

Fractional diffusion equations modeling chemotaxis

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Abstract

In this work, published in [2], we are interested in the microscopic description of fractional diffusion chemotactic models. We will use the kinetic framework of collisional equations having a heavy-tailed distribution as equilibrium state (see [4]) and take an adequate hydrodynamic scaling to deduce the fractional Keller–Segel system for the cell dynamics. In addition, we use this frame to deduce some models for chemotaxis with fractional diffusion including biological effects and non standard drift terms.

Introduction: anomalous diffusion and heavy tail kinetic relaxation model

Classically, **macroscopic diffusion** is obtained as the description of the spatiotemporal distribution of a population density of random walkers. However, in many situations found in Nature, **Lévy flights** are commonly adopted as an efficient search strategy of living organisms to diffuse. The correct description of such a population is given by the substitution of the Laplacian operator by a fractional operator of the Riesz type, defined from its Fourier transform [3]:

$$\widehat{(-\Delta_x)^{\frac{\alpha}{2}}}\rho := -|k|^\alpha \hat{\rho}, \quad 1 < \alpha < 2. \quad (1)$$

The **microscopic description** of these phenomena consists in describing the movement of cells/bacteria by a “run & tumble” process. They move along a straight line in the running phase and make reorientation as a reaction to the surrounding chemicals during the tumbling phase. The kinetic equation reads:

$$\partial_t f + v \cdot \nabla_x f = L(S, f) := \overbrace{\frac{1}{\tau_0} (F(v)\rho - f)}^{\text{Relaxation}} + \overbrace{\frac{1}{\tau_1} \int_{\mathbb{R}^N} (T[S]_{v' \rightarrow v} f(v') - T[S]_{v \rightarrow v'} f(v)) dv'}^{\text{Turning depending on } S} + \overbrace{\widehat{R(f, S)}}^{\text{Biol. interact.}}$$

$$\partial_t S = D \Delta_x S + \beta \rho - \mu S = \text{classical diffusion} + \text{production term due to bacteria} + \text{natural destruction.}$$

The operator L =relaxation+turning+biological interaction, models the change of direction of cells and S stands for the chemical concentration. For our purposes, the **equilibrium function** $F(v)$ correspond to a heavy tailed function with **infinite kinetic energy**:

$$F(-v) = F(v), \quad F(v) \stackrel{|v| > c_0}{=} \frac{K_0}{|v|^{N+\gamma+1}}, \quad 0 < \gamma < 1, \quad \int_{\mathbb{R}^N} F(v) dv = 1. \quad (2)$$

Anomalous “parabolic” scaling of the model

The non-dimensional version of the kinetic system reads:

$$\partial_t f + \alpha v \cdot \nabla_x f = \frac{\alpha}{\beta} (\rho F - f) + \theta \int_{\mathbb{R}^N} \overbrace{(T[S_\varepsilon]_{v' \rightarrow v} f_\varepsilon(v') - T[S_\varepsilon]_{v \rightarrow v'} f_\varepsilon(v))}^{L_1(S_\varepsilon, f_\varepsilon)} dv' + \theta_2 \text{ Biol. interac.},$$

$$\partial_t S = \tilde{D} \Delta_x S + \rho - \tilde{\nu} S.$$

where α is the scaled root-mean-square velocity, and β is the scaled mean free path associated to the main relaxation time τ_0 . θ is the dimensionless secondary frequency,

Following [1] we can fix the hydrodynamical “hyperbolic” scale by calling $\beta = \varepsilon$ and $\alpha = \frac{1}{\varepsilon^\gamma}$ (the typical velocity is **small, at an intermediate order**, compared with the r.m.s velocity c_0). Taking finally the secondary frequency (as in the parabolic case): $(\tau_1)^{-1} = \varepsilon^\gamma (\tau_0)^{-1}$, the kinetic eq. reads:

$$\varepsilon^{1+\gamma} \partial_t f_\varepsilon + \varepsilon v \cdot \nabla_x f_\varepsilon = (\rho_\varepsilon F - f_\varepsilon) + \varepsilon^\gamma L_1(S_\varepsilon, f_\varepsilon) + \varepsilon^{\gamma+1} R(f_\varepsilon, S_\varepsilon), \quad (\text{APS})$$

Actually in the **pure limiting hyperbolic case**, $\gamma = 0$, they are equivalent velocities and, in the other limiting case, $\gamma = 1$, we arrive to the **classical parabolic limit** (where the equilibrium F has finite energy).

Formal limit via Fourier transform

Aim: pass to the limit on the continuity equation (obtained by integration on (APS) with respect to dv),

$$\partial_t \rho_\varepsilon + \text{div}_x j_\varepsilon = \int_{\mathbb{R}^N} R(f_\varepsilon, S_\varepsilon) dv, \quad \text{where the current } j_\varepsilon \text{ is} \quad j_\varepsilon = \frac{1}{\varepsilon^\gamma} \int_{\mathbb{R}^N} v f_\varepsilon dv.$$

by identifying the limit of the current from the first order moment eq. (integrating (APS) w.r. to $\frac{v dv}{\varepsilon^\gamma}$):

$$-j_\varepsilon = \underbrace{\varepsilon^{1-\gamma} \text{Div}_x \int_{\mathbb{R}^N} v \otimes v f_\varepsilon dv}_{\downarrow} - \underbrace{\int_{\mathbb{R}^N} v L_1(S_\varepsilon, f_\varepsilon) dv}_{\downarrow} + \underbrace{\varepsilon^{1+\gamma} \partial_t j_\varepsilon + \varepsilon R(f_\varepsilon, S_\varepsilon)}_{\downarrow} \quad (3)$$

[0 ∞] \mapsto fractional diffusion chemotaxis (drift) cancel.

This becomes workable by taking **Fourier transform** ($\mathcal{F}_{x \rightarrow k}$) in (3) and (APS), obtaining

$$\hat{j}_\varepsilon = \hat{\rho}_\varepsilon \int_{\mathbb{R}^N} \varepsilon^{1-\gamma} \frac{i(v \cdot k) v F(v)}{1 - \varepsilon v \cdot k i} dv + \int_{\mathbb{R}^N} v \mathcal{F}(L_1(S_\varepsilon, \frac{\hat{\rho}_\varepsilon F(v)}{1 - \varepsilon v \cdot k i})) dv + \mathcal{O}(\varepsilon^\gamma) = A_1 + A_2 + \mathcal{O}(\varepsilon^\gamma). \quad (4)$$

Then, we can prove rigorously the following convergence results:

Lemma: Let $0 < \gamma < 1$, $k \in \mathbb{R}^N$, and assume F is a positive continuous function verifying (2). Then

- $A_1 \rightarrow D_\rho i k |k|^{\gamma-1}$ with “diffusion” coefficient given by $D_\rho = \int_{\mathbb{R}^N} \frac{y_1^2}{1 + y_1^2} \frac{1}{|y|^{N+\gamma+1}} dy$.
- $A_2 \rightarrow \Psi(\rho, S) := \int_{\mathbb{R}^N} v \mathcal{F}(L_1(S, \rho F)) dv$.
- $\int_{\mathbb{R}^N} R(f_\varepsilon, S_\varepsilon) dv \rightarrow \Gamma(\rho, S) = \int_{\mathbb{R}^N} R(\rho F(v), S) dv$.

We can then pass to the limit in the expression (4) after taking **Inverse Fourier transform** denoted by \mathcal{F}^{-1} :

$$\partial_t \rho = -D_\rho \text{div}_x \left(\mathcal{F}^{-1} \left(i \hat{\rho} k |k|^{\gamma-1} \right) \right) - \text{div}_x \left(\mathcal{F}^{-1} (\Psi(\rho, S)) \right) + \Gamma(\rho, S).$$

To compute the first term on the r.h.s. we take again Fourier transform to write:

$$\mathcal{F} \left(\text{div}_x \left(\mathcal{F}^{-1} \left(i \hat{\rho}_\varepsilon k |k|^{\gamma-1} \right) \right) \right) = -i k \cdot \mathcal{F} \left(\mathcal{F}^{-1} \left(i \hat{\rho} k |k|^{\gamma-1} \right) \right) = |k|^{\gamma+1} \hat{\rho},$$

that is, the **fractional diffusion operator** (1) in Fourier coordinates: Finally, noting that

$$\mathcal{F}^{-1} (\Psi(\rho, S)) = \mathcal{F}^{-1} \int_{\mathbb{R}^N} v \mathcal{F}(L_1(S, \rho F)) dv = \int_{\mathbb{R}^N} v L_1(S, \rho F) dv = \rho \int_{\mathbb{R}^N} v L_1(S, F) dv =: H(\rho, S),$$

we obtain the **main Theorem**, the limiting macroscopic equation.

$$\partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho - \text{div}_x (H(\rho, S)) + \Gamma(\rho, S). \quad (5)$$

Some fundamentals of fractional Chemotaxis

Let us present several choices of functions T_1 and R , and thus of H and Γ , which will produce a fractional diffusion macroscopic system corresponding to some known models of chemotaxis. We will examine several forms for the dependence of the kernel on S and its gradient, some of which lead to the **fractional Keller–Segel chemotaxis model**. Precisely, we investigate how the classical chemotaxis equations can be obtained from the microscopic description delivered by our model, as well as some more precise approaches to the several phenomena described in the literature.

Fractional Keller–Segel type models. The choice $\overline{T[S]_{v' \rightarrow v}} = \phi(v, v', S) \cdot \nabla_x S$, where $\phi(v, v', S)$ is a vector valued function, leads to the chemotactic term $H(\rho, S) = \rho \chi(S) \nabla_x S$, where the chemotactic sensitivity $\chi(S)$ is given by the matrix $\chi(S) = \int_{\mathbb{R}^N} \int_{\mathbb{R}^N} v \otimes \left(F(v') \phi(v, v', S) - F(v) \phi(v', v, S) \right) dv dv'$. Therefore, (5) coupled with the equation for S becomes the fractional Keller–Segel (type) model

$$\begin{cases} \partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho - \text{div}_x (\rho \chi(S) \nabla_x S) + \Gamma(\rho, S), \\ \partial_t S = D_S \Delta_x S + \beta \rho - \mu S, \end{cases} \quad (6)$$

with D_ρ , and Γ given by **Lemma**. Let us see some **particular cases** of (6) existing on the literature (see [2]).

<p>In 1–D, with $\phi(v, v', S)$ independent of S and $R(f, S) = 0$, the chemotactic sensitivity becomes constant, and we obtain the following system,</p> $\begin{cases} \partial_t \rho + \chi \partial_x (\rho \partial_x S) = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho \\ \partial_t S = D_S \Delta_x S + \beta \rho - \mu S. \end{cases}$	<p>In 2–D with $\phi(v, v', S)$ independent of S and $R(f, S) = 0$, and considering the stationary equation of Poisson type for S: $-\Delta_x S = \rho$, then, system (6) becomes</p> $\partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho + \text{div}_x \left(\rho \chi \nabla_x (\Delta_x^{-1} \rho) \right).$
<p>Taking $R(f, S) = r \left(1 - \frac{f}{\int_{\mathbb{R}^N} F^2(v) dv} \right) f$, then Γ becomes a logistic growing term $\Gamma(\rho, S) = r \rho (1 - \rho)$:</p> $\partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho - \text{div}_x (\rho \chi(S) \nabla_x S) + r \rho (1 - \rho), \quad \partial_t S = D_S \Delta_x S + \beta \rho - \mu S,$ <p>which generalizes a cell kinetic model describing a pattern formation of moving and growing bacteria.</p>	
<p>Taking $R(f, S) = \left(a_0 + a_1 \frac{f}{\int_{\mathbb{R}^N} F^2(v) dv} - a_2 \int_{\mathbb{R}^N} \rho dx \right) f$, for constants $a_0, a_1 \geq 0$, and $a_2 \in \mathbb{R}$, (6) becomes:</p> $\partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho - \text{div}_x (\rho \chi(S) \nabla_x S) + \rho \left(a_0 + a_1 \rho - a_2 \int_{\mathbb{R}^N} \rho dx \right), \quad \partial_t S = D_S \Delta_x S + \beta \rho - \mu S,$ <p>which describe a competitive system under chemotactic effects with non-local reaction terms. The coefficient a_0, sometimes also called Malthusian parameter, induces an exponential growth for low density populations. At the time that the population grows, the competitive effect of the local term $a_1 \rho^2$ becomes more influential. The non-local term $\rho a_2 \int_{\mathbb{R}^N} \rho dx$ describes the influence of the total mass of the species in the growth of the population.</p>	

Optimal drift following the chemoattractant Finally, The choice $\overline{T_1(S, v, v')} = \phi(v, v', S) \cdot Q(\nabla_x S)$, with a smooth bounded flux function $Q: \mathbb{R}^N \rightarrow \mathbb{R}^N$, satisfying $Q(0) = 0$, and $\partial_{y_i} Q_i > 0$, produces a chemosensitive term of the form $H(\rho, S) = \rho \chi(S) Q(\nabla_x S)$, where $\chi(S)$ is still given by the expression above. The model then reads:

$$\begin{cases} \partial_t \rho = -D_\rho (-\Delta_x)^{\frac{\gamma+1}{2}} \rho - \text{div}_x (\rho \chi(S) Q(\nabla_x S)) + \Gamma(\rho, S), \\ \partial_t S = D_S \Delta_x S + G(\rho, S). \end{cases} \quad (7)$$

So, we obtain a more general model of fractional Keller–Segel type, which includes the **boundedness of the chemotactic flux function**. A typical example is: where y^* is a threshold parameter defining a small gradient value under which the system (7) reduces to the original fractional Keller–Segel (6), whereas the effect of saturation is felt at large gradient regimes only. Note finally that for $y^* = 0$, the flux becomes a mean curvature type function: $Q(\nabla_x S) = \frac{\nabla_x S}{\sqrt{1 + |\nabla_x S|^2}}$.

Generalization of the result

We can generalize the convergence result for a more general class of relaxation (turning type) operators, following Ref. [4]. We the consider the following kinetic equation, still coupled with a macroscopic equation for the chemical concentration S , (we omit the biological interactions $R(f, S)$):

$$\partial_t f + v \cdot \nabla_x f = \overbrace{\left(K(f) - \nu(v) f(v) \right)}^{L_0(f)} + \overbrace{\left(L_1(S, f) \right)}^{\text{turning}}, \quad K(f) := \int_{\mathbb{R}^N} T_0(v, v') f(v') dv', \quad \nu(v) := \int_{\mathbb{R}^N} T_0(v', v) dv'.$$

Assumptions: Detailed balance principle: $T_0(v, v') F(v') = T_0(v', v) F(v)$, $\forall v, v' \in \mathbb{R}^N$, for a certain function F . In particular, $K(F) = \nu(v) F(v)$. There exist $\beta \geq 0$, $\gamma, \kappa_0, \nu_0 > 0$, a positive function $F_0(v)$ and a slow varying function l such that $F(v) = F_0(v) l(|v|)$, satisfying $|v|^{N+\gamma+1} F_0 \rightarrow \kappa_0$ and $|v|^{-\beta} \nu(v) \rightarrow \nu_0$, as $|v| \rightarrow \infty$ +integrability, symmetry and positivity conditions

We can now define the scaling, $m(\varepsilon) = \varepsilon^r l(\varepsilon^{\frac{-1}{1-\beta}})$, where $r = \frac{1+\gamma-\beta}{1-\beta} = 1 + \frac{\gamma}{1-\beta}$, and l is the slow varying function given in the assumptions. In this case, the kinetic equation reads

$$m(\varepsilon) \partial_t f_\varepsilon + \varepsilon v \cdot \nabla_x f_\varepsilon = L_0(f_\varepsilon) + \frac{m(\varepsilon)}{\varepsilon} L_1(S_\varepsilon, f_\varepsilon),$$

and the limit can be performed, obtaining

$$\partial_t \rho + \text{div}_x \mathcal{H}(\rho, S) = -D_\rho (-\Delta_x)^{\frac{\gamma}{2}} \rho, \quad \mathcal{H}(\rho, S) = \rho \int_{\mathbb{R}^N} v L_1(S, F) \frac{dv}{\nu(v)}, \quad D_\rho = \frac{\kappa_0 \nu_0}{1 - \beta} \int_{\mathbb{R}^N} \frac{(y_1)^2}{\nu_0^2 + (y_1)^2}.$$

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