_k - 2n_{k-1} + \frac{1}{2} n_{k-2} \right) = \operatorname{div} \left(\nabla n_k - n_k (\nabla B_\alpha * n_k) \right) \quad \text{in } \mathbb{R}^2$$

for $k \geq 2$, where n_0 is given and n_1 is computed from n_0 using the implicit Euler scheme.

Lemma 4 (Existence for the BDF-2 scheme). Let $\alpha \geq 0$, n_{k-2} , $n_{k-1} \in L^1(\mathbb{R}^2) \cap L^{\infty}(\mathbb{R}^2)$, and

$$\tau \le \frac{3}{2} \frac{1}{(\pi + 1/2)^2} \frac{1}{(1 + \|2n_{k-1} - \frac{1}{2}n_{k-2}\|_X)^4}.$$

Then there exists a weak solution $n_k \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ to (23) with the following properties:

- conservation of mass: ∫_{ℝ²} n_kdx = ∫_{ℝ²} n_{k-1}dx,
 control of second moment: if ∫_{ℝ²} n_{k-1}|x|²dx < ∞ then ∫_{ℝ²} n_k|x|²dx < ∞.

Proof. The proof is exactly as for Theorem 1 since we can formulate scheme (23) as

$$-\Delta n_k + \frac{3}{2\tau} n_k = \frac{1}{\tau} \left(2n_{k-1} - \frac{1}{2} n_{k-2} \right) - \operatorname{div}(n_k \nabla B_\alpha * n_k),$$

and the first term on the right-hand side plays the role of n_{k-1} in the implicit Euler scheme. The only difference to the proof of Theorem 1 is that we replace n_k^+ in (6) by n_k , since the truncation was only needed to show the nonnegativity of n_k , which we are not able to show for the BDF-2 scheme.

Theorem 5 (Blow-up for the BFD-2 scheme). Assume that $\alpha \geq 0$ and

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi.$$

Let $(n_k) \subset L^1(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ be a sequence of nonnegative weak solutions to (23). Then this sequence is finite with maximal index k_{max} , where k_{max} is bounded from above according to (17) (if $\alpha = 0$) or (18) (if $\alpha > 0$ and additionally $I_0 \leq I^*$ and $\tau \leq \tau^*$, where I^* and τ^* are defined in (16)).

Proof. The proof is similar to that one of Theorem 2 but the iteration argument is different. First, let $\alpha = 0$. We know from the proof of Theorem 2 that

$$(24) I_1 - I_0 = -\tau\gamma,$$

where we recall that $\gamma = M(M - 8\pi)/(2\pi)$. Using the same approximation of $|x|^2$ as in step 5 of the proof of Theorem 2, we can justify the weak formulation (see (15))

$$\int_{\mathbb{R}^2} (n_j - n_{j-1}) |x|^2 dx = \frac{1}{3} \int_{\mathbb{R}^2} (n_{j-1} - n_{j-2}) |x|^2 dx + \frac{8}{3} \tau \int_{\mathbb{R}^2} n_j dx$$

$$+\frac{2}{3}\tau\int_{\mathbb{R}^2}n_k(\nabla B_\alpha*n_k)\cdot xdx.$$

The last integral can be calculated as in the proof of Theorem 2 and we end up with

$$I_k - I_{k-1} = \frac{1}{3}(I_{k-1} - I_{k-2}) + \frac{2}{3}\frac{\tau}{2\pi}M(8\pi - M).$$

We iterate this identity and insert (24):

$$I_k - I_{k-1} = \frac{1}{3^{k-1}}(I_1 - I_0) - \frac{2}{3}\tau\gamma \sum_{j=1}^{k-1} \frac{1}{3^j} = -\frac{\tau\gamma}{3^{k-1}} - \tau\gamma \left(1 - \frac{1}{3^{k-1}}\right) = -\tau\gamma.$$

As in the proof of Theorem 2, this leads to a contradiction for large values of k.

Next, let $\alpha > 0$. As the first step is computed with the implicit Euler scheme, the proof of Theorem 2 gives the estimate

$$I_1 - I_0 \le \tau f(I_1),$$

where $f(s) = \beta \sqrt{s} - \gamma$ and $\beta = \sqrt{\alpha} M^{3/2} / \pi$. Moreover, since $f(I_0) \leq 0$, we know that $I_1 \leq I_0$, and this gives $f(I_1) \leq 0$.

For the following time steps, we obtain

(25)
$$I_k - I_{k-1} \le \frac{1}{3}(I_{k-1} - I_{k-2}) + \frac{2\tau}{3}f(I_k), \quad k \ge 2$$

Let us assume, by induction, that $I_{k-1} \leq I_{k-2}$ and $f(I_{k-1}) \leq 0$ for $k \geq 2$. We will prove that $I_k \leq I_{k-1}$ and $f(I_k) \leq 0$. Assume by contradiction that $f(I_k) > 0$, which is equivalent to $I_k^{1/2} > \gamma/\beta$. Then, using $I_{k-1} - I_{k-2} \leq 0$, we reformulate (25) as

$$\frac{I_k^{1/2} - I_{k-1}^{1/2}}{I_k^{1/2} - \gamma/\beta} \frac{I_k^{1/2} + I_{k-1}^{1/2}}{\beta} \le \frac{2\tau}{3}.$$

Since $f(I_{k-1}) \leq 0$, the first factor is larger than or equal to one, so

$$\frac{I_k^{1/2} + I_{k-1}^{1/2}}{\beta} \le \frac{2\tau}{3},$$

and $\tau \leq \gamma/\beta^2$ leads to

$$\frac{I_k^{1/2}}{\beta} \le \frac{I_k^{1/2} + I_{k-1}^{1/2}}{\beta} \le \frac{2\tau}{3} \le \frac{2}{3}\frac{\gamma}{\beta^2}$$

or $I_k^{1/2} < \gamma/\beta$, which contradicts $f(I_k) > 0$. We conclude that $f(I_k) \le 0$ and therefore, by (25), $I_k \le I_{k-1} \le 0$, showing the claim.

We infer that $f(I_k) \leq f(I_{k-1}) \leq \cdots \leq f(I_0)$, since f is nondecreasing. Hence, again from (25) and using $I_1 - I_0 \leq \tau f(I_0)$,

$$I_{k} - I_{k-1} \le \frac{1}{3}(I_{k-1} - I_{k-2}) + \frac{2\tau}{3}f(I_{0}) \le \frac{1}{3^{k-1}}(I_{1} - I_{0}) + 2\tau \sum_{j=1}^{k-1} \frac{1}{3^{j}}f(I_{0})$$

$$\leq \frac{\tau}{3^{k-1}}f(I_0) + \tau \left(1 - \frac{1}{3^{k-1}}\right)f(I_0) = \tau f(I_0).$$

Thus, $I_k \leq I_0 + \tau \sum_{j=1}^k f(I_0) = I_0 + \tau k f(I_0)$, and this leads to the contradiction $I_k < 0$ for sufficiently large $k \in \mathbb{N}$, completing the proof.

3.2. **BDF-3 scheme.** The finite-time blow-up can be also shown for solutions to higherorder BDF schemes, at least in the case $\alpha = 0$. As an example, let us consider the BDF-3 scheme

(26)
$$\frac{1}{6\tau}(11n_k - 18n_{k-1} + 9n_{k-2} - 2n_{k-3}) = \operatorname{div}(\nabla n_k - n_k \nabla B_0 * n_k) \quad \text{in } \mathbb{R}^2,$$

where n_{k-1} , n_{k-2} , and n_{k-3} are given. The existence of solutions can be shown as in Lemma 4. First, we prove that the scheme preserves the mass.

Lemma 6 (Conservation of mass). Let n_0 , n_1 , and n_2 be given and having the same mass M. Then the solution n_k has the same mass, $\int_{\mathbb{R}^2} n_k dx = M$, for $k \ge 3$.

Proof. We proceed by induction. Employing the mollified version of the cut-off function (13) as a test function in (26) and passing to the limits $\varepsilon \to 0$ and $R \to \infty$, we arrive at

$$\frac{1}{6\tau} \int_{\mathbb{R}^2} (11n_k - 18n_{k-1} + 9n_{k-2} - 2n_{k-3}) dx = 0$$

If k = 3, this is equivalent to

$$\int_{\mathbb{R}^2} n_3 dx = \int_{\mathbb{R}^2} \left(\frac{18}{11} n_2 - \frac{9}{11} n_1 + \frac{2}{11} n_0 \right) dx = M_1$$

since n_2 , n_1 , and n_0 have the same mass M. For the induction step, if n_{k-1} , n_{k-2} , and n_{k-3} for k > 4 have the same mass, the same argument as above shows that $\int_{\mathbb{R}^2} n_k = M$.

We recall that $I_k = \int_{\mathbb{R}^2} n_k |x|^2 dx$ for $k \in \mathbb{N}_0$ and $\gamma = M(M - 8\pi)/(2\pi)$.

Theorem 7 (Blow-up for the BDF-3 scheme). Assume that $\alpha = 0$, $I_2 - I_1 = I_1 - I_0 = -\tau \gamma$, and

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi.$$

Let $(n_k) \subset L^1(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ be a sequence of nonnegative weak solutions to (26). Then this sequence is finite with maximal index k_{\max} , where k_{\max} is bounded from above according to (17) (if $\alpha = 0$) or (18) (if $\alpha > 0$ and additionally $I_0 \leq I^*$ and $\tau \leq \tau^*$, where I^* and τ^* are defined in (16)).

Proof. We claim that $I_k - I_{k-1} = -\tau\gamma$. To prove this, we proceed by induction. Let k = 3. We take an approximation of $|x|^2$ as a test function in (26). Then, arguing as in the previous sections, we find that

$$\frac{11}{6}(I_3 - I_2) - \frac{7}{6}(I_2 - I_1) + \frac{1}{3}(I_1 - I_0) = \frac{1}{6}(11I_3 - 18I_2 + 9I_1 - 2I_0) = \frac{\tau}{2\pi}M(8\pi - M) = -\tau\gamma.$$

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Since $I_2 - I_1 = I_1 - I_0 = -\tau\gamma$, it follows that

$$\frac{11}{6}(I_3 - I_2) = -\frac{7}{6}\tau\gamma + \frac{1}{3}\tau\gamma - \tau\gamma = -\frac{11}{6}\tau\gamma$$

For the induction step, we assume that $I_{k-1} - I_{k-2} = I_{k-2} - I_{k-3} = -\tau\gamma$ for k > 3. Then, as above,

$$\frac{11}{6}(I_k - I_{k-1}) - \frac{7}{6}(I_{k-1} - I_{k-2}) + \frac{1}{3}(I_{k-2} - I_{k-3}) = -\tau\gamma.$$

which shows that $I_k - I_{k-1} = -\tau \gamma$. As in the proof of Theorem 2, this leads to a contradiction for large values of k.

The previous proof can be generalized to all BDF-m methods

$$\frac{1}{\tau} \sum_{i=0}^{m} a_i n_{k-i} = \operatorname{div}(\nabla n_k - \nabla B_\alpha * n_k),$$

where $a_i \in \mathbb{R}$ satisfy $\sum_{i=0}^{m} a_i = 1$. Note, however, that only the BDF-*m* schemes with $m \leq 6$ are $A(\alpha)$ -stable, while they are instable for m > 6.

3.3. Runge-Kutta schemes. The Runge-Kutta scheme reads as follows:

(27)
$$\frac{1}{\tau}(n_k - n_{k-1}) = \sum_{i=1}^s b_i K_i, \quad K_i = \operatorname{div}(\nabla m_i - m_i \nabla B_\alpha * m_i),$$
$$m_i = n_{k-1} + \tau \sum_{j=1}^s a_{ij} K_j, \quad i = 1, \dots, s,$$

where $s \in \mathbb{N}$ is the number of stages, $b_i \geq 0$ are the weights, and a_{ij} are the Runge-Kutta coefficients. We assume that $\sum_{i=1}^{s} b_i = 1$. The existence of solutions is only shown for two particular Runge-Kutta schemes; see below.

First, we claim that the mass is conserved in the following sense.

Lemma 8 (Conservation of mass). Let $n_k \in L^1(\mathbb{R}^2)$ be a solution to (27) such that $m_i \in L^1(\mathbb{R}^2)$ and

$$\frac{1}{\tau} \int_{\mathbb{R}^2} (n_k - n_{k-1})\phi dx = \sum_{i=1}^s \int_{\mathbb{R}^2} b_i (m_i \Delta \phi + m(\nabla B_\alpha * m) \cdot \nabla \phi) dx$$

for all $\phi \in C_0^{\infty}(\mathbb{R}^2)$. Then

$$\int_{\mathbb{R}^2} m_i dx = \int_{\mathbb{R}^2} n_k dx = \int_{\mathbb{R}^2} n_{k-1} dx, \quad i = 1, \dots, s.$$

Note, however, that we do not know whether $m_i \ge 0$ in \mathbb{R}^2 . Although we expect physically that n_k is nonnegative, this cannot be generally expected for m_i .

Proof. Using the mollifier ρ^{ε} and the cut-of function $\phi_R(x) = \phi(|x|/R)$, where ϕ is defined in (13), as a test function in the weak formulation of the equation for K_i and performing the limit $\varepsilon \to 0$, we find that

$$\int_{\mathbb{R}^2} K_i \phi_R dx = \int_{\mathbb{R}^2} m_i \Delta \phi_R dx + \int_{\mathbb{R}^2} m_i (\nabla B_\alpha * m_i) \cdot \nabla \phi_R dx.$$

According to (14), the first term on the right-hand side can be estimated as

$$\left|\int_{\mathbb{R}^2} m_i \Delta \phi_R dx\right| \le \frac{C_2}{R^2} \|m_i\|_{L^1(\mathbb{R}^2)}.$$

For the second term, we use formulation (8) of ∇B_{α} , the symmetry argument, and the Lipschitz estimate (14) for $\nabla \phi_R$, which leads to

$$\left| \int_{\mathbb{R}^2} m_i(\nabla B_\alpha * m_i) \cdot \nabla \phi_R dx \right|$$

= $\frac{1}{2} \left| \int_{\mathbb{R}^2} m_i(x) \int_{\mathbb{R}^2} \left(\nabla \phi_R(x) - \nabla \phi_R(y) \right) \cdot \frac{x - y}{|x - y|} g_\alpha(|x - y|) m_i(y) dy dx \right|$
 $\leq \frac{C_1}{2R^2} \int_{\mathbb{R}^2} |m_i(x)| \int_{\mathbb{R}^2} |m_i(y)| dy dx = \frac{C_1}{2R^2} ||m_i||_{L^1(\mathbb{R}^2)}^2.$

We deduce that for $R \to \infty$, $\int_{\mathbb{R}^2} K_i dx = 0$. Hence,

$$\int_{\mathbb{R}^2} m_i dx = \int_{\mathbb{R}^2} n_{k-1} dx + \tau \sum_{j=1}^s a_{ij} \int_{\mathbb{R}^2} K_j dx = \int_{\mathbb{R}^2} n_{k-1} dx,$$
$$\int_{\mathbb{R}^2} n_k dx = \int_{\mathbb{R}^2} n_{k-1} + \tau \sum_{i=1}^s b_i \int_{\mathbb{R}^2} K_i dx = \int_{\mathbb{R}^2} n_{k-1} dx,$$

which concludes the proof.

We are able to show finite-time blow-up for all Runge-Kutta schemes if $\alpha = 0$.

Theorem 9 (Blow-up for Runge-Kutta schemes). Let $\alpha = 0$. Assume that

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi.$$

Let $(n_k) \subset L^1(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ be a sequence of nonnegative weak solutions to (27). Then this sequence is finite with maximal index k_{\max} defined in (17).

Proof. Using an approximation of $|x|^2$ as a test function in (27) and passing to the deregularization limit (see step 5 of the proof of Theorem 2), we find that

$$I_k - I_{k-1} = \tau \sum_{i=1}^s b_i \bigg(4 \int_{\mathbb{R}^2} m_i dx - \frac{1}{\pi} \int_{\mathbb{R}^2} m_i(x) \int_{\mathbb{R}^2} \frac{x \cdot (x-y)}{|x-y|^2} m_i(y) dy dx \bigg).$$

By Lemma 8, the symmetry argument, and $\sum_{i=1}^{s} b_i = 1$,

$$I_k - I_{k-1} = \tau \sum_{i=1}^s b_i \left(4M - \frac{1}{2\pi} \int_{\mathbb{R}^2} m_i(x) \int_{\mathbb{R}^2} m_i(y) dy dx \right)$$
$$= \tau \sum_{i=1}^s b_i \left(4M - \frac{M^2}{2\pi} \right) = \frac{M}{2\pi} (8\pi - M).$$

Now, we argue as in the proof of Theorem 2 to conclude.

The case $\alpha > 0$ is more delicate since $m_i \ge 0$ is generally not guaranteed. Indeed, it follows that (see (19) and (20))

$$I_{k} - I_{k-1} = \tau \sum_{i=1}^{s} b_{i} \left(\frac{M}{2\pi} (8\pi - M) + \frac{1}{2\pi} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} \left(1 - g_{\alpha}(|x - y|) \right) m_{i}(x) m_{i}(y) dy dx \right)$$

$$\leq \tau \sum_{i=1}^{s} b_{i} \left(-\gamma + \frac{\sqrt{\alpha}}{2\pi} M \int_{\mathbb{R}^{2}} |y| |m_{i}(y)| dy \right),$$

where we recall that $\gamma = M(M - 8\pi)/(2\pi)$. By the Cauchy-Schwarz inequality,

$$I_{k} - I_{k-1} \le \tau \sum_{i=1}^{s} b_{i} \bigg\{ -\gamma + \frac{\sqrt{\alpha}}{2\pi} M \bigg(\int_{\mathbb{R}^{2}} |m_{i}(y)| dy \bigg)^{1/2} \bigg(\int_{\mathbb{R}^{2}} |y|^{2} |m_{i}(y)| dy \bigg)^{1/2} \bigg\},$$

and this cannot be estimated further as $m_i \ge 0$ may not hold. However, for the midpoint and trapezoidal rule, we are able to give a result. The reason is that these schemes can be reformulated in terms of n_k , n_{k-1} , etc. without the use of m_i . Clearly, we still need to assume that $n_k \ge 0$ but this is expected physically.

Implicit midpoint rule. The implicit midpoint rule is defined by s = 1, $a_{11} = 1/2$, and $b_1 = 1$. Then (27) becomes

$$\frac{1}{\tau}(n_k - n_{k-1}) = \operatorname{div}(\nabla m_1 - m_1 \nabla B_\alpha * m_1),$$
$$m_1 = n_{k-1} + \frac{\tau}{2} \operatorname{div}(\nabla m_1 - m_1 \nabla B_\alpha * m_1),$$

and since $m_1 = \frac{1}{2}(n_k + n_{k-1})$, this can be rewritten as

(28)
$$\frac{1}{\tau}(n_k - n_{k-1}) = \operatorname{div}\left(\nabla\left(\frac{n_k + n_{k-1}}{2}\right) - \frac{n_k + n_{k-1}}{2}\nabla B_{\alpha} * \frac{n_k + n_{k-1}}{2}\right).$$

Lemma 10 (Existence for the midpoint scheme). Let $\alpha \ge 0$, $n_{k-1} \in W^{1,1}(\mathbb{R}^2) \cap W^{1,\infty}(\mathbb{R}^2)$, and

$$\tau \leq \frac{2}{(\pi + \frac{1}{2})^2} \frac{1}{(\|n_{k-1}\|_X + \frac{\pi b}{2}\|n_{k-1}\|_X^2 + \frac{\pi}{2}\|\nabla n_{k-1}\|_X + 1)^4}.$$

Then there exists a unique weak solution $n_k \in L^1(\mathbb{R}^2) \cap L^\infty(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ to (28) with the following properties:

• conservation of mass: $\int_{\mathbb{R}^2} n_k dx = \int_{\mathbb{R}^2} n_{k-1} dx$,

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• control of second moment: if $\int_{\mathbb{R}^2} n_{k-1} |x|^2 dx < \infty$ then $\int_{\mathbb{R}^2} n_k |x|^2 dx < \infty$. Moreover, if $\alpha > 0$ and $n_{k-1} \in Y := W^{1,1}(\mathbb{R}^2) \cap W^{1,\infty}(\mathbb{R}^2) \cap H^3(\mathbb{R}^2)$, then $n_k \in Y$.

Note that our technique of proof requires higher regularity for n_{k-1} compared to the implicit Euler scheme. For general Runge-Kutta schemes, the regularity requirement becomes even stronger, which is the reason why we show existence results only in special cases.

Proof. We set $n := n_k$ and $n_0 := n_{k-1}$. For given $\tilde{n} \in X$, we solve the linear problem

$$\left(-\Delta + \frac{2}{\tau}\right)n = \frac{2}{\tau}n_0 + \operatorname{div}\left(\nabla n_0 - \frac{1}{2}(\widetilde{n} + n_0)\nabla B_\alpha * (\widetilde{n} + n_0)\right) \quad \text{in } \mathbb{R}^2.$$

By Lemma 16, this problem has a unique solution $n \in H^1(\mathbb{R}^2)$, and it can be represented by

(29)
$$T[\tilde{n}] := n = \frac{2}{\tau} B_{2/\tau} * n_0 + \nabla B_{2/\tau} * \nabla n_0 - \frac{1}{2} \nabla B_{2/\tau} * \left((\tilde{n} + n_0) \nabla c[\tilde{n} + n_0] \right),$$

writing $\nabla c[n] = \nabla B_{\alpha} * n$ as in section 2. This defines the fixed-point operator $T: S \to S$, where $S = \{n \in X : ||n||_X \leq C_B\}$ and

$$C_B = \|n_0\|_X + \frac{\pi b}{2} \|n_0\|_X^2 + \frac{\pi}{2} \|\nabla n_0\|_X + 1.$$

It holds $T(S) \subset S$ since, using similar arguments as in the proof of Theorem 1 and the smallness condition on τ ,

$$\|T[n]\|_{X} \leq \frac{2}{\tau} \|B_{2/\tau}\|_{L^{1}(\mathbb{R}^{2})} \|n_{0}\|_{X} + \|\nabla B_{2/\tau}\|_{L^{1}(\mathbb{R}^{2})} \|\nabla n_{0}\|_{X} + \frac{1}{2} \|\nabla B_{2/\tau}\|_{L^{1}(\mathbb{R}^{2})} \|n+n_{0}\|_{X} \|\nabla c[n+n_{0}]\|_{X} \leq \|n_{0}\|_{X} + \frac{\pi\sqrt{\tau}}{2\sqrt{2}} \|\nabla n_{0}\|_{X} + \frac{\pi b\sqrt{\tau}}{4\sqrt{2}} \|n+n_{0}\|_{X}^{2} \leq C_{B}.$$

We claim that $T: S \to S$ is a contraction. Indeed, let $n, m \in S$. Then

$$\begin{aligned} \|T[n] - T[m]\|_{X} &\leq \frac{1}{2} \left\| \nabla B_{2/\tau} * (n+n_{0}) \nabla B_{\alpha} * (n+n_{0}) - \nabla B_{2/\tau} * (m+n_{0}) \nabla B_{\alpha} * (m+n_{0}) \right\|_{X} \\ &\leq \frac{\pi \sqrt{\tau}}{4\sqrt{2}} \| (n+n_{0}) \nabla B_{\alpha} * (n+n_{0}) - (m+n_{0}) \nabla B_{\alpha} * (m+n_{0}) \|_{X} \\ &\leq \frac{\pi \sqrt{\tau}}{4\sqrt{2}} \Big(\|n \nabla B_{\alpha} * n - m \nabla B_{\alpha} * m\|_{X} \\ &+ \|n_{0} \nabla B_{\alpha} * (n-m)\|_{X} + \|(n-m) \nabla B_{\alpha} * n_{0}\|_{X} \Big) \end{aligned}$$

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$$\leq \frac{\pi b \sqrt{\tau}}{\sqrt{2}} (C_B + 1) \|n - m\|_X,$$

and we have $\pi b \sqrt{\tau} (C_B + 1)/2 < 1$. The Banach fixed-point theorem now implies that there exists a unique fixed point $n \in X$.

By the same arguments used in step 2 of the proof of Theorem 1, we infer that $n_k \in H^1(\mathbb{R}^2)$. Steps 4 and 5 show the conservation of mass and the finiteness of the second moment.

It remains to show that if $n_{k-1} \in Y$ then n_k has the same regularity. By Lemma 14, $n_k \in H^1(\mathbb{R}^2)$ implies that $\nabla B_{\alpha} * n_k \in H^2(\mathbb{R}^2)$. Therefore,

$$\left(-\Delta + \frac{2}{\tau}\right)n_k = \frac{2}{\tau}n_{k-1} + \Delta n_{k-1} - \operatorname{div}\left((n_k + n_{k-1})\nabla c[n_k]\right) \in L^2(\mathbb{R}^2).$$

Elliptic regularity then gives $n_k \in H^2(\mathbb{R}^2)$. We bootstrap this argument to find that $n_k \in H^3(\mathbb{R}^2) \hookrightarrow W^{1,\infty}(\mathbb{R}^2)$. Taking the L^1 norm of the gradient of $n = n_k$ in (29) shows that $\|\nabla n_k\|_{L^1(\mathbb{R}^2)}$ can be estimated in terms of the H^3 norms of n_k , n_{k-1} , and $c[n_k]$. We conclude that $n_k \in W^{1,1}(\mathbb{R}^2)$, finishing the proof.

Lemma 11 (Blow-up for the midpoint scheme). Let $\alpha > 0$. Assume that

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi.$$

Let $(n_k) \subset L^1(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ be a sequence of nonnegative weak solutions to (28). Suppose that $I_0 \leq I^*$ and $\tau \leq 2\tau^*$ (see (16)). Then this sequence is finite with maximal index k_{\max} defined in (18).

Proof. Approximating $|x|^2$ as in step 5 of the proof of Theorem 2 and using the nonnegativity of n_k and n_{k-1} , we can estimate as

$$\begin{split} I_{k} - I_{k-1} &= \int_{\mathbb{R}^{2}} (n_{k} - n_{k-1}) |x|^{2} dx \\ &= 4\tau M - \frac{\tau}{2} \int_{\mathbb{R}^{2}} (n_{k} + n_{k-1}) \nabla B_{\alpha} * (n_{k} + n_{k-1}) dx \\ &= -\tau \gamma + \frac{\tau}{4\pi} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} \left(1 - g_{\alpha} (|x - y|) \right) (n_{k} + n_{k-1}) (x) (n_{k} + n_{k-1}) (y) dy dx \\ &\leq -\tau \gamma + \frac{\tau}{4\pi} \sqrt{\alpha} \int_{\mathbb{R}^{2}} \int_{\mathbb{R}^{2}} |x - y| (n_{k} + n_{k-1}) (x) (n_{k} + n_{k-1}) (y) dy dx \\ &\leq -\tau \gamma + \frac{\tau}{4\pi} \sqrt{\alpha} (2M) M^{1/2} \left(I_{k}^{1/2} + I_{k-1}^{1/2} \right) = -\tau \gamma + \frac{\beta}{2} \left(I_{k}^{1/2} + I_{k-1}^{1/2} \right). \end{split}$$

Setting again $f(s) = \beta \sqrt{s} - \gamma$, it follows that

$$I_k - I_{k-1} \le \frac{\tau}{2} (f(I_k) + f(I_{k-1})).$$

Again, since $f(I^*) = 0$ and f is increasing, we have $f(I_0) \leq 0$. Let $f(I_{k-1}) \leq 0$. Then

$$I_k - I_{k-1} \le \frac{\tau}{2} f(I_k),$$

and we can proceed as in the proof of Theorem 2.

Trapezoidal rule. The (implicit, two-stage) trapezoidal rule is defined by s = 2, $a_{11} = a_{12} = \frac{1}{2}$, $b_1 = b_2 = \frac{1}{2}$, which gives the scheme

(30)
$$\frac{1}{\tau}(n_k - n_{k-1}) = \frac{1}{2} \operatorname{div} \left(\nabla (n_k + n_{k-1}) + n_k \nabla B_\alpha * n_k + n_{k-1} \nabla B_\alpha * n_{k-1} \right).$$

The existence of weak solutions can be shown exactly as in the proof of Lemma 10, therefore we leave the details to the reader.

Proposition 12 (Finite-time blow-up for the trapezoidal rule). Let $\alpha > 0$. Assume that

$$n_0 \ge 0, \quad I_0 := \int_{\mathbb{R}^2} n_0(x) |x|^2 dx < \infty, \quad M := \int_{\mathbb{R}^2} n_0 dx > 8\pi.$$

Let (n_k) be a sequence of nonnegative weak solutions to (30). Suppose that $I_0 \leq I^*$ and $\tau \leq \tau^*$ (see (16)). Then this sequence is finite with maximal index k_{\max} defined in (18).

Proof. Arguing as in the previous blow-up proofs, we obtain

$$\begin{split} I_k - I_{k-1} &= 4\tau M - \frac{\tau}{2} \int_{\mathbb{R}^2} n_k \nabla B_\alpha * n_k dx - \frac{\tau}{2} \int_{\mathbb{R}^2} n_{k-1} \nabla B_\alpha * n_{k-1} dx \\ &\leq -\tau \gamma + \frac{\tau}{4\pi} \sqrt{\alpha} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |x - y| n_k(y) n_k(x) dy dx \\ &+ \frac{\tau}{4\pi} \sqrt{\alpha} \int_{\mathbb{R}^2} \int_{\mathbb{R}^2} |x - y| n_{k-1}(y) n_{k-1}(x) dy dx \\ &\leq -\tau \gamma + \frac{\tau}{4\pi} \sqrt{\alpha} M^{3/2} \left(I_k^{1/2} + I_{k-1}^{1/2} \right). \end{split}$$

Now, we proceed as in the proof of Proposition 11.

Remark 13 (Explicit schemes). One may ask to what extent explicit schemes may be considered too. The implicit Euler schemes provides the nonnegativity of the cell density n_k , which generally cannot be proven for the explicit Euler scheme. Clearly, we assumed nonnegativity of n_k for higher-order implicit schemes, so, this argument does not apply to higher-order explicit schemes. In fact, the virial argument can be applied to explicit Runge-Kutta schemes as well, with the same blow-up conditions (for $\alpha = 0$), since the analysis applies to *all* (explicit or implicit) Runge-Kutta schemes. On the other hand, BDF schemes are always implicit. Practically, implicit schemes help to handle the stiff part of the differential equation; recall, however, that there do not exist SSP *implicit* higher-order Runge-Kutta or multistep methods.

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4. Numerical examples

The numerical experiments are performed by using the finite-element method introduced by Saito in [37] and analyzed in [39]. In contrast to [37], we choose higher-order temporal approximations. The scheme uses a first-order upwind technique for the drift term, the lumped mass method, and a decoupling procedure. We take $\alpha = 1$ in (1) and consider bounded domains only. Equations (1) are supplemented with no-flux boundary conditions. In the first example, the domain is large enough to avoid effects arising from boundary conditions. The second example, on the other hand, illustrates blow-up at the boundary.

4.1. Numerical scheme. Let \mathcal{T}_h be a triangulation of the bounded set $\Omega \subset \mathbb{R}^2$, where $h = \max\{\operatorname{diam}(K) : K \in \mathcal{T}_h\}$, and let D_i be the barycentric domain associated with the vertex P_i ; see [37, Section 2] for the definition. Let χ_i be the characteristic function on D_i and let Y_h be the span of all χ_i . Furthermore, let X_h be the space of linear finite elements. The lumping operator $M_h : X_h \to Y_h$ is defined by $M_h v_h = \sum_i v_h(P_i)\chi_i$, where $v_h \in X_h$, and the mass-lumped inner product is given by

$$(v_v, w_h)_h = (M_h v_h, M_h w_h)_2, \quad v_h, w_h \in X_h,$$

where $(\cdot, \cdot)_2$ is the L^2 inner product.

For the discretization of the drift term, we define the discrete Green operator $G_h: X_h \to X_h$ as the unique solution $v_h = G_h f_h \in X_h$ to

$$(\nabla v_h, \nabla w_h)_2 + (v_h, w_h)_2 = (f_h, w_h)_2 \text{ for } w_h \in X_h$$

(Recall that $\alpha = 1$.) The drift term is approximated by the trilinear form $b_h : X_h^3 \to \mathbb{R}$,

$$b_h(u_h, v_h, w_h) = \sum_i w_h(P_i) \sum_{P_j \in \Lambda_i} \left(v_h(P_i) \beta_{ij}^+(u_h) - v_h(P_j) \beta_{ij}^-(u_h) \right),$$

where Λ_i is the set of vertices P_j that share an edge with P_i . For the definition of β_{ij}^{\pm} , we first introduce the set S_h^{ij} of all elements $K \in \mathcal{T}_h$ such that $P_i, P_j \in K$ and the exterior normal vector ν_{ij} to $\partial D_i \cap \partial D_j$ with respect to D_i . Then

$$\beta_{ij}^{\pm}(u_h) = \sum_{K \in S_h^{ij}} \operatorname{meas}\left((\partial D_i \cap \partial D_j) |_K \right) \left[(\nabla G_h u_h) |_K \cdot \nu_{ij} |_K \right]_{\pm},$$

where $[s]_{\pm} = \max\{0, \pm s\}$ for $s \in \mathbb{R}$. It is explained in [37] that the trilinear form approximates the integral $\int_{\Omega} v \nabla(Gu) \cdot \nabla w dx$, where Gu is the Green operator associated with $-\Delta + 1$ on L^2 .

Equation (2) is solved in a semi-implicit way. This means, for the BDF-2 scheme and for given u_h , that we solve the linear problem

(31)
$$\frac{1}{\tau} \left(\frac{3}{2} n_h^k - 2n_h^{k-1} + \frac{1}{2} n_h^{k-2}, w_h \right)_h + (\nabla n_h^k, \nabla w_h)_2 + b_h(u_h, n_h^k, w_h) = 0$$

for all $w_h \in X_h$. Here, n_h^k is an approximation of $n(\cdot, \tau k)$. This defines the solution operator $N(u_h) = n_h$ and the scheme is completed by choosing u_h . Saito has taken $u_h = n_h^{k-1}$, giving the usual semi-implicit scheme of first order. For higher-order schemes, we need to iterate.

For this, we introduce the iteration $u_h^{(0)} := n_h^{k-1}$ and $u_h^{(m)} := N(u_h^{(m-1)})$ for $m \ge 1$. The iteration stops when $\|u_h^{(m)} - u_h^{(m-1)}\|_{L^{\infty}(\mathbb{R}^2)} < \varepsilon$ for some tolerance $\varepsilon > 0$ or if $m \ge m_{\max}$ for a maximal number m_{\max} of iterations. For later reference, we write scheme (31) as

(32)
$$\frac{1}{\tau}M_h(3n_h^k - 4n_h^{k-1} + n_h^{k-2}) = 2(A_h + B_h(n_h^k))n_h^k,$$

where M_h is the lumped mass matrix, A_h the stiffness matrix, $B_h(n_h^k)$ the upwind matrix, and n_h^k is the solution vector at time step k after the Picard iteration has terminated.

In a similar way, we define the scheme with the midpoint discretization:

$$\frac{1}{\tau}(n_h^k - n_h^{k-1}, w_h)_h + \frac{1}{2}(\nabla(n_h^k + n_h^{k-1}), \nabla w_h)_2 + \frac{1}{4}b_h(u_h + n_{k-1}, n_h^k + n_h^{k-1}, w_h) = 0$$

for all $w_h \in X_h$. The resulting linear systems are computed by using MATLAB. We choose the domain $\Omega = (0, 1)^2$, which is triangulated uniformly by $2a^2$ triangles with maximal size $h = \sqrt{2}/a$. The numerical parameters are a = 64, $\tau = 5 \cdot 10^{-5}$, $\varepsilon = 10^{-4}$, and $m_{\text{max}} = 500$ if not stated otherwise. (In all presented simulations, the maximal number of iterations was m = 17, i.e., m_{max} was never reached.)

4.2. Numerical results. To illustrate the behavior of the solutions, we choose the initial data as a linear combination of the shifted Gaussians

$$W_{x_0,y_0}(x,y) = \frac{M}{2\pi\theta} \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{2\theta}\right),$$

where $(x_0, y_0) \in (0, 1)^2$, M > 0, and $\theta > 0$. Clearly, the mass of W_{x_0, y_0} equals M. For the first example, we choose $\theta = 1/500$, $M = 6\pi$, and

$$n_0 = W_{0.33,0.33} + W_{0.33,0.66} + W_{0.66,0.33} + W_{0.66,0.66}$$

The initial mass is $24\pi > 8\pi$ and thus, we expect the solutions to blow up in finite time.

Figure 1 shows the cell density n(x, t) at various time instances computed from the BDF-2 scheme. As expected, the solution blows up in finite time in the center of the domain. Note that the numerical solution is always nonnegative and conserve the total mass.

A nonsymmetric situation is given by the initial data

$$n_0 = \frac{1}{3}W_{0.33,0.66} + \frac{1}{2}W_{0.33,0.33} + W_{0.66,0.66},$$

taking $\theta = 1/500$, $M = 6\pi$, and the same numerical parameters as above. The total mass of n_0 is 11π , so we expect again blow up of the solutions. This is illustrated in Figure 2. The solution aggregates, moves to the boundary and blows up. Again, the discrete solution stays nonnegative and conserves the mass.

We remark that boundary blow-up was analyzed in [41]; also see the presentation in [46, Theorem 5.1]. The proof uses a localized symmetrization argument, which possibly can be extended to a semi-discrete implicit Euler scheme.

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FIGURE 1. Cell density computed from the BDF-2 scheme at times t = 0 (top left), t = 0.005 (top right), t = 0.007 (bottom left), t = 0.02 (bottom right).

4.3. Convergence rate. To calculate the temporal convergence rates and to show that the schemes are indeed of second order, we compute a reference solution n_{ref} with the very small time step $\tau = 10^{-6}$ and compare it in various L^p norms with the solutions n_{τ} using larger time step sizes τ . We choose the same initial datum as in the first example with $M = 24\pi$. Figure 3 shows the L^p error

$$e_p = \|n_\tau(\cdot, T) - n_{\mathrm{ref}}(\cdot, T)\|_{L^p(\Omega)}$$

where the end time T = 0.01 is chosen such that the density already started to aggregate but blow up still did not happen. As expected, the L^p errors are approximately of second order.

4.4. Numerical blow-up. We demonstrate that the bound for the blow-up time $T^* = \tau k_{\text{max}}$ derived in the time-discrete situation can serve as a bound for the numerical blow up. It is well known that the computation of the numerical blow-up time is rather delicate. For



FIGURE 2. Cell density computed from the BDF-2 scheme at times t = 0 (top left), t = 0.005 (top right), t = 0.02 (bottom left), t = 0.1001 (bottom right).

instance, Chertock et al. [15] use the L^{∞} norm of the density as a measure of the numerical blow-up time, since $||n||_{L^{\infty}(\Omega)}$ is proportional to h^2 (recall that h is the spatial grid size). Numerical blow-up may be reached, for instance, when the numerical solution becomes negative [14, 44] or when the second moment becomes negative [23]. However, since our scheme conserves the mass and the grid is finite, the numerical solution cannot blow up in the L^{∞} norm. Instead, the solution converges to a state where the mass concentrates at certain points and no further growth is possible. Moreover, the second moment cannot become negative, provided nonnegativity is preserved (also see below). A lower bound for the blow-up time was derived in, for instance, [19, Theorem 2.2] in two space dimensions (but with a nonexplicit bound) and in [11, Prop. 3.1] in three space dimensions.

For the numerical test, we choose the initial datum $n_0 = W_{1,1}$ on the domain $\Omega = (0, 2)^2$ with parameters $\theta = 1/500$, $M = 30\pi$, and $\tau = 10^{-5}$. The grid sizes are h = 0.02, 0.04, 0.08. The initial density and the density at k = 44 are displayed in Figure 4. The density almost does not change for time steps k > 44.



FIGURE 3. L^p error e_p for $p = 1, 2, 4, \infty$ at time T = 0.01 for various time step sizes $\tau_k = \tau$ (left: BDF-2 discretization; right: midpoint discretization).



FIGURE 4. Cell density at time step k = 0 (left) and $k = k_{\text{max}} = 44$. The mesh size is h = 0.02.

It seems that the solution to the fully discrete semi-implicit scheme exists numerically for all time. Saito observed in [38, p. 144] that his finite-element solution never blows up in finite time, and he argued that this is because of the preservation of the L^1 norm. Note that he employed scheme (31) with $u_h = n_h^{k-1}$, while we used a Picard iteration in order to achieve second-order convergence. In fact, the solution in Figure 4 (right) seems to be the steady state of the discrete nonlinear system (32). This is indicated by the behavior of the residuum $R_k = 2 ||A_h n_h^k + B_h(n_h^k) n_h^k||_{\ell^{\infty}}$, illustrated in Figure 5. The residuum tends to zero for increasing time steps k. This behavior is in contrast to the analytical results, where finite-time blow up occurs for *semi-discrete* solutions. Figure 6 illustrates the evolution of $||n_k||_{L^{\infty}(\Omega)}$ and I_k . The vertical line marks the bound k_{\max} from (18). We observe that the L^{∞} norm and the second moment reach a limit close to k_{\max} .



FIGURE 5. The residuum R_k for time steps 1 to 81 (left) and time steps 30 to 81 (right) versus time steps k.



FIGURE 6. L^{∞} norm $||n_k||_{L^{\infty}(\Omega)}$ (left) and second moment I_k (right) versus time. The vertical line marks the upper bound k_{\max} defined in (18).

For coarse meshes or large time steps, the numerical scheme may produce solutions with negative values. As an example, we take $\tau = 10^{-3}$ and h = 0.02 and choose an initial datum with steep gradients,

$$n_0(x,y) = \begin{cases} 250\pi & \text{for } \frac{1}{3} < x, y < \frac{2}{3}, \\ 0 & \text{else;} \end{cases}$$

see Figure 7 (top left). For small times, the solution becomes negative around the steep gradient, but the regions with negative values disappear for larger times. This is confirmed in the plot L^1 norm over time, where the L^1 norm is larger than the total mass in a certain time interval due to the negative values (note that $||n||_{L^1(\Omega)} \neq \int_{\Omega} ndx$ for functions $n: \Omega \to \mathbb{R}$). The total mass stays constant over time. It seems to be natural to obtain negative values, since higher-order in time schemes usually require a CFL-type condition to remain nonnegative [8]. However, after some time, the L^1 norm stabilizes and equals the total mass again.



FIGURE 7. Cell density computed from the BDF-2 scheme with a coarse mesh at times t = 0 (top left), t = 0.006 (top right), t = 0.021 (bottom left) and the L^1 norm of n_k (bottom right).

APPENDIX A. SOME AUXILIARY RESULTS

We recall that the function

$$B_{\alpha}(x) = \begin{cases} -\frac{1}{2\pi} \log |x| & \text{for } \alpha = 0, \\ \frac{1}{(4\pi)^{n/2}} \int_0^\infty t^{-n/2} e^{-\alpha t - |x|^2/(4t)} dt & \text{for } \alpha > 0, \end{cases}$$

defined for $x \in \mathbb{R}^n$, is called the Newton potential if $\alpha = 0$ and the Bessel potential if $\alpha \neq 0$. We need the following properties of the Bessel potential.

Lemma 14 (Bessel potential). Let $\alpha > 0$ and $k \in \mathbb{N}_0$. Then B_{α} is a fundamental solution of the operator $-\Delta + \alpha$. For given $f \in H^k(\mathbb{R}^n)$, the function $u = B_{\alpha} * f \in H^{k+2}(\mathbb{R}^n)$ solves

$$-\Delta u + \alpha u = f \quad in \ \mathbb{R}^n.$$

Furthermore, it holds that $D^{\beta}(B_{\alpha} * f) = B_{\alpha} * D^{\beta}f$ for all multi-indices $\beta \in \mathbb{N}^{n}$, $|\beta| \leq k$ and

(33)
$$B_{\alpha} \ge 0, \quad \|B_{\alpha}\|_{L^{1}(\mathbb{R}^{n})} = \frac{1}{\alpha}$$

(34)
$$\|\nabla B_{\alpha}\|_{L^{1}(\mathbb{R}^{n})} = \frac{C(n)}{\pi^{(n-1)/2}\alpha^{1/2}}, \quad \|\nabla B_{\alpha}\|_{L^{1}(\mathbb{R}^{2})} = \frac{\pi}{2\alpha^{1/2}},$$

where the constant C(n) > 0 only depends on n.

Proof. We only prove (34), since the other properties are standard; see, e.g., Theorem 1.7.1, Corollary 1.7.2, and Examples 12.5.8 in [27]. By Fubini's theorem and the substitution $u = x/\sqrt{4t}$, we find that

$$\begin{aligned} \|\nabla B_{\alpha}\|_{L^{1}(\mathbb{R}^{n})} &= \frac{1}{2(4t)^{n/2}} \int_{0}^{\infty} t^{n/2+1} e^{-\alpha t} \int_{\mathbb{R}^{n}} e^{-|x|^{2}/(4t)} |x| dx dt \\ &= \frac{1}{\pi^{n/2}} \int_{0}^{\infty} t^{-1/2} e^{-\alpha t} dt \int_{R^{n}} e^{-|u|^{2}} |u| du = \frac{1}{\pi^{(n-1)/2}} \alpha^{-1/2} C(n), \end{aligned}$$

where $C(n) = \int_{\mathbb{R}^n} e^{-|u|^2} |u| du$. In particular, when n = 2, we obtain

$$C(2) = \int_0^\infty \int_0^{2\pi} e^{-r^2} r^2 d\phi dr = \frac{\pi^{3/2}}{2},$$

ending the proof.

Lemma 15 (Young's inequality). Let $g \in L^q(\mathbb{R}^n)$, $h \in L^r(\mathbb{R}^n)$ for $1 \leq q, r \leq \infty$, and 1/q + 1/r = 1/p + 1. Then $g * h \in L^p(\mathbb{R}^n)$ and

$$||g * h||_{L^{p}(\mathbb{R}^{n})} \le ||g||_{L^{q}(\mathbb{R}^{n})} ||h||_{L^{r}(\mathbb{R}^{n})}$$

Lemma 16 (Elliptic problem). Let $\tau > 0$, $f \in L^2(\mathbb{R}^2)^2$, and $g \in L^2(\mathbb{R}^2)$. Then there exists a unique weak solution $n \in H^1(\mathbb{R}^2)$ to

(35)
$$-\Delta n + \tau^{-1}(n-g) = -\operatorname{div} f \quad in \mathbb{R}^2,$$

and this solution can be represented as

(36)
$$n = \frac{1}{\tau} B_{1/\tau} * g - \nabla B_{1/\tau} * f \quad in \ \mathbb{R}^2.$$

Equation (35) correspond to the implicit Euler discretization of a parabolic problem with n being the solution at the actual time step and g being the solution at the previous time step. Although the result is standard, we give proof for the sake of completeness.

Proof. Let $f_k \in C_0^{\infty}(\mathbb{R}^2)^2$ be such that $f_k \to f$ in $L^2(\mathbb{R}^2)^2$ as $k \to \infty$. By Lemma 14, there exists a unique solution $n_k \in H^1(\mathbb{R}^2)$ to

$$(37) \qquad -\Delta n_k + \tau^{-1} n_k = \tau^{-1} g - \operatorname{div} f_k,$$

and, by the variation-of-constants formula and integration by parts,

(38)
$$n_k(x) = \frac{1}{\tau} (B_{1/\tau} * g)(x) - \int_{\mathbb{R}^2} (\nabla B_{1/\tau})(x-y) \cdot f_k(y) dy.$$

Taking the test function $n_k - n_\ell$ in the difference of the weak formulations for n_k , n_ℓ corresponding to f_k , f_ℓ , respectively, it follows that

$$\begin{aligned} \|\nabla(n_k - n_\ell)\|_{L^2(\mathbb{R}^2)}^2 + \frac{1}{\tau} \|n_k - n_\ell\|_{L^2(\mathbb{R}^2)}^2 &= \int_{\mathbb{R}^2} (f_k - f_\ell) \cdot \nabla(n_k - n_\ell) dx \\ &\leq \frac{1}{2} \|f_k - f_\ell\|_{L^2(\mathbb{R}^2)}^2 + \frac{1}{2} \|\nabla(n_k - n_\ell)\|_{L^2(\mathbb{R}^2)}^2. \end{aligned}$$

Since (f_k) is a Cauchy sequence, (n_k) is a Cauchy sequence in $H^1(\mathbb{R}^2)$ and hence there exists a $\tilde{n} \in H^1(\mathbb{R}^2)$, such that $n_k \to \tilde{n}$ strongly in $H^1(\mathbb{R}^2)$ as $k \to \infty$. Therefore, we can perform the limit $k \to \infty$ in the weak formulation of (37) leading to (35).

It remains to show (36). Let $n = (1/\tau)B_{1/\tau} * g - \nabla B_{1/\tau} * f$. Then, by Lemma 15 and (38),

$$\begin{aligned} \|\widetilde{n} - n\|_{L^{2}(\mathbb{R}^{2})} &\leq \|\widetilde{n} - n_{k}\|_{L^{2}(\mathbb{R}^{2})} + \|n_{k} - n\|_{L^{2}(\mathbb{R}^{2})} \\ &\leq \|\widetilde{n} - n_{k}\|_{L^{2}(\mathbb{R}^{2})} + \|\nabla B_{1/\tau}\|_{L^{2}(\mathbb{R}^{2})} \|f_{k} - f\|_{L^{2}(\mathbb{R}^{2})}. \end{aligned}$$

The right-hand side can be made arbitrarily small by choosing k sufficiently large. This shows that $\tilde{n} = n$ in \mathbb{R}^2 .

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