ON NONNEGATIVITY PRESERVATION IN FINITE ELEMENT METHODS FOR SUBDIFFUSION EQUATIONS

BANGTI JIN, RAYTCHO LAZAROV, VIDAR THOMÉE, AND ZHI ZHOU

Abstract. We consider three types of subdiffusion models, namely single-term, multi-term and distributed order fractional diffusion equations, for which the maximum-principle holds and which, in particular, preserve nonnegativity. Hence the solution is nonnegative for nonnegative initial data. Following earlier work on the heat equation, our purpose is to study whether this property is inherited by certain spatially semidiscrete and fully discrete piecewise linear finite element methods, including the standard Galerkin method, the lumped mass method and the finite volume element method. It is shown that, as for the heat equation, when the mass matrix is nondiagonal, nonnegativity is not preserved for small time or time-step, but may reappear after a positivity threshold. For the lumped mass method nonnegativity is preserved if and only if the triangulation in the finite element space is of Delaunay type. Numerical experiments illustrate and complement the theoretical results.
Keywords: subdiffusion, finite element method, nonnegativity preservation, Caputo derivative
Mathematics Subject Classification (2010): 65M12, 65M60

1. Introduction

In this work we consider the numerical analysis of mathematical models arising in subdiffusion. One simple example is the single-term subdiffusion, for which the governing equation is given by

$$\partial_t^\alpha u - \Delta u = 0, \quad \text{in } \Omega, \quad t > 0, \quad \text{with } 0 < \alpha < 1, \tag{1.1}$$

under the initial-boundary conditions

$$u = 0, \quad \text{on } \partial\Omega, \quad t > 0, \quad \text{with } u(0) = v, \quad \text{in } \Omega, \tag{1.2}$$

where Ω is a bounded domain in $\mathbb{R}^2$ which for simplicity we assume to be polygonal, and where v is a given function on Ω. Here $\partial_t^\alpha u$ denotes the Caputo fractional derivative of order $\alpha \in (0,1)$ with respect to t, defined by the convolution (see [12])

$$\partial_t^\alpha u(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t (t-s)^{-\alpha} \frac{d}{ds} u(s) ds, \tag{1.3}$$

where $\Gamma(x) = \int_0^\infty s^{x-1} e^{-s} ds$ is the Gamma function. By continuity we may include the standard heat equation for $\alpha = 1$. The fractional derivative is often used to describe anomalous diffusion, in which the mean square variance grows sublinearly with time t, at a rate slower than that in a Gaussian process. It occurs in many applied disciplines, e.g., electron transport in Xerox copiers, molecule transport in membranes, and thermal diffusion on fractal domains.

By the maximum principle, the solution $u(t)$ of the heat equation satisfies the nonnegativity preservation property

$$v = u(0) \geq 0 \quad \text{in } \Omega \quad \text{implies} \quad u(t) \geq 0 \quad \text{in } \Omega, \quad \text{for } t \geq 0. \tag{1.4}$$

It is natural to ask to what extent this property extends to numerical approximations, and for piecewise linear finite element methods over regular triangulations this question has attracted some attention. Fujii [7] showed that for the lumped mass (LM) method, with backward Euler time-stepping, nonnegativity is preserved when the angles in the triangulation are acute. Thomée and Wahlbin [29] showed that for the semidiscrete standard Galerkin (SG) method, nonnegativity is not preserved for small $t > 0$, but for the LM method, it is preserved if and only if the triangulation is of Delaunay type. Later, Schatz, Thomée and Wahlbin [25] analyzed several fully discrete methods and showed that, in particular, these properties carry over to the backward Euler method. Recently, Thomée [28] and Chatzipantelidis, Horváth and

Thomée [1] extended these results to cover also the finite volume element (FVE) method and further discussed the existence of a threshold $t_0 > 0$, such that nonnegativity is preserved for $t \geq t_0$.

Our purpose in this paper is to discuss the nonnegativity preservation property for a class of piecewise linear finite element approximations, including the SG, LM and FVE methods described briefly in Section 3, for the more general initial–boundary value problem

$$
\begin{aligned}
&P(\partial_t)u - \Delta u = 0, \quad \text{in } \Omega, \qquad \text{for } t > 0, \\
&u = 0, \quad \text{on } \partial\Omega, \quad \text{for } t > 0, \quad \text{and} \quad u(0) = v, \quad \text{in } \Omega,
\end{aligned} \tag{1.5}
$$

where $P(\partial_t)u$ denotes a fractional order differential operator of the form

$$
P(\partial_t)u(t) = \int_0^1 \partial_t^\alpha u(t) d\nu(\alpha), \tag{1.6}
$$

with $\nu(\alpha)$ a positive measure on $[0, 1]$. These more general models, including in addition to (1.1) multi-term and distributed order models, are reviewed briefly in Section 2. There we also introduce the solution operator $E(t)$ of (1.5) and discuss its analytic properties, including asymptotic behavior. In a series of interesting works, Luchko [18, 19, 20] established that the solution $u(t)$ of problem (1.5) also satisfies the property (1.4).

Numerical methods for the model (1.5) and their analysis have received considerable interest, cf., e.g., [8, 9, 10, 11, 16, 21]. The weak formulation of (1.5) is to find $u(t) \in H_0^1(\Omega)$ for $t > 0$ such that

$$
(P(\partial_t)u(t), \varphi) + a(u(t), \varphi) = 0, \quad \forall \varphi \in H_0^1(\Omega), \quad t \geq 0, \quad \text{with } u(0) = v,
$$

where $a(u, \chi) = (\nabla u, \nabla \chi)$ and $(\cdot, \cdot)$ is the inner product in $L^2(\Omega)$. The spatially semidiscrete finite element approximation of (1.5) is based on a family of shape regular quasi-uniform triangulations $\{\mathcal{T}_h\}_{0<h<1}$ of Ω into triangles, with h the maximal length of the sides of the triangulation $\mathcal{T}_h$, and the associated finite element space X_h of continuous piecewise linear functions over $\mathcal{T}_h$,

$$
X_h = \left\{ \chi \in H_0^1(\Omega) : \ \chi \text{ linear in } K, \quad \forall K \in \mathcal{T}_h \right\}.
$$

The spatially semidiscrete approximation of (1.5) is then to find $u_h(t) \in X_h$ for $t \geq 0$ such that

$$
[P(\partial_t)u_h(t), \chi] + a(u_h(t), \chi) = 0, \quad \forall \chi \in X_h, \ t > 0, \quad \text{with } u_h(0) = v_h, \tag{1.7}
$$

where $v_h \in X_h$ is an approximation of the initial data v, and $[\cdot, \cdot]$ is a suitable inner product on X_h. With $\{P_j\}_{j=1}^N$ the interior nodes of $\mathcal{T}_h$, and $\{\phi_j\}_{j=1}^N$ the corresponding nodal basis, we may write

$$
u_h(t) = \sum_{j=1}^N u_j(t)\phi_j(x) \quad \text{and} \quad v_h = \sum_j^N v_j \phi_j(x). \tag{1.8}
$$

Setting $U(t) := (u_1(t), \ldots, u_N(t))^T$ and $V = (v_1, \ldots, v_N)^T$, the semidiscrete problem (1.7) reads

$$
P(\partial_t)U(t) + \mathcal{H}U(t) = 0, \quad \text{for } t > 0, \quad \text{with } U(0) = V, \quad \text{where } \mathcal{H} = \mathcal{M}^{-1}\mathcal{S}. \tag{1.9}
$$

Here $\mathcal{M} = (m_{ij})$, with $m_{ij} = [\phi_j, \phi_i]$, and $\mathcal{S} = (s_{ij})$, with $s_{ij} = a(\phi_j, \phi_i)$, denote the mass and stiffness matrices, respectively, and are both symmetric and positive definite. The case of the semidiscrete SG method was first developed and analyzed by Jin et al. [10] for the single-term problem on a convex polygonal domain, and then extended to multi-term and distributed-order cases in [8, 9], where optimal error estimates with respect to the regularity of initial data v were established.

Following the analysis in the case of the heat equation, we discuss nonnegativity preservation for the spatially semidiscrete methods in Section 3. Introducing the solution matrix $\mathcal{E}(t)$ by writing $U(t) = \mathcal{E}(t)V$, nonnegativity preservation may be expressed as $\mathcal{E}(t) \geq 0$, elementwise. In Theorem 3.1 we show that if the mass matrix $\mathcal{M}$ is nondiagonal, which holds for the SG and FVE methods, then this cannot happen for small $t > 0$. However for the LM method this happens if and only if $\mathcal{T}_h$ is Delaunay. In Theorem 3.2, we show that if $\mathcal{H}^{-1} > 0$, then there exists $t_0 > 0$ such that $U(t) \geq 0$ for all $t \geq t_0$, if $V \geq 0$.

In Section 4 we discuss positivity preservation for fully discrete time stepping methods with a time step τ, for (1.9), based on convolution quadrature generated by the backward Euler method, or

$$
Q_n(U) + \mathcal{H}U^n = Q_n(1)V, \quad \text{for } n \geq 1, \quad \text{with } U^0 = V, \quad \text{where } U^n \approx u_h(t_n), \ t_n = n\tau.
$$

Here $Q_n(U) = \sum_{j=0}^{n} \omega_{n-j} U^j$ denotes the convolution quadrature approximation to $P(\partial_t)U(t_n)$; see Section 4. This gives the fully discrete solution in the form

$$U^n = \mathcal{E}_{n,\tau}\, V := (\omega_0\, \mathcal{I} + \mathcal{H})^{-1}\Big(\sum_{j=0}^{n-1}\omega_j\ V - \sum_{j=1}^{n-1}\omega_{n-j}U^j\Big), \quad \text{for } n \ge 1, \quad \text{with } U^0 = V.$$

This method was developed and analyzed in [9, 11] for the SG approximation, and the convergence of the fully discrete solution to the corresponding spatially semidiscrete one, which is needed below, is shown in the general case in Appendix A. We show time discrete analogues of the results in Section 3, and also, in Theorem 4.3, we give an upper bound of the positivity threshold for special triangulations.

In the final Section 5 we present numerical examples for various domains Ω, with Delaunay and non-Delaunay triangulations $\mathcal{T}_h$, to illustrate and complement our theoretical results.

As a result of the maximum principle, in addition to (1.4), it also follows that the solution operator $E(t)$ is a contraction in the maximum-norm, i.e., $\|E(t)\|_\infty \le 1$. The question about analogues of this for the numerical methods was also discussed in [25, 29] for the heat equation, and in Appendix B we show that the analogue of this holds in the present case for semidiscrete and fully discrete LM approximations, provided that the stiffness matrix $\mathcal{S}$ is diagonally dominant, which is not equivalent to $\mathcal{T}_h$ being Delaunay.

2. Preliminaries

In this section we present preliminary material concerning the subdiffusion model (1.5) and its analytical properties. In particular we introduce the solution operator $E(t)$ for $t \ge 0$ and the associated scalar kernel function $u_\lambda(t)$, and study its asymptotic behavior for small and large t, which will be needed later.

As indicated in Section 1, in addition to the single-term model (1.1), several more complex models for subdiffusion have been proposed, with (1.3) replaced by a weighted linear combination $P(\partial_t)u$, defined in (1.6). We will specifically study two cases, the discrete case (denoted by case I below), with point masses $\{\alpha_j\}_{j=1}^m \subset (0,1),\ m \ge 1$, where $\alpha_m < \alpha_{m-1} < \ldots < \alpha_1$, and the distributed case (denoted by case II below), in which ν is completely continuous, i.e., $d\nu(\alpha) = \mu(\alpha)d\alpha$, with μ smooth and nonnegative. For the characteristic function of $P(\partial_t)$, the complex function $P(z) = \int_0^1 z^\alpha d\nu(\alpha)$, we then have

$$P(z) = \begin{cases} \displaystyle\sum_{i=1}^m b_i z^{\alpha_i} & \text{in case I,} \\ \displaystyle\int_0^1 z^\alpha \mu(\alpha)d\alpha & \text{in case II.} \end{cases}.$$

In the discrete case, the constants b_i are positive, with $b_1 = 1$, which ensures the well-posedness of the problem (1.5), cf. [14]. It reduces to the single-term subdiffusion model (1.1) when $m = 1$. In the distributed case, the nonnegative weight function $\mu(\alpha)$ is assumed to be Hölder continuous, with $\mu(0)\mu(1) > 0$. These conditions are sufficient for the positivity of the solution and are different from the ones used in the existing literature, cf. [13, 15], The general model was proposed in order to extend the flexibility of the single-term model, in that the underlying stochastic process may contain a host of different Hurst exponents, cf. [3].

For the convenience of the reader we prove the positivity preservation property (1.4) for problem (1.5), using arguments in [18, 19, 20]. We first show an extremal principle for the fractional differential operator $P(\partial_t)$.

Lemma 2.1. *Assume $f \in C[0,T] \cap C^1(0,T]$, and let f attain its minimum at $t_0 \in (0,T]$. Then $P(\partial_t)f(t_0) \le 0$.*

Proof. Setting $g(s) = f(s) - f(t_0)$, we have by integration by parts, since $0 \le g(s) = O(t_0 - s)$ as $s \to t_0$,

$$\int_0^{t_0}(t_0-s)^{-\alpha}g'(s)ds = -t_0^{-\alpha}g(0) - \alpha\int_0^{t_0}(t_0-s)^{-\alpha-1}g(s)ds \le 0, \quad \text{for any } \alpha \in (0,1).$$

Since $f'(s) = g'(s)$ we thus have $\partial_t^\alpha f(t_0) \le 0$, and hence $P(\partial_t)f(t_0) = \int_0^1 \partial_t^\alpha f(t_0)d\nu(\alpha) \le 0$. □

Theorem 2.1. *The solution operator $E(t)$ for (1.5) is nonnegative, i.e., $E(t)v \ge 0$ for $t \ge 0$, if $v \ge 0$.*

Proof. Assume that the minimum of $u(t) = E(t)v$ is negative and achieved at $(x_0, t_0) \in \Omega \times (0, T]$. With $\epsilon = -u(x_0, t_0) > 0$ we set $w(x, t) = u(x, t) - \frac{1}{2}\epsilon(1 - t/T) \geq u(x, t) - \frac{1}{2}\epsilon$. Then, for $x \in \partial\Omega$ or $t = 0$,

$$w(x_0, t_0) \leq u(x_0, t_0) = -\epsilon \leq -\epsilon + u(x, t) \leq -\epsilon + w(x, t) + \tfrac{1}{2}\epsilon = w(x, t) - \tfrac{1}{2}\epsilon.$$

Hence $w(x, t)$ cannot attain its minimal value at $t = 0$ of for $x \in \partial\Omega$. Now let the minimum of w be taken at $(x_1, t_1) \in \Omega \times (0, T]$. Then by Lemma 2.1, $P(\partial_t)w(x_1, t_1) \leq 0$, and clearly $-\Delta w(x_1, t_1) \leq 0$. Noting the identity $\partial_t^\alpha t = t^{1-\alpha}/\Gamma(2 - \alpha)$, we find

$$(P(\partial_t) - \Delta)u(x_1, t_1) = (P(\partial_t) - \Delta)w(x_1, t_1) - \frac{\epsilon}{2T}\int_0^1 \frac{t_1^{1-\alpha}}{\Gamma(2 - \alpha)} d\nu(\alpha) < 0,$$

contradicting the fact that $u(t)$ is a solution of (1.5). □

Next we derive an expression for the solution operator $E(t)$ for problem (1.5) by means of Laplace transformation, denoting the Laplace transform of u by $\widehat{u}(z) = (\mathcal{L}u)(z)$. Recall that [12, Lemma 2.24],

$$\mathcal{L}(\partial_t^\alpha u)(z) = z^\alpha \widehat{u}(z) - z^{\alpha-1}u(0),$$

and consequently

$$\begin{aligned}\mathcal{L}P(\partial_t)u(z) &= \int_0^1 \mathcal{L}\partial_t^\alpha u(z) d\nu(\alpha) = \int_0^1 z^\alpha d\nu(\alpha)\widehat{u}(z) - \int_0^1 z^{\alpha-1} d\nu(\alpha)u(0)\\ &= P(z)\widehat{u}(z) - z^{-1}P(z)u(0).\end{aligned}$$

After Laplace transformation of (1.5), with $A = -\Delta$, the negative Laplacian with a zero Dirichlet boundary condition, and the initial condition $u(0) = v$, we therefore obtain

$$P(z)\widehat{u}(z) + A\widehat{u}(z) = z^{-1}P(z)v,$$

or

$$\widehat{u}(z) = J(z)v, \quad \text{where } J(z) = z^{-1}P(z)(P(z)I + A)^{-1},$$

where I is the identity operator. Hence we find for the solution operator, defined by $u(t) = E(t)v$,

$$E(t)v = (\mathcal{L}^{-1}J)(t)v = \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_\sigma} e^{zt}J(z)dzv, \tag{2.1}$$

where $\Gamma_\sigma = \{z = \sigma + \mathrm{i}\eta : \sigma > 0,\ \eta \in \mathbb{R}\}$. Letting $\{\lambda_j\}_{j=1}^\infty$ be the eigenvalues (counting according to the multiplicities) in nondecreasing order and $\{\varphi_j\}_{j=1}^\infty$ the corresponding $L^2(\Omega)$ orthonormal eigenfunctions of the operator A, we may also write

$$E(t)v = \sum_{j=1}^\infty u_{\lambda_j}(t)(v, \varphi_j)\varphi_j, \tag{2.2}$$

where

$$u_\lambda(t) = (\mathcal{L}^{-1}J_\lambda)(t) = \frac{1}{2\pi \mathrm{i}}\int_{\Gamma_\sigma} e^{zt}J_\lambda(z)\,dz, \quad J_\lambda(z) = z^{-1}P(z)(P(z) + \lambda)^{-1}. \tag{2.3}$$

The scalar kernel function $u_\lambda = u_\lambda(t)$ solves the fractional order initial-value problem

$$P(\partial_t)u_\lambda + \lambda u_\lambda = 0, \quad \text{with } u_\lambda(0) = 1. \tag{2.4}$$

Since $P(z)$ is analytic in the complex plane, cut along the negative real axis, we obtain, after deforming the contour Γ_σ in (2.3), and noting that, for small $\delta > 0$,

$$\int_{|z|=\delta} |J_\lambda(z)|\,|dz| \leq C\delta^{-1}\int_{|z|=\delta} P(\delta)\,|dz| = 2\pi\, C\, P(\delta) \to 0, \quad \text{as } \delta \to 0,$$

and hence we find that

$$u_\lambda(t) = \frac{1}{\pi}\int_0^\infty e^{-st}K_\lambda(s)\,ds, \quad K_\lambda(s) = \operatorname{Im} J_\lambda(-s) = \frac{\lambda \operatorname{Im} P(-s)}{s|P(-s) + \lambda|^2} > 0, \tag{2.5}$$

where we have used

$$\operatorname{Im} P(-s) = \operatorname{Im} \int_0^1 e^{\mathrm{i}\alpha\pi} s^\alpha \, d\nu(\alpha) = \int_0^1 \sin \alpha\pi \, s^\alpha \, d\nu(\alpha) > 0.$$

Since $K_\lambda(s)$ in (2.5) is positive, $u_\lambda(t)$ is completely monotone, and, in particular, monotone for $t \geq 0$.

We now study the asymptotic behavior of the function $u_\lambda(t)$ defined in (2.3). Our main tool will be a special case of the Karamata-Feller Tauberian theorem (see [6, Theorems 2–4, pp. 445–466]), which we state as the following lemma. Recall that a positive function $L(t)$ defined on $(0, \infty)$ varies slowly at infinity if for every fixed x, $L(tx)/L(t) \to 1$ as $t \to \infty$.

Lemma 2.2. *Let $u(t)$ be a monotone function with its Laplace transform $\widehat{u}(z) = \mathcal{L}u(z)$ defined for $z = s > 0$, $L(t)$ be slowly varying at infinity, and $\rho > 0$. Then*

$$\widehat{u}(s) \sim \frac{1}{s^\rho} L\left(\frac{1}{s}\right) \quad \text{as } s \to 0 \qquad \text{implies} \qquad u(t) \sim \frac{1}{\Gamma(\rho)} t^{\rho-1} L(t) \quad \text{as } t \to \infty.$$

The statement is also valid when the roles of the origin and infinity are interchanged.

We can now determine the asymptotic behavior for the kernel function $u_\lambda(t)$.

Lemma 2.3. *Let $\mu \in \mathcal{C}^\gamma([0,1])$ and $\mu(0)\mu(1) > 0$, $\lambda > 0$. Then*

$$u_\lambda(t) = 1 - \lambda\beta_0(t)(1 + o(1)) \quad \text{as } t \to 0, \quad \text{where } \beta_0(t) = \begin{cases} t^{\alpha_1}/\Gamma(1+\alpha_1) & \text{in case I,} \\ t/(\mu(1)\log(t^{-1})) & \text{in case II,} \end{cases} \tag{2.6}$$

and

$$u_\lambda(t) = \lambda^{-1}\beta_\infty(t)(1 + o(1)) \quad \text{as } t \to \infty, \text{ where } \beta_\infty(t) = \begin{cases} b_m t^{-\alpha_m}/\Gamma(1-\alpha_m), & \text{in case I,} \\ \mu(0)/\log t, & \text{in case II.} \end{cases} \tag{2.7}$$

Proof. Since $u_\lambda(t)$ is monotone, Lemma 2.2 applies. First, we show the assertion as $t \to 0$, which is determined by the behavior of $\widehat{u}_\lambda(s) = J_\lambda(s)$ for large s. In case I (recall $b_1 = 1$), we have

$$J_\lambda(s) = s^{-1}\left(1 + \lambda\Big(\sum_{i=1}^m b_i s^{\alpha_i}\Big)^{-1}\right)^{-1} = s^{-1} - \lambda s^{-\alpha_1 - 1} + o(s^{-\alpha_1-1}).$$

By Lemma 2.2 this shows the first part of assertion (2.6). In case II, we have

$$P(s) = \int_0^1 e^{\alpha \log s}\mu(1)d\alpha + \int_0^1 e^{\alpha\log s}(\mu(\alpha) - \mu(1))d\alpha = \frac{\mu(1)(s-1)}{\log s} + \int_0^1 (\mu(\alpha)-\mu(1))e^{\alpha\log s}d\alpha.$$

Since $\mu \in \mathcal{C}^\gamma([0,1])$ we obtain, after integration by parts,

$$\Big|\int_0^1 (\mu(\alpha) - \mu(1))e^{\alpha\log s}d\alpha\Big| \leq C\int_0^1 (1-\alpha)^\gamma e^{\alpha\log s}d\alpha \leq C\frac{s}{(\log s)^{1+\gamma}}.$$

Hence, $P(s) = \mu(1)s(\log s)^{-1} + O(s(\log s)^{-1-\gamma})$ and $P(s)^{-1} = \log s/(s\mu(1))(1 + o(1))$ as $s \to \infty$. Thus

$$J_\lambda(s) = \frac{1}{s}\frac{1}{1 + \lambda/P(s)} = \frac{1}{s}\sum_{k=0}^\infty (-1)^k\lambda^k P(s)^{-k} = s^{-1} - \frac{\lambda\log s}{s^2\mu(1)} + o(s^{-2}\log s) \quad \text{as } s \to \infty,$$

and now the second part of assertion (2.6) follows from Lemma 2.2.

Next we show the asymptotic behavior as $t \to \infty$. In case I we have for $s \to 0$

$$J_\lambda(s) = \sum_{i=1}^m b_i s^{\alpha_i - 1} L(1/s) \quad \text{with} \quad L(t) = 1/(\sum_{i=1}^m b_i t^{-\alpha_i} + \lambda) \sim \lambda^{-1} \quad \text{as } t \to \infty.$$

The function $L(t)$ is slowly varying at infinity. Hence, by Lemma 2.2,

$$u_\lambda(t) \sim L(t)\frac{b_m t^{-\alpha_m}}{\Gamma(1-\alpha_m)} \quad \text{as } t \to \infty,$$

which shows the first part of assertion (2.7).

We finally consider the large time asymptotic behavior in case II. It follows from the splitting and using the Hölder continuity of $\mu(\alpha)$ that

$$P(s) = \int_0^1 s^\alpha \mu(\alpha) d\alpha = \mu(0) \int_0^1 s^\alpha d\alpha + \int_0^1 s^\alpha (\mu(\alpha) - \mu(0)) d\alpha = -\frac{\mu(0)}{\log s} + O\Big((\log s)^{-1-\gamma}\Big)$$

(see also [13, Proposition 2.2] for a related estimate). Consequently,

$$J_\lambda(s) = \lambda^{-1} s^{-1} P(s) \sum_{k=0}^\infty \lambda^{-k} P(s)^k = \lambda^{-1} s^{-1} \left(-\mu(0)(\log s)^{-1}(1 + o(1))\right) \quad \text{as } s \to 0.$$

Thus $J_\lambda(s) = \mu(0)\lambda^{-1}s^{-1}L(1/s)(1+o(1))$ with $L(s) = 1/\log s$ slowly varying at infinity, and Lemma 2.2 completes the proof of the lemma. □

3. Nonnegativity preservation in spatially semidiscrete methods

In this section we describe a general class of spatially semidiscrete methods for (1.5), and review three specific examples of such methods mentioned in the introduction. We then analyze their nonnegativity preservation properties.

As described in Section 1, we consider semidiscrete approximations for problem (1.5) of the form (1.7), where $[\cdot,\cdot]$ is an inner product in X_h, approximating the usual L^2 inner product $(\cdot,\cdot)$. We denote the stiffness matrix by $\mathcal{S} = (s_{ij})$, with $s_{ij} = a(\phi_j, \phi_i)$, and the mass matrix by $\mathcal{M} = (m_{ij})$, with $m_{ij} = [\phi_j, \phi_i]$. The semidiscrete problem (1.7) may then be written in matrix form as

$$\mathcal{M} P(\partial_t) U + \mathcal{S} U = 0, \quad \forall\, t > 0, \quad \text{with } U(0) = V,$$

or, equivalently, after multiplication by $\mathcal{M}^{-1}$,

$$P(\partial_t) U + \mathcal{H} U = 0, \quad \forall\, t > 0, \quad \text{with } U(0) = V, \quad \text{where } \mathcal{H} = \mathcal{M}^{-1}\mathcal{S}. \tag{3.1}$$

In analogy with (2.1), we find, for the solution matrix of (3.1),

$$\mathcal{E}(t) = (\mathcal{L}^{-1}\mathcal{J})(t) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_\sigma} e^{zt} \mathcal{J}(z) dz, \quad \text{with } \mathcal{J}(z) = z^{-1}P(z)(P(z)\mathcal{I} + \mathcal{H})^{-1},$$

where $\mathcal{I}$ is the identity matrix. Since both the stiffness matrix $\mathcal{S}$ and the mass matrix $\mathcal{M}$ are symmetric positive definite, the eigenvalue problem $\mathcal{S}\varphi = \lambda \mathcal{M} \varphi$ has a complete system of eigenvectors φ_i with positive eigenvalues λ_i, so that $\mathcal{H} = \mathcal{M}^{-1}\mathcal{S} = \mathcal{Q}^{-1}\mathcal{D}\mathcal{Q}$, where the rows of $\mathcal{Q}$ are the eigenvectors φ_i and the diagonal elements of the diagonal matrix $\mathcal{D}$ are the eigenvalues λ_i. Thus, corresponding to the eigenfunction expansion (2.2), we have

$$\mathcal{E}(t) = \mathcal{Q}^{-1}\mathcal{D}_{\Lambda(t)}\mathcal{Q}, \quad \text{with } \mathcal{D}_{\Lambda(t)} = \mathrm{diag}(u_{\lambda_i}(t)). \tag{3.2}$$

We now briefly review our three examples of finite element methods and the corresponding inner products $[\cdot,\cdot]$ in X_h. The first example is the standard Galerkin (SG) method, with the standard $L^2(\Omega)$ inner product, i.e., we choose $[\cdot,\cdot] = (\cdot,\cdot)$.

Our second example is the lumped mass (LM) method, using

$$[w, \chi] = (w, \chi)_h = \sum_{K \in \mathcal{T}_h} Q_{K,h}(w\chi), \quad \text{with } Q_{K,h}(f) = \tfrac{1}{3}\,|K| \sum_{j=1}^3 f(P_j^K) \approx \int_K f dx, \tag{3.3}$$

where P_j^K, $j = 1, 2, 3$, are the vertices of the triangle $K \in \mathcal{T}_h$ and $|K|$ is its area. In this case the mass matrix $\mathcal{M}$ is diagonal with positive diagonal elements.

Our third example is the finite volume element (FVE) method, cf. [2, 4], which is based on a discrete version of the local conservation law

$$\int_V P(\partial_t) u(t) dx - \int_{\partial V} \frac{\partial u}{\partial n} ds = 0 \quad \text{for } t \geq 0, \tag{3.4}$$

valid for any $V \subset \Omega$ with a piecewise smooth boundary ∂V, with n the unit outward normal to ∂V. The discrete method then requires (3.4) to be satisfied for $V = V_j,\ j = 1,\dots,N$, which are disjoint so called *control volumes* associated with the nodes P_j of $\mathcal{T}_h$. It can be recast as a Galerkin method, by letting

$$Y_h = \left\{\varphi \in L^2(\Omega) : \varphi|_{V_j} = \text{constant},\ j = 1,2,...,N;\ \varphi = 0 \text{ outside } \cup_{j=1}^N V_j\right\},$$

introducing the interpolation operator $J_h : \mathcal{C}(\Omega) \to Y_h$ by $(J_h v)(P_j) = v(P_j),\ j = 1,\dots,N$, and then defining the inner product $\langle \chi, \psi\rangle = (\chi, J_h\psi)$ for all $\chi, \psi \in X_h$. The FVE method then corresponds to (1.7) with $[\cdot,\cdot] = \langle\cdot,\cdot\rangle$.

We recall that an edge e of the triangulation $\mathcal{T}_h$ is called a Delaunay edge if the sum of the angles ψ_1 and ψ_2 opposite e is $\le \pi$, and that $\mathcal{T}_h$ is a *Delaunay triangulation* if all interior edges are Delaunay. A node of $\mathcal{T}_h$ is said to be *strictly interior* if all its neighbors are interior nodes, and $\mathcal{T}_h$ is *normal* if it has a strictly interior node, P_j say, such that any neighbor of P_j has a neighbor which is not a neighbor of P_j. A symmetric, positive definite matrix with non-positive off diagonal entries is called a *Stieltjes* matrix.

We now turn to our main goal, to determine whether the nonnegativity preservation property (1.4) remains valid for the semidiscrete problem, i.e., if $\mathcal{E}(t) \ge 0$ for $t \ge 0$. We shall first discuss the general case, and then the LM method. Our first result states that the semidiscrete method (3.1) does not satisfy (1.4) in general, if the mass matrix $\mathcal{M}$ is *nondiagonal*, in the sense that $m_{ij} > 0$ for all neighbors P_i, P_j.

Theorem 3.1. *Assume that the triangulation $\mathcal{T}_h$ is normal and that the mass matrix $\mathcal{M}$ is nondiagonal. Then the solution matrix $\mathcal{E}(t)$ cannot be nonnegative for all $t > 0$.*

Proof. Assume that $\mathcal{E}(t) \ge 0$ for $t \ge 0$. By (3.2) and Lemma 2.3, we have

$$\mathcal{E}(t) = \mathcal{I} - \beta_0(t)\mathcal{H}(1 + o(1)) \quad \text{as } t \to 0, \tag{3.5}$$

and, since $\beta_0(t) > 0$ for small t, the nonnegativity of $\mathcal{E}(t)$ implies $h_{ij} \le 0$ for all $i \ne j$. Let P_j be a strictly interior node as in the definition of $\mathcal{T}_h$ being normal. We shall show that $h_{ij} = 0$ for $i \ne j$. Consider first the case that P_i is not a neighbor of P_j, so that $m_{ij} = s_{ij} = 0$. Since $\mathcal{S} = \mathcal{M}\mathcal{H}$,

$$0 = s_{ij} = \sum_{k=1}^N m_{ik}h_{kj} = \sum_{k=1,k\ne j}^N m_{ik}h_{kj}.$$

Since $h_{kj} \le 0$ for $k \ne j$, we have $m_{ik}h_{kj} \le 0,\ k \ne j$, and thus $m_{ik}h_{kj} = 0$ for $k \ne j$, and in particular, $h_{ij} = 0$. When P_i is a neighbor of P_j, it has a neighbor P_k which is not a neighbor of P_j, and hence $s_{kj} = \sum_{l\ne j} m_{kl}h_{lj} = 0$, which implies $h_{ij} = 0$ since $m_{ki} > 0$, in view of the assumption that $\mathcal{M}$ is nondiagonal. Thus,

$$s_{ij} = \sum_{k=1}^N m_{ik}h_{kj} = m_{ij}h_{jj}, \quad i = 1,\dots,N,$$

i.e., the jth columns of $\mathcal{S}$ and $\mathcal{M}$ are proportional, which contradicts the facts that $\sum_{i=1}^N s_{ij} = 0$ for a strictly interior node P_j and $\sum_{i=1}^N m_{ij} > 0$. □

Next we show a nonnegativity preservation result in the general case, for large time.

Theorem 3.2. *Suppose $\mathcal{H}^{-1} > 0$. Then there exists a $t_0 > 0$ such that $\mathcal{E}(t) > 0$ for all $t > t_0$.*

Proof. As before, it follows from the asymptotic behavior of the function $u_\lambda(t)$, cf. Lemma 2.3, that

$$\mathcal{E}(t) = \beta_\infty(t)\mathcal{H}^{-1}(1 + o(1)) \quad \text{as } t \to \infty.$$

Since by assumption $\mathcal{H}^{-1} > 0$, we find that $\mathcal{E}(t)$ is positive for large t. □

Theorem 3.1 covers the SG and FVE methods, and Theorem 3.2 applies also to the LM case. We recall from [1] that $\mathcal{S}^{-1} > 0$ if $\mathcal{S}$ is a Stieltjes matrix, and that $\mathcal{S}$ is a Stieltjes matrix if and only if $\mathcal{T}_h$ is a Delaunay triangulation. In particular, if $\mathcal{T}_h$ is Delaunay, then $\mathcal{S}^{-1} > 0$, and hence also $\mathcal{H}^{-1} > 0$, but $\mathcal{H}^{-1}$ may be positive also for some non-Delaunay triangulations.

In the case of the LM method we may prove the following sharper result.

Theorem 3.3. *Let $\mathcal{E}(t)$ be the solution matrix of the LM approximation. Then $\mathcal{E}(t) \geq 0$ for all $t \geq 0$ if and only if the triangulation $\mathcal{T}_h$ is Delaunay.*

Proof. If $\mathcal{E}(t) \geq 0$ for all $t \geq 0$ we conclude as in the proof of Theorem 3.1 that $h_{ij} \leq 0$ for all $i \neq j$, Consequently, since $\mathcal{M}$ is a positive diagonal matrix, $s_{ij} \leq 0$ for all $i \neq j$, so that $\mathcal{S}$ is Stieltjes and hence $\mathcal{T}_h$ Delaunay. The proof of the converse statement requires the corresponding result for the fully discrete solution matrix $\mathcal{E}_{n,\tau}$, and the convergence of the fully discrete solution matrix to the semidiscrete one. These two results are shown in Theorem 4.4 and Lemma A.1, respectively, and assuming their validity we find $\mathcal{E}(t) = \lim_{n\to\infty} \mathcal{E}_{n,t/n} \geq 0$. □

We remark that in the single-term case, the converse part of Theorem 3.3 also follows from the representation $\mathcal{E}(t) = E_\alpha(-t^\alpha \mathcal{H})$ of the solution shown in [24], where $E_\alpha(z) = \sum_{k=0}^\infty z^k/\Gamma(k\alpha+1)$ is the Mittag-Leffler function. Since, by [23], $E_\alpha(-t)$ is completely monotone, Bernstein's theorem implies that $E_\alpha(-y) = \int_0^\infty e^{-xy}\, d\sigma(x)$, with $\sigma(x)$ a positive measure. Recalling from [1] that $e^{-t\mathcal{H}} \geq 0$ for $t \geq 0$ when $\mathcal{T}_h$ is Delaunay, we conclude

$$\mathcal{E}(t) = E_\alpha(-t^\alpha \mathcal{H}) = \int_0^\infty e^{-x\, t^\alpha\, \mathcal{H}} d\sigma(x) \geq 0, \quad \text{for } t \geq 0.$$

4. Nonnegativity preservation of a fully discrete method

Now we discuss the preservation of nonnegativity for a fully discrete method for the subdiffusion model (1.5), developed in [11, 9], based on applying convolution quadrature [17] to the semidiscrete problem (3.1).

Using the definition of the Caputo fractional derivative, we deduce that $P(\partial_t)\varphi(t) = P(\partial_t)\,(\varphi(t) - \varphi(0))$, and hence problem (3.1) may then be rewritten as

$$P(\partial_t)(U(t) - V) + \mathcal{H}U(t) = 0, \quad \text{for } t > 0, \quad \text{with } U(0) = V. \tag{4.1}$$

For the discretization in time of (4.1) we introduce a time step $\tau > 0$, and set $t_n = n\tau$, $n \geq 0$. For a smooth function φ, the approximation $Q_n(\varphi)$, of $P(\partial_t)\varphi(t_n)$, is then given by

$$Q_n(\varphi) = \sum_{j=0}^{n} \omega_{n-j}\varphi^j, \quad \text{for } n \geq 0, \quad \text{where } \varphi^j = \varphi(t_j).$$

The weights $\{\omega_j\}$ are generated by the characteristic polynomial $(1-\xi)/\tau$ of the backward Euler (BE) method, i.e., $\sum_{j=0}^\infty \omega_j \xi^j = P((1-\xi)/\tau)$. The fully discrete scheme is then given by [11]:

$$Q_n(U) + \mathcal{H}U^n = Q_n(1)V, \quad \text{for } n \geq 1, \quad \text{with } U^0 = V.$$

Noting that $\omega_n(U^0 - V) = 0$, the fully discrete solution U^n can be explicitly represented by

$$U^n = \mathcal{E}_{n,\tau}\, V := (\omega_0\, \mathcal{I} + \mathcal{H})^{-1}\Big(\sum_{j=0}^{n-1} \omega_j V - \sum_{j=1}^{n-1} \omega_{n-j} U^j\Big), \quad \text{for } n \geq 1, \quad \text{with } U^0 = V. \tag{4.2}$$

Clearly this relation defines a sequence of rational functions $r_{n,\tau}(\lambda)$, $n = 0, 1, 2, \ldots$, such that $\mathcal{E}_{n,\tau} = r_{n,\tau}(\mathcal{H})$, and analogously to (3.2) we may write, with λ_j the eigenvalues of $\mathcal{H}$,

$$\mathcal{E}_{n,\tau} = \mathcal{Q}^{-1}\mathcal{D}_{\Pi^n}\,\mathcal{Q}, \quad \text{with } \mathcal{D}_{\Pi^n} = \mathrm{diag}(r_{n,\tau}(\lambda_i)). \tag{4.3}$$

We now turn to nonnegativity preservation property for the method (4.2). We first show some properties of the quadrature weights $\{\omega_j\}$.

Lemma 4.1. *Let the weights $\{\omega_j\}$ be generated by the backward Euler method. Then*

$$(i) \quad \omega_0 > 0 \ \text{ and } \ \omega_j < 0 \quad \text{for } j \geq 1, \quad \text{and} \quad (ii) \quad \sum_{j=0}^{n} \omega_j > 0, \quad \text{for } n \geq 1.$$

Proof. It suffices to show the assertion for the single-term model ($m = 1$ and $\alpha_1 = \alpha$), since the more general case follows by linearity. Property (i) follows directly from the explicit formula

$$\omega_j = \tau^{-\alpha}(-1)^j \binom{\alpha}{j} = \tau^{-\alpha}(-1)^j \frac{\alpha(\alpha-1)\dots(\alpha-j+1)}{j!}.$$

For (ii), we claim that the partial sum satisfies the relation

$$\sum_{j=0}^{n} \omega_j = \tau^{-\alpha} \frac{(n+1)(-1)^n}{\alpha} \binom{\alpha}{n+1}, \quad \text{for } n \geq 0. \tag{4.4}$$

We show the claim by mathematical induction. First, we note that $\omega_0 = \tau^{-\alpha}$ satisfies (4.4) with $n = 0$. Next, assuming (4.4) holds up to $n-1$, we find

$$\sum_{j=0}^{n} \omega_j = \sum_{j=0}^{n-1} \omega_j + \omega_n = \tau^{-\alpha} \frac{n(-1)^{n-1}}{\alpha} \binom{\alpha}{n} + \tau^{-\alpha}(-1)^n \binom{\alpha}{n} = \tau^{-\alpha} \frac{(n+1)(-1)^n}{\alpha} \binom{\alpha}{n+1}.$$

Thus the relation (4.4) holds for all $n \geq 0$, which completes the proof of the lemma. □

Lemma 4.2. *Let $\mathcal{E}_{1,\tau} = \omega_0 (\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$, where $\omega_0 = P(\tau^{-1})$. Then $\mathcal{E}_{n,\tau} \geq 0$ for $n \geq 1$.*

Proof. Let $U^0 = V \geq 0$ and let U^n be defined by (4.2) for $n \geq 1$. For a proof by induction, assume that $U^j \geq 0$ for $j \leq n-1$. By assumption, $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$, and by Lemma 4.1 we have $\sum_{j=0}^{n-1} \omega_j V - \sum_{j=1}^{n-1} \omega_{n-j} U^j \geq 0$. Hence $U^n = \mathcal{E}_{n,\tau} V \geq 0$, which completes the proof. □

Next we state the following fully discrete analogue of Theorem 3.1.

Theorem 4.1. *Assume that the triangulation $\mathcal{T}_h$ is normal and the mass matrix $\mathcal{M}$ is nondiagonal. Then the solution matrix $\mathcal{E}_{1,\tau}$ cannot be nonnegative for small $\tau > 0$.*

Proof. From the proof of Lemma 2.3 we find as $\tau \to 0$

$$\omega_0^{-1} = P(\tau^{-1})^{-1} = \widetilde{\beta}_0(\tau)(1 + o(1)) \quad \text{where} \quad \widetilde{\beta}_0(\tau) = \begin{cases} \tau^{\alpha_1}, & \text{in case I,} \\ \mu(1)^{-1} \tau \log(\tau^{-1}), & \text{in case II,} \end{cases}$$

and hence

$$\mathcal{E}_{1,\tau} = (\mathcal{I} + \omega_0^{-1} \mathcal{H})^{-1} = \mathcal{I} - \widetilde{\beta}_0(\tau) \mathcal{H} \, (1 + o(1)). \tag{4.5}$$

Since $\widetilde{\beta}_0(\tau) > 0$, the argument in the proof of Theorem 3.1 then completes the proof. □

We now show some results concerning positivity thresholds for the fully discrete method.

Theorem 4.2. *The following statements hold.*

(i) *If $\mathcal{H}^{-1} > 0$, then there exists a $\tau_0 > 0$ such that $\mathcal{E}_{n,\tau} \geq 0$ for $\tau \geq \tau_0, \ n \geq 1$.*
(ii) *If $\mathcal{E}_{1,\tau_0} \geq 0$, then $\mathcal{E}_{n,\tau} \geq 0$ for $\tau \geq \tau_0, \ n \geq 1$, and $\mathcal{H}^{-1} \geq 0$.*

Proof. If $\mathcal{H}^{-1} > 0$, then by continuity, $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$ for ω_0 small, i.e., for τ large. In particular, there exists $\tau_0 \geq 0$ such that $\mathcal{E}_{1,\tau} \geq 0$ for $\tau \geq \tau_0$, and hence $\mathcal{E}_{n,\tau} \geq 0$ for $\tau \geq \tau_0, \ n \geq 1$, by Lemma 4.2.

For part (ii), we note that if $\mathcal{E}_{1,\tau_0} \geq 0$, then $(\widetilde{\omega}_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$, with $\widetilde{\omega}_0 = P(\tau_0^{-1})$. We show that then $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$ for $\omega_0 \in [0, \tilde{\omega}_0]$. In fact, with $\delta = \tilde{\omega}_0 - \omega_0 > 0$, we may write

$$(\omega_0 \mathcal{I} + \mathcal{H})^{-1} = (\tilde{\omega}_0 \mathcal{I} + \mathcal{H} - \delta \mathcal{I})^{-1} = (\tilde{\omega}_0 \mathcal{I} + \mathcal{H})^{-1} (\mathcal{I} - \mathcal{K})^{-1}, \quad \text{with } \mathcal{K} = \delta (\tilde{\omega}_0 \mathcal{I} + \mathcal{H})^{-1}.$$

Note that $\mathcal{K} \geq 0$ by assumption, and if δ is so small that for some matrix norm $|\cdot|$, $|\mathcal{K}| = \delta |(\tilde{\omega}_0 \mathcal{I} + \mathcal{H})^{-1}| < 1$, then $(\mathcal{I} - \mathcal{K})^{-1} = \sum_{j=0}^{\infty} \mathcal{K}^j \geq 0$, and therefore, $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$. But if $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$ for $\omega_0 \in (\tilde{\tilde{\omega}}_0, \tilde{\omega}_0]$, with $\tilde{\tilde{\omega}}_0 \geq 0$, then $(\tilde{\tilde{\omega}}_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$. Hence, by repeating the argument, we deduce $(\omega_0 \mathcal{I} + \mathcal{H})^{-1} \geq 0$ for some $\omega_0 < \tilde{\tilde{\omega}}_0$, and thus the smallest such $\tilde{\tilde{\omega}}_0$ has to be 0. Since $P(\tau^{-1})$ is monotone, this means that $\mathcal{E}_{1,\tau} \geq 0$ for $\tau \geq \tau_0$, and thus shows the first part of (ii), by Lemma 4.2. The last part of (ii) now follows from $\mathcal{H}^{-1} = \lim_{\omega_0 \to 0} (\omega_0 \mathcal{I} + \mathcal{H})^{-1}$. □

We note that if $\mathcal{H}^{-1} > 0$ and ω_0 is the largest number such that $(\omega_0\mathcal{I} + \mathcal{H})^{-1} \geq 0$, then in the single-term case the positivity threshold equals $\omega_0^{-1/\alpha}$. For $\omega_0 > 1$, this number increases with $\alpha \in (0, 1]$, with its largest value for $\alpha = 1$, i.e., for the heat equation, and tends to zero as $\alpha \to 0$.

The following result gives a somewhat more precise estimate for the positivity threshold ω_0, in the case of "strictly" Delaunay triangulations.

Theorem 4.3. *If $s_{ij} < 0$ for all neighbors P_i, P_j and $\mathcal{M}$ is nondiagonal, then $\mathcal{E}_{n,\tau} \geq 0$ for all $n \geq 1$ if $\omega_0 \leq \max_{\mathcal{N}} |s_{ij}|/m_{ij}$, where $\mathcal{N} = \{(i,j) :\ P_i, P_j \text{ neighbors}\}$.*

Proof. If the assumptions hold, we have $\omega_0\, m_{ij} + s_{ij} < 0$ for $j \neq i$, so that $\omega_0\, \mathcal{M} + \mathcal{S}$ is a Stieltjes matrix. Hence $(\omega_0\, \mathcal{I} + \mathcal{H})^{-1} = (\omega_0\, \mathcal{M} + \mathcal{S})^{-1}\mathcal{M} \geq 0$, and thus $\mathcal{E}_{n,\tau} \geq 0$ for $n \geq 1$, by Lemma 4.2. □

In particular, for the single-term model, in the case of a quasiuniform family of triangulation $\mathcal{T}_h$, with $\psi_1 + \psi_2 \leq \gamma < \pi$ for all edges P_iP_j, we have $\mathcal{E}_{n,\tau} \geq 0$ for $n \geq 1$, if $\tau \geq c_\alpha h^{2/\alpha}$, with $c_\alpha > 0$.

We finally show the following fully discrete analogue of Theorem 3.3 for the LM method.

Theorem 4.4. *Let $\mathcal{E}_{n,\tau}$ be the solution matrix of the LM method. Then $\mathcal{E}_{n,\tau} \geq 0$ for all $\tau > 0$, $n \geq 1$, if $\mathcal{T}_h$ is Delaunay, and, conversely, if $\mathcal{E}_{1,\tau} \geq 0$ for all $\tau > 0$, then $\mathcal{T}_h$ is Delaunay.*

Proof. If $\mathcal{T}_h$ is Delaunay, then the stiffness matrix $\mathcal{S}$ is Stieltjes, and so is $\omega_0\mathcal{M} + \mathcal{S}$, for any $\omega_0 \geq 0$. Hence $(\omega_0\mathcal{I}+\mathcal{H})^{-1} = (\omega_0\mathcal{M}+\mathcal{S})^{-1}\mathcal{M} \geq 0$. and, by Lemma 4.2, $\mathcal{E}_{n,\tau} \geq 0$ for all $\tau > 0, n \geq 1$. Conversely, if $\mathcal{E}_{1,\tau} \geq 0$ for all $\tau > 0$, then (4.5) holds for τ small. Hence $h_{ij} \leq 0$ and thus $s_{ij} \leq 0$ for $P_i.P_j$ neighbors, so that $\mathcal{S}$ is Stieltjes and $\mathcal{T}_h$ is Delaunay. □

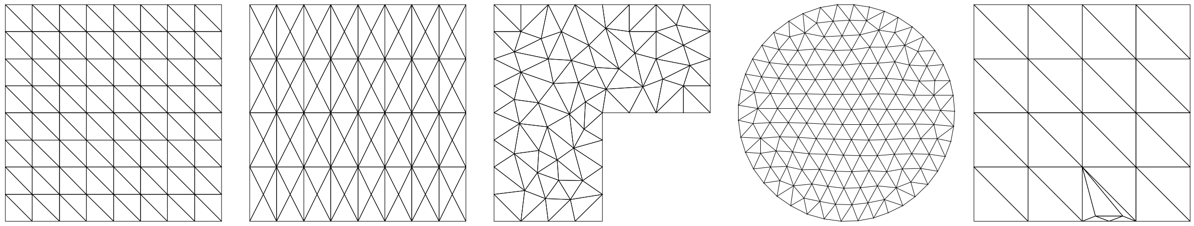
5. Numerical experiments and discussions

In this section we present numerical experiments to illustrate and to complement our theoretical findings. We consider the following five domains with different triangulations, cf. Fig 1:

(a) The unit square $\Omega = (0, 1)^2$, partitioned by uniform Delaunay triangulations;
(b) The unit square $\Omega = (0, 1)^2$, partitioned into a structured family of non-Delaunay triangulations;
(c) The L-shaped domain $\Omega = (0, 1)^2\backslash([1/2, 1) \times (0, 1/2])$, partitioned by unstructured Delaunay triangulations;
(d) The unit disk $\Omega = \{(x, y) : x^2 + y^2 < 1\}$, partitioned by unstructured Delaunay triangulations;
(e) The unit square $\Omega = (0, 1)^2$, partitioned into non-Delaunay triangulations, obtained from the uniform triangulations in Example (a) with an additional subdivision of one boundary triangle.

Our numerical experiments cover single-term ($m = 1$, $\alpha_1 = \alpha \in (0, 1)$), multi-term (with $m = 2$, $1 > \alpha_1 > \alpha_2 > 0$), and distributed order cases of problem (1.5), to be made specific below. For each example, we investigate the preservation of nonnegativity for the spatially semidiscrete and the fully discrete SG, FVE and LM methods. In the third case, of course, calculations are only needed for the non-Delaunay triangulations in (b) and (e). For our numerical calculations of the solution matrices $\mathcal{E}(t)$ we use the eigenvalue decomposition (3.2), where the $u_{\lambda_j}(t)$ are defined as inverse Laplace transforms in (2.3). For the latter we employ a numerical algorithm from [30], deforming the contour Γ_σ to the left branch of a hyperbola in the complex plane with the parametric representation $z(\xi) := \lambda(1+\sin(\mathrm{i}\xi - \psi))$, $\lambda > 0$, $\psi \in (0, \pi/2)$ and $\xi \in \mathbb{R}$. The resulting integral is then approximated by a truncated trapezoidal rule, which, for an appropriate choice of the parameters λ and ψ, is exponentially convergent. The positivity thresholds t_0 and τ_0 are computed using a bisection method. In the semidiscrete case we start with an upper bound t_+, with $\mathcal{E}(t_+) \geq 0$, and a lower bound t_-, with $\mathcal{E}(t_-) \not\geq 0$, and refine these bounds by successive bisection, till the appropriate accuracy. This assumes that $\mathcal{E}(t_0) \geq 0$ implies $\mathcal{E}(t) \geq 0$ for $t > t_0$, which was numerically verified in our experiments, but has not been mathematically proven. In the fully discrete case the corresponding result holds by Theorem 4.2(ii).

Example (a). As in [1] we begin by studying a family of uniform triangulations $\mathcal{T}_h$, constructed as follows. For given $M > 0$ we divide the sides of Ω into M equal subintervals of length $h_0 = 1/M$, thus dividing Ω into M^2 small squares. By means of parallel diagonals in the small squares we then obtain a uniform triangulation, with $h = \sqrt{2}h_0$. Note that for such triangulations, the stiffness matrix $\mathcal{S} = (s_{ij})$ has $s_{ii} = 4$ and $s_{ij} = -1$ if P_iP_j are vertical or horizontal neighbors, with $s_{ij} = 0$ otherwise. In particular

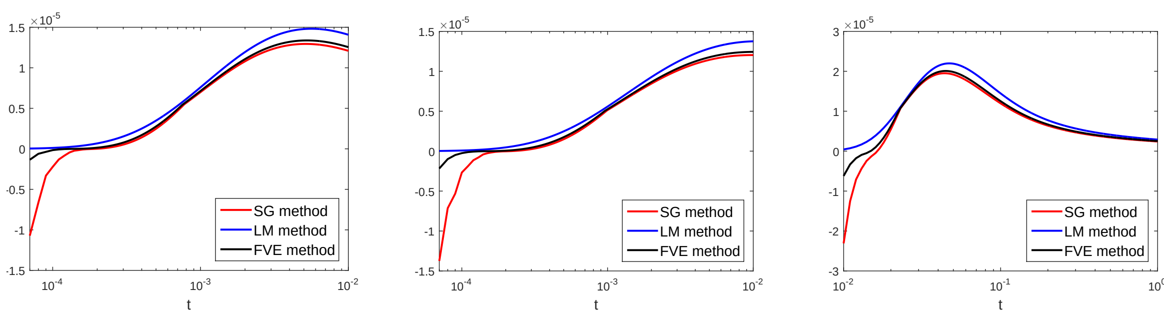


(a) uniform mesh (b) nonDelaunay mesh (c) L-shape domain (d) unit disk (e) nonDelaunay mesh

FIGURE 1. The domains with triangulations of Examples (a), (b), (c), (d) and (e).

$\mathcal{S}$ is Stieltjes, with $\mathcal{S}^{-1} > 0$, and hence $\mathcal{H}^{-1} = \mathcal{S}^{-1}\mathcal{M} > 0$ for the SG, LM and FVE methods. Thus the results in Sections 3 and 4 concerning nonnegativity preservation for large t and τ apply.

In Fig. 2, we plot the smallest entry of the solution matrix $\mathcal{E}(t)$ for the semidiscrete SG, LM and FVE methods with $h_0 = 0.100$. The LM method preserves nonnegativity, and in Table 1 we present threshold values $\hat{t}_0$ and $\tilde{t}_0$ for the semidiscrete SG and FVE methods, respectively, for $M = 10$, 20 and 40. Their behavior is in agreement with Theorems 3.1, 3.2 and 3.3. Like in [1] the thresholds are smaller for the FVE methods than for the SG methods and decrease with the fractional order α in the single-term case. We also observe that the thresholds decrease with h. For the fully discrete method, the positivity thresholds $\hat{\tau}_0$ and $\tilde{\tau}_0$ of $\mathcal{E}_{1,\tau}$ are also given in Table 1. Note that the triangulations do not satisfy the condition in Theorem 4.3. Nevertheless, following the argument in [1, Section 5.1], lower bounds for the positivity thresholds may be derived in the fully discrete case. By Table 1 it appears that, for the single-term model, this is of order $O(h^{2/\alpha})$, and the multi-term model shows a similar behavior.



(a) single-term, $\alpha = 0.5$ (b) multi-term, $\alpha_1 = 0.5$, $\alpha_2 = 0.2$ (c) distributed order, $\mu(\alpha) = e^{\alpha}$

FIGURE 2. The evolution of the smallest entry of $\mathcal{E}(t)$ for the semidiscrete SG, LM and FVE methods for Example (a), with $h_0 = 0.100$.

Example (b). We next consider a family of non-Delaunay triangulations $\mathcal{T}_h$ from [1, Section 5.2], constructed as follows. Let M be a positive integer, $h_0 = 1/(2M)$, and set $x_i = ih_0$, $i = 0, \ldots, 2M$, and $y_j = 2jh_0$ for $j = 0, \ldots, M$. This divides the domain Ω into small rectangles $(x_i, x_{i+1}) \times (y_j, y_{j+1})$, and we now connect the nodes (x_i, y_j) with (x_{i+1}, y_{j+1}), and (x_{i+1}, y_j) with (x_i, y_{j+1}). For this triangulation, $h = 2h_0$, and all vertical edges are non-Delaunay, cf., Fig. 1(b). The stiffness and mass matrices are given analytically in [1].

Since $\mathcal{T}_h$ is non-Delaunay, the LM solution matrices $\mathcal{E}(t)$ and $\mathcal{E}_{1,\tau}$ cannot be nonnegative for small $t > 0$ and $\tau > 0$, by Theorems 3.3 and 4.4, respectively. However, even though the stiffness matrix $\mathcal{S}$ is not Stieltjes, in our computations $\mathcal{S}^{-1} > 0$, and hence by Theorems 3.2 and 4.2, there exist positivity thresholds for all three methods, cf. Table 2. For all three subdiffusion models, the positivity thresholds are still smallest for the LM method and largest for the SG method, and the thresholds decrease with h.

TABLE 1. Positivity thresholds for Example (a), for the semidiscrete and fully discrete SG and FVE methods.

	h_0	h	single-term (α)				multi-term (α_1,α_2)				distributed ($\mu(\alpha)$)	
			0.5		0.75		$(0.5,0.2)$		$(0.75,0.2)$		e^α	
			$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$
SD	0.100	0.141	1.96e-4	1.46e-4	7.42e-3	6.41e-3	2.11e-4	1.56e-4	7.56e-3	6.51e-3	1.64e-2	1.48e-2
	0.050	0.071	3.74e-5	2.74e-5	3.54e-3	2.98e-3	3.86e-5	2.82e-5	3.57e-3	3.00e-3	1.03e-2	9.12e-3
	0.025	0.035	1.36e-5	1.29e-5	1.44e-3	1.19e-3	1.41e-5	1.16e-5	1.43e-3	1.23e-3	5.42e-3	4.64e-3
FD	0.100	0.141	2.85e-5	1.98e-5	9.33e-4	7.32e-4	3.11e-5	2.14e-5	9.61e-4	7.50e-4	2.01e-3	1.63e-3
	0.050	0.071	1.81e-6	1.26e-6	1.49e-4	1.17e-4	1.88e-6	1.30e-6	1.50e-4	1.18e-4	4.17e-4	3.39e-4
	0.025	0.035	1.37e-7	8.24e-8	2.65e-5	1.89e-5	1.39e-7	8.36e-8	2.67e-5	1.90e-5	9.80e-5	7.42e-5

TABLE 2. Positivity thresholds for Example (b) for the semidiscrete and fully discrete SG, LM and FVE methods.

	h_0	h	single-term (α)			multi-term (α_1,α_2)			distributed ($\mu(\alpha)$)		
			0.5			$(0.5,0.2)$			e^α		
			$\hat t_0\backslash\hat\tau_0$	$\bar t_0\backslash\bar\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\bar t_0\backslash\bar\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\bar t_0\backslash\bar\tau_0$	$\tilde t_0\backslash\tilde\tau_0$
SD	0.100	0.200	2.59e-4	1.17e-4	2.26e-4	2.99e-4	1.30e-4	2.58e-4	1.09e-2	7.02e-3	1.03e-2
	0.050	0.100	3.97e-5	1.15e-5	3.14e-5	4.13e-5	1.20e-5	3.27e-5	7.85e-3	3.52e-3	7.13e-3
	0.025	0.050	1.77e-5	1.27e-5	1.68e-5	1.78e-5	1.38e-5	1.74e-5	4.70e-3	3.55e-3	4.41e-3
FD	0.100	0.200	6.20e-4	2.21e-4	5.21e-4	7.73e-4	2.60e-4	6.42e-4	1.25e-2	6.71e-2	1.13e-2
	0.050	0.100	3.88e-5	1.38e-5	3.26e-5	4.26e-5	1.48e-5	3.57e-5	2.41e-3	1.32e-3	2.17e-3
	0.025	0.050	2.42e-6	8.64e-7	2.03e-6	2.52e-5	8.90e-7	2.12e-6	4.91e-4	2.74e-4	4.44e-4

Examples (c) and (d). In these examples unstructured Delaunay triangulations are generated using the public domain mesh generators `Triangle` [26] and `DistMesh` [22] for (c) and (d), respectively. The LM method preserves nonnegativity for $t \geq 0$, and the positivity thresholds for the SG and FVE methods, in Tables 3 and 4, exhibit a behavior similar to that for the uniform triangulations in Example (a). For example, in the single-term subdiffusion, the positivity threshold for the fully discrete schemes shows a $O(h^{2/\alpha})$ dependence on h.

TABLE 3. Positivity thresholds for Example (c) for the semidiscrete and fully discrete SG and FVE methods.

	h	single-term (α)				multi-term (α_1,α_2)				distributed ($\mu(\alpha)$)	
		0.5		0.75		$(0.5,0.2)$		$(0.75,0.2)$		e^α	
		$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$
SD	0.198	1.17e-4	8.52e-5	5.04e-3	4.17e-3	1.25e-4	8.72e-5	5.13e-3	4.23e-3	1.17e-2	1.02e-2
	0.101	2.05e-5	1.47e-5	2.28e-3	1.83e-3	2.12e-5	1.51e-5	2.29e-3	1.83e-3	7.38e-3	6.12e-3
	0.051	1.21e-5	1.05e-5	1.26e-3	1.09e-3	1.23e-5	1.12e-5	1.27e-3	1.11e-3	4.11e-3	3.63e-3
FD	0.198	4.36e-5	3.03e-5	1.24e-3	9.72e-4	4.81e-5	3.31e-5	1.28e-3	1.00e-3	2.57e-3	2.08e-3
	0.101	3.07e-6	2.09e-6	2.11e-4	1.64e-4	3.21e-6	2.18e-6	2.14e-4	1.65e-4	5.61e-4	4.52e-5
	0.051	2.50e-7	1.73e-7	3.97e-5	3.10e-5	2.55e-7	1.76e-7	3.99e-5	3.12e-5	1.38e-4	1.12e-4

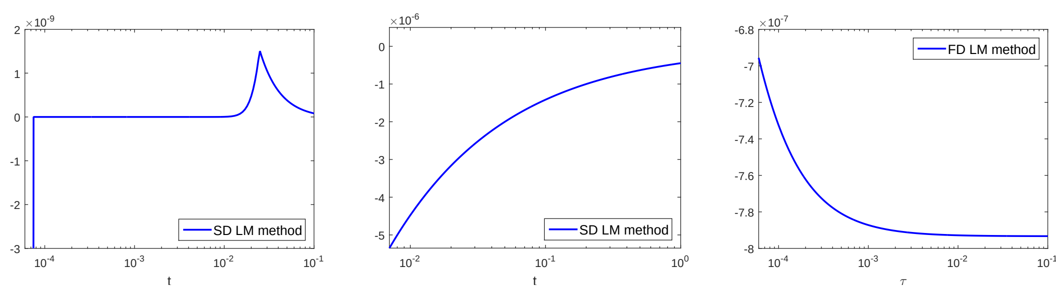
Example (e). We finally consider a family of non-Delaunay triangulations $\mathcal{T}_h$ of the unit square, studied in Drăgănescu et al. [5]. Using the uniform triangulation of Ω in Example (a) with $h_0 = 1/M$, we further subdivide one triangle at the boundary by introducing three extra nodes, $Q = (1/2 + h_0/4, h_0\epsilon)$, $R = (1/2 + 3h_0/4, h_0\epsilon)$ with $\epsilon = 10^{-3}$, and $P = (h_0/2, 0)$, cf. Fig. 1(e).

TABLE 4. Positivity thresholds for Example (d) for the semidiscrete and fully discrete SG and FVE methods.

	h	single-term (α)				multi-term (α_1, α_2)				distributed ($\mu(\alpha)$)	
		0.5		0.75		(0.5, 0.2)		(0.75, 0.2)		e^α	
		$\hat{t}_0\backslash\hat{\tau}_0$	$\tilde{t}_0\backslash\tilde{\tau}_0$	$\hat{t}_0\backslash\hat{\tau}_0$	$\tilde{t}_0\backslash\tilde{\tau}_0$	$\hat{t}_0\backslash\hat{\tau}_0$	$\tilde{t}_0\backslash\tilde{\tau}_0$	$\hat{t}_0\backslash\hat{\tau}_0$	$\tilde{t}_0\backslash\tilde{\tau}_0$	$\hat{t}_0\backslash\hat{\tau}_0$	$\tilde{t}_0\backslash\tilde{\tau}_0$
SD	0.20	6.68e-4	4.29e-4	1.78e-2	1.38e-2	7.38e-4	4.67e-4	1.83e-2	1.41e-2	3.66e-2	2.99e-2
	0.10	9.11e-5	6.12e-5	7.12e-3	5.42e-3	9.46e-5	6.42e-5	7.18e-3	5.46e-3	1.95e-2	1.58e-2
	0.05	5.68e-5	5.24e-5	3.58e-3	3.29e-3	6.00e-5	5.53e-5	3.59e-3	3.34e-3	1.02e-2	9.36e-3
FD	0.20	9.39e-5	5.95e-5	2.07e-3	1.53e-3	1.06e-4	6.64e-5	2.16e-3	1.58e-3	4.04e-3	3.09e-3
	0.10	6.06e-6	3.88e-6	3.32e-4	2.47e-4	6.40e-6	4.07e-6	3.38e-4	2.50e-4	8.25e-4	6.40e-4
	0.05	4.03e-7	2.50e-7	5.45e-5	3.96e-5	4.12e-7	2.55e-7	5.46e-5	3.98e-5	1.80e-4	1.37e-4

Since $\mathcal{T}_h$ is non-Delaunay, by Theorems 3.3 and 4.4 the LM methods do not preserve nonnegativity for small positive t and τ. It was shown in [5] that $\mathcal{S}^{-1} \not\geq 0$, and hence $\mathcal{H}^{-1} \not\geq 0$ for the LM methods. In particular, by Theorem 4.2, the fully discrete method cannot preserve positivity for large τ. It can be seen that $\mathcal{H}^{-3} > 0$, i.e., that $\mathcal{H}^{-1}$ is eventually positive, which is sufficient to ensure the existence of a positivity threshold for $\mathcal{E}(t)$ in the case of the heat equation (see [1]). In contrast, in the fractional case, no positivity threshold appears to exist for the semidiscrete LM method for the single-term model, which shows a drastic difference between anomalous and normal diffusion. The evolution of the smallest entry of $\mathcal{E}(t)$ for the single-term case with $\alpha = 0.5$ and $e^{-\mathcal{H}t}$ (corresponding to the heat equation) for the semidiscrete methods is shown in Fig. 3.

However, even for this somewhat pathological triangulation, in our computations the matrix $\mathcal{H}^{-1}$ turns out to be positive for the SG and FVE methods, and hence, by Theorems 3.2 and 4.2, both the semidiscrete and the fully discrete methods preserve nonnegativity for large t and τ. Table 5 shows positivity thresholds for the FVE and SG methods, and we note that again they are smaller for the FVE method than for the SG method and decrease with h.



(a) $\mathcal{E}(t) = e^{-\mathcal{H}t}$ (b) $\mathcal{E}(t) = E_\alpha(-\mathcal{H}t^\alpha)$, $\alpha = 0.5$ (c) $(\tau^\alpha I + \mathcal{H})^{-1}$, $\alpha = 0.5$

FIGURE 3. The evolution of the smallest entry of $\mathcal{E}(t)$ for the semidiscrete and fully discrete LM methods for Example (e), with $h = 0.141$.

APPENDIX A. CONVERGENCE OF THE TIME STEPPING SCHEME

In the proof of Theorem 3.3 and also in Appendix B we need the convergence of the fully discrete solution matrix to the semidiscrete one as the time step τ tends to zero, as shown in the following lemma.

Lemma A.1. *Let $\mathcal{E}(t)$ and $\mathcal{E}_{n,\tau}$ be the semidiscrete and fully discrete solution matrices, defined by (3.1) and (4.2), respectively. Then, with the norm defined by the inner product $\mathcal{M}V \cdot W$, we have*

$$\|\mathcal{E}(t) - \mathcal{E}_{n,t/n}\| \leq Cn^{-1}, \quad \text{for } n \geq 1.$$

TABLE 5. Positivity thresholds for Example (e) for the semidiscrete and fully discrete SG and FVE methods.

	h_0	h	single-term (α)		multi-term (α_1, α_2)		distributed ($\mu(\alpha)$)	
			0.5		$(0.5, 0.2)$		e^α	
			$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$	$\hat t_0\backslash\hat\tau_0$	$\tilde t_0\backslash\tilde\tau_0$
SD	0.100	0.141	1.96e-4	1.47e-4	2.11e-4	1.56e-4	1.64e-2	1.49e-2
	0.050	0.071	3.75e-5	2.75e-5	3.87e-5	2.83e-5	1.04e-2	9.12e-3
	0.025	0.035	1.58e-5	1.20e-5	1.66e-5	1.24e-5	5.43e-3	4.72e-3
FD	0.100	0.141	2.86e-5	1.98e-5	3.11e-5	2.14e-5	2.02e-3	1.63e-3
	0.050	0.071	1.82e-6	1.26e-6	1.89e-6	1.31e-6	4.17e-4	3.40e-4
	0.025	0.035	1.36e-7	8.21e-8	1.41e-7	8.31e-8	9.80e-5	7.42e-5

Proof. By eigenvector expansion, cf. (3.2) and (4.3), and Parseval's formula we have

$$\|\mathcal{E}(t) - \mathcal{E}_{n,t/n}\| = \max_j |u_{\lambda_j} - r_{n,t/n}(\lambda_j)|,$$

where $r_{n,\tau}(\lambda),\ n \geq 1$, with $\tau = t/n$, are the rational functions for which $\mathcal{E}_{n,\tau} = r_{n,\tau}(\mathcal{H})$, and the λ_j are the eigenvalues of $\mathcal{H}$. So it remains to show the inequality

$$|u_\lambda(t) - r_{n,t/n}(\lambda)| \leq Cn^{-1}, \quad \text{for } \lambda > 0,\ n \geq 1.$$

We recall from (2.3) that

$$u_\lambda(t) = \frac{1}{2\pi \mathrm{i}} \int_{\Gamma_\sigma} J_\lambda(z) e^{zt}\, dz \quad \text{with } J_\lambda(z) = z^{-1} P(z)(P(z) + \lambda)^{-1}. \tag{A.1}$$

To determine a corresponding representation of $r_{n,\tau}(\lambda)$ we consider the fully discrete solution $u^n = r_{n,\tau}(\lambda),\ n \geq 0$, of the scalar problem (2.4) for $u_\lambda(t)$, which is given by

$$\sum_{j=0}^{n} \omega_{n-j} u^j + \lambda u^n = \sum_{j=0}^{n} \omega_{n-j} \quad \text{for } n \geq 1, \quad \text{with } u^0 = 1. \tag{A.2}$$

Multiplying both sides by ξ^n and summing over n from 1 to ∞, we obtain

$$\sum_{n=1}^{\infty} \xi^n \sum_{j=0}^{n} \omega_{n-j} u^j + \lambda \sum_{n=1}^{\infty} u^n \xi^n = \sum_{n=1}^{\infty} \xi^n \sum_{j=0}^{n} \omega_{n-j}.$$

Upon adding ω_0 to both sides, the summation in the double sums may start at $n = 0$, so that they are both discrete convolutions, and hence, with $\widetilde{u}(\xi)$ the generating function of the u^j (i.e., $\widetilde{u}(\xi) = \sum_{j=0}^{\infty} u^j \xi^j$), $\delta_\tau(\xi) = (1 - \xi)/\tau$ that of the backward Euler method, and $(1 - \xi)^{-1}$ that of the sequence $(1, 1, 1, \ldots)$, we obtain

$$P(\delta_\tau(\xi))\widetilde{u}(\xi) + \lambda(\widetilde{u}(\xi) - 1) = P(\delta_\tau(\xi))(1 - \xi)^{-1},$$

or

$$(P(\delta_\tau(\xi)) + \lambda)(\widetilde{u}(\xi) - 1) = P(\delta_\tau(\xi))((1 - \xi)^{-1} - 1).$$

Consequently, we have

$$\widetilde{u}(\xi) - 1 = (P(\delta_\tau(\xi)) + \lambda)^{-1} P(\delta_\tau(\xi)) \xi (1 - \xi)^{-1} = \tau^{-1} \xi J_\lambda(\delta_\tau(\xi)),$$

Hence, the nth term in $\widetilde{u}(\xi)$ is given by

$$u^n = \frac{1}{2\pi \mathrm{i}} \int_{|\xi| = \epsilon} \tau^{-1} J_\lambda(\delta_\tau(\xi)) \xi^{-n}\, d\xi, \quad \text{for } n \geq 1,$$

and changing variables with $z = (1 - \xi)/\tau$ yields, with small $\epsilon > 0$,

$$r_{n,\tau}(\lambda) = u^n = \frac{1}{2\pi \mathrm{i}} \int_{|1 - z\tau| = \epsilon} J_\lambda(z)(1 - z\tau)^{-n}\, d\xi. \tag{A.3}$$

Since $J_\lambda(\xi)$ is analytic in the complement of the negative real axis we may deform the contour of integration into Γ_σ and, with the change of variables $z = \zeta/\tau,\ \tau = t/n$, we obtain the error representation

$$u_\lambda(t) - r_{n,\tau}(\lambda) = \frac{1}{2\pi\mathrm{i}} \int_{\Gamma_\sigma} J_\lambda(z) \left(e^{zt} - (1 - z\tau)^{-n}\right) dz = \frac{1}{2\tau\pi\mathrm{i}} \int_{\Gamma_\sigma} J_\lambda(\zeta/\tau) \left(e^{n\zeta} - (1-\zeta)^{-n}\right) d\zeta.$$

We now deform Γ_σ into $\Gamma = \Gamma_0 \cup \Gamma_1$, with $\Gamma_0 = \{e^{\mathrm{i}\varphi}/(2n) : \varphi \in [-\theta, \theta]\}$ a circular arc and $\Gamma_1 = \{\rho e^{\pm \mathrm{i}\theta} : \rho \geq 1/(2n)\}$, a pair of rays in the left half-plane, where $\theta \in (\pi/2, \pi)$. On Γ_0, we have $|\zeta| = 1/(2n)$ and $|(1-\zeta)^{-1}| \leq e^{c|\zeta|}$ and hence

$$|e^{n\zeta} - (1-\zeta)^{-n}| = \left| \left(e^{\zeta} - (1-\zeta)^{-1}\right) \sum_{j=0}^{n-1} (1-\zeta)^{-j} e^{(n-1-j)\zeta} \right| \leq C|\zeta|^2\, n\, e^{cn|\zeta|} \leq Cn^{-1}.$$

Next, we write $\Gamma_1 = \Gamma_R \cup \Gamma^R$ where $\Gamma_R = \{\rho e^{\pm\mathrm{i}\theta} : \rho \in [1/(2n), R]\}$ and $\Gamma^R = \{\rho e^{\pm\mathrm{i}\theta} : \rho \geq R\}$. With $c > 0$ and R large enough such that $|(1-\zeta)^{-1}| \leq e^{-c}$ on Γ^R, using also $|(1-\zeta)^{-1}| \leq |\zeta|^{-1}$ on Γ_1, we have

$$|e^{n\zeta} - (1-\zeta)^{-n}| \leq |e^{n\zeta}| + |1-\zeta|^{-n} \leq C|\zeta|^{-1} e^{-cn}, \quad \text{for } \zeta \in \Gamma^R.$$

Further, with $R > 0$ given, we have $|(1-\zeta)^{-1}| \leq e^{-c|\zeta|}$ for $\zeta \in \Gamma_R$ and $c > 0$ small enough, and hence

$$|e^{n\zeta} - (1-\zeta)^{-n}| = \big| \left(e^{\zeta} - (1-\zeta)^{-1}\right) \sum_{j=0}^{n-1} (1-\zeta)^{-j} e^{(n-1-j)\zeta} \big| \leq C|\zeta|^2\, n\, e^{-cn|\zeta|}, \quad \text{for } \zeta \in \Gamma_R.$$

We also note that $|J_\lambda(z)| \leq C/|z|$ for $z \in \Sigma_\theta := \{z : z \neq 0, |\arg z| \leq \theta\}$ with $\theta < \pi$. In fact, if $z \in \Sigma_\theta$, with $\operatorname{Im} z \geq 0$, say, then the same holds for z^α if $\alpha \in [0,1]$ and $w = P(z) = \int_0^1 z^\alpha\, d\nu(\alpha)$, and it hence suffices to show $|w/(w+\lambda)| \leq C$ for $w \in \Sigma_\theta$. For $\operatorname{Re} w \geq 0$ we have $|w/(w+\lambda)| \leq 1$, and for $\operatorname{Re} w < 0$, $|w/(w+\lambda)| \leq |w|/|\operatorname{Im} w| \leq 1/|\cos\theta|$. Together these inequalities yield

$$\begin{aligned} |u_\lambda(t) - r_{n,t/n}(\lambda)| &\leq C\Big(n^{-1} \int_{\Gamma_0} |\zeta|^{-1}\, |d\zeta| + n \int_{\Gamma_R} |\zeta| e^{-cn|\zeta|}\, |d\zeta| + e^{-cn} \int_{\Gamma^R} |\zeta|^{-2}\, |d\zeta|\Big) \\ &\leq C\Big(n^{-1} \int_{-\theta}^{\theta} d\psi + \int_{1/2n}^{R} nre^{-cnr}\, dr + e^{-cn} \int_R^\infty r^{-2}\, dr\Big) \leq Cn^{-1}. \end{aligned}$$

This completes the proof of the lemma. □

We observe from (A.3) that by Cauchy's integral formula, $r_{n,\tau}(\lambda) = (-1)^{n-1}\tau^{-n} J_\lambda^{(n-1)}(1/\tau)$.

Appendix B. Maximum-norm contractivity of the lumped mass method

The maximum principle for (1.5) ensures the maximum-norm contractivity, i.e.,

$$\|E(t)v\|_{L^\infty(\Omega)} \leq \|v\|_{L^\infty(\Omega)} \quad \forall t \geq 0. \tag{B.1}$$

It is natural to ask if this property remains valid for discrete methods, and in [29, 25] this problem was discussed for the SG and LM methods for the heat equation. It turned out that, in contrast to the continuous case, the discrete analogue of (B.1) is not equivalent to the preservation of nonnegativity. In this appendix, we discuss maximum-norm contractivity for the LM method. In this case the desired property holds when the stiffness matrix $\mathcal{S}$ is diagonally dominant.

We first show a contraction property for the fully discrete method, and write $\|V\|_\infty = \max_i |V_i|$.

Theorem B.1. *The solution matrix $\mathcal{E}_{n,\tau}$ of the fully discrete LM method is contractive in the maximum-norm if the matrix $\mathcal{S}$ is diagonally dominant. If $\mathcal{E}_{1,\tau}$ is contractive in the maximum-norm, then $\mathcal{S}$ is diagonally dominant.*

Proof. Assume that $\mathcal{S}$ is diagonally dominant. Since $\mathcal{M}$ is positive and diagonal, $\mathcal{H} = \mathcal{M}^{-1}\mathcal{S}$ is row diagonally dominant. Let $V \in \mathbb{R}^N$, set $U^1 = \mathcal{E}_{1,\tau}V = (\mathcal{I} + \omega_0^{-1}\mathcal{H})^{-1}V$, and let $|U_j^1| = \|U^1\|_\infty$. Then

$$(1 + \omega_0^{-1}h_{jj})|U_j^1| = |V_j - \omega_0^{-1} \sum_{l \neq j} h_{jl} U_l^1| \leq \|V\|_\infty + \omega_0^{-1} h_{jj} \|U^1\|_\infty,$$

and hence $\|U^1\|_\infty \le \|V\|_\infty$, i.e., $\|(\mathcal{I}+\omega_0^{-1}\mathcal{H})^{-1}\|_\infty \le 1$.

We now prove that $\mathcal{E}_{n,\tau}$ is a contraction, by showing by induction that, for all $V \in \mathbb{R}^N$, $\|\mathcal{E}_{n,\tau}V\|_\infty = \|V^n\|_\infty \le \|V\|_\infty$. To this end, assume that this holds for all $j \le n-1$. Using Lemma 4.1, we then find

$$\|\sum_{j=0}^{n-1}\omega_j\ V - \sum_{j=1}^{n-1}\omega_{n-j}U^j\|_\infty \le \sum_{j=0}^{n-1}\omega_j\ \|V\|_\infty + \sum_{j=1}^{n-1}(-\omega_j)\|V\|_\infty = \omega_0\|V\|_\infty,$$

and hence, cf. (4.2), we get

$$\|U^n\|_\infty = \Big\|(\omega_0\mathcal{I}+\mathcal{H})^{-1}\Big(\sum_{j=0}^{n-1}\omega_j\ V - \sum_{j=1}^{n-1}\omega_{n-j}U^j\Big)\Big\|_\infty \le \|(\mathcal{I}+\omega_0^{-1}\mathcal{H})^{-1}\|_\infty\|V\|_\infty \le \|V\|_\infty,$$

which shows our claim.

Now, suppose that $\mathcal{E}_{1,\tau}$ is a contraction. In view of (4.5), we have

$$\|\mathcal{E}_{1,\tau}\|_\infty = \max_i \sum_j |(\mathcal{E}_{1,\tau})_{ij}| = \max_i \Big(1 - \widetilde{\beta}_0(\tau)\big(h_{ii} - \sum_{j\ne i}|h_{ij}|\big) + o(\widetilde{\beta}_0(\tau))\Big), \quad \text{as } \tau \to 0.$$

If $\|\mathcal{E}_{1,\tau}\|_\infty \le 1$, by taking τ small we find $\sum_{j\ne i}|h_{ij}| \le h_{ii}$ for $i = 1,\ldots,N$. Hence $\mathcal{H}$ is row diagonally dominant. Since $\mathcal{M}$ is a positive diagonal matrix, $\mathcal{S} = \mathcal{M}\mathcal{H}$ is also row diagonally dominant and hence, since it is symmetric, diagonally dominant. ☐

The next result gives the contractivity of the semidiscrete LM method.

Theorem B.2. *The semidiscrete LM solution matrix $\mathcal{E}(t)$ is contractive in the maximum norm if $\mathcal{S}$ is diagonally dominant. Conversely, if $\mathcal{E}(t)$ is contractive for small t then $\mathcal{S}$ is diagonally dominant.*

Proof. By Theorem B.1, $\mathcal{E}_{n,\tau}$ is a contraction in the maximum-norm, and, by Lemma A.1, converges to the semidiscrete solution matrix in the sense that $\mathcal{E}(t) = \lim_{n\to\infty}\mathcal{E}_{n,t/n}$. Hence also $\mathcal{E}(t)$ is a contraction. Conversely, if $\mathcal{E}(t)$ is a contraction in $\|\cdot\|_\infty$ for small t, then by (3.5) we have

$$\|\mathcal{E}(t)\|_\infty = \max_i \Big(1 - \beta_0(t)\big(h_{ii} - \sum_{j\ne i}|h_{ij}|\big) + o(\beta_0(t))\Big) \quad \text{as } t \to 0.$$

The rest of the proof is then identical to that of Theorem B.1. ☐

Acknowledgements

The work of the first author (B. Jin) is partly supported by UK Engineering and Physical Sciences Research Council grant EP/M025160/1.

References

[1] P. Chatzipantelidis, Z. Horváth, and V. Thomée. On positivity preservation in some finite element methods for the heat equation. *Comput. Methods Appl. Math.*, 15(4): 417–437, 2015.
[2] P. Chatzipantelidis, R. Lazarov, and V. Thomée. Some error estimates for the finite volume element method for a parabolic problem. *Comput. Methods Appl. Math.*, 13(3):251–279, 2013.
[3] A. V. Chechkin, R. Gorenflo, and I. M. Sokolov. Retarding subdiffusion and accelerating superdiffusion governed by distributed-order fractional diffusion equations. *Phys. Rev. E*, 66:046129, 2002.
[4] S.-H. Chou and Q. Li. Error estimates in L^2, H^1 and L^∞ in covolume methods for elliptic and parabolic problems: a unified approach. *Math. Comp.*, 69(229):103–120, 2000.
[5] A. Drăgănescu, T. Dupont, and L. Scott. Failure of the discrete maximum principle for an elliptic finite element problem. *Math. Comp.*, 74(249):1–23, 2005.
[6] W. Feller. *An Introduction to Probability Theory and its Applications*, Vol. 2. John Wiley & Sons, 1971.
[7] H. Fujii. Some remarks on finite element analysis of time-dependent field problems. In. Theory and Practice in Finite Element Structural Analysis (Y. Yamada, R. H. Gallagher & N. K. Kyokai eds). Tokyo, Japan: University of Tokyo Press, pp. 91–106., 1973.
[8] B. Jin, R. Lazarov, Y. Liu, and Z. Zhou. The Galerkin finite element method for a multi-term time-fractional diffusion equation. *J. Comput. Phys.*, 281:825–843, 2015.
[9] B. Jin, R. Lazarov, D. Sheen, and Z. Zhou. Error estimates for approximations of distributed order time fractional diffusion with nonsmooth data. Fract. Calc. Appl. Anal., 19(1):69–93, 2016.

[10] B. Jin, R. Lazarov, and Z. Zhou. Error estimates for a semidiscrete finite element method for fractional order parabolic equations. *SIAM J. Numer. Anal.*, 51(1):445–466, 2013.
[11] B. Jin, R. Lazarov, and Z. Zhou. On two schemes for fractional diffusion and diffusion wave equations. *SIAM J. Sci. Comput.* 38(1): A146–A170, 2016.
[12] A. Kilbas, H. Srivastava, and J. Trujillo. *Theory and Applications of Fractional Differential Equations*. Elsevier, Amsterdam, 2006.
[13] A. N. Kochubei. Distributed order calculus and equations of ultraslow diffusion. *J. Math. Anal. Appl.*, 340(1):252–281, 2008.
[14] Z. Li, Y. Liu, and M. Yamamoto. Initial-boundary value problems for multi-term time-fractional diffusion equations with positive constant coefficients. *Appl. Math. Comput.*, 257:381–397, 2015.
[15] Z. Li, Y. Luchko, and M. Yamamoto. Asymptotic estimates of solutions to initial-boundary-value problems for distributed order time-fractional diffusion equations. *Fract. Calc. Appl. Anal.*, 17(4):1114–1136, 2014.
[16] Y. Lin and C. Xu. Finite difference/spectral approximations for the time-fractional diffusion equation. *J. Comput. Phys.*, 225(2):1533–1552, 2007.
[17] C. Lubich. Convolution quadrature and discretized operational calculus. I. *Numer. Math.*, 52(2):129–145, 1988.
[18] Y. Luchko. Boundary value problems for the generalized time fractional diffusion equation of distributed order. *Frac. Cal. Appl. Anal.*, 12(4):409–422, 2009.
[19] Y. Luchko. Maximum principle for the generalized time-fractional diffusion equation. *J. Math. Anal. Appl.*, 351(1):218–223, 2009.
[20] Y. Luchko. Initial-boundary problems for the generalized multi-term time-fractional diffusion equation. *J. Math. Anal. Appl.*, 374(2):538–548, 2011.
[21] K. Mustapha, B. Abdallah, and K. M. Furati. A discontinuous Petrov-Galerkin method for time-fractional diffusion equations. *SIAM J. Numer. Anal.*, 52(5):2512–2529, 2014.
[22] P. Persson and G. Strang. A simple mesh generator in MATLAB, *SIAM Rev.*, 46(2):329–345, 2004.
[23] H. Pollard. The completely monotonic character of the Mittag-Leffler function $E_a(-x)$. *Bull. Amer. Math. Soc.*, 54:1115–1116, 1948.
[24] K. Sakamoto and M. Yamamoto. Initial value/boundary value problems for fractional diffusion-wave equations and applications to some inverse problems. *J. Math. Anal. Appl.*, 382(1):426–447, 2011.
[25] A. H. Schatz, V. Thomée, and L. B. Wahlbin. On positivity and maximum-norm contractivity in time stepping methods for parabolic equations. *Comput. Methods Appl. Math.*, 10(4):421–443, 2010.
[26] J. R. Shewchuk. Triangle: Engineering a 2D quality mesh generator and delaunay triangulator. In M. C. Lin and D. Manocha, editors, *Applied Computational Geometry: Towards Geometric Engineering*, pages 203–222. Springer, 1996.
[27] V. Thomée. *Galerkin Finite Element Methods for Parabolic Problems*, Springer-Verlag, Berlin, 2006.
[28] V. Thomée. On positivity preservation in some finite element methods for the heat equation. In I. Dimov et al., editor, *NMA 2014, LNCS 8962*, pp. 13–24. 2015.
[29] V. Thomée and L. B. Wahlbin. On the existence of maximum principles in parabolic finite element equations. *Math. Comp.*, 77(261):11–19, 2008.
[30] J. A. C. Weideman and L. N. Trefethen. Parabolic and hyperbolic contours for computing the Bromwich integral. *Math. Comp.*, 76(259):1341–1356, 2007.

Department of Computer Science
University College London
Gower Street, London WC1E 6BT, UK
e-mail: (bangti.jin@gmail.com,b.jin@ucl.ac.uk)

Department of Mathematics
Texas A&M University
College Station, TX 77843-3368, USA
e-mail: lazarov@math.tamu.edu

Mathematical Sciences
Chalmers University of Technology and the University of Gothenburg
SE-412 96 Göteborg, Sweden
e-mail: thomee@chalmers.se

Department of Applied Physics and Applied Mathematics
Columbia University
500 W. 120th Street, New York, NY 10027, USA

e-mail: zhizhou0125@gmail.com