ON THE NECESSARY CONDITIONS FOR PRESERVING THE NONNEGATIVE CONE: MIXED DIFFUSION

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Abstract: The article 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 mixed diffusion when the standard Laplacian in the first m variables is added to the Laplace operator in the rest of the variables in a fractional power in the space of an arbitary dimension. This necessary condition is crucial for the applied analysis community since it imposes the necessary form of the system of equations that must be treated mathematically.

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1. Introduction

The solutions of various 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. Hence, a natural property to require for the solutions is their nonnegativity. Models that do not guarantee the nonnegativity are not valid or break down for small values of the solution. In many situations, showing that a particular model fails to 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) which correspond 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 [9], [10]. For systems including the standard diffusion, transport and general interaction terms (not necessarily monotone) the necessary and sufficient conditions for preserving the nonnegative cones were obtained in [2].

In the present work 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-mixed 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 system of reaction-diffusion equations in the space of an arbitrary dimension $d \in \mathbb{N},\ d \geq 2$, namely

$$\frac{\partial u}{\partial t} = A[\alpha \Delta_{x,m} - \beta(-\Delta_{x,d-m})^s]u + \sum_{l=1}^{d} \Gamma^l \frac{\partial u}{\partial x_l} - F(u), \tag{1.1}$$

where the Laplace operators

$$\Delta_{x,m} := \sum_{l=1}^{m} \frac{\partial^2}{\partial x_l^2}, \quad \Delta_{x,d-m} := \sum_{l=m+1}^{d} \frac{\partial^2}{\partial x_l^2}, \quad 1 \leq m \leq d-1, \quad 0 < s < 1,$$

$A,\ \Gamma^l,\ 1 \leq l \leq d$ are $N \times N$ matrices with constant coefficients, which is relevant to the cell population dynamics in Mathematical Biology. Here $\alpha, \beta > 0$ are constants as well. The case of $\beta = 0$ corresponds to the normal diffusion treated in [2]. The situation when $\alpha = 0$ corresponds to the anomalous diffusion studied recently in [3]. As distinct from the present article, the power of the negative Laplace operator in [3] was restricted to $0 < s < \frac{1}{4}$ due to the solvability conditions for the Poisson type equation involving the fractional Laplacian in one dimension (see [14]). Note that the model analogous to (1.1) can be used to study such branches of science as the Damage Mechanics, the temperature distribution in Thermodynamics. In the present work 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 $(-\Delta_{x,d-m})^s$ in system (1.1) describes a particular case of the anomalous diffusion actively treated in the context of different applications in plasma physics and turbulence [1], [4], 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 the anomalous diffusion. Asymptotic behavior at infinity of the probability density function determines the value s of the power of the negative Laplacian [6]. The operator $(-\Delta_{x,d-m})^s$ is defined by virtue of the spectral calculus. Front propagation problems with anomalous diffusion were treated actively in recent years (see e.g. [11], [12]). The solvability of the single equation involving the Laplacian with drift relevant to the fluid mechanics was studied in [13]. Let us assume here that (1.1) contains the square matrices with the entries constant in space and time

$$(A)_{k,j} := a_{k,j}, \quad (\Gamma^l)_{k,j} := \gamma^l_{k,j}, \quad 1 \le k, j \le N, \quad 1 \le l \le d$$

and that the given matrix A is an $N \times N$ matrix with a positive symmetric part $A + A^* > 0$ (parabolicity assumption) for the sake of the well posedness of problem (1.1). Here A^* denotes the adjoint of matrix A. Hence, system (1.1) can be rewritten in the form

$$\frac{\partial u_k}{\partial t} = \sum_{j=1}^{N} a_{k,j}[\alpha \Delta_{x,m} - \beta(-\Delta_{x,d-m})^s] u_j + \sum_{l=1}^{d}\sum_{j=1}^{N} \gamma^l_{k,j} \frac{\partial u_j}{\partial x_l} - F_k(u), \tag{1.2}$$

where $1 \le k \le N$ and $0 < s < 1$. In the present article the interaction of species term

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

which in principle can be linear, nonlinear or even nonlocal. Let us assume its smoothness in the theorem below for the sake of the well posedness of our problem (1.1), although, we are not focused on the well posedness issue in the present work. From the perspective of applications, the space dimension can be chosen arbitrarily, $d \in \mathbb{N}, \ d \ge 2$ since the space variable here corresponds to the cell genotype but not to the usual physical space. Let us denote the inner product as

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

As for the vector functions, their inner product is defined using their components as

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

Obviously, (1.4) induces the norm

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

By the nonnegativity of a vector function below we mean the nonnegativity of the each of its components. Our concern is not the study of the existence of solutions but their qualitative behavior. Hence, in the sequel we assume that for any initial data

$$u_0 \in K^+ := \{u : \mathbb{R}^d \to \mathbb{R}^N \mid u_i(x,t) \geq 0 \; a.e. \; in \; \mathbb{R}^d, \; i = 1, ..., N\}$$

there exists a unique solution (satisfying the appropriate estimates) to carry out our calculations. Our main proposition is as follows.

Theorem 1. *Let $F : \mathbb{R}^N \to \mathbb{R}^N$, such that $F \in C^1$, the initial condition for problem (1.1) is $u(x,0) = u_0(x) \geq 0$ and $u_0(x) \in L^2(\mathbb{R}^d, \mathbb{R}^N), \; d, N \in \mathbb{N}, \; d, N \geq 2$. Then in order to preserve the non-negative cone for system (1.1) the necessary condition is that the matrices A and Γ are diagonal and for all $1 \leq k \leq N$*

$$F_k(s_1, ..., s_{k-1}, 0, s_{k+1}, ..., s_N) \leq 0 \tag{1.5}$$

holds , where $s_l \geq 0$ and $1 \leq l \leq N, \; l \neq k$.

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 yields that, the necessary condition for preserving the non-negative 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 density-dependent diffusion matrix,
c) the stochastic perturbation of the deterministic case,
d) the effect of the delay term in the cases a), b) and c).

Remark 4. *Note that in the present work as distinct from [3] we do not assume the nonnegativity of the off diagonal elements of the matrix A.*

We proceed to the proof of our main statement.

2. The preservation of the nonnegativity of the solution of the system with mixed diffusion

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

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

By virtue of the continuity of the inner product, the right side of the equality above is equal to

$$\lim_{t\to 0^+}\frac{(u(x,t),v(x))_{L^2(\mathbb{R}^d,\mathbb{R}^N)}}{t} - \lim_{t\to 0^+}\frac{(u_0(x),v(x))_{L^2(\mathbb{R}^d,\mathbb{R}^N)}}{t}. \tag{2.6}$$

We 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 $L^2(\mathbb{R}^d, \mathbb{R}^N)$. This can be achieved, for example for

$$u_0(x) = (\tilde{u}_1(x), ..., \tilde{u}_{k-1}(x), 0, \tilde{u}_{k+1}(x), ..., \tilde{u}_N(x)), \quad v_j(x) = \tilde{v}(x)\delta_{j,k}, \tag{2.7}$$

with $1 \leq j \leq N$, where $\delta_{j,k}$ is the Kronecker symbol and $1 \leq k \leq N$ is fixed. Hence, the second term in (2.6) vanishes and (2.6) is equal to

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

by means of the nonnegativity of all the components $u_k(x,t)$ and $v_k(x)$ involved in the formula above. Hence, we obtain

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

By means of (2.7), only the k th component of the vector function $v(x)$ is nontrivial. This gives us

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

Therefore, by means of (1.2) we derive

$$\int_{\mathbb{R}^d}\Bigg[\sum_{j=1,\ j\neq k}^N a_{k,j}[\alpha\Delta_{x,m} - \beta(-\Delta_{x,d-m})^s]\tilde{u}_j(x) + \sum_{l=1}^d \sum_{j=1,\ j\neq k}^N \gamma_{k,j}^l \frac{\partial \tilde{u}_j}{\partial x_l} -$$

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

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

$$\sum_{j=1,\ j\neq k}^{N} a_{k,j}[\alpha\Delta_{x,m} - \beta(-\Delta_{x,d-m})^s]\tilde{u}_j(x) + \sum_{l=1}^{d}\sum_{j=1,\ j\neq k}^{N} \gamma_{k,j}^l \frac{\partial \tilde{u}_j}{\partial x_l} -$$

$$-F_k(\tilde{u}_1(x), ..., \tilde{u}_{k-1}(x), 0, \tilde{u}_{k+1}(x), ..., \tilde{u}_N(x)) \geq 0 \quad a.e. \tag{2.8}$$

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

$$\sum_{j=1,\ j\neq k}^{N} a_{k,j}\left[\frac{\alpha}{\varepsilon^2}\Delta_{y,m} - \frac{\beta}{\varepsilon^{2s}}(-\Delta_{y,d-m})^s\right]\tilde{u}_j(y) + \sum_{l=1}^{d}\sum_{j=1,\ j\neq k}^{N} \frac{\gamma_{k,j}^l}{\varepsilon}\frac{\partial \tilde{u}_j(y)}{\partial y_l} -$$

$$-F_k(\tilde{u}_1(y), ..., \tilde{u}_{k-1}(y), 0, \tilde{u}_{k+1}(y), ..., \tilde{u}_N(y)) \geq 0 \quad a.e. \tag{2.9}$$

Obviously, the $\frac{1}{\varepsilon^2}$ term in the left side of (2.9) is the leading one as $\varepsilon \to 0$. In the case of $a_{k,j} < 0$ we can choose here $\tilde{u}_j(y) = e^{y^2}$ in a neighborhood of the origin, smooth and decaying to zero at the infinity. A trivial calculation yields that $\Delta_{y,m}\tilde{u}_j(y) > 0$ near the origin. If $a_{k,j} > 0$, then we can consider $\tilde{u}_j(y) = e^{-y^2}$ around the origin, smooth and tending to zero at the infinity. An easy computation shows that $\Delta_{y,m}\tilde{u}_j(y) < 0$ in a neighborhood the origin. Thus, the left side of (2.9) can be made as negative as possible which will violate inequality (2.9). Note that the last term in the left side of (2.9) will remain bounded. Therefore, for the matrix A involved in system (1.1), the off diagonal terms should vanish, such that

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

Hence, from (2.9) we arrive at

$$\sum_{l=1}^{d}\sum_{j=1,\ j\neq k}^{N} \frac{\gamma_{k,j}^l}{\varepsilon}\frac{\partial \tilde{u}_j(y)}{\partial y_l} -$$

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

In the case of $\gamma_{k,j}^l < 0$ involved in the sum in the left side of (2.10), we can choose $\tilde{u}_j(y) = e^{\sqrt{y^2+1}}$ in a neighborhood of the origin, smooth and decaying to zero at the infinity, such that

$$\frac{\partial \tilde{u}_j(y)}{\partial y_l} = \frac{y_l}{\sqrt{y^2+1}}e^{\sqrt{y^2+1}} > 0, \quad y_l > 0$$

near the origin. If $\gamma_{k,j}^l > 0$, we consider $\tilde{u}_j(y) = e^{-\sqrt{y^2+1}}$ near the origin, smooth and decaying to zero at the infinity, such that

$$\frac{\partial \tilde{u}_j(y)}{\partial y_l} = -\frac{y_l}{\sqrt{y^2+1}} e^{-\sqrt{y^2+1}} < 0, \quad y_l > 0$$

in a neighborhood of the origin. By making the parameter ε sufficiently small, we can violate the inequality in (2.10). This yields for $1 \le l \le d$ that

$$\gamma_{k,j}^l = 0, \quad 1 \le k, j \le N, \quad k \ne j.$$

Therefore, by virtue of (2.8) we arrive at

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

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

Remark 5. *Let us assume that the components of the reaction term satisfy for all* $1 \le k \le N$

$$F_k(t, s_1, ..., s_{k-1}, 0, s_{k+1}, ..., s_N) \le 0,$$

where $s_l \ge 0$ *with* $1 \le l \le N,\ l \ne k$ *and* $F \in C^1_{t,x},\ t \in [0, \tau],\ x \in \mathbb{R}^d$ *for some* $\tau > 0$. *Then it is not difficult to see that the analog of Theorem 1 holds.*

References

[1] B. Carreras, V. Lynch, G. Zaslavsky. *Anomalous diffusion and exit time distribution of particle tracers in plasma turbulence model*, Phys. Plasmas, **8** (2001), 5096–5103.

[2] M. A. Efendiev. *Evolution equations arising in the modelling of life sciences. International Series of Numerical Mathematics*, **163**, Birkhäuser/Springer, Basel, (2013), 217 pp.

[3] M. A. Efendiev, V. Vougalter. *Verification of biomedical processes with anomalous diffusion, transport and interaction of species*, to appear as a Springer book chapter.

[4] T. Solomon, E. Weeks, H. Swinney. *Observation of anomalous diffusion and Lévy flights in a two-dimensional rotating flow*, Phys. Rev. Lett., **71** (1993), 3975–3978.

[5] P. Manandhar, J. Jang, G.C. Schatz, M.A. Ratner, S. Hong. *Anomalous surface diffusion in nanoscale direct deposition processes*, Phys. Rev. Lett., **90** (2003), 4043–4052.

[6] R. Metzler, J. Klafter. *The random walk's guide to anomalous diffusion: a fractional dynamics approach*, Phys. Rep., **339** (2000), 1–77.

[7] J. Sancho, A. Lacasta, K. Lindenberg, I. Sokolov, A. Romero. *Diffusion on a solid surface: Anomalous is normal*, Phys. Rev. Lett., **92** (2004), 250601.

[8] H. Scher, E. Montroll. *Anomalous transit-time dispersion in amorphous solids*, Phys. Rev. B, **12** (1975), 2455–2477.

[9] H. Smith. *Monotone Dynamical Systems. An Introduction to the Theory of Competitive and Cooperative Systems*, Mathematical Surveys and Monographs, **41**, American Mathematical Society, (2008).

[10] A.I. Volpert, V.A. Volpert, V.A. Volpert. *Traveling wave solutions of parabolic systems*, Translations of Mathematical Monographs, **140**. American Mathematical Society, Providence, RI, (1994), 448pp.

[11] V.A. Volpert, Y. Nec, A.A. Nepomnyashchy. *Exact solutions in front propagation problems with superdiffusion*, Phys. D, **239** (2010), No.3–4, 134–144.

[12] V.A. Volpert, Y. Nec, A.A. Nepomnyashchy. *Fronts in anomalous diffusion-reaction systems*, Philos. Trans. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci., **371** (2013), No. 1982, 20120179, 18pp.

[13] V. Vougalter, V. Volpert. *On the solvability conditions for the diffusion equation with convection terms*, Commun. Pure Appl. Anal., **11** (2012), No. 1, 365–373.

[14] V. Vougalter, V. Volpert. *Solvability of some integro-differential equations with anomalous diffusion. Regularity and stochasticity of nonlinear dynamical systems*, Nonlinear Syst. Complex., **21** Springer, Cham, (2018), 1–17.