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A finite volume scheme for the Patlak–Keller–Segel chemotaxis model

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Abstract A finite volume method is presented to discretize the Patlak–Keller–Segel (PKS) modeling chemosensitive movements. First, we prove existence and uniqueness of a numerical solution to the proposed scheme. Then, we give a priori estimates and establish a threshold on the initial mass, for which we show that the numerical approximation converges to the solution to the PKS system when the initial mass is lower than this threshold. Numerical simulations are performed to verify accuracy and the properties of the scheme. Finally, in the last section we investigate blow-up of the solution for large mass.

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1 Introduction

Chemotaxis is a process by which cells change their state of movement reacting to the presence of a chemical substance, approaching chemically favorable environments and avoiding unfavorable ones.

Different aspects of chemotactic motility, especially for the model organisms *Escherichia Coli*, have been studied in great detail. These cells have several extracellular helical thread-like structures called flagella. Each flagellum has a rotary motor at its base, which can rotate in a clockwise or counterclockwise direction. When individual flagella rotate counterclockwise, they assemble into a coherent rotating bundle, and this bundle propels the bacterium forward. These runs are terminated by tumbles, which are short episodes of erratic motion without net translation. Tumbles are caused by the disintegration of the flagellar bundle, which

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results from the reversal in the rotation direction of the individual flagella from counterclockwise to clockwise. After each tumble the bacterium moves in a new, almost random direction.

Another example is the *Dictyostelium* (amoebae), which has been extensively studied for its ability to climb gradients of cAMP, a signaling molecule involved in the development of the slug. Then, cells produce cAMP and interact themselves (adhesion) and with the spatial gradients of cAMP concentration (chemotaxis). The interplay of these processes causes the amoebae to spatially self-organize leading to the complex behavior of stream and mound formation, cell sorting and slug migration all without any change of parameters.

In the simple situation where we only consider cells and a chemical substance (the chemo-attractant), a model for the space and time evolution of the density $n = n(t, x)$ of cells and the chemical concentration $c = c(t, x)$ at time t and position $x \in \Omega \subset \mathbb{R}^2$ has been introduced by Patlak [22] and Keller and Segel [17] (PKS) and reads

$$\frac{\partial n}{\partial t} - \operatorname{div}(\nabla n - \chi\, n \nabla c) = 0, \quad x \in \Omega,\ t \in \mathbb{R}_+, \tag{1}$$

$$\frac{\partial c}{\partial t} - \Delta c = n - c, \quad x \in \Omega,\ t \in \mathbb{R}_+, \tag{2}$$

where Ω is assumed to be a convex, bounded and open set of $\mathbb{R}^2$, the chemotactic sensitivity function χ is constant with respect to the chemical concentration c. Concerning initial conditions, we choose

$$n(t = 0, x) = n^0(x), \;\; c(t = 0, x) = c^0(x); \quad x \in \Omega$$

and for boundary conditions, we will consider zero flux boundary conditions i.e.,

$$\nabla n \cdot \nu = \nabla c \cdot \nu = 0, \quad x \in \partial\Omega,\ t \in \mathbb{R}_+,$$

where ν is the unit normal to the boundary $\partial\Omega$.

A different version of the PKS model consists in replacing the Eq. (2) by an elliptic equation

$$-\Delta c = n - c, \quad x \in \Omega,\ t \in \mathbb{R}_+. \tag{3}$$

Before describing more precisely our results, let us recall that the PKS systems (1),(2) and (1),(3) have been the object of several studies recently. Briefly speaking, these models exhibit singular pattern formation, and in particular blow-up patterns. For the PKS parabolic model (1),(2), the density n of cells concentrates in the neighborhood of isolated points, these concentration regions becoming more and more narrow and ultimately leading to finite time point-wise blow-up. We refer to [12] for mathematical proofs for spherically symmetric solutions in a ball, the blow-up point being the center of the ball (and these are the only possible singularities). In the nonsymmetric case blow-up results are established in [14,15], the blow-up points being located on the boundary. Numerical evidence of this fact may be found in [19].

The purpose of this work is to present and study a numerical scheme for the PKS systems (1),(3) and to investigate numerically the occurrence of blow-up, when it takes place, and the time evolution behavior otherwise. Numerical methods have already been developed to solve (1),(3); see, e.g., [19] for finite element methods, [16] for finite difference methods, and the references therein. However, it seems that none of the above-mentioned numerical approaches have been studied theoretically to understand if they give the correct behavior of the solution when it is effectively smooth and when it blows-up. Indeed, as we will explain later, there exists a ratio on the initial mass, which determines if either the solution is smooth (when the mass is small enough) or it blows-up (when the mass is large enough). Then, we propose a fully implicit finite volume scheme to the PKS system and prove its convergence to the solution of the PKS system when the initial mass is small enough.

We now briefly outline the contents of the paper. In the next section, we introduce the numerical approximation of (1),(3) and state the convergence result for small density initial datum which we prove in Sects. 3 and 4. Two points are worth mentioning here. First, one difficulty in the analysis of the PKS model, is related to the existence of a threshold on the global mass $\int_\Omega n^0 \mathrm{d}x$ (in dimension 2) for which either there exist global solutions or solutions blow-up at finite time. At the discrete level, our approximation also enjoys a similar property and we prove the convergence of the approximation under a smallness condition on the initial mass. Secondly, an important step of the convergence proof is the derivation of uniform estimate on the density n. Indeed, we cannot directly find $L^\infty(\Omega)$ estimates, which are usually established for finite volume approximations of parabolic problems [7], since the main argument leading to global existence is based on the estimation of $L^p(\Omega)$ norms and standard interpolation techniques [11,23]. The final section is devoted to numerical simulations performed with the numerical scheme presented in Sect. 2. We investigate numerically the blow-up problem in a bounded domain.

2 Numerical scheme and main results

Before describing our numerical scheme and stating a convergence result, we first introduce some notations and assumptions and recall previous results on (1),(3). As already mentioned, we focus on the approximation of the boundary value problem (1),(3) with Neumann boundary conditions and assume that the initial datum n^0 satisfies:

$$n^0 \in L^2(\Omega) \quad \text{and} \quad n^0 \geq a^0 > 0 \quad \forall x \in \Omega. \tag{4}$$

Moreover, the initial density n^0 satisfies a smallness contition: there exists a constant $C_\Omega^{\mathrm{GNS}} > 0$ such that

$$C_\Omega^{\mathrm{GNS}}\, \chi\, \|n^0\|_{L^1(\Omega)} < 1,$$

where C_Ω^{GNS} represents the best constant in the Gagliardo–Nirenberg–Sobolev inequality

$$\|u - \overline{u}\|^2_{L^2(\Omega)} \;\leq\; C_\Omega^{\mathrm{GNS}}\, \|\nabla u\|^2_{L^1(\Omega)}; \quad u \in W^{1,1}(\Omega) \quad \overline{u} = \frac{1}{\mathrm{m}(\Omega)} \int_\Omega u(x)\,\mathrm{d}x.$$

As a consequence of [11], there is at least a couple of nonnegative function (n, c) satisfying

$$n \in \mathcal{C}([0,T]; L^2(\Omega)) \cap L^2(0,T; H^1(\Omega)), \quad c \in L^2((0,T); H^1(\Omega))$$

for each $T \in \mathbb{R}_+$ and (1), (3). Moreover, mass is conserved with respect to time,

$$\int_\Omega n(t,x)\,\mathrm{d}x = \int_\Omega n^0(x)\,\mathrm{d}x. \tag{5}$$

Now, we define the finite volume scheme to the problem (1), (3). An admissible mesh of Ω is given by a family $\mathcal{T}$ of control volumes (open and convex polygons in 2D), a family $\mathcal{E}$ of edges and a family of points $(x_K)_{K\in\mathcal{T}}$ which satisfy Definition 5.1 in [7]. It implies that the straight line between two neighboring centers of cells (x_K, x_L) is orthogonal to the edge $\sigma = K|L$. In the set of edges $\mathcal{E}$, we distinguish the interior edges $\sigma \in \mathcal{E}_{\mathrm{int}}$ and the boundary edges $\sigma \in \mathcal{E}_{\mathrm{ext}}$. For a control volume $K \in \mathcal{T}$, we denote by $\mathcal{E}_K$ the set of its edges, $\mathcal{E}_{\mathrm{int}} K$, the set of its interior edges, $\mathcal{E}_{\mathrm{ext}}, K$ the set of edges of K included in $\Gamma = \partial\Omega$.

In the sequel, we denote by d the distance in $\mathbb{R}^2$, m the measure in $\mathbb{R}^2$ or $\mathbb{R}$. We assume that the family of mesh considered satisfies the following regularity constraint: there exists $\xi > 0$ such that

$$d(x_K, \sigma) \;\geq\; \xi\, d(x_K, x_L), \quad \text{for } K \in \mathcal{T},\ \text{for } \sigma \in \mathcal{E}_{\mathrm{int}} K,\ \sigma = K|L. \tag{6}$$

The size of the mesh is defined by

$$\delta \;=\; \max_{K\in\mathcal{T}} (\mathrm{diam(K)})\,. \tag{7}$$

For all $\sigma \in \mathcal{E}$, we define the transmissibility coefficient:

$$\tau_\sigma = \begin{cases} \dfrac{m(\sigma)}{d(x_K, x_L)}, & \text{for } \sigma \in \mathcal{E}_{\mathrm{int}},\ \sigma = K|L, \\[2ex] \dfrac{m(\sigma)}{d(x_K, \sigma)}, & \text{for } \sigma \in \mathcal{E}_{\mathrm{ext}} K. \end{cases}$$

Next, $X(\mathcal{T})$ will be the set of functions from Ω to $\mathbb{R}$ which are constant over each control volume $K \in \mathcal{T}$.

We define the approximation $n^0_{\mathcal{T}}$ of the initial datum n^0 as usual by

$$n^0_{\mathcal{T}} = \sum_{K\in\mathcal{T}} n^0_K\, \mathbf{1}_K, \quad \text{with} \quad n^0_K = \frac{1}{m(K)} \int_K n^0(x)\,\mathrm{d}x\,,$$

where $\mathbf{1}_E$ denotes the characteristic function of the subset E of Ω. Finally, let $T \in \mathbb{R}_+$ be some final time, M_T the number of time iterations and put

$$\Delta t = \frac{T}{M_T}\,, \quad t^k = k\,\Delta t\,, \quad 0 \leq k \leq M_T\,.$$

Denoting by n_K^k an approximation of the mean value of $n(t^k)$ on K and by c_K^k an approximation of the mean value of $c(t^k)$ on K for $K \in \mathcal{T}$, the numerical scheme to be studied in this paper reads

$$m(K)\frac{n_K^{k+1}-n_K^k}{\Delta t} - \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dn_{K,\sigma}^{k+1} + \chi \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(Dc_{K,\sigma}^{k+1}\right)^+ n_K^{k+1} - \left(Dc_{K,\sigma}^{k+1}\right)^- n_L^{k+1}\right] = 0 \tag{8}$$

and

$$-\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc_{K,\sigma}^{k+1} = m(K)\left(n_K^{k+1} - c_K^{k+1}\right), \tag{9}$$

for all $K \in \mathcal{T}$ and $0 \le k \le M_T - 1$, where $v^+ = \max(v, 0)$, $v^- = \max(-v, 0)$ and

$$Dc_{K,\sigma}^k = \begin{cases} c_L^k - c_K^k, & \text{if } \sigma = K|L \in \mathcal{E}_{\mathrm{int},K}, \\ 0, & \text{if } \sigma \in \mathcal{E}_{\mathrm{ext},K}, \end{cases} \tag{10}$$

for all $K \in \mathcal{T}$ and $0 \le k \le M_T$.

Before stating some properties on the scheme (8)–(10), let us briefly comment on its derivation which relies obviously on a fully implicit Euler scheme for the time variable and on a finite volume approach for the volume variable (see, e.g., [7]). The implicit scheme allows here to establish $L^2(\Omega)$ estimates, which are not valid with explicit schemes (see Proposition 3.1 below). Under the condition (23), the solution (n_K^k, c_K^k) enjoys similar properties to (n, c) (see Propositions 3.1 and 3.2).

We next define the numerical approximation $(n_\mathcal{T}, c_\mathcal{T})$ of (n, c) by

$$n_\mathcal{T}(t,x) = \sum_{K\in\mathcal{T}} n_K^{k+1}\,\mathbf{1}_K(x), \quad c_\mathcal{T}(t,x) = \sum_{K\in\mathcal{T}} c_K^{k+1}\,\mathbf{1}_K(x); \quad t \in (t^k, t^{k+1}] \tag{11}$$

for $k \in \{0, \ldots, M_T - 1\}$. We also define an approximation of the gradient $Dc_\mathcal{T}$ (as well as $Dn_\mathcal{T}$) following [3]. For $K \in \mathcal{T}$ and $\sigma = K|L \in \mathcal{E}_K$ with common vertexes $(y_{K,L}^j)_{1\le j\le J}$, $(J \in \mathbb{N})$. Let T_σ (respectively $T_{K,\sigma}$, $\sigma \in \mathcal{E}_{\mathrm{ext},K}$) be the open and convex polygon built by taking the convex envelope of vertexes (x_K, x_L) (respectively x_K) and $(y_{K,L}^j)_{1\le j\le J}$. Then, the domain Ω can be decomposed as

$$\overline{\Omega} = \bigcup_{K\in\mathcal{T}} \left(\left(\cup_{\sigma\in\mathcal{E}_K} \overline{T}_\sigma\right) \cup \left(\cup_{\sigma\in\mathcal{E}_{\mathrm{ext},K}} \overline{T}_{K,\sigma}\right)\right).$$

The approximation of the gradient $Dc_\mathcal{T}$ is then given by

$$Dc_\mathcal{T}(t,x) = \begin{cases} \frac{m(\sigma)}{m(T_\sigma)}\, Dc_{K,\sigma}^{k+1}\, \nu_{K,\sigma} & \text{if } (t,x) \in (t^k, t^{k+1}] \times T_\sigma \text{ and } \sigma = K|L \\ \\ 0 & \text{if } (t,x) \in (t^k, t^{k+1}] \times T_{K,\sigma}, \end{cases} \tag{12}$$

for all $K \in \mathcal{T}$ and $0 \leq k \leq M_T - 1$, where $\nu_{K,\sigma}$ stands for the unit normal to σ outward from K.

Finally, for any function $u \in X(\mathcal{T})$ with zero flux boundary condition, we define the discrete $H^1(\Omega)$-norm

$$\|u\|_{1,\mathcal{T}}^2 := \sum_{K\in\mathcal{T}} m(K)|u_K|^2 + \sum_{\substack{\sigma\in\mathcal{E}_{\text{int}}\\ \sigma=K|L}} \tau_\sigma |u_L - u_K|^2.$$

We first establish an existence and uniqueness theorem for the numerical solution $(n_{\mathcal{T}}(t^k), c_{\mathcal{T}}(t^k))$, for all $k \geq 0$.

Theorem 2.1 *Assume that the following CFL condition*

$$\chi\, \Delta t\, \mathcal{D}_{\mathcal{T},1} < 1, \quad \textit{with} \quad \mathcal{D}_{\mathcal{T},1} := \frac{2\,||n^0||_{L^1(\Omega)}}{\min_{K\in\mathcal{T}}\{m(K)\}} \tag{13}$$

is fulfilled and that the initial datum n^0 satisfies (4)*. Then, there exists a unique solution $(n_{\mathcal{T}}, c_{\mathcal{T}})$ to the scheme* (8)–(10)*, which satisfies*

$$n_K^k \geq a^k := \frac{a^0}{(1+\mathcal{D}_{\mathcal{T},1}\,\chi\,\Delta t)^k} > 0 \quad \textit{and} \quad c_K^k \geq 0 \tag{14}$$

for all $k \geq 0$, $K \in \mathcal{T}$ and

$$\sum_{K\in\mathcal{T}} m(K)\, n_K^k = \sum_{K\in\mathcal{T}} m(K)\, n_K^0 = \|n^0\|_{L^1(\Omega)}. \tag{15}$$

Moreover, the numerical approximation of the chemical concentration $c_{\mathcal{T}}$ is such that

$$c_{\mathcal{T}}(t^k) \in \mathcal{H} := \left\{ u \in X(\mathcal{T});\ \sup_{K\in\mathcal{T}} \left| \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Du_{K,\sigma} \right| \leq 2\,||n^0||_{L^1(\Omega)};\ ||u||_{1,\mathcal{T}} \leq \mathcal{D}_{\mathcal{T},2} \right\} \tag{16}$$

with $\mathcal{D}_{\mathcal{T},2} := \frac{\|n^0\|_{L^1(\Omega)}}{\sqrt{\min_{K\in\mathcal{T}}\{m(K)\}}}$ *for all $k \geq 0$.*

Proof The proof is based on the application of the Brower fixed point theorem.

Let us proceed by induction on $k \in \{0, \ldots, M_T - 1\}$ and first consider the case $k = 0$. The assertions (14) and (15) are obvious in that case while (16) follows from a classical discrete $H^1(\Omega)$ estimate for a finite volume approximation to an elliptic equation (see [7, Chapt. 3])

$$||c_{\mathcal{T}}(t^0)||_{1,\mathcal{T}} \leq ||n_{\mathcal{T}}(t^0)||_{L^2(\Omega)} \leq \frac{\|n_{\mathcal{T}}(t^0)\|_{L^1(\Omega)}}{\sqrt{\min_{K\in\mathcal{T}}\{m(K)\}}} = D_{\mathcal{T},2}.$$

Thus, we have checked that Theorem 2.1 is valid for $k = 0$.

Assume now $k \in \{0, \ldots, M_T - 1\}$ such that the assertions (14)–(16) hold true. To prove the existence of a couple $(n_{\mathcal{T}}(t^{k+1}), c_{\mathcal{T}}(t^{k+1}))$, we will construct an application based on the linearization of the scheme (8)–(10). We first choose a nonnegative function c such that $c \in \mathcal{H}$ and solve the following linearized problem: we construct n^* using the linear scheme

$$m(K)\frac{n_K^\star - n_K^k}{\Delta t} - \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \, Dn^\star_{K,\sigma}$$
$$+ \chi \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(Dc_{K,\sigma}\right)^+ n_K^\star - \left(Dc_{K,\sigma}\right)^- n_L^\star\right] = 0.$$

We next compute $c^\star$ from $n^\star$ by solving the discrete Poisson equation

$$-\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \, Dc^\star_{K,\sigma} = m(K)\, \left(n_K^\star - c_K^\star\right), \tag{17}$$

for all $K \in \mathcal{T}$ supplemented by zero flux boundary conditions for (17) and (17).

On the one hand, using classical arguments on finite volume approximations for a parabolic equation [7, Chap. 4] and [3], we set $n^\star_{K_0} := \min_{K\in\mathcal{T}}\{n^\star_K\}$ and obtain

$$m(K_0)(n^\star_{K_0} - n^k_{K_0}) \geq -\chi \, \Delta t \sum_{\sigma\in\mathcal{E}_{K_0}} \tau_\sigma \, Dc_{K_0,\sigma} \, n^\star_{K_0}.$$

Under the CFL condition (13) and the assumption that $c \in \mathcal{H}$, we know that

$$\chi \, \Delta t \sum_{\sigma\in\mathcal{E}_{K_0}} \tau_{K_0,\sigma} \, Dc_{K_0,\sigma} < m(K_0)$$

and then using the assumption (14) on n^k, we deduce a lower bound on the density $n^\star$

$$n^\star_{K_0} \geq \frac{n^k_{K_0}}{1 + \chi \, \Delta t \, \mathcal{D}_{\mathcal{T},1}} \geq \frac{a^0}{(1 + \chi \, \Delta t \, \mathcal{D}_{\mathcal{T},1})^{k+1}} > 0, \tag{18}$$

which shows the assertion (14) for $n^\star$. On the other hand, using zero flux boundary conditions in (17), we easily obtain the mass conservation

$$\sum_{K\in\mathcal{T}} m(K)\, n^\star_K = \sum_{K\in\mathcal{T}} m(K)\, n^k_K = \|n^0\|_{L^1(\Omega)}. \tag{19}$$

Gathering (18) and (19), we get a $L^1(\Omega)$ estimate on $n^\star$.

Now, we turn on the estimates to $c^\star$. First, using Neumann boundary conditions on the discrete Poisson equation, we get by summing over $K \in \mathcal{T}$

$$\sum_{K\in\mathcal{T}} m(K)\, c^\star_K = \sum_{K\in\mathcal{T}} m(K)\, n^\star_K \leq ||n^0||_{L^1(\Omega)}. \tag{20}$$

Moreover, setting $c^\star_{K_0} = \min_{K\in\mathcal{T}}\left\{c^\star_K\right\}$, and using the scheme (17), we have

$$m(K_0)\,c^\star_{K_0} = \sum_{\sigma\in\mathcal{E}_{K_0}} \tau_\sigma\, Dc^\star_{K_0,\sigma} \;+\; m(K_0)\,n^\star_{K_0} \;\geq\; m(K_0)\,n^\star_{K_0} \;\geq\; 0, \tag{21}$$

which proves that $c^\star_K$ is nonnegative for all $K\in\mathcal{T}$.

Next, multiplying the scheme (17) by $c^\star_K$ and performing a discrete integration by part, we easily obtain the second estimate of (16)

$$\begin{aligned}\sum_{K\in\mathcal{T}} m(K)\,|c^\star_K|^2 + \sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_\mathcal{K}} \tau_\sigma\,|Dc^\star_{K,\sigma}|^2 \;&\leq\; \sum_{K\in\mathcal{T}} m(K)|n^\star_K|^2 \\ &\leq\; \frac{||n^\star||^2_{L^1(\Omega)}}{\min_{K\in\mathcal{T}}\{m(K)\}} \;\leq\; \mathcal{D}^2_{\mathcal{T},2}.\end{aligned} \tag{22}$$

Finally, from the scheme (17) and using the previous estimates (20) and (21) on $c^\star$, we get the first estimate of (16)

$$\left|\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc^\star_{K,\sigma}\right| \;\leq\; m(K)\;\left(|n^\star_K| + |c^\star_K|\right) \leq 2\,||n^0||_{L^1(\Omega)}.$$

Thus, following this algorithm we have defined an application $\mathcal{S}$, such that

$$\mathcal{S}\;:\;\begin{array}{l}\mathcal{H}\longrightarrow\mathcal{H}\\ c\;\;\longrightarrow c^\star = \mathcal{S}\,(c).\end{array}$$

Now, in order to apply the Brower fixed point theorem, it remains to prove that this application is continuous. We consider a sequence $(c^\alpha)_{\alpha\in\mathbb{N}}$ such that $c^\alpha\to c$ as α goes to infinity, we want to show that $(c^{\alpha\,\star})_{\alpha\in\mathbb{N}}$ converges to $c^\star$ as $\alpha\to\infty$ where $c^{\alpha\,\star} = \mathcal{S}(c^\alpha)$ and $c^\star = \mathcal{S}(c)$. Using the scheme (17), we first construct $n^{\alpha\,\star}$ (respectively $n^\star$) from c^α (respectively c) and then from the discrete scheme for the Poisson equation (17); we get $c^{\alpha\,\star}$ (respectively $c^\star$).

We first prove that $n^{\alpha\,\star} - n^\star \to 0$, as $\alpha\to\infty$. Indeed, denoting by $p^\star = n^{\alpha\,\star} - n^\star$, we have

$$\begin{aligned} m(K)\,p^\star_K = \Delta t \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma\,(p^\star_L - p^\star_K) \\ &- \chi\,\Delta t \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(Dc^\alpha_{K,\sigma}\right)^+\; p^\star_K - \left(Dc^\alpha_{K,\sigma}\right)^-\; p^\star_L\right] \\ &- \chi\,\Delta t \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(\left(Dc^\alpha_{K,\sigma}\right)^+ - \left(Dc_{K,\sigma}\right)^+\right)\, n^\star_K\right] \\ &+ \chi\,\Delta t \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(\left(Dc^\alpha_{K,\sigma}\right)^- - \left(Dc_{K,\sigma}\right)^-\right)\, n^\star_L\right].\end{aligned}$$

Thus, we multiply the latter equality by $\mathrm{sign}(p_K^\star)$ and sum over $K \in \mathcal{T}$ to get

$$\begin{aligned}\sum_{K\in\mathcal{T}} m(K)\,|p_K^\star| \le -\Delta t &\sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(|p_L^\star| - |p_K^\star|\right)\\ &- \chi\,\Delta t \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(\left(Dc^\alpha_{K,\sigma}\right)^+ |p_K^\star| - \left(Dc^\alpha_{K,\sigma}\right)^- |p_L^\star|\right)\\ &+ \chi\,\Delta t \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left\{\left|\left(Dc^\alpha_{K,\sigma}\right)^+ - \left(Dc_{K,\sigma}\right)^+\right| n_K^\star\right\}\\ &+ \chi\,\Delta t \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left\{\left|\left(Dc^\alpha_{K,\sigma}\right)^- - \left(Dc_{K,\sigma}\right)^-\right| n_L^\star\right\}.\end{aligned}$$

On the one hand, we use the following identity

$$\sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(|p_K^\star| - |p_L^\star|\right) = 0$$

to cancel the first term of the right-hand side of the latter inequality. On the other hand, since for $\sigma = K|L$, $\left(Dc^\alpha_{K,\sigma}\right) = -\left(Dc^\alpha_{L,\sigma}\right)$ we have $\left(Dc^\alpha_{L,\sigma}\right)^+ = \left(Dc^\alpha_{K,\sigma}\right)^-$, which yields

$$\begin{aligned}&\sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(\left(Dc^\alpha_{K,\sigma}\right)^+ |p_K^\star| - \left(Dc^\alpha_{K,\sigma}\right)^- |p_L^\star|\right)\\ &\quad= \frac{1}{2}\sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(\left(Dc^\alpha_{K,\sigma}\right)^+ |p_K^\star| - \left(Dc^\alpha_{K,\sigma}\right)^- |p_L^\star|\right)\\ &\quad= 0.\end{aligned}$$

Finally, using that $|a^+ - b^+| \le |a-b|$ and the Cauchy–Schwarz inequality, we only have

$$\sum_{K\in\mathcal{T}} m(K)\,|p_K^\star| \le \chi\,\Delta t \left(\sum_{K\in\mathcal{T}} |n_K^\star|^2\right)^{1/2} \left(\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \,|D(c^\alpha - c)_{K,\sigma}|^2\right)^{1/2}.$$

Since $n^\star$ is uniformly bounded with respect to α in $L^1(\Omega)$ (the mesh $\mathcal{T}$ is fixed here) and c^α converges to c, as α goes to infinity; we have proven that $n^{\alpha,\star}$ converges to $n^\star$, as α goes to infinity.

Now, using the numerical scheme (9) for the chemical concentrations $c^{k\,\star}$ and $c^\star$ with the source term $n^{\alpha\,\star}$ and $n^\star$, we easily show that

$$\sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \left(Dc^{\alpha\,\star}_{K,\sigma} - Dc^\star_{K,\sigma}\right) = m(K)\left[(n_K^{\alpha\,\star} - n_K^\star) - \left(c_K^{\alpha\,\star} - c_K^\star\right)\right].$$

From a classical discrete $H^1(\Omega)$ estimate and using that $n_K^{\alpha\star} - n_K^\star$ goes to zero as α goes to infinity, we easily prove that $c_K^{\alpha\star}$ converges to $c_K^\star$, as $\alpha \to \infty$ and then the application $\mathcal{S}$ is continuous.

Moreover, $\mathcal{H}$ is a convex, closed and bounded set of $X(\mathcal{T})$. Thus, applying the Brower fixed point, the application $\mathcal{S}$ admits a fixed point. We denote it by $c_{\mathcal{T}}(t^{k+1})$ and it satisfies (16). Finally, from $c_{\mathcal{T}}(t^{k+1})$, we construct $n_{\mathcal{T}}(t^{k+1})$ using the scheme (17) with $c = c_{\mathcal{T}}(t^{k+1})$ and easily check that it satisfies (14) and (15). Using the same strategy as for the continuity of $\mathcal{S}$, the uniqueness of the solution at each time step follows directly. □

Remark 2.1 The CFL condition given in (13) is unusual for a fully implicit scheme. However, it is only due to the lack of estimates we get on the linearized scheme (17)–(17). In fact, we only need that

$$\chi\,\Delta t \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc_{K,\sigma}^k < m(K); \quad K \in \mathcal{T}, \quad k \in \mathbb{N}. \tag{23}$$

Then, this CFL condition will be sensitively improved using the estimates of the next section and it will be shown in the sequel that the time step is not sensitive to the mesh size but depends on the smoothness of the solution (L^∞ bound on $n_{\mathcal{T}}$ is enough).

We may now state our main result.

Theorem 2.2 *Assume that the CFL condition* (23) *on the time step is fulfilled and that the initial datum n^0 satisfies* (4). *Moreover, n^0 satisfies the smallness assumption: there exists a constant $C_\Omega > 0$, only depending on the domain Ω, such that*

$$\sum_{K\in\mathcal{T}} m(K)\, n_K^0 < \frac{2\,\xi}{9\,C_\Omega\,\chi}, \tag{24}$$

where ξ is given by (6). *Then, the solution $(n_{\mathcal{T}}, c_{\mathcal{T}})$ given by the finite volume scheme* (8)–(10) *satisfies*

$$\begin{aligned} n_{\mathcal{T}} &\longrightarrow n \quad in \quad L^2(\Omega_T)\,, \\ c_{\mathcal{T}} &\rightharpoonup c \quad in \quad L^\infty(0,T;L^2(\Omega))\,, \\ Dc_{\mathcal{T}} &\rightharpoonup \nabla c \quad in \quad L^\infty(0,T;L^2(\Omega))\,, \end{aligned}$$

with $\Omega_T = (0,T)\times\Omega$ and (n,c) is the weak solution to the PKS system (1), (3) *on* $[0,T]$ *with initial datum n^0. More precisely, (n,c) is a couple of nonnegative functions satisfying*

$$\begin{cases} n \in \mathcal{C}([0,T];L^2(\Omega)) \cap L^2\left(0,T;H^1(\Omega)\right)\,, \\ c \in L^\infty(0,T;H^1(\Omega))\,, \end{cases}$$

and for all test functions $\psi \in C^1(\overline{\Omega}_T)$,

$$\int_{\Omega_T} n \frac{\partial \psi}{\partial t} \; - \; \nabla n \cdot \nabla \psi \; + \; \chi\, n \nabla c \cdot \nabla \psi \; \mathrm{d}x\mathrm{d}t + \int_{\Omega} n^0 \, \psi(0,x) \; \mathrm{d}x = 0, \quad (25)$$

$$\int_{\Omega_T} \nabla c \cdot \nabla \psi \; \mathrm{d}x\mathrm{d}t = \int_{\Omega_T} (n-c)\, \psi \; \mathrm{d}x\mathrm{d}t. \quad (26)$$

In addition, mass is conserved with respect to time (5).

3 A priori estimates

This section is devoted to the proof of uniform a priori estimates with respect to the mesh $\mathcal{T}$ on the numerical solution $(n_{\mathcal{T}}, c_{\mathcal{T}})$. The aim is to prove strong compactness in $L^2(\Omega_T)$ on the density $n_{\mathcal{T}}$ while $L^2(\Omega_T)$ uniform estimates on $Dc_{\mathcal{T}}$ are sufficient.

Lemma 3.1 *Let* $\phi : \mathbb{R} \to \mathbb{R}$ *be an increasing* C^1*-function. Then, the solution to the numerical scheme* (8)–(10) *satisfies for all* $k \in \mathbb{N}$

$$\sum_{K\in\mathcal{T}} m(K) \left(n_K^{k+1} - n_K^k\right) \phi(n_K^{k+1}) \le -\frac{\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \left[Dn_{K,\sigma}^{k+1} \sqrt{\phi'\left(\tilde{n}_\sigma^{k+1}\right)} \right]^2 + \frac{\chi\, \Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \, \tilde{n}_\sigma^{k+1} \, \phi'\left(\tilde{n}_\sigma^{k+1}\right) \times Dc_{K,\sigma}^{k+1}\, Dn_{K,\sigma}^{k+1},$$

where $\sigma = K|L$ *and* $\tilde{n}_\sigma^{k+1} = t_\sigma\, n_K^{k+1} + (1-t_\sigma)\, n_L^{k+1}$ *and* $t_\sigma \in (0,1)$.

Proof Multiplying the scheme (8) by $\Delta t\, \phi(n_K^{k+1})$ and summing for $K \in \mathcal{T}$, we obtain

$$\sum_{K\in\mathcal{T}} m(K) \left(n_K^{k+1} - n_K^k\right) \phi(n_K^{k+1}) \; = \; -\left(G_1 + G_2\right),$$

where

$$G_1 = \Delta t \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K \\ \sigma=K|L}} \tau_\sigma \left[n_K^{k+1} - n_L^{k+1} \right] \phi(n_K^{k+1}),$$

$$G_2 = \chi\, \Delta t \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K \\ \sigma=K|L}} \tau_\sigma \left[(Dc_{K,\sigma}^{k+1})^+ n_K^{k+1} - (Dc_{K,\sigma}^{k+1})^- n_L^{k+1} \right] \phi(n_K^{k+1}).$$

We first deal with the term G_1. We set $\sigma = K|L$ and using a Taylor expansion of $\phi(.)$ at n_K^{k+1}, we show that there exists $t_\sigma \in (0,1)$ such that $\tilde{n}_\sigma^{k+1} = t_\sigma\, n_K^{k+1} + (1-t_\sigma)\, n_L^{k+1}$ and

$$\left[n_K^{k+1} - n_L^{k+1} \right] \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1}) \right] \; = \; \left[n_K^{k+1} - n_L^{k+1} \right]^2 \phi'\left(\tilde{n}_\sigma^{k+1}\right). \quad (27)$$

Next, using the symmetry of τ_σ and the Taylor expansion of the function ϕ, we get

$$\begin{aligned} G_1 &= \frac{\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[n_K^{k+1} - n_L^{k+1}\right] \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right] \\ &= \frac{\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left[\left(n_L^{k+1} - n_K^{k+1}\right) \sqrt{\phi'\left(\tilde{n}_\sigma^{k+1}\right)}\right]^2. \end{aligned} \tag{28}$$

Now, we perform a discrete integration by part (using the symmetry of τ_σ) and estimate the term G_2

$$\begin{aligned} G_2 = \frac{\chi\,\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma &\left[(Dc_{K,\sigma}^{k+1})^+\, n_K^{k+1} - (Dc_{K,\sigma}^{k+1})^-\, n_L^{k+1}\right] \\ &\times \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right]. \end{aligned}$$

Then, we set

$$G_2^\star = \frac{\chi\,\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma\, \tilde{n}_\sigma^{k+1}\, Dc_{K,\sigma}^{k+1} \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right],$$

where $\tilde{n}_\sigma^{k+1}$ is given by the Taylor expansion (27); and let us show that $G_2 \geq G_2^\star$.

Indeed, reordering the sum and using the expression of $\tilde{n}$, it yields

$$\begin{aligned} \frac{2\,(G_2 - G_2^\star)}{\chi\,\Delta t} &= \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(Dc_{K,\sigma}^{k+1}\right)^+ \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right] \left(n_K^{k+1} - \tilde{n}_\sigma^{k+1}\right) \\ &\quad + \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(Dc_{K,\sigma}^{k+1}\right)^- \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right] \\ &\quad \times \left(\tilde{n}_\sigma^{k+1} - n_L^{k+1}\right) \\ &= \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(Dc_{K,\sigma}^{k+1}\right)^+ (1 - t_\sigma) \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right] \\ &\quad \times \left(n_K^{k+1} - n_L^{k+1}\right) \\ &\quad + \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} \tau_\sigma \left(Dc_{K,\sigma}^{k+1}\right)^- t_\sigma \left[\phi(n_K^{k+1}) - \phi(n_L^{k+1})\right] \\ &\quad \times \left(n_K^{k+1} - n_L^{k+1}\right). \end{aligned}$$

Finally, since ϕ is an increasing function, we show that

$$G_2 - G_2^\star \geq 0. \tag{29}$$

Thus, gathering (28) and (29), we get

$$\begin{aligned}\sum_{K\in\mathcal{T}} m(K)\left(n_K^{k+1}-n_K^k\right)\,\phi(n_K^{k+1}) &= -G_1 - G_2 + G_2^\star - G_2^\star\\ &\le -G_1 - G_2^\star,\\ &= -\frac{\Delta t}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\left[Dn_{K,\sigma}^{k+1}\sqrt{\phi'\left(\tilde{n}_\sigma^{k+1}\right)}\right]^2\\ &\quad+\frac{\chi\,\Delta t}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,\tilde{n}_\sigma^{k+1}\,Dc_{K,\sigma}^{k+1}\,D\\ &\quad\times\left[\phi(n^{k+1})\right]_{K,\sigma}.\end{aligned}$$

Finally, using the Taylor expansion (27), we obtain the final result

$$\begin{aligned}\sum_{K\in\mathcal{T}} m(K)\left(n_K^{k+1}-n_K^k\right)\,\phi(n_K^{k+1}) &\le -\frac{\Delta t}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\left[Dn_{K,\sigma}^{k+1}\sqrt{\phi'\left(\tilde{n}_\sigma^{k+1}\right)}\right]^2\\ &\quad+\frac{\chi\,\Delta t}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,\tilde{n}_\sigma^{k+1}\,\phi'\left(\tilde{n}_\sigma^{k+1}\right)\\ &\quad\times Dc_{K,\sigma}^{k+1}\,Dn_{K,\sigma}^{k+1}.\end{aligned}$$

□

We also give a discrete version of the Poincaré–Wirtinger inequality.

Lemma 3.2 *Let Ω be an open convex bounded polygonal (Lipschitz domain) subset of $\mathbb{R}^2$ and $\mathcal{T}$ be an admissible mesh of Ω satisfying (6). Then, there exists a constant $C_\Omega > 0$, only depending on Ω, such that for all admissible meshes $\mathcal{T}$ and all $u \in X(\mathcal{T})$, $u \ge 0$,*

$$\begin{aligned}\sum_{K\in\mathcal{T}} m(K)|u_K|^2 \;\le\; \frac{4\,C_\Omega}{\xi}&\left(\sum_{K\in\mathcal{T}} m(K)u_K\right)\left(\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}}\tau_\sigma\,|D(\sqrt{u})_{K,\sigma}|^2\right)\\ &+\;m(\Omega)\,\overline{u}^2,\end{aligned}\tag{30}$$

where $\overline{u}$ is the average of u in Ω and C_Ω corresponds to the best constant in the BV version of the Gagliardo–Nirenberg–Sobolev inequality

$$\sum_{K\in\mathcal{T}} m(K)|u_K-\overline{u}|^2 \;\le\; C_\Omega\left[\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left|Du_{K,\sigma}\right|\right]^2.\tag{31}$$

Proof Let $\mathcal{T}$ be an admissible mesh and $u \in X(\mathcal{T})$, since the function u is piecewise constant and has a finite number of jumps (which corresponds to the number of edges), we get that $u \in BV(\Omega)$. Moreover, in dimension $d = 2$ and for a

Lipschitz domain Ω, the space $BV(\Omega)$ is continuously embedded in $L^2(\Omega)$ [6, Theorem 3.5]. Then, there exists a constant C_Ω, only depending on the shape of Ω, such that

$$\int_\Omega |u(x)-\overline{u}|^2 \mathrm{d}x \;=\; \int_\Omega |u(x)|^2 \mathrm{d}x \;-\; m(\Omega)\,\overline{u}^2 \;\le\; C_\Omega\;[BV_\Omega(u)]^2\,,$$

where

$$\overline{u} \;=\; \frac{1}{m(\Omega)} \int_\Omega u(x)\mathrm{d}x,$$

and

$$BV_\Omega(u) \;=\; \sup\left\{ \int_\Omega u(x)\;\mathrm{div}\varphi(x)\mathrm{d}x, \quad \varphi \in C_o^\infty(\Omega), \quad |\varphi(x)| \le 1, \quad \forall x \in \Omega \right\}.$$

Applying this latter result to the function $u \in X(\mathcal{T})$, we get

$$\sum_{K\in\mathcal{T}} m(K)|u_K - \overline{u}|^2 \;=\; \|u-\overline{u}\|^2_{L^2(\Omega)} \;\le\; C_\Omega\,[BV_\Omega(u)]^2$$

and since u is piecewise contant, for all $\varphi \in C_o^\infty(\Omega)$

$$\int_\Omega u(x)\;\mathrm{div}\varphi(x)\mathrm{d}x = \sum_{K\in\mathcal{T}} u_K \int_K \mathrm{div}\varphi(x)\mathrm{d}x.$$

Thus, applying the Green formula to the smooth and compactly supported function φ

$$\int_\Omega u(x)\;\mathrm{div}\varphi(x)\mathrm{d}x \;=\; \sum_{K\in\mathcal{T}} u_K \sum_{\sigma\in\mathcal{E}_K} \int_\sigma \varphi(\gamma)\cdot \nu_{K,\sigma}\mathrm{d}\gamma,$$

where $\nu_{K,\sigma}$ is the unit external normal to the edge σ. Next, we perform a discrete integration by part

$$\begin{aligned}
\int_\Omega u(x)\,\mathrm{div}\varphi(x)\mathrm{d}x &= \frac{1}{2}\sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} (u_K - u_L) \int_\sigma \varphi(\gamma)\cdot\nu_{K,\sigma}\mathrm{d}\gamma,\\
&\le \frac{1}{2}\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,|Du_{K,\sigma}|\,||\varphi||_\infty,\\
&= \frac{1}{2}\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,|Du_{K,\sigma}|.
\end{aligned}$$

Finally, we have proven the discrete version of a Gagliardo–Nirenberg–Sobolev inequality: there exists a constant C_Ω such that

$$\sum_{K\in\mathcal{T}} m(K)|u_K - \overline{u}|^2 \;\le\; C_\Omega \left[\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\left|Du_{K,\sigma}\right|\right]^2.$$

On the other hand, by definition of Du we have

$$\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)|Du_{K,\sigma}| = \frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} m(\sigma)|u_K - u_L|$$

and since $u \ge 0$

$$|u_K - u_L| = |\sqrt{u_K} - \sqrt{u_L}|\;(\sqrt{u_K} + \sqrt{u_L}),$$

it follows that

$$\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)|Du_{K,\sigma}| \;=\; \sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\sqrt{\frac{m(\sigma)}{d_{K,\sigma}}}|D(\sqrt{u})_{K,\sigma}|\,\sqrt{m(\sigma)\,d_{K,\sigma}}\sqrt{u_K}.$$

Hence, we apply the Cauchy–Schwarz inequality and since in dimension $2\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,d(K,\sigma) \le 2\,m(K)$ and (6); we get

$$\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)|Du_{K,\sigma}| \;\le\; \frac{2}{\sqrt{\xi}}\left(\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma|D(\sqrt{u})_{K,\sigma}|^2\right)^{1/2} \times\left(\sum_{K\in\mathcal{T}} m(K)u_K\right)^{1/2}. \tag{32}$$

Finally, gathering the two inequalities (31) and (32), we obtain the result: there exists a constant $C_\Omega > 0$ such that

$$\sum_{K\in\mathcal{T}} m(K)\,|u_K|^2 \le \frac{4\,C_\Omega}{\xi}\left(\sum_{K\in\mathcal{T}} m(K)\,u_K\right)\left(\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,|D(\sqrt{u})_{K,\sigma}|^2\right) + m(\Omega)\,\overline{u}^2.$$

□

Proposition 3.1 *Assume the initial datum fulfills (4) and satisfies the smallness condition (24), where C_Ω corresponds to the best constant in Lemma 3.2. Then, the solution (n_K^k, c_K^k), $K \in \mathcal{T}$ and $k \in \mathbb{N}$ to the scheme (8)–(10) satisfies there* *exists a constant* $\mathcal{C} > 0$*, only depending on* n^0*,* χ*,* T*,* Ω *and* ξ *[given by (6)], such that for all* $k \in \{0, \dots, M_T - 1\}$

$$\sum_{K \in \mathcal{T}} m(K) n_K^{k+1} \log(n_K^{k+1}) + \frac{1}{2}\left(1 - \chi\, \frac{4\, C_\Omega}{\xi}\, \|n^0\|_{L^1}\right) \sum_{l=0}^{k} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \Delta t\, \tau_\sigma \left| D(\sqrt{n^{l+1}})_{K,\sigma} \right|^2 \leq \mathcal{C} \tag{33}$$

and

$$\sum_{K \in \mathcal{T}} m(K) |n_K^{k+1}|^2 + \left(1 - \chi\, \frac{9\, C_\Omega}{2\,\xi}\, \|n^0\|_{L^1}\right) \sum_{l=0}^{k} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \Delta t\, \tau_\sigma |D n_{K,\sigma}^{l+1}|^2 \leq \mathcal{C}. \tag{34}$$

Proof To prove (33), we start with the identity

$$\frac{n_K^{k+1} \log(n_K^{k+1}) - n_K^k \log(n_K^k)}{\Delta t} = \frac{n_K^{k+1} - n_K^k}{\Delta t} \log(n_K^{k+1}) + n_K^k \frac{\log(n_K^{k+1}) - \log(n_K^k)}{\Delta t}. \tag{35}$$

From a Taylor expansion of $x \mapsto \log(x)$ at $x = n_K^k$, we get

$$n_K^k \frac{\log(n_K^{k+1}) - \log(n_K^k)}{\Delta t} \leq \frac{n_K^{k+1} - n_K^k}{\Delta t},$$

which gives an upper bound of the second term of (35). Then, multiplying (35) by $m(K)$, summing over $K \in \mathcal{T}$ and using the conservation of mass, we obtain the following inequality

$$\sum_{K \in \mathcal{T}} m(K) \frac{n_K^{k+1} \log(n_K^{k+1}) - n_K^k \log(n_K^k)}{\Delta t} \leq \sum_{K \in \mathcal{T}} m(K) \frac{n_K^{k+1} - n_K^k}{\Delta t} \log(n_K^{k+1}). \tag{36}$$

Now, applying Lemma 3.1 with $\phi(n) = \log(n)$, it yields

$$\sum_{K \in \mathcal{T}} m(K) \frac{n_K^{k+1} - n_K^k}{\Delta t} \log(n_K^{k+1}) \leq -\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \left[\frac{D n_{K,\sigma}^{k+1}}{\sqrt{\tilde{n}_\sigma^{k+1}}} \right]^2 + \frac{\chi}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma\, D c_{K,\sigma}^{k+1}\, D n_{K,\sigma}^{k+1}. \tag{37}$$

Let us estimate the right-hand side of the latter inequality. Using a discrete integration by part of the latter term and the numerical scheme for the Poisson equation (9), we get

$$\begin{aligned}\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\, Dc^{k+1}_{K,\sigma}\, Dn^{k+1}_{K,\sigma} &= -\sum_{K\in\mathcal{T}}\left(\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\, Dc^{k+1}_{K,\sigma}\right) n^{k+1}_K\\ &= \sum_{K\in\mathcal{T}} m(K)\,|n^{k+1}_K|^2 - \sum_{K\in\mathcal{T}} m(K)\, n^{k+1}_K\, c^{k+1}_K.\end{aligned}$$

Hence, applying Lemma 3.2 with $u = n^{k+1}$, we estimate the $L^2(\Omega)$ norm of n^{k+1} with respect to the $L^2(\Omega)$ norm of $D\sqrt{n^{k+1}}$

$$\begin{aligned}\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\, Dc^{k+1}_{K,\sigma}\, Dn^{k+1}_{K,\sigma} &\le \sum_{K\in\mathcal{T}} m(K)\,|n^{k+1}_K|^2\\ &\le \frac{2\,C_\Omega}{\xi}\,\|n^0\|_{L^1}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\left|D(\sqrt{n^{k+1}})_{K,\sigma}\right|^2\\ &\quad + m(\Omega)\,\left|\overline{n}^0\right|^2.\end{aligned}\tag{38}$$

Gathering inequalities (36),(37) and (38), it yields

$$\begin{aligned}&\sum_{K\in\mathcal{T}} m(K)\frac{n^{k+1}_K\log(n^{k+1}_K) - n^k_K\log(n^k_K)}{\Delta t}\\ &\quad\le -\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\left\{\left[\frac{Dn^{k+1}_{K,\sigma}}{\sqrt{\tilde{n}^{k+1}_\sigma}}\right]^2 - \chi\,\frac{4\,C_\Omega}{\xi}\,\|n^0\|_{L^1}\,\left|D(\sqrt{n^{k+1}})_\sigma\right|^2\right\}\\ &\qquad + m(\Omega)\,\chi\,\left|\overline{n}^0\right|^2.\end{aligned}$$

Moreover, we set $\sigma = K|L$ and use that

$$\begin{aligned}-\frac{|n^{k+1}_L - n^{k+1}_K|}{\sqrt{\tilde{n}^{k+1}_\sigma}} &= -\frac{\sqrt{n^{k+1}_K}+\sqrt{n^{k+1}_L}}{\sqrt{\tilde{n}^{k+1}_\sigma}}\left|\sqrt{n^{k+1}_L}-\sqrt{n^{k+1}_K}\right|\\ &\le -\left|\sqrt{n^{k+1}_L}-\sqrt{n^{k+1}_K}\right|\end{aligned}$$

to get the following estimate

$$\begin{aligned}&\sum_{K\in\mathcal{T}} m(K)\frac{n^{k+1}_K\log(n^{k+1}_K) - n^k_K\log(n^k_K)}{\Delta t}\\ &\quad\le -\frac{1}{2}\left(1-\chi\,\frac{4\,C_\Omega}{\xi}\,\|n^0\|_{L^1}\right)\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,\left|D(\sqrt{n^{k+1}})_{K,\sigma}\right|^2\\ &\qquad + m(\Omega)\,\chi\,\left|\overline{n}^{\,0}\right|^2.\end{aligned}$$

Finally, multiplying the latter inequality by Δt and summing over $l \in \{0, \dots, k\}$ with $k \leq M_T - 1$, we get the first result (33): there exists a constant $\mathcal{C} > 0$, only depending on n^0, χ, T, Ω and ξ, such that

$$\sum_{K \in \mathcal{T}} m(K) n_K^{k+1} \log(n_K^{k+1}) + \frac{1}{2}\left(1 - \chi \frac{4\, C_\Omega}{\xi} \|n^0\|_{L^1}\right) \sum_{l=0}^{k} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \Delta t\, \tau_\sigma \left| D(\sqrt{n^{l+1}})_{K,\sigma}\right|^2 \leq \mathcal{C}.$$

To prove (34), we first proceed as in the proof of Lemma 3.1 with $\phi(n) = n$ and get that

$$\begin{aligned}
\sum_{K \in \mathcal{T}} m(K) \frac{n_K^{k+1} - n_K^k}{\Delta t} n_K^{k+1} &\leq -\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \left[D n_{K,\sigma}^{k+1}\right]^2 \\
&\quad + \frac{\chi}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma\, n_K^{k+1}\, D c_{K,\sigma}^{k+1}\, D n_{K,\sigma}^{k+1}, \\
&\leq -\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \left[D n_{K,\sigma}^{k+1}\right]^2 \\
&\quad - \frac{\chi}{2} \sum_{K \in \mathcal{T}} \left(\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma\, D c_{K,\sigma}^{k+1}\right) \left| n_K^{k+1}\right|^2.
\end{aligned}$$

Using the numerical scheme (9) for the Poisson equation, we easily obtain

$$\begin{aligned}
\sum_{K \in \mathcal{T}} m(K) \frac{n_K^{k+1} - n_K^k}{\Delta t} n_K^{k+1} &\leq -\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \left[D n_{K,\sigma}^{k+1}\right]^2 \\
&\quad + \frac{\chi}{2} \sum_{K \in \mathcal{T}} m(K) |n_K^{k+1}|^3.
\end{aligned} \tag{39}$$

From this last inequality, we need to control the $L^3(\Omega)$ norm of n^{k+1} with respect to the discrete $H^1(\Omega)$ norm of n^{k+1}. Therefore, we apply the discrete Sobolev–Gagliardo–Nirenberg inequality (31) with $u = |n^{k+1}|^{3/2}$

$$\begin{aligned}
\sum_{K \in \mathcal{T}} m(K)\, |n_K^{k+1}|^3 &\leq C_\Omega \left(\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} m(\sigma)\, D\left(|n^{k+1}|^{3/2}\right)_{K,\sigma} \right)^2 \\
&\quad + \frac{1}{m(\Omega)} \left(\sum_{K \in \mathcal{T}} m(K)\, |n_K^{k+1}|^{3/2}\right)^2.
\end{aligned}$$

Now, since for $\sigma = K|L$, $|n_K^{3/2} - n_L^{3/2}| \leq \frac{3}{2}\,(n_K^{1/2} + n_L^{1/2})\,|n_K - n_L|$; we have

$$\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^3 \leq \frac{9\,C_\Omega}{4}\left(\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\sqrt{n_K^{k+1}}\,|Dn_{K,\sigma}^{k+1}|\right)^2 + \frac{1}{m(\Omega)}\left(\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^{3/2}\right)^2.$$

Then, applying the Cauchy–Schwarz inequality; we deduce that

$$\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^3 \leq \frac{9\,C_\Omega}{4}\left(\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,d_{K,\sigma}\,|n_K^{k+1}|\right) \times \left(\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\frac{|Dn_{K,\sigma}^{k+1}|^2}{d_{K,\sigma}}\right) + \frac{\|n^0\|_{L^1}}{m(\Omega)}\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^2.$$

Since $\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,d_{K,\sigma} \leq 2m(K)$ and using the condition (6), this gives

$$\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^3 \leq \frac{9\,C_\Omega}{2\,\xi}\|n^0\|_{L^1}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,|Dn_{K,\sigma}^{k+1}|^2 + \frac{\|n^0\|_{L^1}}{m(\Omega)}\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^2. \tag{40}$$

Substituting this latter inequality in (39), it yields

$$\begin{aligned}\frac{1}{2}\sum_{K\in\mathcal{T}} m(K)\frac{|n_K^{k+1}|^2 - |n_K^k|^2}{\Delta t} &\leq \sum_{K\in\mathcal{T}} m(K)\frac{n_K^{k+1} - n_K^k}{\Delta t}\,n_K^{k+1}\\ &\leq -\frac{1}{2}\left(1 - \chi\,\frac{9\,C_\Omega}{2\,\xi}\,\|n^0\|_{L^1}\right)\\ &\quad\times\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma\,\left|Dn_{K,\sigma}^{k+1}\right|^2\\ &\quad+\frac{\chi\,\|n^0\|_{L^1}}{2\,m(\Omega)}\sum_{K\in\mathcal{T}} m(K)\,|n_K^{k+1}|^2.\end{aligned}$$

Next, multiplying the latter inequality by Δt and summing over $l \in \{0,\dots,k\}$, we get

$$\sum_{K\in\mathcal{T}} m(K)|n_K^{k+1}|^2 + \left(1-\chi\,\frac{9\,C_\Omega}{2\,\xi}\,\|n^0\|_{L^1}\right)\sum_{l=0}^{k}\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\Delta t\,\tau_\sigma\left|Dn_{K,\sigma}^{l+1}\right|^2$$
$$\le\ \frac{1}{2}\sum_{K\in\mathcal{T}} m(K)\,|n_K^0|^2 + \frac{\chi\,\|n^0\|_{L^1}}{2\,m(\Omega)}\sum_{l=0}^{k}\sum_{K\in\mathcal{T}}\Delta t\,m(K)\,|n_K^{l+1}|^2 \tag{41}$$

The last step consists in controlling the last term $n_\mathcal{T}$ in $L^2(0,T;L^2(\Omega))$ that is

$$\sum_{l=0}^{M_T}\sum_{K\in\mathcal{T}}\Delta t\,m(K)\,|n_K^l|^2.$$

Thus, we apply Lemma 3.2 to the density $n_\mathcal{T}(t^l,\cdot)$ and get for all $l\in\{0,\dots,M_T\}$

$$\sum_{K\in\mathcal{T}} m(K)\,|n_K^l|^2 \le \frac{4\,C_\Omega}{\xi}\,\|n^0\|_{L^1}\left(\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\tau_\sigma|D\sqrt{n^l}_{K,\sigma}|^2\right) + \frac{||n^0||_{L^1}^2}{m(\Omega)}.$$

Therefore, from (33), we control the right-hand side i.e., there exists a constant $\mathcal{C}>0$, only depending on n^0, χ, T, Ω and ξ, such that

$$\sum_{l=0}^{k+1}\sum_{K\in\mathcal{T}}\Delta t\,m(K)\,|n_K^l|^2 \le \frac{4\,C_\Omega}{\xi}\,\|n^0\|_{L^1}\left(\frac{1}{2}\sum_{l=0}^{k+1}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\Delta t\,\tau_\sigma|D\sqrt{n^l}_{K,\sigma}|^2\right)$$
$$+\frac{T\,||n^0||_{L^1}^2}{m(\Omega)} \le \mathcal{C}. \tag{42}$$

Finally, gathering (41) and (42), there exists a constant $\mathcal{C}>0$, only depending on n^0, χ, T, Ω and ξ, such that

$$\sum_{K\in\mathcal{T}} m(K)|n_K^{k+1}|^2+\left(1-\chi\,\frac{9\,C_\Omega}{2\,\xi}\,\|n^0\|_{L^1}\right)\sum_{l=0}^{k+1}\frac{1}{2}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\Delta t\,\tau_\sigma\left|Dn_{K,\sigma}^{l}\right|^2\le\mathcal{C},$$

which concludes the proof. □

From this last result, we are now able to prove a uniform estimate on the discrete $H^1(\Omega)$ norm of the chemical concentration $c_\mathcal{T}(t,x)$

Proposition 3.2 *Assume the initial datum fulfills* (4) *and satisfies the smallness condition* (24)*, where C_Ω corresponds to the best constant in Lemma 3.2. Then, the concentration $c_\mathcal{T}$ solution to the discrete Poisson equation* (9) *satisfies, there exists a constant $\mathcal{C} > 0$ such that*

$$\sum_{k=0}^{M_T} \sum_{K \in \mathcal{T}} \Delta t\, m(K) |c_K^k|^2 + \frac{1}{2} \sum_{k=0}^{M_T} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \Delta t\, \tau_\sigma |Dc_{K,\sigma}^k|^2 \leq \sum_{k=0}^{M_T} \sum_{K \in \mathcal{T}} \Delta t\, m(K) |n_K^k|^2 \leq \mathcal{C}. \tag{43}$$

Proof We multiply the discrete scheme (9) by c_K^{k+1}, sum over $K \in \mathcal{T}$ and apply a discrete integration by part

$$\frac{1}{2} \sum_{K \in \mathcal{T}} \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma \, |Dc_{K,\sigma}^{k+1}|^2 + \sum_{K \in \mathcal{T}} m(K)\, |c_K^{k+1}|^2 \leq \left(\sum_{K \in \mathcal{T}} m(K)\, |n_K^{k+1}|^2 \right)^{1/2} \left(\sum_{K \in \mathcal{T}} m(K)\, |c_K^{k+1}|^2 \right)^{1/2}.$$

Then, the uniform estimate (34) on $n_\mathcal{T}$ obtained in Proposition 3.1 allows to conclude. □

4 Convergence of the finite volume scheme

In this section, we show the convergence of the approximate solutions $(n_\mathcal{T}, c_\mathcal{T})_\mathcal{T}$ to a global solution (n, c) to the PKS system (1),(3). The key point is to pass to the limit in the numerical scheme (8) and to treat the nonlinear term. For this purpose the strong compactness of $(n_\mathcal{T})_\mathcal{T}$ is required.

Proposition 4.1 *There are a subsequence of $(n_\mathcal{T}, c_\mathcal{T})_\mathcal{T}$ (not relabeled) and a couple of nonnegative functions $n \in L^2(0, T;\ H^1(\Omega))$ and $c \in L^\infty(0, T;\ H^1(\Omega))$ such that*

$$c_\mathcal{T} \rightharpoonup c, \quad \textit{weakly in } L^\infty(0, T;\ L^2(\Omega)),$$
$$Dc_\mathcal{T} \rightharpoonup \nabla c, \quad \textit{weakly in } L^\infty(0, T;\ L^2(\Omega))$$

and

$$n_\mathcal{T} \to n, \quad \textit{strongly in } L^2(\Omega_T))$$
$$Dn_\mathcal{T} \rightharpoonup \nabla n, \quad \textit{weakly in } L^2(\Omega_T);$$

as the parameter δ (mesh size) goes to zero.

Proof We first introduce the space

$$X_p(\Omega) = \left\{ u \in L^p(\Omega); \quad \forall \omega \subset \Omega, \quad \sup_\eta \left\| \frac{u(\cdot + \eta) - u(\cdot)}{|\eta|^{1/2}} \right\|_{L^2(\omega)} < +\infty \right\}. \tag{44}$$

From [2, Corollary IV.26], we can prove that $X_p(\Omega)$ is included in $L^2(\Omega)$ with compact embedding for $p > 2$.

Let us first consider the set of approximate solutions $(n_\mathcal{T})_\mathcal{T}$ and prove that it is bounded in $L^2(0, T;\ X_3(\Omega))$. On the one hand we have shown in Proposition 3.1 that $n_\mathcal{T}$ is bounded in $L^\infty(0, T;\ L^2(\Omega))$ uniformly with respect to the mesh size δ and from the discrete Sobolev–Gagliardo–Nirenberg inequality established in (40), there exists a constant $\mathcal{C} > 0$, only depending on Ω and n_0, such that

$$\|n_\mathcal{T}(\cdot, \cdot)\|_{L^3(\Omega_T)} \ \leq \ \mathcal{C}.$$

On the other hand, following the classical proof of [7, Theorem 3.7], we show that for all compact set $\overline{\omega} \subset \Omega$ and η such that $|\eta| < d(\overline{\omega}, \Omega^c)$

$$\sum_{k=0}^{M_T-1} \Delta t \|n_\mathcal{T}(t, \cdot + \eta) - n_\mathcal{T}(t, \cdot)\|^2_{L^2(\omega)} \leq |\eta| \, (|\eta| + 2\,h) \sum_{k=0}^{M_T-1} \Delta t \ \|n_\mathcal{T}\|^2_{1,\mathcal{T}}.$$

Thus, using the uniform estimate on the discrete $H^1(\Omega)$-norm of $n_\mathcal{T}$ (34) given in Proposition 3.1, we prove that there exists a constant $\mathcal{C} > 0$, only depending on Ω and n_0, such that for $|\eta|$ small enough

$$\sum_{k=0}^{M_T-1} \Delta t \ \|n_\mathcal{T}(t, \cdot + \eta) - n_\mathcal{T}(t, \cdot)\|^2_{L^2(\omega)} \ \leq \ \mathcal{C}\,|\eta|.$$

Therefore, the set of approximate solutions $n_\mathcal{T}$ for all admissible mesh $\mathcal{T}$ is bounded in $L^2(0, T;\ X_3(\Omega))$. Moreover, using the discrete scheme (8) and for all $\varphi \in H^4(\Omega)$; we denote by φ_K the average of φ in the control volume K and show that

$$\begin{aligned}
\sum_{K\in\mathcal{T}} m(K)(n_K^{k+1} - n_K^k)\,\varphi_K &\leq \frac{\Delta t}{2} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma \Big(|Dn^{k+1}_{K,\sigma}| \\
&\qquad + \chi\, n_K^{k+1} |Dc^{k+1}_{K,\sigma}| \Big) \, |D\varphi_{K,\sigma}| \\
&\leq \Delta t \ \big(\|n_\mathcal{T}\|_{1,\mathcal{T}} \|\varphi_\mathcal{T}\|_{1,\mathcal{T}} \\
&\qquad + \chi \ \|n_\mathcal{T}\|_{L^3(\Omega_T)} \|c_\mathcal{T}\|_{1,\mathcal{T}} \|D\varphi_\mathcal{T}\|_{L^6(\Omega_T)} \big) \\
&\leq \Delta t \big(\|n_\mathcal{T}\|_{1,\mathcal{T}} + \chi \|n_\mathcal{T}\|_{L^3(\Omega_T)} \|c_\mathcal{T}\|_{1,\mathcal{T}} \big) \ ||\varphi||_{H^4(\Omega)}.
\end{aligned}$$

Then, we sum over $k \in \{0, \ldots, M_T - 1\}$ and apply the Holder inequality with the results (34) of Proposition 3.1 and (43) of Proposition 3.2, which establish uniform bounds on $n_{\mathcal{T}}$ and $c_{\mathcal{T}}$. Finally, we get the following estimate: there exists a constant $\mathcal{C} > 0$, only depending on Ω and n_0, such that

$$\sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} m(K)(n_K^{k+1} - n_K^k)\,\varphi_K \leq \mathcal{C} \left(\int_0^T ||\varphi(t)||^2_{H^4(\Omega)} \mathrm{d}t \right)^{1/2}. \tag{45}$$

Using a time translate estimate on $n_{\mathcal{T}}$ and this latter inequality, we prove that there exists a constant $\mathcal{C} > 0$, only depending on Ω and n_0, such that for all $\tau \in (0, T)$

$$\int_0^{T-\tau} \int_\Omega [n_{\mathcal{T}}(t+\tau, x) - n_{\mathcal{T}}(t, x)]\ \varphi(t, x)\,\mathrm{d}x\mathrm{d}t \leq \mathcal{C}\ \tau\ \|\varphi\|_{L^2(0,T;\ H^4(\Omega))},$$

which gives a uniform estimate of the time translation of $n_{\mathcal{T}}$ in $L^2(0, T;\ (H^4(\Omega))')$. Now, since $n_{\mathcal{T}}$ is bounded in $L^2(0, T;\ X_3(\Omega))$, where $X_3(\Omega)$ is included in $L^2(\Omega)$ with compact embedding and the uniform estimates of time translation of $n_{\mathcal{T}}$ in $L^2(0, T;\ (H^4(\Omega))')$ with $L^2(\Omega) \subset (H^4(\Omega))'$; we can apply the compactness result of Simon [24] showing that there exists a subsequence of $(n_{\mathcal{T}})_{\mathcal{T}}$ (still labeled $(n_{\mathcal{T}})_{\mathcal{T}}$) such that

$$n_{\mathcal{T}} \to n, \quad \text{strongly in } L^2(\Omega_T).$$

Moreover, $Dn_{\mathcal{T}}$ is also bounded in $L^2(\Omega_T)$, then there exist a subsequence of $(Dn_{\mathcal{T}})_{\mathcal{T}}$ (still labeled $(Dn_{\mathcal{T}})_{\mathcal{T}}$) and a function $\Theta \in L^2(\Omega_T)$ such that

$$Dn_{\mathcal{T}} \rightharpoonup \Theta, \quad \text{weakly in } L^2(\Omega_T).$$

We refer to [3, Lemma 4.4] to prove that $\Theta = \nabla n$.

Finally, the uniform bound on the discrete $L^2(0, T;\ H^1(\Omega))$ norm of $c_{\mathcal{T}}$, obtained in Proposition 3.2, gives compactness in $L^2(\Omega_T)$ for $c_{\mathcal{T}}$ and $Dc_{\mathcal{T}}$ given by the definitions (11) and (12). Thus, there exist a subsequence of $(c_{\mathcal{T}})_{\mathcal{T}}$ (still labeled $(c_{\mathcal{T}})_{\mathcal{T}}$) and a couple of functions $(c, \gamma) \in (L^\infty(0, T;\ L^2(\Omega)))^2$ such that

$$c_{\mathcal{T}} \rightharpoonup c,\ \text{ weakly in } L^\infty(0, T; L^2(\Omega)),\ \ Dc_{\mathcal{T}} \rightharpoonup \gamma,\ \text{ weakly in} L^\infty(0, T;\ L^2(\Omega)).$$

We also refer to [3, Lemma 4.4] to prove that $\gamma = \nabla c$. □

From Proposition 4.1, the convergence of the scheme is now the main task. It will be achieved for the Poisson equation and the continuity equations in Propositions 4.2 and 4.3 separately. In particular, it implies the results of Theorem 2.2.

Proposition 4.2 *The nonnegative functions n and c defined in Proposition* 4.1 *satisfy the Poisson equation in the sense of* (26) *with Neumann boundary condition.*

Proof Let $\psi \in \mathcal{C}^2(\overline{\Omega}_T)$ be a test function and $\psi_K^k = \psi(t^k, x_K)$ for all $K \in \mathcal{T}$ and $k = 0,\ldots,M_T - 1$. We introduce:

$$F_{10}(\delta) = -\int_{\Omega_T} Dc_{\mathcal{T}} \cdot \nabla\psi\ \mathrm{d}x\mathrm{d}t \quad \text{and} \quad F_{20}(\delta) = \int_{\Omega_T} (n_{\mathcal{T}} - c_{\mathcal{T}})\,\psi\ \mathrm{d}x\mathrm{d}t$$

On the one hand, from the weak convergence of $(Dc_{\mathcal{T}})_{\mathcal{T}}$ to ∇c and the weak convergence of $n_{\mathcal{T}} - c_{\mathcal{T}}$ to $n - c$ in $L^2(\Omega_T)$, as δ goes to zero, obtained in Proposition 4.1, we have

$$F_{10}(\delta) + F_{20}(\delta) \to -\int_{\Omega_T} \nabla c \cdot \nabla \psi \,\mathrm{d}x\mathrm{d}t + \int_{\Omega_T} (n - c)\,\psi \,\mathrm{d}x\mathrm{d}t, \quad \text{as } \delta \to 0.$$

On the other hand, multiplying the scheme (9) by $\Delta t\, \psi_K^k$ and summing for K and k, we get

$$F_1(\delta) + F_2(\delta) = 0,$$

with

$$F_1(\delta) = \Delta t \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc_{K,\sigma}^{k+1}\, \psi_K^k,$$

$$F_2(\delta) = \Delta t \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} m(K)(n_K^{k+1} - c_K^{k+1})\, \psi_K^k.$$

Now, we prove the limits $F_j(\delta) - F_{j0}(\delta) \to 0$ as $\delta \to 0$ for $j = 1, 2$, which imply that the functions (n, c) satisfy the Poisson equation (26). We start with $j = 2$.

A straightforward computation gives

$$F_2(\delta) - F_{20}(\delta) = \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \int_{t^k}^{t^{k+1}} \int_K (n_K^{k+1} - c_K^{k+1})\,(\psi_K^k - \psi(t,x)) \,\mathrm{d}x\mathrm{d}t.$$

Since $(n_{\mathcal{T}})_{\mathcal{T}}$ and $(c_{\mathcal{T}})_{\mathcal{T}}$ are uniformly bounded in $L^2(\Omega_T)$ and ψ is smooth, it is easy to obtain

$$|F_2(\delta) - F_{20}(\delta)| \le \left(T\, \|\psi\|_{\mathcal{C}^1(\Omega_T)} \left[\|n_{\mathcal{T}}\|_{L^2(\Omega_T)} + \|c_{\mathcal{T}}\|_{L^2(\Omega_T)}\right]\right) \delta,$$

which yields $F_2(\delta) - F_{20}(\delta) \to 0$ as $\delta \to 0$.

Next, using the definition of $Dc_{K|L}^{k+1}$ and the symmetry of $K|L$, we have

$$F_1(\delta) = -\frac{\Delta t}{2} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc_{K,\sigma}^{k+1}\, D\psi_{K,\sigma}^k.$$

Let us rewrite $F_{10}(\delta)$ as

$$F_{10}(\delta) = -\frac{1}{2} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \int_{t^k}^{t^{k+1}} \int_{T_\sigma} Dc_{\mathcal{T}} \cdot \nabla\psi \,\mathrm{d}x\mathrm{d}t.$$

Therefore, by the definition of τ_σ and $Dc_{\mathcal{T}}$,

$$\begin{aligned}
&F_1(\delta) - F_{10}(\delta)\\
&\quad = -\frac{1}{2}\sum_{k=0}^{M_T-1}\sum_{K\in\mathcal{T}}\sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} m(\sigma)\, Dc_{K,\sigma}^{k+1}\int_{t^k}^{t^{k+1}}\Bigg(\frac{D\psi_{K,\sigma}^k}{d(x_K,x_L)}\\
&\qquad - \frac{1}{m(T_\sigma)}\int_{T_\sigma}\nabla\psi\cdot\nu_{K,\sigma}\,\mathrm{d}x\Bigg)\mathrm{d}t.
\end{aligned}$$

On the one hand, since the straight line (x_K,x_L) is orthogonal to σ, we have $x_K - x_L = d(x_K,x_L)\,\nu_{L,K}$. It follows from the regularity of ψ that

$$\begin{aligned}
\frac{D\psi_{K,\sigma}^k}{d(x_K,x_L)} &= \nabla\psi(t^k,x_L) + O(h) = \nabla\psi(t,x)\cdot\nu_{K,\sigma}\\
&\quad + O(\delta), \quad (t,x)\in[t^k,t^{k+1})\times T_\sigma.
\end{aligned}$$

By taking the mean value over T_σ, there exists a constant $\mathcal{C}>0$, only depending on ψ, such that

$$\left|\int_{t^k}^{t^{k+1}}\left(\frac{D\psi_{K,\sigma}^k}{d(x_K,x_L)} - \frac{1}{m(T_\sigma)}\int_{T_\sigma}\nabla\psi\cdot\nu_{K,\sigma}\,\mathrm{d}x\right)\mathrm{d}t\right| \le \mathcal{C}\Delta t\,\delta.$$

On the other hand, since the mesh $\mathcal{T}$ is regular, there exists a constant $\mathcal{C}>0$, only depending on the dimension of the domain and the geometry of $\mathcal{T}$, such that for $\sigma = K|L$

$$d(x_K,x_L)m(\sigma) \le \mathcal{C}m(T_\sigma).$$

Using the definition of τ_σ, we then have

$$\begin{aligned}
m(\sigma)|c_L^{k+1} - c_K^{k+1}| &= \sqrt{\tau_\sigma}|c_L^{k+1} - c_K^{k+1}|\sqrt{d(x_K,x_L)m(\sigma)},\\
&\le \sqrt{\tau_\sigma}|c_L^{k+1} - c_K^{k+1}|\sqrt{\mathcal{C}\,m(T_\sigma)}.
\end{aligned}$$

Hence, applying the Cauchy–Schwarz inequality and using the discrete $L^\infty(0,T;H^1(\Omega))$ estimate established in Proposition 3.2, we obtain

$$|F_1(\delta) - F_{10}(\delta)| \le \mathcal{C}\,\delta,$$

where $\mathcal{C}>0$ is a constant. This shows that $F_1(\delta) - F_{10}(\delta)\to 0$ as $\delta\to 0$. □

Proposition 4.3 *The functions n and c defined in Proposition* 4.1 *satisfy the continuity equation in the sense of* (25) *with Neumann boundary conditions. Moreover,*

$$\int_\Omega n(t,x)\mathrm{d}x = \int_\Omega n^0(x)\mathrm{d}x; \quad t\in\mathbb{R}_+.$$

Proof Let $\psi \in \mathcal{C}^2(\Omega_T)$ be a test function. We define

$$G_{10}(\delta) = -\int_{\Omega_T} n_{\mathcal{T}} \frac{\partial \psi}{\partial t} \mathrm{d}x\mathrm{d}t - \int_{\Omega} n_{\mathcal{T}}(0,x)\psi(0,x)\,\mathrm{d}x,$$

$$G_{20}(\delta) = \int_{\Omega_T} Dn_{\mathcal{T}} \cdot \nabla\psi \,\mathrm{d}x\,\mathrm{d}t,$$

$$G_{30}(\delta) = -\chi \int_{\Omega_T} n_{\mathcal{T}}\, Dc_{\mathcal{T}} \cdot \nabla\psi \,\mathrm{d}x\mathrm{d}t$$

and

$$\varepsilon(\delta) = -\left[G_{10}(\delta) + G_{20}(\delta) + G_{30}(\delta)\right].$$

Let $\psi_K^k = \psi(t^k, x_K)$ for all $K \in \mathcal{T}$ and $k = 0,1,...,M_T$. Multiplying the scheme (8) by $\Delta t\, \psi_K^k$ and summing for K and k, we obtain

$$G_1(\delta) + G_2(\delta) + G_3(\delta) = 0,$$

where

$$G_1(\delta) = \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} m(K)(n_K^{k+1} - n_K^k)\psi_K^k,$$

$$G_2(\delta) = -\Delta t \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dn_{K,\sigma}^{k+1}\, \psi_K^k,$$

$$G_3(\delta) = \Delta t\, \chi \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K \\ \sigma=K|L}} \tau_\sigma \left[(Dc_{K,\sigma}^{k+1})^+ n_K^{k+1} - (Dc_{K,\sigma}^{k+1})^- n_L^{k+1}\right] \psi_K^k.$$

From the weak convergence of the sequences $(Dc_{\mathcal{T}})_{\mathcal{T}}$ to ∇c and the strong convergence of the sequence $(n_{\mathcal{T}})_{\mathcal{T}}$ to n in $L^2(\Omega_T)$, it is easy to see that,

$$\varepsilon(\delta) \to \int_{\Omega_T} \left(n \frac{\partial \psi}{\partial t} - \nabla n \cdot \nabla\psi + n\nabla c \cdot \nabla\psi\right) \mathrm{d}x\mathrm{d}t$$
$$+ \int_{\Omega} n_0(x)\psi(0,x)\mathrm{d}x, \text{ as } \delta \to 0.$$

Therefore, it remains to show that $\varepsilon(\delta)$ converges to zero as δ goes to zero, which will be achieved from the limits: $G_j(\delta) - G_{j0}(\delta)$ converges to zero for $j = 1,2,3$.

In view of the expression of $G_2(\delta)$ and $G_{20}(\delta)$, it is easy to see that the proof of $G_2(\delta) - G_{20}(\delta)$ converges to zero is similar to the study of $F_1(\delta) - F_{10}(\delta)$ in Proposition 4.2. Hence, we only show $G_1(\delta) - G_{10}(\delta)$ and $G_3(\delta) - G_{30}(\delta)$ go to zero.

For the first limit, we have

$$G_1(\delta) = \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} m(K) n_K^{k+1}(\psi_K^k - \psi_K^{k+1}) - \sum_{K\in\mathcal{T}} m(K)\, n_K^0 \psi_K^0$$

$$= -\sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \int_{t^k}^{t^{k+1}} \int_K n_K^{k+1} \frac{\partial\psi}{\partial t}(t, x_K) \mathrm{d}x\mathrm{d}t - \sum_{K\in\mathcal{T}} \int_K n_K^0 \psi(0, x_K)\mathrm{d}x,$$

$$G_{10}(\delta) = -\sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \int_{t^k}^{t^{k+1}} \int_K n_K^{k+1} \frac{\partial\psi}{\partial t} \mathrm{d}x\mathrm{d}t - \sum_{K\in\mathcal{T}} \int_K n_K^0 \psi(0, x)\mathrm{d}x.$$

Hence, it follows from the regularity of ψ that

$$|G_1(\delta) - G_{10}(\delta)| \le \left[(T+1)\, m(\Omega)\ \|n_{\mathcal{T}}\|_{L^2(\Omega_T)}\ \|\psi\|_{\mathcal{C}^2(\Omega_T)}\right] h \to 0, \text{ as } \delta \to 0.$$

For the second limit, we set $\sigma = K|L$ and using the relation

$$(Dc_{K,\sigma}^{k+1})^+ n_K^{k+1} - (Dc_{K,\sigma}^{k+1})^- n_L^{k+1} = \frac{1}{2}|Dc_{K,\sigma}^{k+1}|\,(n_K^{k+1} - n_L^{k+1}) + \frac{1}{2} Dc_{K,\sigma}^{k+1}(n_K^{k+1} + n_L^{k+1}),$$

we may write $G_3(\delta) = G_{31}(\delta) + G_{32}(\delta)$, with

$$G_{31}(\delta) = -\frac{\chi\,\Delta t}{2} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, |Dc_{K,\sigma}^{k+1}|\, Dn_{K,\sigma}^{k+1}\, \psi_K^k,$$

$$= \frac{\chi\,\Delta t}{4} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, |Dc_{K,\sigma}^{k+1}| Dn_{K,\sigma}^{k+1})\, D\psi_{K,\sigma}^k,$$

$$G_{32}(\delta) = \frac{\chi\,\Delta t}{2} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\substack{\sigma\in\mathcal{E}_K \\ \sigma=K|L}} \tau_\sigma\, Dc_{K,\sigma}^{k+1}(n_K^{k+1} + n_L^{k+1})\, \psi_K^k,$$

$$= -\frac{\chi\,\Delta t}{2} \sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \tau_\sigma\, Dc_{K,\sigma}^{k+1}\, n_K^{k+1}\, D\psi_{K,\sigma}^k.$$

From the definition of $n_{\mathcal{T}}$, we also have

$$G_{30}(\delta) = -\sum_{k=0}^{M_T-1} \sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_K} \int_{t^k}^{t^{k+1}} \int_{T_\sigma} n_{\mathcal{T}}\, Dc_{\mathcal{T}} \cdot \nabla\psi \,\mathrm{d}x\mathrm{d}t,$$

$$= G_{310}(\delta) + G_{320}(\delta)$$

with

$$G_{310}(\delta) = -\frac{1}{2}\sum_{k=0}^{M_T-1}\sum_{K\in\mathcal{T}}\sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}}\int_{t^k}^{t^{k+1}}\int_{S_{L,\sigma}} Dn_{K,\sigma}^{k+1} - Dc_{\mathcal{T}}\cdot\nabla\psi\,\mathrm{d}x\mathrm{d}t,$$

$$G_{320}(\delta) = -\frac{1}{2}\sum_{k=0}^{M_T-1}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K}\int_{t^k}^{t^{k+1}}\int_{T_\sigma} n_K^{k+1}\, Dc_{\mathcal{T}}\cdot\nabla\psi\,\mathrm{d}x\mathrm{d}t,$$

where $S_{L,\sigma} = L\cap T_\sigma$. Therefore, the convergence result follows if we prove that G_{31}, $G_{310}(\delta)\to 0$ and $|G_{32}(\delta)-G_{320}(\delta)|\to 0$ as $\delta\to 0$. First of all, by the Cauchy–Schwarz inequality and using the results of Propositions 3.1 and 3.2, we obtain

$$|G_{31}(\delta)| \le \frac{\chi\, h}{4}\|\psi\|_{C^1}\,\|n_{\mathcal{T}}\|_{1,\mathcal{T}}\,\|c_{\mathcal{T}}\|_{1,\mathcal{T}} \to 0,\ \text{as } \delta\to 0.$$

Next, noting that from (12), $Dc_{\mathcal{T}} = \frac{d(x_K,x_L)}{m(T_\sigma)}Dc_{K,\sigma}\cdot\nu_{K,\sigma}$ in T_σ and $S_{L,\sigma}\subset T_\sigma$, we obtain again from the Cauchy–Schwarz inequality,

$$\begin{aligned}|G_{310}(\delta)| &\le \frac{\chi}{2}\sum_{k=0}^{M_T-1}\sum_{K\in\mathcal{T}}\sum_{\substack{\sigma\in\mathcal{E}_K\\ \sigma=K|L}} d(x_K,x_L)\,\tau_\sigma\,|Dc_{K,\sigma}^{k+1}|\,|Dn_{K,\sigma}^{k+1}|\,\|\psi\|_{C^1},\\ &\le \chi\, h\,\|\psi\|_{C^1}\,\|n_{\mathcal{T}}\|_{1,\mathcal{T}}\,\|c_{\mathcal{T}}\|_{1,\mathcal{T}}, \quad \text{as } \delta\to 0.\end{aligned}$$

Finally,

$$\begin{aligned}G_{32}(\delta)-G_{320}(\delta) = -\frac{\chi}{2}\sum_{k=0}^{M_T-1}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} m(\sigma)\,n_K^{k+1}\,Dc_{K,\sigma}^{k+1}\int_{t^k}^{t^{k+1}}\Bigg(&\frac{D\psi_{K,\sigma}^k}{d(x_K,x_L)}\\ &-\frac{1}{m(T_\sigma)}\int_{T_\sigma}\nabla\psi\cdot\nu_{K,\sigma}\mathrm{d}x\Bigg)\mathrm{d}t.\end{aligned}$$

Using the $L^2(0,T;\ X_3(\Omega))$ bound for $n_{\mathcal{T}}$ and $c_{\mathcal{T}}$, we obtain $G_{32}(\delta)-G_{320}(\delta)$ converges to zero as δ goes to zero similarly to that of $F_1(\delta)$-$F_{10}(\delta)\to 0$. This ends the proof of Theorem 2.2. □

5 Numerical Simulations

In [4,21], the authors formulated the following conjecture for the solution to (1),(2) in dimension 2:

- the density n cannot form a δ function if the total density in Ω is less than a critical number d_Ω.
- density n can form a δ function singularity if the total density in Ω is larger than a critical number D_Ω.

In the recent years, one was led to believe that the equality $d_\Omega = D_\Omega$ should hold for the critical values mentioned in the conjecture. In [13], Herrero and Velazquez showed the existence of radially symmetric solutions to (1),(2), which blow-up at the center of the disk in finite time provided that

$$\overline{n_0}\,\chi > 8\,\pi, \quad \overline{n_0} = \frac{1}{|\Omega|}\int\limits_{\Omega} n_0(x)\,\mathrm{d}x.$$

Moreover in the $2D$ case, assuming that $4\,\pi < \chi\,\overline{n_0} < 8\,\pi$, Hortsmann showed that under the additional assumption that the solution to (1)–(2) blows-up, the function c has to blow-up at the boundary of the domain.

We present several numerical results to observe the evolution of cell density bumps under the influence of a chemoattractant given by the system (1),(2) in dimension two using the finite volume method (8)–(10). The initial datum is a Gaussian function

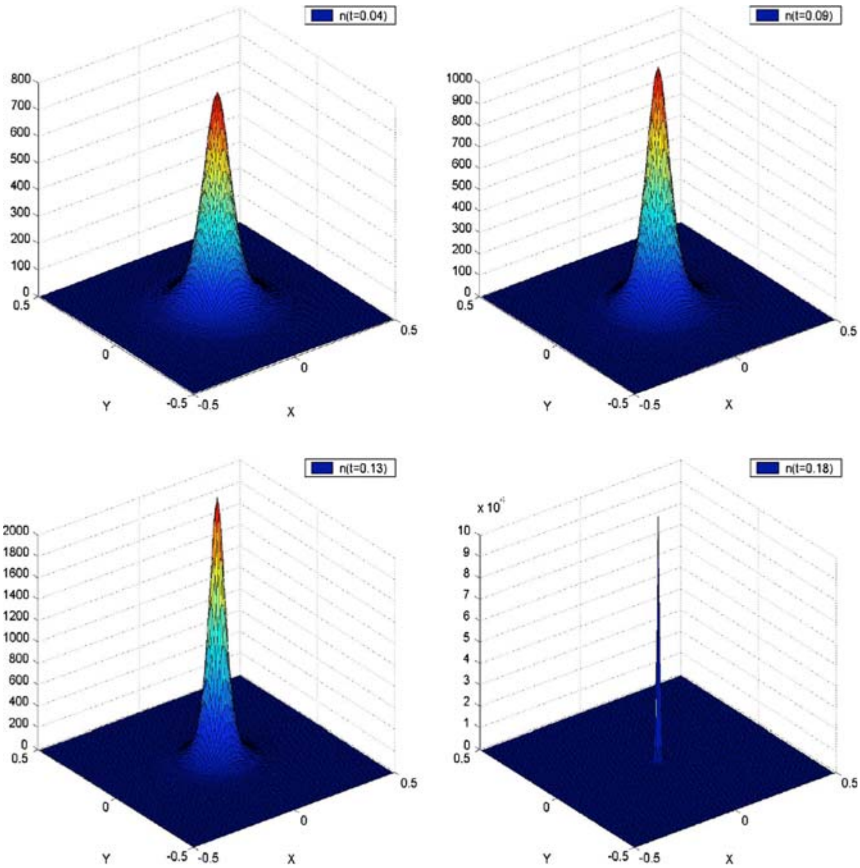

Fig. 1 Initial datum with a radial symmetry: $\overline{n_0} = 10\pi$, evolution of the numerical solution at time $t = 0.04$, $t = 0.09$, $t = 0.13$ and $t = 0.18$

$$n^0(x, y) = \frac{n_0}{2\pi T} \exp\left(-\frac{(x-x_0)^2 + (y-y_0)^2}{2T}\right),$$

where $T = 5 \times 10^{-3}$, the total mass is $n_0 = 10\pi$ and the domain is the box $(-1/2, 1/2) \times (-1/2, 1/2)$. The time step is $\Delta t = 1 \times 10^{-3}$ and the number of points is 100×100.

On the one hand, we choose a radially symmetric solution $(x_0, y_0) = (0, 0)$, for which we know that the solution blows-up at finite time. We solve the system (1),(2) without boundary conditions. (We choose the domain large enough to avoid boundary condition effect.) This first test is performed to check the ability of the method to recover blowing-up solutions. In Fig. 1, the cell density is plotted at different times and we observe that, as expected, the solution blows-up at the center of the domain (0, 0).

On the other hand, we choose a nonsymmetric initial Gaussian $(x_0, y_0) = (0.1, 0.1)$ with the same initial mass as before. In this case, the solution moves to

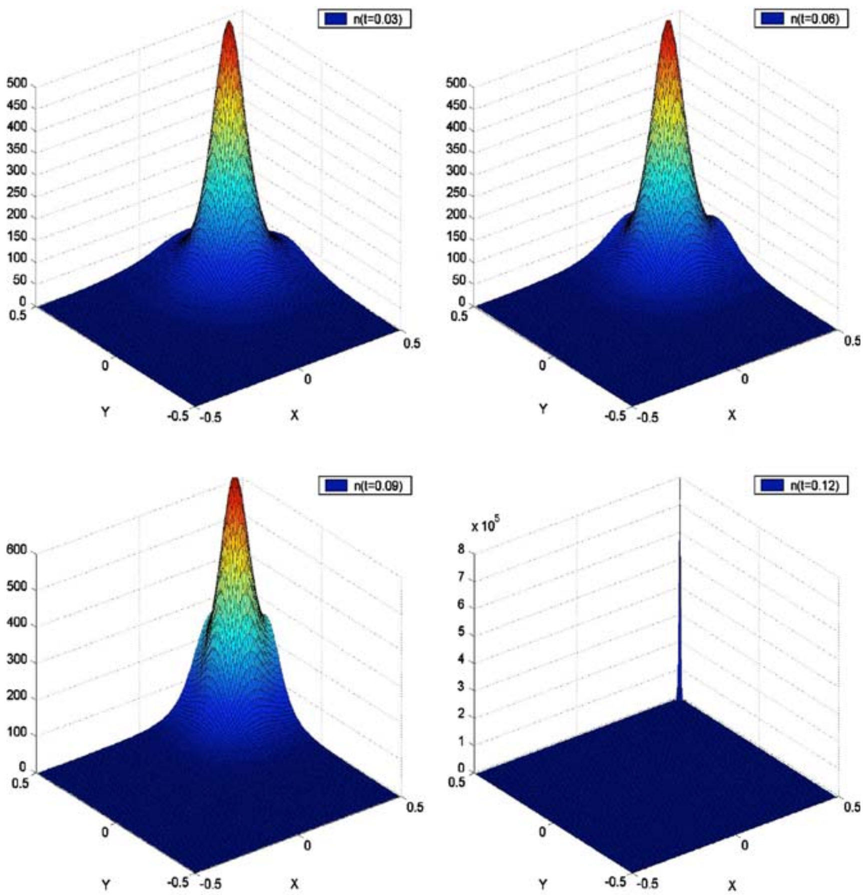

Fig. 2 Nonsymmetric initial datum: $\overline{n_0} = 10\pi$, evolution of the cell density n at time $t = 0.03$, $t = 0.06$, $t = 0.09$ and $t = 0.12$

the boundary and finally also blows-up, but now at the boundary (see Fig. 2). Let us remark that in [19], the author solved the same system with Dirichlet boundary conditions for c and observed that the solution always blows-up inside the domain but not at the center. We also have performed such simulations which agree well with these results. Thus, from these different numerical results, it seems that boundary conditions have a strong influence on the solution and on the localization of the blow-up.

Finally, in [13] it is proven that for intermediate mass

$$4\pi \ \leq \ \overline{n_0} \ \leq \ 8\pi,$$

if the solution blows-up it is necessary at the boundary. We illustrate this result in Fig. 3 with the same nonsymmetric initial datum as before, but with the total mass $\overline{n_0} = 6\pi$. Then, the solution first hesitates between converging to a steady state or blowing-up and finally moves to the boundary to blow-up. We also observe that

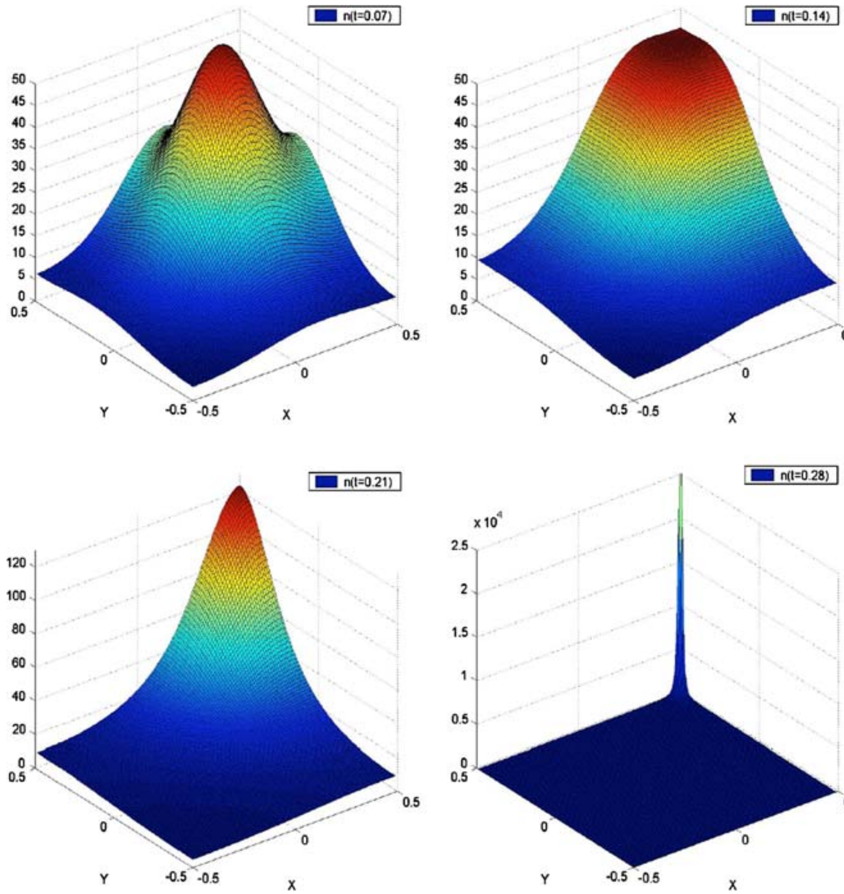

Fig. 3 Blow-up at the boundary for $\overline{n_0} = 6\pi$: time evolution of the cell density at time $t = 0.07$, $t = 0.14$, $t = 0.21$ and $t = 0.28$

the blow-up is always point-wise for this system. Moreover, the corners seem to be more attractive for the blow-up.

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