VERIFICATION OF BIOMEDICAL PROCESSES WITH ANOMALOUS DIFFUSION, TRANSPORT AND INTERACTION OF SPECIES

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Abstract: The paper deals with the easily verifiable necessary condition of the preservation of the nonnegativity of the solutions of a system of parabolic equations in the case of the anomalous diffusion with the Laplace operator in a fractional power in one dimension. This necessary condition is vitally important for the applied analysis society because it imposes the necessary form of the system of equations that must be studied mathematically.

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1. Introduction

The solutions of many systems of convection-diffusion-reaction equations arising in biology, physics or engineering describe such quantities as population densities, pressure or concentrations of nutrients and chemicals. Thus, a natural property to require for the solutions is the nonnegativity. Models that do not guarantee the nonnegativity are not valid or break down for small values of the solution. In many cases, showing that a particular model does not preserve the nonnegativity leads to the better understanding of the model and its limitations. One of the first steps in analyzing ecological or biological or bio-medical models mathematically is to test whether solutions originating from the nonnegative initial data remain nonnegative (as long as they exist). In other words, the model under consideration ensures that the nonnegative cone is positively invariant. We recall that if the solutions (of a given evolution PDE) corresponding to the nonnegative initial data remain nonnegative as long as they exist, we say that the system satisfies the nonnegativity property.

For scalar equations the nonnegativity property is a direct consequence of the maximum principle (see [2] and the references therein). However, for systems of equations the maximum principle is not valid. In the particular case of monotone systems the situation resembles the case of scalar equations, sufficient conditions for preserving the nonnegative cone can be found in [2].

In this paper we aim to prove a simple and easily verifiable criterion, that is, the necessary condition for the nonnegativity of solutions of systems of nonlinear convection-anomalous diffusion-reaction equations arising in the modelling of life sciences. We believe that it could provide the modeler with a tool, which is easy to verify, to approach the question of positive invariance of the model.

The present article deals with the preservation of the nonnegativity of solutions of the following system of reaction-diffusion equations

$$\frac{\partial u}{\partial t} = -A(-\Delta_x)^s u + \sum_{l=1}^{m} \Gamma^l \frac{\partial u}{\partial x_l} - F(u), \tag{1.1}$$

where $A,\ \Gamma^l,\ 1 \le l \le m$ are $N \times N$ matrices with constant coefficients, which is relevant to the cell population dynamics in Mathematical Biology. We call system (1.1) as a (N, m) one. Note that the analogous model can be used to study such branches of science as the Damage Mechanics, the temperature distribution in Thermodynamics. In the present article the space variable x corresponds to the cell genotype, $u_k(x,t)$ stands for the cell density distributions for various groups of cells as functions of their genotype and time,

$$u(x,t) = (u_1(x,t), u_2(x,t), ..., u_N(x,t))^T.$$

The operator $(-\Delta_x)^s$ in problem (1.1) describes a particular case of anomalous diffusion actively treated in the context of different applications in plasma physics and turbulence [4], [1], surface diffusion [5], [7], semiconductors [8] and so on. Anomalous diffusion can be described as a random process of particle motion characterized by the probability density distribution of jump length. The moments of this density distribution are finite in the case of normal diffusion, but this is not the case for superdiffusion. Asymptotic behavior at infinity of the probability density function determines the value s of the power of the Laplacian [6]. The operator $(-\Delta_x)^s$ is defined by virtue of the spectral calculus. For the simplicity of presentation we will treat the case of the one spatial dimension with $0 < s < 1/4$. Front propagation problems with anomalous diffusion were studied actively in recent years (see e.g. [9], [10]). The solvability of the single equation containing the Laplacian with drift relevant to the fluid mechanics was treated in [11]. We assume here that (1.1) contains the square matrices with the entries constant in space and time

$$(A)_{k,j} := a_{k,j}, \quad (\Gamma)_{k,j} := \gamma_{k,j}, \quad 1 \le k, j \le N$$

and that the matrix $A + A^* > 0$ for the sake of the global well posedness of system (1.1). Here A^* stands for the adjoint of matrix A. Hence, problem (1.1) can be rewritten in the form

$$\frac{\partial u_k}{\partial t} = -\sum_{j=1}^{N} a_{k,j}\left(-\frac{\partial^2}{\partial x^2}\right)^s u_j + \sum_{j=1}^{N} \gamma_{k,j}\frac{\partial u_j}{\partial x} - F_k(u), \quad 1 \le k \le N, \tag{1.2}$$

with $0 < s < \dfrac{1}{4}$. In the present work the interaction of species term

$$F(u) = (F_1(u), F_2(u), ..., F_N(u))^T,$$

which can be linear, nonlinear or in principle even nonlocal. We assume its smoothness in the theorem below for the sake of the well posedness of our system (1.1), although, we are not focused on the well posedness issue in the present article. Let us choose the space dimension $d = 1$, which is related to the solvability conditions for the linear Poisson type problem (4.14) stated in Lemma 2 below. From the perspective of applications, the space dimension is not restricted to $d = 1$ because the space variable corresponds to cell genotype but not to the usual physical space. We denote the inner product as

$$(f(x), g(x))_{L^2(\mathbb{R})} := \int_{-\infty}^{\infty} f(x)\bar{g}(x)dx, \tag{1.3}$$

with a slight abuse of notations when the functions involved in (1.3) are not square integrable, like for example the one present in orthogonality relations (4.17) and (4.18) of Lemma 2 below. Indeed, if $f(x) \in L^1(\mathbb{R})$ and $g(x)$ is bounded , then the integral in the right side of (1.3) makes sense. As for the vector functions, their inner product is defined using their components as

$$(u, v)_{L^2(\mathbb{R},\mathbb{R}^N)} := \sum_{k=1}^{N} (u_k, v_k)_{L^2(\mathbb{R})}. \tag{1.4}$$

Clearly, (1.4) induces the norm

$$\|u\|^2_{L^2(\mathbb{R},\mathbb{R}^N)} = \sum_{k=1}^{N} \|u_k\|^2_{L^2(\mathbb{R})}.$$

We use the Sobolev spaces

$$H^{2s}(\mathbb{R}) := \left\{ u(x) : \mathbb{R} \to \mathbb{R} \mid u(x) \in L^2(\mathbb{R}),\ \left(-\frac{d^2}{dx^2}\right)^s u \in L^2(\mathbb{R}) \right\}, \quad 0 < s \le 1$$

equipped with the norm

$$\|u\|^2_{H^{2s}(\mathbb{R})} := \|u\|^2_{L^2(\mathbb{R})} + \left\| \left(-\frac{d^2}{dx^2} \right)^s u \right\|^2_{L^2(\mathbb{R})}. \tag{1.5}$$

By the nonnegativity of a vector function below we mean the nonnegativity of the each of its components. Our main statement is as follows.

Theorem 1. *Let $F : \mathbb{R}^N \to \mathbb{R}^N$, such that $F \in \mathbb{C}^1$, the initial condition for system (1.1) is $u(x,0) = u_0(x) \geq 0$ and $u_0(x) \in L^2(\mathbb{R}, \mathbb{R}^N)$. We also assume that the off diagonal element of the matrix A, are nonnegative, such that*

$$a_{k,l} \geq 0, \quad 1 \leq k,l \leq N, \quad k \neq l. \tag{1.6}$$

Then the necessary condition for problem (1.1) to admit a solution $u(x,t) \geq 0$ for all $t \in [0,\infty)$ is that the matrices A and Γ are diagonal and for all $1 \leq k \leq N$

$$F_k(u_1(x), ..., u_{k-1}(x), 0, u_{k+1}(x), ..., u_N(x)) \leq 0 \tag{1.7}$$

holds a.e., where $u_l(x) \geq 0$ and $u_l(x) \in L^2(\mathbb{R})$ with $1 \leq l \leq N, \ l \neq k$.

Remark 1. *In the case of the linear interaction of species, namely when $F(u) = Lu$, where L is a matrix with elements $b_{i,j}, \ 1 \leq i,j \leq N$ constant in space and time, our necessary condition leads to the condition that the matrix L must be essentially nonpositive, that is $b_{i,j} \leq 0$ for $i \neq j, \ 1 \leq i,j \leq N$.*

Remark 2. *Our proof implies that, the necessary condition for preserving the nonnegative cone is carried over from the ODE (the spatially homogeneous case, as described by the ordinary differential equation $u'(t) = -F(u)$) to the case of the anomalous diffusion and the convective drift term.*

Remark 3. *In the forthcoming papers we intend to consider the following cases:*
a) the necessary and sufficient conditions of the present work,
b) the nonautonomous version of the present work,
c) the density-dependent diffusion matrix,
d) the effect of the delay term in the cases a), b) and c).

Let us proceed to the proof of our main result.

2. The preservation of the nonnegativity of the solution of the system of parabolic equations

Proof of Theorem 1. Let us note that the maximum principle actively used for the studies of solutions of single parabolic equations does not apply to systems of such equations. We consider a time independent, square integrable vector function $v(x)$ and estimate

$$\left(\frac{\partial u}{\partial t}\bigg|_{t=0}, v\right)_{L^2(\mathbb{R},\mathbb{R}^N)} = \left(\lim_{t\to 0}\frac{u(x,t)-u_0(x)}{t}, v(x)\right)_{L^2(\mathbb{R},\mathbb{R}^N)}.$$

By means of the continuity of the inner product, the right side of the identity above equals to

$$\lim_{t\to 0}\frac{(u(x,t),v(x))_{L^2(\mathbb{R},\mathbb{R}^N)}}{t} - \lim_{t\to 0}\frac{(u_0(x),v(x))_{L^2(\mathbb{R},\mathbb{R}^N)}}{t}. \tag{2.8}$$

Let us choose the initial condition for our system $u_0(x) \geq 0$ and the constant in time vector function $v(x) \geq 0$ to be orthogonal to each other in $L^2(\mathbb{R},\mathbb{R}^N)$. This can be achieved, for instance for

$$u_0(x) = (\tilde{u}_1(x), ..., \tilde{u}_{k-1}(x), 0, \tilde{u}_{k+1}(x), ..., \tilde{u}_N(x)), \quad v_j(x) = \tilde{v}(x)\delta_{j,k}, \tag{2.9}$$

with $1 \leq j \leq N$, where $\delta_{j,k}$ is the Kronecker symbol and $1 \leq k \leq N$ is fixed. Therefore, the second term in (2.8) vanishes and (2.8) equals to

$$\lim_{t\to 0}\frac{\sum_{k=1}^N \int_{-\infty}^{\infty} u_k(x,t)v_k(x)dx}{t} \geq 0$$

due to the nonnegativity of all the components $u_k(x,t)$ and $v_k(x)$ involved in the formula above. Thus, we arrive at

$$\sum_{j=1}^N \int_{-\infty}^{\infty} \frac{\partial u_j}{\partial t}\bigg|_{t=0} v_j(x)dx \geq 0.$$

By virtue of (2.9), only the k th component of the vector function $v(x)$ is nontrivial. This yields

$$\int_{-\infty}^{\infty} \frac{\partial u_k}{\partial t}\bigg|_{t=0} \tilde{v}(x)dx \geq 0.$$

Hence, via (1.2) we arrive at

$$\int_{-\infty}^{\infty}\Bigg[-\sum_{j=1,\, j\neq k}^N a_{k,j}\left(-\frac{\partial^2}{\partial x^2}\right)^s \tilde{u}_j(x) + \sum_{j=1,\, j\neq k}^N \gamma_{k,j}\frac{\partial \tilde{u}_j}{\partial x} -$$

$$-F_k(\tilde{u}_1(x), ..., \tilde{u}_{k-1}(x), 0, \tilde{u}_{k+1}(x), ..., \tilde{u}_N(x))\Bigg]\tilde{v}(x)dx \geq 0.$$

Since the nonnegative, square integrable function $\tilde{v}(x)$ can be chosen arbitrarily, we obtain

$$-\sum_{j=1,\ j\neq k}^{N} a_{k,j}\left(-\frac{\partial^2}{\partial x^2}\right)^s \tilde{u}_j(x)+\sum_{j=1,\ j\neq k}^{N} \gamma_{k,j}\frac{\partial \tilde{u}_j}{\partial x}-$$

$$-F_k(\tilde{u}_1(x),...,\tilde{u}_{k-1}(x),0,\tilde{u}_{k+1}(x),...,\tilde{u}_N(x))\geq 0 \quad a.e. \tag{2.10}$$

For the purpose of the scaling, let us replace all the $\tilde{u}_j(x)$ by $\tilde{u}_j\left(\dfrac{x}{\varepsilon}\right)$ in the inequality above, where $\varepsilon>0$ is a small parameter. This yields

$$-\sum_{j=1,\ j\neq k}^{N} \frac{a_{k,j}}{\varepsilon^{2s}}\left(-\frac{\partial^2}{\partial y^2}\right)^s \tilde{u}_j(y)+\sum_{j=1,\ j\neq k}^{N} \frac{\gamma_{k,j}}{\varepsilon}\frac{\partial \tilde{u}_j(y)}{\partial y}-$$

$$-F_k(\tilde{u}_1(y),...,\tilde{u}_{k-1}(y),0,\tilde{u}_{k+1}(y),...,\tilde{u}_N(y))\geq 0 \quad a.e. \tag{2.11}$$

Clearly, the second term in the left side of (2.11) is the leading one as $\varepsilon\to 0$. In the case of $\gamma_{k,j}>0$ we can choose here $\tilde{u}_j(y)=e^{-y}$ in a neighborhood of the origin, smooth and decaying to zero at the infinities. If $\gamma_{k,j}<0$, then we can pick $\tilde{u}_j(y)=e^{y}$ around the origin and tending to zero at the infinities. Then the left side of (2.11) can be made as negative as possible which will violate inequality (2.11). Note that the last term in the left side of (2.11) will remain bounded. Therefore, for the matrix Γ involved in problem (1.1), the off diagonal terms should vanish, such that

$$\gamma_{k,j}=0, \quad 1\leq k,j\leq N, \quad k\neq j.$$

Therefore, from (2.11) we obtain

$$-\sum_{j=1,\ j\neq k}^{N} \frac{a_{k,j}}{\varepsilon^{2s}}\left(-\frac{\partial^2}{\partial y^2}\right)^s \tilde{u}_j(y)-$$

$$-F_k(\tilde{u}_1(y),...,\tilde{u}_{k-1}(y),0,\tilde{u}_{k+1}(y),...,\tilde{u}_N(y))\geq 0 \quad a.e. \tag{2.12}$$

Let us suppose that some of the $a_{k,j}$ involved in the sum in the left side of (2.12) are strictly positive. We choose here all the $\tilde{u}_j(y),\ 1\leq j\leq N,\ j\neq k$ to be identical. For the equation

$$-\left(-\frac{\partial^2}{\partial x^2}\right)^s \tilde{u}_j(x)=\tilde{v}_j(x), \quad 0<s<\frac{1}{4}, \tag{2.13}$$

we assume that its right side belongs to $C_c^\infty(\mathbb{R})$. Clearly, $\tilde{v}_j(x)\in L^1(\mathbb{R})\cap L^2(\mathbb{R})$ as well. Then by means of the part 1 of Lemma 2 below, (2.13) admits a unique solution $\tilde{u}_j(x)\in H^{2s}(\mathbb{R})$. Suppose the right side of (2.13) is nonnegative on the whole real line. By virtue of Section 5.9 of [3] we have the explicit formula

$$\tilde{u}_j(x)=-c_s\int_{-\infty}^{\infty}|x-y|^{2s-1}\tilde{v}_j(y)dy,$$

where $c_s > 0$ is a constant. Then $\tilde{u}_j(x)$ is negative on $\mathbb{R}$, which contradicts to our original assumption. Therefore, $\tilde{v}_j(x)$ has the points of negativity on the real line. By making the parameter ε small enough, we can violate the inequality in (2.12). Since the negativity of the off diagonal elements of the matrix A is ruled out due to assumption (1.6), we arrive at

$$a_{k,j} = 0, \quad 1 \le k, j \le N, \quad k \ne j.$$

Therefore, by means of (2.10) we obtain

$$F_k(\tilde{u}_1(x), ..., \tilde{u}_{k-1}(x), 0, \tilde{u}_{k+1}(x), ..., \tilde{u}_N(x)) \le 0 \quad a.e.,$$

where $\tilde{u}_j(x) \ge 0$ and $\tilde{u}_j(x) \in L^2(\mathbb{R})$ with $1 \le j \le N,\ j \ne k$. ∎

4. Auxiliary results

Below we state the solvability conditions for the linear Poisson type equation with a square integrable right side

$$\left(-\frac{d^2}{dx^2}\right)^s u = f(x), \quad x \in \mathbb{R}, \quad 0 < s < 1. \tag{4.14}$$

We have the following technical proposition. It can be easily derived by applying the standard Fourier transform

$$\widehat{\phi}(p) := \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(x) e^{-ipx} dx. \tag{4.15}$$

to both sides of problem (4.14) (see Lemma 1.6 of [13]). For the similar results in three dimensions see Lemma 5 of [12]. We will use the obvious upper bound

$$\|\widehat{\phi}(p)\|_{L^\infty(\mathbb{R})} \le \frac{1}{\sqrt{2\pi}} \|\phi(x)\|_{L^1(\mathbb{R})}. \tag{4.16}$$

We will provide the proof below for the convenience of the readers.

Lemma 2. *Let $f(x) : \mathbb{R} \to \mathbb{R}$ and $f(x) \in L^2(\mathbb{R})$.*
1) When $0 < s < \frac{1}{4}$ and in addition $f(x) \in L^1(\mathbb{R})$, equation (4.14) admits a unique solution $u(x) \in H^{2s}(\mathbb{R})$.

2) When $\frac{1}{4} \le s < \frac{3}{4}$ and additionally $|x|f(x) \in L^1(\mathbb{R})$, problem (4.14) possesses a unique solution $u(x) \in H^{2s}(\mathbb{R})$ if and only if the orthogonality relation

$$(f(x), 1)_{L^2(\mathbb{R})} = 0 \tag{4.17}$$

holds.

3) When $\frac{3}{4} \leq s < 1$ and in addition $x^2 f(x) \in L^1(\mathbb{R})$, equation (4.14) has a unique solution $u(x) \in H^{2s}(\mathbb{R})$ if and only if orthogonality conditions (4.17) and

$$(f(x), x)_{L^2(\mathbb{R})} = 0 \tag{4.18}$$

hold.

Proof. First, let us observe that by virtue of norm definition (1.5) along with the square integrability of the right side of (4.14), it would be sufficient to establish the solvability of equation (4.14) in $L^2(\mathbb{R})$. Clearly, the solution $u(x) \in L^2(\mathbb{R})$ will belong to $H^{2s}(\mathbb{R}),\ 0 < s < 1$ as well.

We prove the uniqueness of solutions for problem (4.14). If $u_{1,2}(x) \in H^{2s}(\mathbb{R})$ both solve (4.14), then the difference $w(x) := u_1(x) - u_2(x) \in L^2(\mathbb{R})$ satisfies the homogeneous equation

$$\left(-\frac{d^2}{dx^2}\right)^s w = 0.$$

Because the operator $\left(-\frac{d^2}{dx^2}\right)^s$ on the real line does not possess nontrivial square integrable zero modes, $w(x) = 0$ a.e. on $\mathbb{R}$.

We apply (4.15) to both sides of problem (4.14). This yields

$$\widehat{u}(p) = \frac{\widehat{f}(p)}{|p|^{2s}} \chi_{\{p \in \mathbb{R} \ | \ |p| \leq 1\}} + \frac{\widehat{f}(p)}{|p|^{2s}} \chi_{\{p \in \mathbb{R} \ | \ |p| > 1\}}, \tag{4.19}$$

where χ_A is the characteristic function of a set $A \subseteq \mathbb{R}$. Evidently, for all $0 < s < 1$ the second term in the right side of (4.19) is square integrable by means of the bound

$$\int_{-\infty}^{\infty} \frac{|\widehat{f}(p)|^2}{|p|^{4s}} \chi_{\{p \in \mathbb{R} \ | \ |p| > 1\}} dp \leq \|f\|^2_{L^2(\mathbb{R})} < \infty.$$

To establish the square integrability of the first term in the right side of (4.19) for $0 < s < \frac{1}{4}$, we apply inequality (4.16), which yields

$$\int_{-\infty}^{\infty} \frac{|\widehat{f}(p)|^2}{|p|^{4s}} \chi_{\{p \in \mathbb{R} \ | \ |p| \leq 1\}} dp \leq \frac{\|f(x)\|^2_{L^1(\mathbb{R})}}{\pi(1-4s)} < \infty.$$

This completes the proof of part 1) of our lemma.

To prove the solvability of problem (4.14) when $\frac{1}{4} \leq s < \frac{3}{4}$, we apply the formula

$$\widehat{f}(p) = \widehat{f}(0) + \int_0^p \frac{d\widehat{f}(s)}{ds} ds.$$

This enables us to express the first term in the right side of (4.19) as

$$\frac{\widehat{f}(0)}{|p|^{2s}} \chi_{\{p \in \mathbb{R} \ | \ |p| \leq 1\}} + \frac{\int_0^p \frac{d\widehat{f}(s)}{ds} ds}{|p|^{2s}} \chi_{\{p \in \mathbb{R} \ | \ |p| \leq 1\}}. \tag{4.20}$$

By means of definition (4.15)

$$\left|\frac{d\widehat{f}(p)}{dp}\right| \leq \frac{1}{\sqrt{2\pi}} \| |x| f(x) \|_{L^1(\mathbb{R})} < \infty$$

via the one of our assumptions. Thus,

$$\left|\frac{\int_0^p \frac{d\widehat{f}(s)}{ds} ds}{|p|^{2s}} \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}}\right| \leq \frac{1}{\sqrt{2\pi}} \| |x| f(x) \|_{L^1(\mathbb{R})} |p|^{1-2s} \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}} \in L^2(\mathbb{R}).$$

The remaining term in (4.20) $\dfrac{\widehat{f}(0)}{|p|^{2s}} \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}} \in L^2(\mathbb{R})$ if and only if $\widehat{f}(0) = 0$, which gives us orthogonality relation (4.17) in case 2) of the lemma.

Finally, it remains to study the situation when $\dfrac{3}{4} \leq s < 1$. For that purpose, we use the identity

$$\widehat{f}(p) = \widehat{f}(0) + p \frac{d\widehat{f}}{dp}(0) + \int_0^p \Big(\int_0^r \frac{d^2\widehat{f}(q)}{dq^2} dq \Big) dr.$$

This allows us to express the first term in the right side of (4.19) as

$$\left[\frac{\widehat{f}(0)}{|p|^{2s}} + \frac{p\frac{d\widehat{f}}{dp}(0)}{|p|^{2s}} + \frac{\int_0^p \Big(\int_0^r \frac{d^2\widehat{f}(q)}{dq^2} dq \Big) dr}{|p|^{2s}} \right] \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}}. \tag{4.21}$$

Definition (4.15) yields

$$\left|\frac{d^2\widehat{f}(p)}{dp^2}\right| \leq \frac{1}{\sqrt{2\pi}} \| x^2 f(x) \|_{L^1(\mathbb{R})} < \infty$$

as assumed. This enables us to estimate

$$\left|\frac{\int_0^p \Big(\int_0^r \frac{d^2\widehat{f}(q)}{dq^2} dq \Big) dr}{|p|^{2s}} \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}}\right| \leq \frac{1}{2\sqrt{2\pi}} \| x^2 f(x) \|_{L^1(\mathbb{R})} |p|^{2-2s} \chi_{\{p\in\mathbb{R} \mid |p|\leq 1\}},$$

which is clearly square integrable. The sum of the first and the second terms in (4.21) does not belong to $L^2(\mathbb{R})$ unless both $\widehat{f}(0)$ and $\dfrac{d\widehat{f}}{dp}(0)$ are equal to zero. This yields orthogonality relations (4.17) and (4.18) respectively. ∎

Let us note that the left side of relations (4.17) and (4.18) is well defined under the given conditions. For the lower values of the power of the negative second derivative operator $0 < s < \dfrac{1}{4}$ under the assumptions stated above no orthogonality relations are required to solve the linear Poisson type equation (4.14) in $H^{2s}(\mathbb{R})$.

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