Re: *Manuscript KRM 241002*
Title: *From a nonlinear kinetic equation to a volume-exclusion chemotaxis model via asymptotic preserving methods*

Dear Editor,

We would like to thank the reviewers for their careful reading of the article and the helpful comments.

Attached to this letter we submit a revised manuscript, which takes into account the Referees' specific comments. A revised version with changes in blue is also submitted for ease of reading. Below we describe our action with respect to the reviews on a point-by-point basis. We think that thanks to the Referee's suggestions, the work has been further improved.

Yours sincerely,

Gissell Estrada-Rodriguez,
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Xinran Ruan.

From a nonlinear kinetic equation to a volume-exclusion chemotaxis model via asymptotic preserving methods
by G. Estrada-Rodriguez, D. Peurichard, and X. Ruan.

Authors' response to the Reviewers

Report 1

- *The authors study the diffusion limit of a kinetic velocity-jump model, where the transport and turning operator are density-dependent. The limit equation obtained is the volume-exclusion chemotactic equation. The micro-macro decomposition technique is used to derive a micro-macro model equivalent to the kinetic equation. The authors propose an implicit-explicit Finite Difference scheme and prove its Asymptotic-Preserving property. The scheme naturally discretizes the macroscopic volume-exclusion chemotactic equation without strict constraints on the time step. The bound-preserving property of the scheme is also established. Finally, numerical experiments illustrate the method's effectiveness. This work is interesting and presents a novel approach to numerical methods for chemotactic problems. The paper is well-written, but the following points need clarification:*

1. *Introduction (p.3): The function T is written as dependent on ∇c rather than c. Is there a biological motivation for this choice?*

   We thank the reviewer for this remark. We clarified the choice of T in the new version of the manuscript, by adding the following text in the introduction (p3):
   $T(\mathbf{v}, \rho, \nabla c)$ gives the probability of a velocity jump to velocity $\mathbf{v}$, which accounts for cell preference to move up the chemotactic gradient ∇c, and the term $F[\rho](t, \mathbf{x}, \mathbf{v})$ describes the anisotropic transport due to the density limited motion. The fact that the turning operator $T(\mathbf{v}, \rho, c, \nabla c)$ depends on the gradient of chemical concentration ∇c is necessary to obtain the chemotactic behavior described by (2), as discussed thoroughly in [33]. For simplicity, we have assumed here that the turning rate only depends on ∇c but the derivation extends to more general choices $T(\mathbf{v}, \rho, c, \nabla c)$, as briefly discussed in Remark 1.

   And added a remark after the derivation (section 2.2 p7)
   Remark 1. As discussed in [33], the assumption H2 which consists in assuming that the perturbation ψ_1 is linearly dependent on ∇c is necessary to recover the chemotactic term in the limit $\epsilon \to 0$. We note here that the derivation extends easily to perturbations of the form $\psi_1(\mathbf{v}, c, \nabla c) = \tilde{\phi}(\mathbf{v}, c) \cdot \nabla c$. In this case, notice that we would obtain a non constant chemotactic intensity $\chi_0(c) = \langle v \otimes \phi(v, c) \rangle$ in the limit.

2. *Section 2 (p.4): The function ψ appears in T. Could you clarify that ψ will be discussed later?*

   We included a clarifying sentence in p4: '$\psi(\mathbf{v}, \nabla c)$ will be defined later in (6)'.

3. *Section 2.1 (p.5): Define the notation $\langle \cdot \rangle$ generally, as it appears frequently.*

   We clarified the notation p.5:
   We denote by $\langle . \rangle$ the integration in the $\mathbf{v}$ variable, $\langle u \rangle = \int_V u(\mathbf{v}) d\mathbf{v}$, and we will consider that $\langle \psi_\varepsilon \rangle = \int_V \psi_\varepsilon(\mathbf{v}, \nabla c) d\mathbf{v} = 1$, where $\psi_\varepsilon(\mathbf{v}, \nabla c)$ is a non-negative and decreasing function in ∇c. This modeling choice amounts to consider that cells are less likely to tumble when the chemical gradient increases.

4. *Section 2.3 (p.7): Clarify the hypothesis (19) in Proposition 1.*

   We thank the reviewer for this remark, enabling to realize we did not come back to the equation for c before this section. We added a clarifying sentence before Proposition 1 and referred to this equation in the proposition directly (p7):
   Thus far, we could perform the derivation without specifying the equation for the chemoattractant c. From the remaining of the paper, we choose the production and consumption of chemoattractant $g(\rho, c)$ in Eq. (1) to be linear in both variables $g(\rho, c) = \rho - c$. Therefore, c solves:

$$\Delta c + \rho - c = 0. \tag{1}$$

5. *Section 4: Is the finite difference scheme chosen for simplicity?*

   Yes, the finite difference discretization is indeed chosen for its simplicity. We have added an explanation in p10 to clarify the motivation for using the finite difference method:
   To facilitate a more straightforward analysis of the asymptotic preserving property based on the micro-macro decomposition, we adopt the finite difference discretization. This choice enables a fully explicit formulation and simplifies the theoretical verification of the asymptotic preserving property.

6. *Section 4.2 (p.12): How restrictive is the CFL condition (37)?*

The CFL condition (37) is a sufficient condition to ensure the boundedness of the numerical solution, but it is not sharp. It is a guideline for theoretical analysis rather than a strict limitation in computations. We have clarified this in p14:
The CFL condition (37) derived is not sharp. In practice, violating this condition does not necessarily lead to computational breakdown. Nevertheless, it provides useful guidance on the choice of time steps for ensuring stability.

7. *Section 5 (p.14): The kinetic model (21) is referenced, but numerical results are based on (25). Please confirm.*

   Indeed. We solve numerically a micro-macro decomposition given by (25), of the kinetic original model (21). We clarified this in the text p14:
   In particular, we numerically verify the convergence of the kinetic model proposed in (21) (numerically solved with (29) from the micro-macro decomposition (25)), which we denote as $\rho^{\epsilon}_{\text{kinetic}}$, to the volume-exclusion Keller-Segel model (26) (numerically solved with (36)), denoted as ρ_{macro}, as $\varepsilon \to 0$ in one and two dimensions.

8. *Sections 5-6: Have you compared computational times? What motivates the finite difference scheme over a full kinetic scheme?*

   We have added a plot in Figure 1 to illustrate the total computation time of the proposed AP scheme for various values of ε and different time step sizes. However, comparisions with other numerical methods, such as a fully kinetic scheme, are not included in the paper. This is because the main focus of this work is the convergence of the kinetic model to its macroscopic limit and the design of an AP scheme that accurately captures this transition. As such, general computational time comparisons with full kinetic solvers are beyond the scope of this study. To facilitate a more straightforward analysis of the AP property, the finite difference discretization is applied. To clarify the motivation of this choice, we have added the following explanation in p10:
   To facilitate a more straightforward analysis of the asymptotic preserving property based on the macro-micro decomposition, we adopt the finite difference discretization. This choice enables a fully explicit formulation and simplifies the theoretical verification of the asymptotic preserving property.

9. *General: Consider adjusting parenthesis sizes appropriately in equations.*

   We thank the reviewer for this comment. We adjusted the parenthesis sizes everywhere relevant.

Report 2

- *The authors formally derive a volume-exclusion chemotactic equation from a kinetic model with a density-dependent turning operator. The paper is clear and well-written. However, some points need attention:*

1. *Page 4 (lines 21, 27): Why is $q(\rho(t, x+av))$ in $T(v, \rho, \nabla c)$ identical to the function in $F[\rho]$? Is this necessary? Furthermore, $F[\rho](t, x, v) = 0$ when $\rho(t, x) = \bar{\rho}$. How does this affect T? Is it necessary for both T and $F[\rho]$ to be density-dependent?*

   We thank the reviewer for this remark. In general, this is a modelling assumption and other forms of these functions might be considered. Our choice is the relevant one in order to obtain the nonlinear PDE (1). We added the following paragraph at the beginning of p.5 to clarify our choice of T and F:
   We consider that the saturation on both the turning operator T and the density-dependent transport F, is given by the same function q. This is because cells will sense crowded regions in the same way either when they are going to choose the next direction of movement, or when they are in the running phase. This is of course a modeling assumption in our case, but in general, different functions can be considered.

2. *Page 8 (line 14): What difficulty arises from using $q(\rho(x+\alpha v, t))$ directly? The expansion in line 15 holds only for small α. The AP scheme should be accurate for both small and large ϵ, making direct use of $q(\rho(x+\alpha v, t))$ more reasonable.*

   We agree that directly using $q(\rho(x + \alpha v, t))$ would be more accurate, especially for large ε. However, the micro-macro decomposition relies on a linearization of this term. The direct evaluation of $q(\rho(x + \alpha v, t))$ significantly complicates both the algorithm design and the analysis of the AP property. Therefore, we perform a Taylor expansion of $q(\rho(x + \alpha v, t))$ for α small. This is consistent with the scaling $\alpha = O(\epsilon)$ and ensures that the scheme captures the correct macroscopic limit as $\epsilon \to 0$. We acknowledge that this approximation may reduce accuracy when ϵ is large. Developing an accurate and stable AP scheme that remains efficient for all ϵ, including $\epsilon = O(1)$, is an interesting direction for future work.
   For better clarification, we have revised lines 14-18 in p.8 as follows:
   The transport term $F_\varepsilon(\rho)$ and the turning operator T_ε introduced in (5) are highly nonlinear. To facilitate the design and analysis of an asymptotic preserving scheme based on micro-macro decomposition, a linearization of these terms is needed. From now on, we consider a slightly modified version of the kinetic model, where F_ε and T_ε are truncated to the first order in the expansions (9) and (10).

3. *Page 14 (line 27): The time step restriction strengthens as ϵ increases. Please explain and include results illustrating how Δt depends on ϵ. The scheme should function for $\epsilon = O(1)$, but results for large ϵ are lacking.*

   To illustrate the dependency of the time step on ϵ, we have introduced Fig. 1 in the revised manuscript. This figure assesses the stability and boundedness of solutions up to time $T = 40$ in 1D simulations, indicating appropriate time steps. Additionally, a second plot within Fig. 1 shows that the total computational cost increases significantly for large ϵ due to the necessity of using extremely small time steps for stability, resulting in a substantial increase in the number of time steps required. Further explanations are provided in p15:
   Although the numerical scheme (29) works well in the diffusion limit $\varepsilon \to 0$, it is conditionally stable, and numerical experiments show that the restrictions on time step Δt might be quite strong for large ε values. In Figure 1, we evaluate the stability and computational efficiency of the scheme for different time steps and ε values. As demonstrated, maintaining stability for large values of ε requires significantly small time steps, which in turn greatly increases computational costs. Consequently, in subsequent 1D simulations, we limit ε to a maximum of 0.2 to avoid overly restrictive time step constraints. The instability observed for large values of ε is mainly due to the failure of the AP scheme to ensure the boundedness of the kinetic solution. Although it has been proven that the scheme ensures boundedness for the macroscopic limit model with sufficiently small time steps, no such theoretical result exists for the full kinetic model. This highlights a limitation of the current scheme in the kinetic regime with $\varepsilon = O(1)$, and addressing this issue will be an important direction for future work.

4. *Figure 2: The energy defined in (41) decreases for the kinetic model with nonzero ϵ. Does the kinetic model have an energy dissipation structure? Please elaborate.*

   We thank the reviewer for this remark. We added a remark in this direction in p16:
   Consistent with the analysis of Section 2.3, we recover that the energy is decreasing in time for the macroscopic model. It is noteworthy that the energy defined by (41) also decreases along the solutions of the kinetic model for $\epsilon > 0$. These numerical results indicate that the kinetic model may possess an energy dissipation structure, the formal proof of which is left for future work.

5. *Page 16 (Figure 3, left): The claim that frequent interactions delay aggregation is incorrect. Different ϵ values rescale the system differently, affecting physical time recovery. Consider both ϵ and t when discussing aggregation times.*

   We thank the referee for this comment. We moved the interpretation of the aggregation times to p16 together with the following explanation:
   In Figure 4 (left) we see formations of aggregates at $t = 5$ and around $t = 32$, in agreement with Figure 3. For the different values of ε we observe that the formation of the aggregate at $t = 32$ occurs at different times, i.e., the kinetic model seems to converge faster to the "aggregated-state" compared to the macroscopic dynamics. These changes in speed could be a result of the diffusion scaling, where the macroscopic model is obtained in a regime where there are many velocity jumps but small net displacements in one order of time (see [3,35,15,34]] for thorough interpretations of the diffusion scaling).

6. *Section 6: Compare aggregation patterns between kinetic and macroscopic models in 2D simulations. Examining aggregation for varying ϵ in Figure 6 would be more informative than just confirming agreement between kinetic and macroscopic limits.*

   We appreciate the suggestion. To better illustrate the convergence of aggregation patterns as $\varepsilon \to 0$, we have replaced Figure 7 (originally Figure 6), which now offers a clearer visualization of the transition from kinetic to macroscopic regimes. This supports the asymptotic consistency of the proposed scheme.