Discrete maximum principles for nonlinear parabolic PDE systems *

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Abstract: Discrete maximum principles are established for finite element approximations of nonlinear parabolic PDE systems with mixed boundary and interface conditions. The results are based on an algebraic discrete maximum principle for suitable ODE systems.

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1 Introduction

The numerical solution of parabolic partial differential equations or systems is a widespread task in numerical analysis, see, e.g., [29, 30, 32]. The discrete solution is naturally required to reproduce the basic qualitative properties of the exact solution. Such a property for parabolic equations is the (continuous) maximum principle (CMP), see e.g. [14, 28] for its several variants. Its discrete analogues, the so-called discrete maximum principles (DMPs) for linear parabolic problems were first presented in the papers [15, 25], and later developed and analysed in many papers, see e.g. [9, 10, 31] and the references therein. A related important discrete qualitative property is the so-called nonnegativity preservation, analysed in the context of DMPs e.g. in [9].

It is well-known from the above works on linear parabolic equations that the usual relation between the space and time discretization steps is generally

$$\Delta t = O(h^2)$$

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(i.e., the ratio of Δt and $O(h^2)$ should remain between two positive constants as they tend to 0), both to achieve convergence and to satisfy the DMP [9, 10]. We note that mass lumping can be used to avoid the lower bound $\Delta t \geq ch^2$ (which requires sufficiently large time-steps w.r.t. h^2), see [15, 33, 34]; on the other hand, the really important restriction is not the large time steps but the sufficiently small time steps w.r.t. h^2 (i.e. the upper bound $\Delta t \leq ch^2$), which is however inevitable in any work even for linear DMP [9, 10]. The other main assumption to achieve the DMP arises for the space mesh. When using FEM, one has to impose certain geometrical restrictions, e.g. for simplicial elements this means certain acuteness of the mesh in the presence of lower order terms. These conditions also appear in the widely studied elliptic case, see, e.g., [5, 15, 16, 22, 26, 27, 38, 41] and the references therein. A fairly general algebraic condition on the FE basis functions that covers most of these conditions has been given in [24]:

$$\nabla\varphi_i \cdot \nabla\varphi_j \leq 0 \quad \text{on } \Omega \quad \text{and} \quad \int_\Omega \nabla\varphi_i \cdot \nabla\varphi_j \leq -K_0\, h^{d-2}$$

for all i, j, where h is the mesh size, d is the space dimension and $K_0 > 0$ is a constant (independent of h). Under such conditions, the DMP holds for small enough h, namely, for $h < h_0$ where h_0 is a computable bound.

In this paper we prove that proper discrete maximum principles hold for nonlinear parabolic systems of PDEs, discretized in space by FEM, under the same conditions as discussed above. To our knowledge, there have appeared very few papers on nonlinear equations concerning parabolic DMP. A related result in [8, Th. 5.13] shows that FEM for some semilinear reaction-diffusion systems on 2D domains preserves invariant regions under certain assumptions, which is closely related to DMP. Some results on DMP for FEM for certain nonlinear parabolic equations have been given in [13]. Our goal is to extend the result of [13] to systems as general as possible, involving nonsymmetric terms and mixed boundary and interface conditions as well. The coupling of the equations in the system is cooperative and weakly diagonally dominant, similarly to the elliptic case [24].

The CMP itself has been extended for nonlinear parabolic systems of PDEs in different forms, often in the context of invariant sets, see, e.g., [7, 39, 40]. We find it natural to require an analogy of the DMP, known for linear equations, to hold for nonlinear systems as well. First, this is suggested by the physical meaning of such systems, most often in the special form of nonnegativity of the solution. Second, in the elliptic case the same CMP holds for related nonlinear equations as for linear equations [22], and a natural analogue of these holds for systems [24].

An important step in our process is to establish a purely algebraic DMP for systems of ordinary differential equations (ODEs), to which our results on PDE systems can then be reduced. This DMP for ODEs is of independent interest, and can be regarded as a basic property that underlies parabolic PDEs. This is analogous to the algebraic or matrix maximum principle for generalized nonnegative matrices [4, 37] that underlies most elliptic DMP results.

The paper is organized as follows. In Section 2, we formulate the considered class of systems. The discretization scheme is given in detail in Section 3. Section 4 is devoted to the algebraic DMP for ODE systems. The DMP and related nonnegativity preservation for the considered parabolic systems are presented in Section 5. Finally, various examples are given in Section 6.

2 The class of problems

In this paper we consider the following type of nonlinear parabolic systems, involving cooperative and weakly diagonally dominant coupling, nonsymmetric terms and mixed boundary and interface conditions. Find a function $u = u(x,t) = (u_1(x,t), \dots, u_s(x,t))$ such that for all $k = 1, \dots, s$,

$$\frac{\partial u_k}{\partial t} - \operatorname{div}\Big(a_k(x,t,u,\nabla u)\nabla u_k\Big) + \mathbf{w}_k(x,t)\cdot\nabla u_k + q_k(x,t,u) = f_k(x,t)$$
$$\text{in } \; Q_T := (\Omega \setminus \Gamma_{int}) \times (0,T), \qquad (1)$$

where Ω is a bounded domain in $\mathbf{R}^d$ and $T > 0$, further, the boundary, interface and initial conditions are as follows ($k = 1, \dots, s$):

$$u_k(x,t) = g_k(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T], \qquad (2)$$

$$a_k(x,t,u,\nabla u)\tfrac{\partial u_k}{\partial \nu} + s_k(x,t,u) = \gamma_k(x,t) \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T], \qquad (3)$$

$$[\,u_k]_{\Gamma_{int}} = 0 \quad \text{and} \quad \Big[a_k(x,t,u,\nabla u)\tfrac{\partial u_k}{\partial \nu} + s_k(x,t,u)\Big]_{\Gamma_{int}} = \gamma_k(x,t) \quad \text{for} \quad (x,t) \in \Gamma_{int} \times [0,T], \qquad (4)$$

$$u_k(x,0) = u_k^{(0)}(x) \quad \text{for} \quad x \in \Omega, \qquad (5)$$

respectively, where ν is the outer normal vector and $[\,.]_{\Gamma_{int}}$ denotes the jump (i.e., the difference of the limits from the two sides of the interface Γ_{int}) of a function. We impose the following

Assumptions 2.1.

(A1) (Domain.) Ω is a bounded polytopic domain in $\mathbf{R}^d$; $\Gamma_N, \Gamma_D \subset \partial\Omega$ are disjoint open subsets of $\partial\Omega$ such that $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$, and Γ_{int} is a piecewise C^1 surface in Ω.

(A2) (Smoothness.) For all $k = 1, \dots, s$, the scalar functions $a_k : Q_T \times \mathbf{R}^s \times \mathbf{R}^{d\times s} \to \mathbf{R}$, $q_k : Q_T \times \mathbf{R}^s \to \mathbf{R}$ and $s_k : (\Gamma_N \cup \Gamma_{int}) \times [0,T] \times \mathbf{R}^s \to \mathbf{R}$ are measurable and bounded, further, q_k and s_k are continuously differentiable w.r.t. their variables in $\mathbf{R}^s$, on their domains of definition. Further, $\mathbf{w}_k \in W^{1,\infty}(Q_T)$, $f_k \in L^\infty(Q_T)$, $\gamma_k \in L^2((\Gamma_N \cup \Gamma_{int}) \times [0,T])$, $g_k \in L^\infty(\Gamma_D \times [0,T])$ and $u_k^{(0)} \in L^\infty(\Omega)$.

(A3) (Ellipticity for the principal space term.) There exist constants μ_0 and μ_1 such that

$$0 < \mu_0 \le a_k(x,t,\xi,\eta) \le \mu_1 \qquad (6)$$

for all $k = 1, \dots, s$ and all $(x,t,\xi,\eta) \in \Omega \times (0,T) \times \mathbf{R}^s \times \mathbf{R}^{d\times s}$.

(A4) (Coercivity.) For all $k = 1, \dots, s$, we have $\operatorname{div} \mathbf{w}_k \le 0$ on Ω, $\mathbf{w}_k \cdot \nu \ge 0$ on Γ_N, further, $[\mathbf{w}_k]_{\Gamma_{int}} = 0$ and $[\mathbf{w}_k \cdot \nu]_{\Gamma_{int}} \ge 0$.

(A5) (Growth.) Let $2 \le p_1$ if $d = 2$ and $2 \le p_1 < \frac{2d}{d-2}$ if $d > 2$, further, let $2 \le p_2$ if $d = 2$ and $2 \le p_2 < \frac{2d-2}{d-2}$ if $d > 2$. There exist constants $\alpha_1, \alpha_2, \beta_1, \beta_2 \ge 0$ such that for any $x \in \Omega$ (or $x \in \Gamma_N \cup \Gamma_{int}$, resp.), $t \in (0, T)$, $\xi \in \mathbf{R}^s$, and any $k, l = 1, \dots, s$,

$$\left| \frac{\partial q_k}{\partial \xi_l}(x, t, \xi) \right| \le \alpha_1 + \beta_1 |\xi|^{p_1 - 2}, \qquad \left| \frac{\partial s_k}{\partial \xi_l}(x, t, \xi) \right| \le \alpha_2 + \beta_2 |\xi|^{p_2 - 2}. \tag{7}$$

(A6) (Cooperativity.) For all $k, l = 1, \dots, s$, $x \in \Omega$ (or $x \in \Gamma_N \cup \Gamma_{int}$, resp.), $t \in (0, T)$, $\xi \in \mathbf{R}^s$,

$$\frac{\partial q_k}{\partial \xi_l}(x, t, \xi) \le 0, \qquad \frac{\partial s_k}{\partial \xi_l}(x, t, \xi) \le 0, \qquad \text{whenever } k \ne l. \tag{8}$$

(A7) (Weak diagonal dominance.) For all $k = 1, \dots, s$, $x \in \Omega$ (or $x \in \Gamma_N \cup \Gamma_{int}$, resp.), $t \in (0, T)$, $\xi \in \mathbf{R}^s$,

$$\sum_{l=1}^{s} \frac{\partial q_k}{\partial \xi_l}(x, t, \xi) \ge 0. \qquad \sum_{l=1}^{s} \frac{\partial s_k}{\partial \xi_l}(x, t, \xi) \ge 0. \tag{9}$$

Remark 2.1 Assumptions (A6)-(A7) imply for all $k = 1, \dots, s$, $x \in \Omega$ (or $x \in \Gamma_N \cup \Gamma_{int}$, resp.), $t \in (0, T)$, $\xi \in \mathbf{R}^s$ that $\frac{\partial q_k}{\partial \xi_k}(x, t, \xi) \ge 0$, $\frac{\partial s_k}{\partial \xi_k}(x, t, \xi) \ge 0$.

We will define weak solutions in a usual way. The interface conditions are handled similarly to the Neumann boundary, see e.g. [23]; now we can join these two sets and denote

$$\Gamma := \Gamma_N \cup \Gamma_{int}$$

in the sequel. Let

$$H_D^1(\Omega) := \{u \in H^1(\Omega) : \ u_{|\Gamma_D} = 0\}.$$

A function $u : Q_T \to \mathbf{R}^s$ is called the weak solution of the problem (1)–(5) if for all $k = 1, \dots, s$, u_k are continuously differentiable with respect to t and $u_k(., t) \in H_D^1(\Omega)$ for all $t \in (0, T)$, and satisfy the relation

$$\int_\Omega \sum_{k=1}^{s} \frac{\partial u_k}{\partial t} v_k \, dx + \int_\Omega \sum_{k=1}^{s} \Big(a_k(x, t, u, \nabla u) \nabla u_k \cdot \nabla v_k + (\mathbf{w}_k(x, t) \cdot \nabla u_k) v_k + q_k(x, t, u) v_k \Big) \, dx$$
$$+ \int_\Gamma \sum_{k=1}^{s} s_k(x, t, u) v_k \, d\sigma = \int_\Omega \sum_{k=1}^{s} f_k v_k \, dx + \int_\Gamma \sum_{k=1}^{s} \gamma_k v_k \, d\sigma \qquad (\forall v \in H_D^1(\Omega)^s, \quad t \in (0, T)), \tag{10}$$

further,

$$u_k = g_k \quad \text{on} \quad [0, T] \times \Gamma_D, \qquad u_k|_{t=0} = u_k^{(0)} \quad \text{in} \quad \Omega. \tag{11}$$

Here and in the sequel, equality of functions in Lebesgue or Sobolev spaces is understood almost everywhere.

3 Discretization scheme

The full discretization of problem (1)–(5) is built up from two standard steps in space and time; in addition, suitable vector basis functions are involved.

3.1 Semidiscretization in space

Let $\mathcal{T}_h$ be a finite element mesh over the solution domain $\Omega \subset \mathbf{R}^d$, where h stands for the discretization parameter. We choose basis functions in the following way. First, let $\bar{n}_0 \leq \bar{n}$ be positive integers and let us choose basis functions

$$\varphi_1, \dots, \varphi_{\bar{n}_0} \in H^1_D(\Omega), \qquad \varphi_{\bar{n}_0+1}, \dots, \varphi_{\bar{n}} \in H^1(\Omega) \setminus H^1_D(\Omega), \tag{12}$$

which are associated with the homogeneous and inhomogeneous boundary conditions on Γ_D, respectively. These basis functions are assumed to be continuous on $\overline{\Omega}$ and to satisfy

$$\varphi_p \geq 0 \quad (p = 1, \dots, \bar{n}), \qquad \sum_{p=1}^{\bar{n}} \varphi_p \equiv 1, \tag{13}$$

further, that there exist node points $B_p \in \Omega \cup \Gamma_N$ $(p = 1, \dots, \bar{n}_0)$ and $B_p \in \Gamma_D$ $(p = \bar{n}_0 + 1, \dots, \bar{n})$ such that

$$\varphi_p(B_q) = \delta_{pq} \tag{14}$$

where δ_{pq} is the Kronecker symbol. These conditions hold e.g. for standard linear, bilinear or prismatic finite elements. We note that in general $\bar{n} = O(h^d)$. Further, one usually considers a family of subspaces and lets $h \to 0$, hence we will stress the independence of h for certain bounds where applicable.

We in fact need a basis in the corresponding product spaces, which we define by repeating the above functions in each of the s coordinates and setting zero in the other coordinates. That is, let $N_0 := s\bar{n}_0$ and $N := s\bar{n}$. First, for any $1 \leq i \leq N_0$,

$$\text{if } \ i = (k_0 - 1)\bar{n}_0 + p \quad \text{for some } 1 \leq k_0 \leq s \text{ and } 1 \leq p \leq \bar{n}_0, \ \text{ then}$$

$$\phi_i := (0, \dots, 0, \varphi_p, 0, \dots, 0) \qquad \text{where } \ \varphi_p \ \text{ stands at the } k_0\text{th entry}, \tag{15}$$

that is, the mth coordinate of ϕ_i satisfies $(\phi_i)_m = \varphi_p$ if $m = k_0$ and $(\phi_i)_m = 0$ if $m \neq k_0$. From these, we let

$$V_h^0 := \text{span}\{\phi_1, ..., \phi_{N_0}\} \ \subset H^1_D(\Omega)^s. \tag{16}$$

Similarly, for any $N_0 + 1 \leq i \leq N$,

$$\text{if } \ i = N_0 + (k_0 - 1)(\bar{n} - \bar{n}_0) + p - \bar{n}_0 \quad \text{for some } 1 \leq k_0 \leq s \text{ and } \bar{n}_0 + 1 \leq p \leq \bar{n}, \ \text{ then}$$

$$\phi_i := (0, \dots, 0, \varphi_p, 0, \dots, 0)^T \qquad \text{where } \ \varphi_p \ \text{ stands at the } k_0\text{th entry}, \tag{17}$$

that is, the mth coordinate of ϕ_i satisfies $(\phi_i)_m = \varphi_p$ if $m = k_0$ and $(\phi_i)_m = 0$ if $m \neq k_0$. From (16) and these, we let

$$V_h := \text{span}\{\phi_1, ..., \phi_N\} \ \subset H^1(\Omega)^s. \tag{18}$$

Using the above FEM subspaces, one can define the semidiscrete problem for (10) with initial-boundary conditions (11). We look for a vector function $u_h = u_h(x,t)$ that satisfies (10) for all $v_h = (v_1, \ldots, v_s) \in V_h^0$, and the conditions

$$u_k^h(x,0) = u_k^{(0),h}(x) \quad (x \in \Omega), \qquad u_k^h(.,t) - g_k^h(.,t) \in V_0^h \quad (t \in (0,T)), \text{ for all } k = 1, \ldots, s$$

must hold. In the above formulae, the functions $u_k^{(0),h}$ and $g_k^h(.,t)$ (for any fixed t) are suitable approximations of the given functions u_0 and $g(.,t)$, respectively. In particular, we will use the following form to describe the kth coordinate g_k^h:

$$g_k^h(x,t) = \sum_{p=1}^{\bar{n}_\partial} g_p^{(k)}(t)\, \varphi_{\bar{n}_0+p}(x), \qquad \text{where} \qquad \bar{n}_\partial := \bar{n} - \bar{n}_0. \tag{19}$$

We seek the kth coordinate function u_k of the numerical solution in the form

$$u_k^h(x,t) = \sum_{p=1}^{\bar{n}} u_p^{(k)}(t)\, \varphi_p(x) + g_k(x,t) = \sum_{p=1}^{\bar{n}_0} u_p^{(k)}(t)\, \varphi_p(x) + \sum_{p=1}^{\bar{n}_\partial} g_p^{(k)}(t)\, \varphi_{\bar{n}_0+p}(x), \tag{20}$$

where the coefficients $u_p^{(k)}(t)$ $(p = 1, \ldots, \bar{n}_0)$ are unknown. The set of all coefficient functions will be ordered in the following vector:

$$\begin{aligned}\mathbf{u}^h(t) = \big(\, & u_1^{(1)}(t), \ldots,\, u_{\bar{n}_0}^{(1)}(t);\; u_1^{(2)}(t), \ldots,\, u_{\bar{n}_0}^{(2)}(t); \ldots;\; u_1^{(s)}(t), \ldots,\, u_{\bar{n}_0}^{(s)}(t);\\ & g_1^{(1)}(t), \ldots,\, g_{\bar{n}_\partial}^{(1)}(t);\; g_1^{(2)}(t), \ldots,\, g_{\bar{n}_\partial}^{(2)}(t); \ldots;\; g_1^{(s)}(t), \ldots,\, g_{\bar{n}_\partial}^{(s)}(t)\big)^T\end{aligned} \tag{21}$$

(where ^{T} denotes the transposed of a vector), that is, $\mathbf{u}^h(t)$ has $N_0 = s\bar{n}_0$ coordinates from $u_1^{(1)}(t)$ to $u_{\bar{n}_0}^{(s)}(t)$ belonging to the points in the interior or on Γ, and then $N - N_0 = s(\bar{n} - \bar{n}_0)$ coordinates from $g_1^{(1)}(t)$ to $g_{\bar{n}_\partial}^{(s)}(t)$ belonging to the boundary points on Γ_D, such that the upper index from 1 to s gives the number of coordinate in the parabolic system. We will also use the notations

$$\mathbf{u}^{(k_0)}(t) := \big(\, u_1^{(k_0)}(t), \ldots,\, u_{\bar{n}_0}^{(k_0)}(t)\big), \qquad \mathbf{g}^{(k_0)}(t) := \big(\, g_1^{(k_0)}(t), \ldots,\, g_{\bar{n}_\partial}^{(k_0)}(t)\big)$$

for any fixed $k_0 = 1, \ldots, s$, to denote the corresponding sub-$\bar{n}_0$-tuples of $\mathbf{u}^h(t)$ and sub-$\bar{n}_\partial$-tuples of $\mathbf{g}^h(t)$, respectively.

To find the function $\mathbf{u}^h(t)$, first note that it is sufficient that u_h satisfies (10) for $v = \phi_i$ only $(i = 1, 2, \ldots, N_0)$. Writing the index i in the following form as before:

$$i = (k_0 - 1)\bar{n}_0 + p \quad \text{for some } 1 \le k_0 \le s \text{ and } 1 \le p \le \bar{n}_0, \tag{22}$$

the function $v = \phi_i$ has kth coordinates $v_k = \delta_{k,k_0}\varphi_p$ (where δ_{k,k_0} is the Kronecker symbol) for $k = 1, \ldots, s$, hence (10) yields

$$\int_\Omega \frac{\partial u_{k_0}}{\partial t}\varphi_p\, dx + \int_\Omega \Big(a_{k_0}(x,t,u,\nabla u)\nabla u_{k_0} \cdot \nabla\varphi_p + (\mathbf{w}_{k_0}(x,t) \cdot \nabla u_{k_0})\varphi_p + q_{k_0}(x,t,u)\varphi_p \Big)\, dx \tag{23}$$

$$+\int_\Gamma s_{k_0}(x,t,u)\varphi_p \, d\sigma \;=\; \int_\Omega f_{k_0}\varphi_p \, dx + \int_\Gamma \gamma_{k_0}\varphi_p \, d\sigma \qquad (1 \le k_0 \le s, \; 1 \le p \le \bar{n}_0).$$

For fixed k_0, using (20), the first integral in (23) becomes $\bar{\mathbf{M}}\,[\frac{\mathrm{d}\mathbf{u}^{(k_0)}}{\mathrm{d}t}, \frac{\mathrm{d}\mathbf{g}^{(k_0)}}{\mathrm{d}t}]$, where

$$\bar{\mathbf{M}} = [M_{pq}]_{\bar{n}_0 \times \bar{n}}, \quad M_{pq} = \int_\Omega \varphi_p \, \varphi_q \, dx. \tag{24}$$

We shall use the corresponding partition

$$\bar{\mathbf{M}} = [\bar{\mathbf{M}}_0 | \bar{\mathbf{M}}_\partial], \quad \text{where} \quad \bar{\mathbf{M}}_0 \in \mathbf{R}^{\bar{n}_0 \times \bar{n}_0}, \;\; \bar{\mathbf{M}}_\partial \in \mathbf{R}^{\bar{n}_0 \times \bar{n}_\partial}$$

and here $\bar{\mathbf{M}}_0$ is the mass matrix corresponding to the interior of Ω. Let $k_0 = 1, \dots, s$ and let us define the partitioned block matrix

$$\mathbf{M} := \Big[blockdiag_s(\bar{\mathbf{M}}_0, \bar{\mathbf{M}}_0, \dots, \bar{\mathbf{M}}_0) \;\Big|\; blockdiag_s(\bar{\mathbf{M}}_\partial, \bar{\mathbf{M}}_\partial, \dots, \bar{\mathbf{M}}_\partial) \Big] \in \mathbf{R}^{N_0 \times N}. \tag{25}$$

Then we are led to the following Cauchy problem for the system of ordinary differential equations:

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{G}(t, \mathbf{u}^h(t)) = \mathbf{f}(t), \tag{26}$$

$$\mathbf{u}^h(0) = \mathbf{u}_0^h, \tag{27}$$

where using the form of i as in (22),

$$\mathbf{G}(t, \mathbf{u}^h(t)) = [G(t, \mathbf{u}^h(t))_i]_{i=1,\dots,N_0},$$

$$G(t, \mathbf{u}^h(t))_i = \int_\Omega \Big(a_{k_0}(x,t,u,\nabla u)\nabla u_{k_0} \cdot \nabla\varphi_p + (\mathbf{w}_{k_0}(x,t) \cdot \nabla u_{k_0})\varphi_p + q_{k_0}(x,t,u)\varphi_p \Big) \, dx$$

$$+ \int_\Gamma s_{k_0}(x,t,u)\varphi_p \, d\sigma,$$

$$\mathbf{f}(t) = [f_i(t)]_{i=1,\dots,N_0}, \quad f_i(t) = \int_\Omega f_{k_0}(x,t)\varphi_p(x) \, dx + \int_\Gamma \gamma_{k_0}(x,t)\varphi_p(x) \, d\sigma(x),$$

and finally, $\mathbf{u}_0^h$ is defined by setting $t = 0$ in (21) and using that $u_p^{(k)}(0) = u_k^{(0)}(B_p)$ for $k = 1, \dots, s$ and $p = 1, \dots, \bar{n}_0$.

The solution $\mathbf{u}^h = \mathbf{u}^h(t)$ of problem (26)–(27) is called the semidiscrete solution. Here the coefficients $g_p^{(k)}(t)$ are given, hence (26) can be reduced to a system where $\mathbf{M}$ is replaced by the nonsingular square matrix $\mathbf{M}_0 := blockdiag_s(\bar{\mathbf{M}}_0, \bar{\mathbf{M}}_0, \dots, \bar{\mathbf{M}}_0)$ only. Then existence and uniqueness for (26)–(27) is ensured by Assumptions 2.1, since then $\mathbf{G}$ is locally Lipschitz continuous.

3.2 Full discretization

In order to get a fully discrete numerical scheme, we choose a time-step Δt and denote the approximation to $\mathbf{u}^h(t_n)$ and $\mathbf{f}(t_n)$ by $\mathbf{u}^n$ and $\mathbf{f}^n$ (where $t_n := n\Delta t,\ \ n = 0, 1, 2, \ldots, n_T$, $T = n_T \Delta t$), respectively. To discretize (26) in time, we apply the simplest and most commonly used one-step time discretization method, the so-called θ-method [15, 32] with some given parameter

$$\theta \in (0,\, 1].$$

We note that the case $\theta = 0$, which is otherwise also acceptable, will be excluded later by condition (75).

We then obtain a system of nonlinear algebraic equations of the form

$$\mathbf{M}\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \theta \mathbf{G}(t_{n+1},\, \mathbf{u}^{n+1}) + (1-\theta)\mathbf{G}(t_n,\, \mathbf{u}^n) = \mathbf{f}^{(n,\theta)} := \theta \mathbf{f}^{n+1} + (1-\theta)\mathbf{f}^n, \quad (28)$$

$n = 0, 1, \ldots, n_T - 1$, which can be rewritten as a recursion

$$\mathbf{M}\mathbf{u}^{n+1} + \theta \Delta t \mathbf{G}(t_{n+1},\, \mathbf{u}^{n+1}) = \mathbf{M}\mathbf{u}^n - (1-\theta)\Delta t \mathbf{G}(t_n,\, \mathbf{u}^n) + \Delta t\ \mathbf{f}^{(n,\theta)} \quad (29)$$

with $\mathbf{u}^0 = \mathbf{u}^h(0)$. Furthermore, we will use notations

$$\mathbf{P}(\mathbf{u}^{n+1}) := \mathbf{M}\mathbf{u}^{n+1} + \theta \Delta t \mathbf{G}(t_{n+1},\, \mathbf{u}^{n+1}), \qquad \mathbf{Q}(\mathbf{u}^n) := \mathbf{M}\mathbf{u}^n - (1-\theta)\Delta t \mathbf{G}(t_n,\, \mathbf{u}^n), \quad (30)$$

respectively. Then, the iteration procedure (29) can be also written as

$$\mathbf{P}(\mathbf{u}^{n+1}) = \mathbf{Q}(\mathbf{u}^n) + \Delta t\ \mathbf{f}^{(n,\theta)}. \quad (31)$$

Finding $\mathbf{u}^{n+1}$ in (31) requires the solution of a nonlinear algebraic system. Similarly as mentioned before, (31) can be reduced to a system with the first N_0 coefficients, i.e. $\mathbf{M}$ is replaced by the nonsingular square matrix $\mathbf{M}_0 := blockdiag_s(\bar{\mathbf{M}}_0, \bar{\mathbf{M}}_0, \ldots, \bar{\mathbf{M}}_0)$ only, since the other coefficients of $\mathbf{u}^{n+1}$ are given from the $g_p^{(k)}(t)$. Analogously, $\mathbf{P}$ is replaced by $\mathbf{P}_0$. The block mass matrix $\mathbf{M}_0$ is positive definite, and it follows from Assumptions 2.1 that $\mathbf{u} \mapsto \mathbf{G}(\mathbf{u})$ has positive semidefinite derivatives. hence by the definition in (30), the function $\mathbf{u} \mapsto \mathbf{P}_0(\mathbf{u})$ has regular derivatives. This ensures the unique solvability of (31) and, under standard local Lipschitz conditions on the coefficients, also the convergence of the damped Newton iteration, see e.g. [12].

4 An algebraic discrete maximum principle for ODE systems

An important and widely studied special case of our problem is the linear case, in fact, we wish to recast the nonlinear case to that. In this section we establish an algebraic DMP for systems of ordinary differential equations (ODEs), which can be later used for our discretized parabolic PDE system.

The motivation for that is the well-known continuous maximum principle (CMP) for a linear parabolic PDE. Consider the problem

$$\frac{\partial u}{\partial t} - k\Delta u + c(x)u = f(x,t) \quad \text{in } Q_T, \qquad u = g \quad \text{on } [0,T]\times\partial\Omega, \qquad u|_{t=0} = u_0 \text{ in } \Omega \quad (32)$$

where $k > 0$ is constant and $c \geq 0$. If the data and solution are assumed to be sufficiently smooth, then problem (32) satisfies the following CMP [11]:

$$\min\{0; \min_{\overline{\Gamma}_{t_1}} g\} + t_1 \min\{0; \min_{\overline{Q}_{t_1}} f\} \leq u(x,t_1) \leq \max\{0; \max_{\overline{\Gamma}_{t_1}} g\} + t_1 \max\{0; \max_{\overline{Q}_{t_1}} f\} \quad (33)$$

for all $x \in \Omega$ and any fixed $t_1 \in (0,T)$, where $Q_{t_1} := \Omega \times [0,t_1]$, and Γ_{t_1} denotes the parabolic boundary, i.e., $\Gamma_{t_1} := (\partial\Omega \times [0,t_1]) \cup (\Omega \times \{0\})$. A related property, which follows from the above [10], is the *continuous nonnegativity preservation principle*: relations $f \geq 0$, $g \geq 0$ and $u_0 \geq 0$ imply $u(x,t) \geq 0$ for all $(x,t) \in Q_T$.

In the discrete case, the ODE system (26) for (32) becomes linear and has the form

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{K}\mathbf{u}^h(t) = \mathbf{f}. \quad (34)$$

Suitable analogues of (33) have been established e.g. in [11] for such discretized PDEs. Below our goal is to formulate a DMP purely algebraically for such ODE systems, to which our results on PDE systems can then be reduced.

4.1 The Cauchy problem and its discretization

Let us consider the Cauchy problem for the system of linear ordinary differential equations

$$\mathbf{M}\frac{\mathrm{d}\bar{\mathbf{u}}}{\mathrm{d}t} + \mathbf{K}\bar{\mathbf{u}} = \mathbf{f}, \quad (35)$$

where $\mathbf{M} = [\mathbf{M}_0|\mathbf{M}_\partial]$, $\mathbf{K} = [\mathbf{K}_0|\mathbf{K}_\partial] \in \mathbf{R}^{N_0\times N}$ are partitioned matrices with the entries $\mathbf{M}_0, \mathbf{K}_0 \in \mathbf{R}^{N_0\times N_0}$, $\mathbf{M}_\partial, \mathbf{K}_\partial \in \mathbf{R}^{N_0\times N_\partial}$ $(N = N_0 + N_\partial)$, $\mathbf{f}(t) \in \mathbf{R}^{N_0}$ for all $t > 0$ and $\bar{\mathbf{u}}(0) \in \mathbf{R}^N$ are given. Here $\bar{\mathbf{u}}(t) \in \mathbf{R}^N$ has the partitioning $[\mathbf{u}(t)|\mathbf{g}(t)]^T$, where $\mathbf{u}(t) \in \mathbf{R}^{N_0}$, $\mathbf{g}(t) \in \mathbf{R}^{N_\partial}$ and $\mathbf{g}(t)$ for $t \geq 0$ and $\mathbf{u}(0)$ are given. We seek the unknown function $\mathbf{u}(t)$ for $t > 0$.

We impose the following conditions for the matrices $\mathbf{M}$ and $\mathbf{K}$, wherein $i = 1,...,N_0$, $j = 1,...,N$:

(B1) $K_{ij} \leq 0$ for all $i \neq j$; (B2) $\sum_{j=1}^{N} K_{ij} \geq 0$ for all i;

(B3) $M_{ij} \geq 0$ for all i,j; (B4) $\sum_{j=1}^{N} M_{ij} \geq 1$ for all i.

Constructing a full discretization of (35) as in subsection 3.2, we obtain a recursion of algebraic systems analogously to (29):

$$(\mathbf{M}+\theta\Delta t\mathbf{K})\bar{\mathbf{u}}^{n+1}=(\mathbf{M}-(1-\theta)\Delta t\mathbf{K})\bar{\mathbf{u}}^{n}+\Delta t\ \mathbf{f}^{(n,\theta)}, \tag{36}$$

further, the matrices $\mathbf{M}+\theta\Delta t\mathbf{K}$ and $\mathbf{M}-(1-\theta)\Delta t\mathbf{K}$ are denoted by $\mathbf{A}$ and $\mathbf{B}$ respectively. In what follows, we shall use the following partitions of the matrices and vectors:

$$\mathbf{A}=[\mathbf{A}_0|\mathbf{A}_\partial],\quad \mathbf{B}=[\mathbf{B}_0|\mathbf{B}_\partial],\quad \bar{\mathbf{u}}^n=\begin{bmatrix}\mathbf{u}^n\\ \mathbf{g}^n\end{bmatrix}, \tag{37}$$

where, obviously, $\mathbf{A}_0$ and $\mathbf{B}_0$ are quadratic matrices from $\mathbf{R}^{N_0\times N_0}$; $\mathbf{A}_\partial,\mathbf{B}_\partial\in\mathbf{R}^{N_0\times N_\partial}$, $\mathbf{u}^n=[u_1^n,...,u_{N_0}^n]^T\in\mathbf{R}^{N_0}$ and $\mathbf{g}^n=[g_1^n,...,g_{N_\partial}^n]^T\in\mathbf{R}^{N_\partial}$. Then, the iteration (36) can be also written as

$$\mathbf{A}\bar{\mathbf{u}}^{n+1}=\mathbf{B}\bar{\mathbf{u}}^{n}+\Delta t\ \mathbf{f}^{(n,\theta)}, \tag{38}$$

or

$$[\mathbf{A}_0|\mathbf{A}_\partial]\begin{bmatrix}\mathbf{u}^{n+1}\\ \mathbf{g}^{n+1}\end{bmatrix}=[\mathbf{B}_0|\mathbf{B}_\partial]\begin{bmatrix}\mathbf{u}^{n}\\ \mathbf{g}^{n}\end{bmatrix}+\Delta t\ \mathbf{f}^{(n,\theta)}. \tag{39}$$

4.2 A discrete maximum principle

Let us use the following notations:

$$g_{min}^n=\min\{g_1^n,\dots,g_{N_\partial}^n\},\quad g_{max}^n=\max\{g_1^n,\dots,g_{N_\partial}^n\}, \tag{40}$$

$$u_{min}^n=\min\{u_1^n,\dots,u_{N_0}^n\},\quad u_{max}^n=\max\{u_1^n,\dots,u_{N_0}^n\}, \tag{41}$$

$$v_{min}^n=\min\{g_{min}^n,u_{min}^n\},\quad v_{max}^n=\max\{g_{max}^n,u_{max}^n\} \tag{42}$$

$$f_{min}^n=\min\{0,f_1^{(n,\theta)},\dots,f_{N_0}^{(n,\theta)}\},\quad f_{max}^n=\max\{0,f_1^{(n,\theta)},\dots,f_{N_0}^{(n,\theta)}\}, \tag{43}$$

$$\mathbf{e}_0=[1,\dots,1]^T\in\mathbf{R}^{N_0},\ \mathbf{e}_\partial=[1,\dots,1]^T\in\mathbf{R}^{N_\partial},\ \mathbf{e}=[1,\dots,1]^T\in\mathbf{R}^{N,}. \tag{44}$$

We formulate the discrete maximum principle (DMP) for the discrete model (39) as follows:

$$\begin{aligned}&\min\{0,g_{min}^n,g_{min}^{n+1},u_{min}^n\}+\Delta t f_{min}^n\le\\ &\le u_i^{n+1}\le\max\{0,g_{max}^n,g_{max}^{n+1},u_{max}^n\}+\Delta t f_{max}^n,\end{aligned} \tag{45}$$

$(i=1,\dots,N_0;\ n=0,1,2...)$, following [15, p. 100].

In order to satisfy the DMP for the model (39), we also impose conditions for the choice of the time-discretization parameter Δt:

(B5) $\quad A_{ij}=M_{ij}+\theta\Delta t\ K_{ij}\le 0 \qquad (i\ne j,\quad i=1,...,N_0,\ j=1,...,N)$;

(B6) $\quad B_{ii}=M_{ii}-(1-\theta)\Delta t\ K_{ii}\ge 0 \qquad (i=1,...,N_0)$.

The following proposition summarizes some properties of the matrices $\mathbf{A}$ and $\mathbf{B}$.

Lemma 4.1 *Under conditions (B1)–(B6) the following properties are valid:*

P1. $\mathbf{A}_\partial \leq \mathbf{0}$, P2. *$\mathbf{e}_0 \leq \mathbf{Ae}$;*

P3. *$\mathbf{A}_0$ is an invertible matrix and $\mathbf{A}_0^{-1} \geq \mathbf{0}$;* P4. *$\mathbf{A}_0^{-1}\mathbf{A}_\partial \leq \mathbf{0}$;*

P5. *$\mathbf{B} \geq \mathbf{0}$;* P6. *$\mathbf{Ke} \geq \mathbf{0}$;*

P7. *$\mathbf{Ae} \geq \mathbf{Be}$;* P8. $-\mathbf{A}_0^{-1}\mathbf{A}_\partial \mathbf{e}_\partial \leq \mathbf{e}_0$.

Proof. Property P1 follows from assumption (B5). Using assumptions (B2) and (B4), we have

$$(\mathbf{Ae})_i = \sum_{j=1}^{N} \mathbf{A}_{ij} = \sum_{j=1}^{N} \mathbf{M}_{ij} + \theta \Delta t \sum_{j=1}^{N} \mathbf{K}_{ij} \geq 1, \tag{46}$$

which shows the validity of P2.
Condition B5 implies that $A_{ij} \leq 0$ for all $i \neq j$. Moreover, based on P1 and P2, we have the relation

$$\mathbf{A}_0\mathbf{e}_0 \geq \mathbf{A}_0\mathbf{e}_0 + \mathbf{A}_\partial \mathbf{e}_\partial = \mathbf{Ae} \geq \mathbf{e}_0 > \mathbf{0}. \tag{47}$$

Owing to (B5), the off-diagonal elements of $\mathbf{A}_0$ are nonpositive. Moreover, there exists a positive vector $\mathbf{e}_0 > 0$ for which $\mathbf{A}_0\mathbf{e}_0 > 0$. This yields that $\mathbf{A}_0$ is an M-matrix, see e.g. [1, Thm. 2.3]. Hence, the statements P3 and P4 are obvious. Condition (B6) implies that $B_{ii} \geq 0$ for all $i = 1, 2, \dots N_0$. On the other hand, according to (B1) and (B3), we get $B_{ij} \geq 0$ for all $i \neq j$. Hence, P5 also holds. Property P6 follows from (B2). Using P6, we have

$$\mathbf{Ae} = \mathbf{Me} + \theta \Delta t \mathbf{Ke} \geq \mathbf{Me} \geq (\mathbf{M} - (1-\theta)\Delta t \mathbf{K})\mathbf{e} = \mathbf{Be},$$

which proves P7. Finally, due to P2 and P1, we have $\mathbf{A}_0^{-1}\mathbf{e}_0 \leq \mathbf{e}_0 + \mathbf{A}_0^{-1}\mathbf{A}_\partial \mathbf{e}_\partial$. Hence, using P3, we get $-\mathbf{A}_0^{-1}\mathbf{A}_\partial \mathbf{e}_\partial \leq \mathbf{e}_0 - \mathbf{A}_0^{-1}\mathbf{e}_0 \leq \mathbf{e}_0$, which shows the validity of P8. This completes the proof. ■

Now we can prove the following

Theorem 4.1 *Assume that conditions (B1)–(B6) are satisfied. Then the DMP of the form* (45) *holds for the system* (38).

Proof. ¿From (39), using P2, we get

$$\begin{aligned} \mathbf{A}_0\mathbf{u}^{n+1} + \mathbf{A}_\partial \mathbf{g}^{n+1} = \mathbf{A}\bar{\mathbf{u}}^{n+1} = \mathbf{B}\bar{\mathbf{u}}^n + \Delta t\, \mathbf{f}^{(n,\theta)} \leq \\ \leq \mathbf{B}\bar{\mathbf{u}}^n + \Delta t f_{max}^n \mathbf{e}_0 \leq \mathbf{B}\bar{\mathbf{u}}^n + \Delta t f_{max}^n \mathbf{Ae}. \end{aligned} \tag{48}$$

Hence, using P3, and then P5 and P7, respectively, we get

$$\begin{aligned} &\mathbf{u}^{n+1} \leq -\mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{g}^{n+1} + \mathbf{A}_0^{-1}\mathbf{B}\bar{\mathbf{u}}^n + \Delta t f_{max}^n \mathbf{A}_0^{-1}\mathbf{Ae} \leq \\ &\leq -\mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{g}^{n+1} + v_{max}^n \mathbf{A}_0^{-1}\mathbf{Be} + \Delta t f_{max}^n \mathbf{A}_0^{-1}\mathbf{Ae} \leq \\ &\leq -\mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{g}^{n+1} + v_{max}^n \mathbf{A}_0^{-1}\mathbf{Ae} + \Delta t f_{max}^n \mathbf{A}_0^{-1}\mathbf{Ae} = \\ &= -\mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{g}^{n+1} + v_{max}^n \mathbf{A}_0^{-1}[\mathbf{A}_0 |\, \mathbf{A}_\partial]\mathbf{e} + \Delta t f_{max}^n \mathbf{A}_0^{-1}[\mathbf{A}_0 |\, \mathbf{A}_\partial]\mathbf{e} = \\ &= -\mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{g}^{n+1} + v_{max}^n (\mathbf{e}_0 + \mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{e}_\partial) + \\ &+ \Delta t f_{max}^n (\mathbf{e}_0 + \mathbf{A}_0^{-1}\mathbf{A}_\partial\, \mathbf{e}_\partial). \end{aligned} \tag{49}$$

Regrouping the above inequality, we get

$$\mathbf{u}^{n+1} - v^n_{max}\mathbf{e}_0 - \Delta t f^n_{max}\mathbf{e}_0 \le -\mathbf{A}_0^{-1}\mathbf{A}_\partial(\mathbf{g}^{n+1} - v^n_{max}\mathbf{e}_\partial - \Delta t f^n_{max}\mathbf{e}_\partial). \tag{50}$$

Hence, for the i-th coordinate of the both sides of (50), using P4, and finally P8, we obtain

$$\begin{aligned} &u_i^{n+1} - v^n_{max} - \Delta t f^n_{max} \le \textstyle\sum_{j=1}^{N_\partial} \left(-\mathbf{A}_0^{-1}\mathbf{A}_\partial\right)_{ij} (g_j^{n+1} - v^n_{max} - \Delta t\ f^n_{max}) \le \\ &\le \left(\textstyle\sum_{j=1}^{N_\partial} \left(-\mathbf{A}_0^{-1}\mathbf{A}_\partial\right)_{ij}\right) \cdot \max\{0, \max_j\{g_j^{n+1} - v^n_{max}\}\} \le \max\{0, \max_j\{g_j^{n+1} - v^n_{max}\}\}. \end{aligned} \tag{51}$$

Finally, expressing u_i^{n+1} we obtain the required inequality. The inequality on the left-hand side of (45) can be proved similarly. This completes the proof of the theorem. ■

Remark 4.1 The DMP (45) can be equivalently formulated as

$$\begin{aligned} &\min\{0, g^n_{min}, g^{n+1}_{min}, u^n_{min}\} + \Delta t \min\{0, f^n_{min}\} \le \\ &\le u_i^{n+1} \le \max\{0, g^n_{max}, g^{n+1}_{max}, u^n_{max}\} + \Delta t \max\{0, f^n_{max}\}, \end{aligned} \tag{52}$$

$(i = 1, \ldots, N_0;\ n = 0, 1, 2...)$, where

$$f^n_{min} = \min\{f_1^{(n,\theta)}, \ldots, f_{N_0}^{(n,\theta)}\}, \quad f^n_{max} = \max\{f_1^{(n,\theta)}, \ldots, f_{N_0}^{(n,\theta)}\}. \tag{53}$$

4.3 The general case

Now we verify that, without loss of generality, we can replace condition (B4) with the less restrictive assumption $\sum_{j=1}^{N} M_{ij} > 0$ for all i. Further, assumption (B1) can be formally omitted (it will follow from the other ones).

Hence we now impose the following five conditions:

Assumptions 4.3.

(i) $\sum\limits_{j=1}^{N} K_{ij} \ge 0$ for all $i = 1, \ldots, N_0$;

(ii) $M_{ij} \ge 0$ for all $i = 1, \ldots, N_0,\ j = 1, \ldots, N$;

(iii) $\sum\limits_{j=1}^{N} M_{ij} =: m_i > 0$ for all $i = 1, \ldots, N_0$;

(iv) $A_{ij} = M_{ij} + \theta\Delta t\ K_{ij} \le 0$ for all $i = 1, \ldots, N_0,\ j = 1, \ldots, N,\ i \ne j$;

(v) $B_{ii} = M_{ii} - (1-\theta)\Delta t\ K_{ii} \ge 0$ for all $i = 1, ..., N_0$.

Theorem 4.2 *Let Assumptions 4.3 hold for the full discretization of the ODE system* (35)*. Then the discrete solution, obtained from* (38)*, satisfies the following DMP:*

$$\begin{aligned} &\min\{0, g^n_{min}, g^{n+1}_{min}, u^n_{min}\} + \Delta t \min\{0, \tilde{f}^n_{min}\} \le \\ &\le u_i^{n+1} \le \max\{0, g^n_{max}, g^{n+1}_{max}, u^n_{max}\} + \Delta t \max\{0, \tilde{f}^n_{max}\}, \end{aligned} \tag{54}$$

$(i = 1, \ldots, N_0;\ n = 0, 1, 2 \ldots)$, where, using m_i from Assumption 4.3 (iii),

$$\tilde{f}^n_{min} = \min\Big\{\frac{f_1^{(n,\theta)}}{m_1}, \ldots, \frac{f_{N_0}^{(n,\theta)}}{m_{N_0}}\Big\}, \quad \tilde{f}^n_{max} = \max\Big\{\frac{f_1^{(n,\theta)}}{m_1}, \ldots, \frac{f_{N_0}^{(n,\theta)}}{m_{N_0}}\Big\}. \tag{55}$$

PROOF. Introducing the diagonal matrix $\mathbf{D} = \mathrm{diag}[m_1, \ldots m_{N_0}]$, we can rewrite the original equation (35) in the equivalent form

$$\mathbf{D}^{-1}\mathbf{M}\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} + \mathbf{D}^{-1}\mathbf{K}\mathbf{u} = \mathbf{D}^{-1}\mathbf{f}. \tag{56}$$

Assumptions 4.3 (i)-(ii) and (iv)-(v) for the matrices in (35) are equivalent to the properties (B2)-(B3) and (B5)-(B6) for the matrix in (56), and assumption (iii) implies that the matrix $\mathbf{D}^{-1}\mathbf{M}$ satisfies the condition (B4). Finally, assumptions (B3) and (B5) imply that θ must be positive, in which case assumption (B1) follows from (B5). Consequently, Theorem 4.1 can be applied to system (56). By Remark 4.1, this means that (52) holds such that $\mathbf{f}$ is replaced by $\mathbf{D}^{-1}\mathbf{f}$, i.e. f^n_{min} and f^n_{max} are replaced by $\tilde{f}^n_{min}$ and $\tilde{f}^n_{max}$, respectively. ■

The above result still reduces the values of u on the $(n+1)$th time level to the values of u on nth time level. Now, by induction, we obtain a DMP that reduces the values of u only to the input data until the $(n+1)$th time level:

Theorem 4.3 *Let Assumptions 4.3 hold and let us introduce notations*

$$\begin{aligned} g^{(n)}_{min} &:= \min\Big\{g^0_{min}, \ldots, g^{n+1}_{min}\Big\}, \quad \hat{f}^{(n)}_{min} := \min\Big\{\hat{f}^0_{min}, \ldots, \hat{f}^n_{min}\Big\}, \\ g^{(n)}_{max} &:= \max\Big\{g^0_{max}, \ldots, g^{n+1}_{max}\Big\}, \quad \hat{f}^{(n)}_{max} := \max\Big\{\hat{f}^0_{max}, \ldots, \hat{f}^n_{max}\Big\}. \end{aligned} \tag{57}$$

Then we have

$$\min\{0, g^{(n)}_{min}, u^{(0)}_{min}\} + (n+1)\Delta t \min\{0, \hat{f}^{(n)}_{min}\} \le u^{n+1}_i \le \max\{0, g^{(n)}_{max}, u^{(0)}_{max}\} + (n+1)\Delta t \max\{0, \hat{f}^{(n)}_{max}\}. \tag{58}$$

PROOF. The result follows directly from the previous theorem by mathematical induction. ■

Of course, the values in (57) can be further estimated by the global minima and maxima of $\mathbf{g}$ and $\mathbf{f}$ for $n = 0, \ldots, n_T - 1$ independently of n, which shows the analogy with the continuous case (33).

5 The discrete maximum principle for the nonlinear system

5.1 Reformulation of the problem

First we rewrite problem (10) to a problem with nonlinear coefficients. Let us define, for any $k, l = 1, \ldots, s,\ x \in \Omega$ resp. $\Gamma,\ t > 0,\ \xi \in \mathbf{R}^s$,

$$r_{kl}(x, t, \xi) := \int_0^1 \frac{\partial q_k}{\partial \xi_l}(x, t, \alpha\xi)\, d\alpha, \quad z_{kl}(x, t, \xi) := \int_0^1 \frac{\partial s_k}{\partial \xi_l}(x, t, \alpha\xi)\, d\alpha \tag{59}$$

and

$$\hat{f}_k(x,t) := f_k(x,t) - q_k(x,t,0), \qquad \hat{\gamma}_k(x,t) := \gamma_k(x,t) - s_k(x,t,0). \tag{60}$$

Then the Newton-Leibniz formula yields for all x, t, ξ that

$$q_k(x,t,\xi) - q_k(x,t,0) = \sum_{l=1}^{s} r_{kl}(x,t,\xi)\,\xi_l, \qquad s_k(x,t,\xi) - s_k(x,t,0) = \sum_{l=1}^{s} z_{kl}(x,t,\xi)\,\xi_l.$$

Subtracting $q_k(x,t,0)$ and $s_k(x,t,0)$ from (1) and (3), respectively, we thus obtain that problem (10) is equivalent to

$$\int_\Omega \sum_{k=1}^{s} \frac{\partial u_k}{\partial t} v_k\,dx + B(t,u;u,v) = \langle \psi(t), v\rangle \qquad (\forall v \in H_D^1(\Omega)^s, \quad t \in (0,T)), \tag{61}$$

where

$$B(t,y;u,v) := \int_\Omega \sum_{k=1}^{s} \Big(a_k(x,t,y,\nabla y)\nabla u_k \cdot \nabla v_k + (\mathbf{w}_k(x,t)\cdot \nabla u_k)v_k \tag{62}$$

$$+ \sum_{k,l=1}^{s} r_{kl}(x,t,y)\,u_l v_k \Big)\,dx + \int_\Gamma \sum_{k,l=1}^{s} z_{kl}(x,t,y)\,u_l v_k\,d\sigma$$

and $\langle \psi(t), v\rangle := \int_\Omega \sum_{k=1}^{s} \hat{f}_k v_k\,dx + \int_\Gamma \sum_{k=1}^{s} \hat{\gamma}_k v_k\,d\sigma.$

Then the semidiscretization of the problem reads as follows: find a vector function $u_h = u_h(x,t)$ such that

$$u_k^h(x,0) = u_k^{(0),h}(x) \quad (x \in \Omega), \qquad u_k^h(.,t) - g_k^h(.,t) \in V_0^h \quad (t \in (0,T)), \text{ for all } k = 1,\dots,s$$

and

$$\int_\Omega \sum_{k=1}^{s} \frac{\partial u_k^h}{\partial t} v_k^h\,dx + B(t,u_h;u_h,v^h) = \langle \psi(t), v^h\rangle \qquad (\forall v^h \in V_0^h, \quad t \in (0,T)).$$

Proceeding as in (20)–(26), the Cauchy problem for the system of ordinary differential equations (26) takes the following form:

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{K}(t,\mathbf{u}^h)\mathbf{u}^h = \hat{\mathbf{f}}(t), \qquad \mathbf{u}^h(0) = \mathbf{u}_0^h \tag{63}$$

where $\mathbf{M}$ is as in (26),

$$\mathbf{K}(t,\mathbf{u}^h) = [K(t,\mathbf{u}^h)_{ij}]_{N_0 \times N}, \quad K(t,\mathbf{u}^h)_{ij} := B(t,u_h;\phi_j,\phi_i), \tag{64}$$

$$\hat{\mathbf{f}}(t) = [\hat{f}_i(t)]_{i=1,\dots,N_0}, \quad \hat{f}_i(t) = \int_\Omega \hat{f}_{k_0}(x,t)\varphi_p(x)\,dx + \int_\Gamma \hat{\gamma}_{k_0}(x,t)\varphi_p(x)\,d\sigma(x). \tag{65}$$

The full discretization reads as

$$\mathbf{M}\mathbf{u}^{n+1} + \theta\Delta t\mathbf{K}(t_{n+1},\, \mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^{n} - (1-\theta)\Delta t\mathbf{K}(t_n,\, \mathbf{u}^{n})\mathbf{u}^{n} + \Delta t\, \hat{\mathbf{f}}^{(n,\theta)}. \tag{66}$$

Since we have set $\mathbf{G}(t, \mathbf{u}^h) = \mathbf{K}(t, \mathbf{u}^h)\mathbf{u}^h$ in (26), the expressions (30)–(31) become

$$\mathbf{P}(\mathbf{u}^{n+1}) = \big(\mathbf{M} + \theta\Delta t\mathbf{K}(t_{n+1},\, \mathbf{u}^{n+1})\big)\, \mathbf{u}^{n+1}, \qquad \mathbf{Q}(\mathbf{u}^{n}) = \big(\mathbf{M} - (1-\theta)\Delta t\, \mathbf{K}(t_n,\, \mathbf{u}^{n})\big)\, \mathbf{u}^{n},$$

respectively. Then, letting

$$\mathbf{A}(\mathbf{u}^n) := \mathbf{M} + \theta\Delta t\mathbf{K}(t_n,\, \mathbf{u}^n), \quad \mathbf{B}(\mathbf{u}^n) := \mathbf{M} - (1-\theta)\Delta t\mathbf{K}(t_n,\, \mathbf{u}^n) \quad (n = 0, 1, 2, \ldots, n_T), \tag{67}$$

the iteration procedure (66) takes the form

$$\mathbf{A}(\mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{B}(\mathbf{u}^n)\mathbf{u}^n + \Delta t\, \hat{\mathbf{f}}^{(n,\theta)}, \tag{68}$$

which is similar to (38), but now the coefficient matrices depend on $\mathbf{u}^{n+1}$ resp. $\mathbf{u}^n$.

5.2 The DMP: problems with sublinear growth

Let us consider Assumptions 2.1, where we let $p_1 = p_2 = 2$ in assumption (A5), i.e. we have

Assumption (A5'): there exist constants $\alpha_1, \alpha_2 \geq 0$ such that for any $x \in \Omega$ (or $x \in \Gamma$, resp.), $t \in (0, T)$ and $\xi \in \mathbf{R}$, and any $k, l = 1, \ldots, s$,

$$\left|\frac{\partial q_k}{\partial \xi_l}(x, t, \xi)\right| \leq \alpha_1, \qquad \left|\frac{\partial s_k}{\partial \xi_l}(x, t, \xi)\right| \leq \alpha_2. \tag{69}$$

In what follows, we will need the standard notion of (patch-)regularity of the considered meshes.

Definition 5.1 Let $\Omega \subset \mathbf{R}^d$ and let us consider a family of FEM subspaces $\mathcal{V} = \{V_h\}_{h\to 0}$. The corresponding family of FE meshes will be called *quasi-regular* if there exist constants $c_0, c_1 > 0$ and a constant $1 \leq \sigma < 2$ such that for any $h > 0$ and basis function ϕ_p,

$$c_1 h^{\sigma} \leq diam(\operatorname{supp}\phi_p) \leq c_0 h \quad \text{and} \quad meas_{d-1}(\partial(\operatorname{supp}\phi_p)) \leq c_2 h^{d-1} \tag{70}$$

(where *supp* denotes the support, i.e. the closure of the set where the function does not vanish, and $meas_{d-1}$ denotes $(d-1)$-dimensional measure of the boundary of $\operatorname{supp}\phi_p$), further, there exist constants $c_{grad} > 0$ and $1 \leq \varrho \leq \frac{2}{\sigma}$ (independent of the basis functions and h) such that

$$\max|\nabla\varphi_p| \leq \frac{c_{grad}}{diam(\operatorname{supp}\varphi_p)^{\varrho}} \qquad (p = 1, \ldots, \bar{n}). \tag{71}$$

Note that the first inequality in (70) implies

$$meas_d(\operatorname{supp}\phi_p) \leq c_3 h^d, \tag{72}$$

and in fact it also implies the second inequality in (70) under certain natural but additional assumptions, e.g. if $\operatorname{supp}\phi_p$ are convex, as is usually the case for linear, bilinear or prismatic elements.

Theorem 5.1 *Let problem (1)–(5) satisfy Assumptions 2.1 such that we let* $p_1 = p_2 = 2$ *in (7), i.e. (A5) reduces to assumption (A5') above. Let us consider a family of finite element subspaces* $\mathcal{V} = \{V_h\}_{h\to 0}$ *such that the basis functions satisfy (13)–(14), and the family of associated FE meshes is quasi-regular as in Definition 5.1. Let the following assumptions hold:*

(i) for any $p = 1, ..., n_0,\ q = 1, ..., n\ (p \neq q)$, *if* $meas_d(\operatorname{supp}\varphi_p \cap \operatorname{supp}\varphi_q) > 0$ *then*

$$\nabla\varphi_p \cdot \nabla\varphi_q \le 0 \quad on\ \Omega \quad and \quad \int_\Omega \nabla\varphi_p \cdot \nabla\varphi_q \le -K_0\, h^{d-2} \tag{73}$$

with some constant $K_0 > 0$ *independent of* p, q *and* h;

(ii) the mesh parameter h *satisfies* $h < h_0$, *where* $h_0 > 0$ *is the first positive root of the equation*

$$-\frac{\mu_0 K_0}{c_3}\frac{1}{h^2} + \alpha_1 + \frac{\omega}{c_3 h^{\varrho\sigma}} = 0$$

where, using notation $\|\mathbf{w}\|_\infty := \sup_{k,x,t} |\mathbf{w}_k(x,t)|$,

$$\omega := c_2\alpha_2 + c_{grad}\|\mathbf{w}\|_\infty\,; \tag{74}$$

(iii) using ω *from (74), we have*

$$\Delta t \ge \frac{c_3 h^2}{\theta\big(\mu_0 K_0 - \alpha_1 c_3 h^2 - \omega h^{2-\varrho\sigma}\big)}; \tag{75}$$

(iv) if $\theta < 1$ *then*

$$\Delta t \le \frac{1}{(1-\theta)\,R(h)}, \tag{76}$$

using the notations

$$R(h) := (\mu_1 + \frac{\|\mathbf{w}\|_\infty}{2})N(h) + \alpha_2\, G(h) + (\alpha_1 + \frac{\|\mathbf{w}\|_\infty}{2}), \tag{77}$$

$$N(h) := \max_{p=1,\dots,\bar{n}_0} \frac{\int_\Omega |\nabla\varphi_p|^2}{\int_\Omega \varphi_p^2}\,, \qquad G(h) := \max_{p=1,\dots,\bar{n}_0} \frac{\int_{\Gamma_N} \varphi_p^2}{\int_\Omega \varphi_p^2}\,. \tag{78}$$

Then the matrices $\mathbf{M}$, $\mathbf{K}(t_{n+1}, \mathbf{u}^{n+1})$, $\mathbf{A}(\mathbf{u}^{n+1})$ *and* $\mathbf{B}(\mathbf{u}^n)$, *defined via (25), (64) and (67)–(68), respectively, have the following properties:*

(1) $\sum_{j=1}^{N} \mathbf{K}(t_{n+1}, \mathbf{u}^{n+1})_{ij} \ge 0$ *for all* $i = 1, \dots, N_0$;

(2) $\mathbf{M}_{ij} \ge 0$ *for all* $i = 1, \dots, N_0,\ j = 1, \dots, N$;

(3) $\sum_{j=1}^{N} \mathbf{M}_{ij} =: m_i > 0$ *for all* $i = 1, \dots, N_0$;

(4) $\mathbf{A}(\mathbf{u}^{n+1})_{ij} \le 0 \quad (i \ne j,\ \ i = 1, ..., N_0,\ j = 1, ..., N)$*;*

(5) $\mathbf{B}(\mathbf{u}^{n})_{ii} \ge 0 \quad (i = 1, ..., N_0)$*.*

Proof. First we calculate $K(t, \mathbf{u}^h)_{ij} := B(t, u_h; \phi_j, \phi_i)$ for given $i = 1, ..., N_0$, $j = 1, ..., N$. Let us write the indices i, j in the form as in (22):

$$i = (k_0 - 1)\bar{n}_0 + p \quad \text{for some } 1 \le k_0 \le s \text{ and } 1 \le p \le \bar{n}_0, \tag{79}$$

$$\begin{aligned} j &= (l_0 - 1)\bar{n}_0 + q \quad \text{for some } 1 \le l_0 \le s \text{ and } 1 \le q \le \bar{n}_0 \text{ or} \\ j &= N_0 + (l_0 - 1)(\bar{n} - \bar{n}_0) + q - \bar{n}_0 \quad \text{for some } 1 \le l_0 \le s \text{ and } \bar{n}_0 + 1 \le q \le \bar{n}. \end{aligned} \tag{80}$$

Then the functions $u = \phi_j$ and $v = \phi_i$ have lth and kth coordinates $u_l = \delta_{l,l_0}\varphi_q$ and $v_k = \delta_{k,k_0}\varphi_p$ (where $\delta_{\cdot,\cdot}$ is the Kronecker symbol) for $k, l = 1, \dots, s$, hence by (62),

$$K(t, \mathbf{u}^h)_{ij} = \begin{cases} \displaystyle\int_\Omega r_{k_0\, l_0}(x, t, u_h)\, \varphi_p\, \varphi_q\, dx + \int_\Gamma z_{k_0\, l_0}(x, t, u_h)\, \varphi_p\, \varphi_q\, d\sigma \qquad \text{if } k_0 \ne l_0; \\ \displaystyle\int_\Omega \Big(a_{k_0}(x, t, u_h, \nabla u_h)\nabla\varphi_p \cdot \nabla\varphi_q + (\mathbf{w}_{k_0}(x, t) \cdot \nabla\varphi_p)\varphi_q + r_{k_0\, k_0}(x, t, u_h)\, \varphi_p\, \varphi_q\Big)\, dx \\ \qquad\qquad \displaystyle + \int_\Gamma z_{k_0\, k_0}(x, t, u_h)\, \varphi_p\, \varphi_q\, d\sigma \qquad \text{if } k_0 = l_0\,. \end{cases}$$

Similarly,

$$M_{ij} = 0 \qquad \text{if } \ k_0 \ne l_0, \quad \text{and} \qquad M_{ij} = \int_\Omega \varphi_p\, \varphi_q\, dx \qquad \text{if } \ k_0 = l_0\,. \tag{81}$$

Now we can prove the desired properties (1)-(5). Moreover, we prove them in general for all t and $\mathbf{u}^h$ (but will use them later only in the case formulated in the theorem).

(1) Let $i \in \{1, \dots, N_0\}$ be fixed. Then, using the notations of (22),

$$\begin{aligned} \sum_{j=1}^{N} K(t, \mathbf{u}^h)_{ij} = \int_\Omega \Big(& a_{k_0}(x, t, u_h, \nabla u_h)\nabla\varphi_p \cdot \nabla(\sum_{q=1}^{\bar{n}} \varphi_q) + (\mathbf{w}_{k_0}(x, t) \cdot \nabla\varphi_p)(\sum_{q=1}^{\bar{n}} \varphi_q) \\ & + (\sum_{l_0=1}^{s} r_{k_0\, l_0}(x, t, u_h))\, \varphi_p\, (\sum_{q=1}^{\bar{n}} \varphi_q)\Big)\, dx + \int_\Gamma (\sum_{l_0=1}^{s} z_{k_0\, l_0}(x, t, u_h))\, \varphi_p\, (\sum_{q=1}^{\bar{n}} \varphi_q)\, d\sigma\,. \end{aligned}$$

We now use (13) and first estimate the last terms. Using (59), the sums of functions $r_{k\,l}$ and $z_{k\,l}$ inherit the nonnegativity (9), hence from (13) we altogether obtain that the last two integrands are nonnegative. Then, (13) also yields that the first integrand vanishes and the sum in the second integrand equals 1, thus we obtain

$$\sum_{j=1}^{N} K(t, \mathbf{u}^h)_{ij} \ge \int_\Omega \mathbf{w}_{k_0}(x, t) \cdot \nabla\varphi_p\,. \tag{82}$$

For fixed t, using the divergence theorem and Assumption 2.1 (A4),

$$K(t,\mathbf{u}^h)_{ij} \geq \int_\Omega (\mathbf{w}_{k_0}(x,t)\cdot\nabla\varphi_p) = \int_{\Gamma_N} (\mathbf{w}_{k_0}(x,t)\cdot\nu)\,\varphi_p\; d\sigma + \int_{\Gamma_{int}} [\mathbf{w}_{k_0}(x,t)\cdot\nu]\,\varphi_p\; d\sigma$$
$$- \int_\Omega (\operatorname{div}\mathbf{w}_{k_0}(x,t))\,\varphi_p\; dx \geq 0. \tag{83}$$

(2) It is obvious from (81) and (13) that $M_{ij} \geq 0$ for all i,j.

(3) Using the notations (79)-(80), (81) and (13) again, we find

$$m_i := \int\limits_\Omega \varphi_p \qquad \text{if} \quad i = (k_0-1)\bar{n}_0 + p \qquad (1 \leq k_0 \leq s,\ 1 \leq p \leq \bar{n}_0). \tag{84}$$

since $\sum\limits_{j=1}^{N} M_{ij} = \int\limits_\Omega \varphi_p\,(\sum\limits_{q=1}^{\bar{n}} \varphi_q) = \int\limits_\Omega \varphi_p\, > 0.$

(4) We calculate $A(t,\mathbf{u}^h)_{ij} := \mathbf{M}_{ij} + \theta\Delta t\mathbf{K}(t,\,\mathbf{u}^h)_{ij}$ and check its nonpositivity for all t and $\mathbf{u}^h$. If $k_0 \neq l_0$ then

$$\mathbf{A}(t,\mathbf{u}^h)_{ij} =\; \theta\Delta t\,\Big(\int\limits_\Omega r_{k_0\,l_0}(x,t,u_h)\,\varphi_p\,\varphi_q\,dx + \int\limits_\Gamma z_{k_0\,l_0}(x,t,u_h)\,\varphi_p\,\varphi_q\,d\sigma\Big) \leq 0,$$

using (13) and that by (59), $r_{k_0\,l_0}$ and $z_{k_0\,l_0}$ inherit the nonpositivity (8).

If $k_0 = l_0$ then

$$\mathbf{A}(t,\mathbf{u}^h)_{ij} = \int\limits_\Omega \varphi_p\,\varphi_q\,dx + \theta\Delta t\,\int\limits_\Omega \Big(a_{k_0}(x,t,u_h,\nabla u_h)\nabla\varphi_p\cdot\nabla\varphi_q + (\mathbf{w}_{k_0}(x,t)\cdot\nabla\varphi_p)\varphi_q$$
$$+ r_{k_0\,k_0}(x,t,u_h)\,\varphi_p\,\varphi_q\Big)\,dx + \theta\Delta t\,\int\limits_\Gamma z_{k_0\,k_0}(x,t,u_h)\,\varphi_p\,\varphi_q\,d\sigma.$$

Let $\Omega_{pq} := \operatorname{supp}\varphi_p \cap \operatorname{supp}\varphi_q$. Here (13) and (72) yield

$$\int_\Omega \varphi_p\,\varphi_q \leq meas_d(\Omega_{pq}) \leq c_3 h^d\,, \tag{85}$$

and similarly, also using (70),

$$\int_\Omega r_{k_0\,k_0}(x,t,u_h)\,\varphi_p\,\varphi_q \leq \alpha_1 c_3 h^d, \qquad \int\limits_\Gamma z_{k_0\,k_0}(x,t,u_h)\,\varphi_p\,\varphi_q \leq \alpha_2 c_2 h^{d-1} \tag{86}$$

since by (59), $r_{k_0\,k_0}$ and $z_{k_0\,k_0}$ inherit (69). By (6) and (73), resp. (13), (71) and (72),

$$\int_\Omega a_{k_0}(x,t,u_h,\nabla u_h)\nabla\varphi_p\cdot\nabla\varphi_q \leq -\mu_0 K_0\, h^{d-2}\,, \qquad \int_\Omega (\mathbf{w}_{k_0}(x,t)\cdot\nabla\varphi_p)\varphi_q \leq c_{grad}\|\mathbf{w}\|_\infty\, h^{d-\varrho\sigma}. \tag{87}$$

Altogether, we obtain

$$\mathbf{A}(t,\mathbf{u}^h)_{ij} \le c_3 h^d \left[1 + \ \theta\Delta t \left(-\frac{\mu_0 K_0}{c_3}\,\frac{1}{h^2} + \alpha_1 + \frac{c_2\alpha_2 + c_{grad}\|\mathbf{w}\|_{L^\infty(\Omega)^s}}{c_3 h^{\varrho\sigma}} \right)\right].$$

Since $\varrho\sigma < 2$ and $h < h_0$ for h_0 defined in assumption (ii), it follows that we have a negative coefficient of $\theta\Delta t$ above, and from (74) and (75) we obtain that the expression in the large brackets is nonpositive, hence $\mathbf{A}(t,\mathbf{u}^h)_{ij} \le 0$.

(5) We have $B(t,\mathbf{u}^h)_{ii} := M_{ii} - (1-\theta)\Delta t K(t,\mathbf{u}^h)_{ii} \ge 0$ iff

$$\begin{aligned}\int_\Omega \varphi_p^2 \ge\ (1-\theta)\Delta t\Big[\int_\Omega \Big(a_{k_0}(x,t,u_h,\nabla u_h)|\nabla\varphi_p|^2 + (\mathbf{w}_{k_0}(x,t)\cdot\nabla\varphi_p)\varphi_p \\ + r_{k_0\,k_0}(x,t,u_h)\,\varphi_p^2\Big)\,dx + \int_\Gamma z_{k_0\,k_0}(x,t,u_h)\,\varphi_p^2\,d\sigma\Big].\end{aligned} \tag{88}$$

The latter holds for all $\Delta t > 0$ if $\theta = 1$ (i.e. the scheme is implicit). If $\theta < 1$, then we estimate the expresssion in brackets from above by

$$\int_\Omega \Big(\mu_1|\nabla\varphi_p|^2 + \|\mathbf{w}\|_\infty|\nabla\varphi_p|\varphi_p + \alpha_1\varphi_p^2\Big) + \int_\Gamma \alpha_2\,\varphi_p^2$$

$$\le \int_\Omega \Big((\mu_1 + \frac{\|\mathbf{w}\|_\infty}{2})|\nabla\varphi_p|^2 + (\alpha_1 + \frac{\|\mathbf{w}\|_\infty}{2})\varphi_p^2\Big) + \int_\Gamma \alpha_2\,\varphi_p^2 \le\ R(h)\cdot\int_\Omega \varphi_p^2,$$

which shows that (88) holds for all Δt that satisfies (76). ■

Remark 5.1 *(Discussion of the assumptions in Theorem 5.1.)* We may state similar comments as in the scalar case [13]:

(i) Assumption (i) can be ensured by suitable geometric properties of the space mesh, see subsection 5.4 below.

(ii) The value of h_0 can be computed easily since it is defined by an equation containing given or computable constants from the assumptions on the coefficients, the mesh quasi-regularity and geometry.

(iii) It is well-known from the above works on linear parabolic equations that the usual requirement for the relation between the space and time discretization steps is generally to keep their ratio between two positive constants as they tend to 0, i.e.

$$\Delta t = O(h^2) \tag{89}$$

should hold, in order both to achieve convergence in the maximum norm and to satisfy the DMP [9, 10, 32]. We obtain similar properties in Theorem 5.1 for our nonlinear systems. Namely, first, the lower bound in (75) is asymptotically of the form $\Delta t \ge O(h^2)$ as $h \to 0$, and all the constants involved are easily computable. If $\theta = 1$, i.e. the scheme is implicit, then there is no upper restriction on Δt. If $\theta < 1$, then for various popular finite elements one has $R(h) = O(h^{-2})$ in (77), see [13]. (Namely, this has been proved so far for simplicial elements in any dimension, bilinear elements in 2D and prismatic elements in 3D.) Hence $\Delta t \le O(h^2)$ as $h \to 0$, which yields with the other bound the usual condition (89) (as $h \to 0$) for the space and time discretizations.

In addition, the lower bound in (75) must be smaller than the upper bound in (76). In view of the factor $1-\theta$ in the latter, this gives a restriction on θ to be close enough to 1, similarly to the linear case.

Now we can derive the corresponding *discrete maximum principles.* First, based on Theorem 4.2, we obtain

Corollary 5.1 *Let problem (1)–(5) and its FE discretization satisfy the conditions of Theorem 5.1. Then the discrete solution, obtained from (68), satisfies the discrete maximum principles (54) and (58).*

One is more interested in the information containing the original coefficients rather than the discrete values in (54). In this respect we can derive the following result:

Lemma 5.1 *Let problem (1)–(5) and its FE discretization satisfy the conditions of Theorem 5.1.*

If the functions $u_k^{(0)}$, g_k and f_k are also continuous on the closure of their domains, then the discrete solution, obtained from (68), satisfies the following discrete maximum principle*:*

$$u_i^{n+1} \le \max\{0, \max_{k=1,\dots,s} \max_{\overline{\Gamma}^D_{(n+1)\Delta t}} g_k^h, \max_{k=1,\dots,s} \max_{\overline{\Omega}} u_k^{(0),h}\} \\ + (n+1)\Delta t \max\{0, \max_{k=1,\dots,s} \max_{\overline{Q}_{(n+1)\Delta t}} \hat{f}_k + D(h) \max_{k=1,\dots,s} \max_{\overline{\Gamma}_{(n+1)\Delta t}} \hat{\gamma}_k\},$$

where $\Gamma^D_{(n+1)\Delta t} := \Gamma_D \times [0,(n+1)\Delta t]$, $\Gamma_{(n+1)\Delta t} := \Gamma \times [0,(n+1)\Delta t]$, $Q_{(n+1)\Delta t} := \Omega \times [0,(n+1)\Delta t]$*, further, from (60),*

$$\hat{f}_k(x,t) := f_k(x,t) - q_k(x,t,0), \qquad \hat{\gamma}_k(x,t) := \gamma_k(x,t) - s_k(x,t,0)$$

and finally, $D(h) := \max_{p=1,\dots,\bar{n}} \dfrac{\int_{\Gamma_N} \varphi_p \, d\sigma}{\int_\Omega \varphi_p \, dx}$.

*The reverse of the above inequality (*discrete minimum principle*) holds if all maxima are replaced by minima.*

If we do not assume $u_k^{(0)}$, g_k and f_k to be continuous on the closure of their domains, then the above inequalities hold if the corresponding max *and* min *are replaced by* ess sup *and* ess inf.

Proof. We only prove the first, major, statement. (The other two are then obvious.) In view of Corollary 5.1, we must estimate further the r.h.s. of (58):

$$u_i^{n+1} \le \max\{0, g_{max}^{(n)}, u_{max}^{(0)}\} + (n+1)\Delta t \max\{0, \hat{f}_{max}^{(n)}\}.$$

Using the definitions, we first have

$$g_{max}^{(n)} = \max\{\, g_p^{(k)}(j\Delta t) :\ j = 0, \ldots, n+1,\ k = 1, \ldots, s,\ p = 1, \ldots, \bar{n}_\partial\}$$

$$\le \max\{\, g_p^{(k)}(t) :\ 0 \le t \le (n+1)\Delta t,\ \ k = 1, \ldots, s,\ p = 1, \ldots, \bar{n}_\partial\}.$$

Here (14) and (19) imply $g_p^{(k)}(t) = g_k(B_{\bar{n}_0+p}, t)$, hence $g_{max}^{(n)} \le \max\{\, g_k(x,t) :\ x \in \overline{\Gamma}_D,\ 0 \le t \le (n+1)\Delta t,\ \ k = 1, \ldots, s\} = \max\limits_{k=1,\ldots,s} \max\limits_{\overline{\Gamma}^D_{(n+1)\Delta t}} g_k^h$. Second, we similarly obtain

$$u_{max}^{(0)} = \max\{\, u_p^{(k)}(0) :\ k = 1, \ldots, s,\ p = 1, \ldots, \bar{n}_\partial\} = \max\{\, u_k^{(0)}(B_p) :\ k = 1, \ldots, s,\ p = 1, \ldots, \bar{n}_\partial\}$$

$$\le \max\{\, u_k^{(0)}(x) :\ x \in \overline{\Omega},\ k = 1, \ldots, s\} = \max_{k=1,\ldots,s} \max_{\overline{\Omega}} u_k^{(0),h}.$$

Finally, from (28), (55) and (65) we have

$$\hat{f}_{max}^{(n)} = \max_{i=1,\ldots,N} \frac{1}{m_i}(\theta \hat{f}_i((n+1)\Delta t) + (1-\theta)\hat{f}_i(n\Delta t))$$

$$= \max_{i=1,\ldots,N} \frac{1}{m_i}\Big(\int_\Omega (\theta \hat{f}_{k_0}(x,(n+1)\Delta t) + (1-\theta)\hat{f}_{k_0}(x, n\Delta t))\, \varphi_p\, dx$$

$$+ \int_\Gamma (\theta \hat{\gamma}_{k_0}(x,(n+1)\Delta t) + (1-\theta)\gamma_{k_0}(x, n\Delta t))\, \varphi_p\, d\sigma\Big).$$

By definition and (84),

$$\hat{f}_{max}^{(n)} \le \max_{p=1,\ldots,\bar{n}} \frac{1}{\int_\Omega \varphi_p}\Big((\max_{k=1,\ldots,s} \max_{\overline{Q}_{(n+1)\Delta t}} \hat{f}_k) \int_\Omega \varphi_p\ + (\max_{k=1,\ldots,s} \max_{\overline{\Gamma}_{(n+1)Deltat}} \hat{\gamma}_k) \int_\Gamma \varphi_p \Big)$$

$$\le \max_{k=1,\ldots,s} \max_{\overline{Q}_{(n+1)\Delta t}} \hat{f}_k + D(h) \max_{k=1,\ldots,s} \max_{\overline{\Gamma}_{(n+1)\Delta t}} \hat{\gamma}_k\,. \qquad \blacksquare$$

In practical situations the terms with $D(h)$ usually vanish. Namely, one often has $\hat{\gamma}_k \equiv 0$ (namely, $\gamma_k \equiv 0$ and $s_k(x,t,0) \equiv 0$, e.g. for reaction-diffusion problems), in which case the term containing $\max \hat{\gamma}_k$ disappears, and Lemma 5.1 becomes completely analogous to (33). The same holds if there is only Dirichlet boundary. More generally, if the $\hat{\gamma}_k$ do not vanish but have a common sign condition, then we have a one-sided analogy. These are summarized as follows:

Theorem 5.2 *Let problem (1)–(5) and its FE discretization satisfy the conditions of Theorem 5.1.*

If the functions $u_k^{(0)}$, g_k and f_k are also continuous on the closure of their domains, then the discrete solution, obtained from (68), satisfies the following inequalities, where the notations of Lemma 5.1 are used:

(1) If $\hat{\gamma}_k \le 0$ for all $k = 1, \ldots, s$, then

$$u_i^{n+1} \le \max\{0, \max_{k=1,\ldots,s} \max_{\overline{\Gamma}^D_{(n+1)\Delta t}} g_k^h,\ \max_{k=1,\ldots,s} \max_{\overline{\Omega}} u_k^{(0),h}\} + (n+1)\Delta t \max\{0, \max_{k=1,\ldots,s} \max_{\overline{Q}_{(n+1)\Delta t}} \hat{f}_k\}.$$

(2) If $\hat{\gamma}_k \geq 0$ for all $k = 1, \ldots, s$, then

$$u_i^{n+1} \geq \min\{0, \min_{k=1,\ldots,s} \min_{\overline{\Gamma}^D_{(n+1)\Delta t}} g_k^h, \min_{k=1,\ldots,s} \min_{\overline{\Omega}} u_k^{(0),h}\} + (n+1)\Delta t \min\{0, \min_{k=1,\ldots,s} \min_{\overline{Q}_{(n+1)\Delta t}} \hat{f}_k\}.$$

(3) If $\hat{\gamma}_k \equiv 0$ for all $k = 1, \ldots, s$, or $\Gamma_N \cup \Gamma_{int} = \emptyset$, then both of the above inequalities are valid.

If we do not assume $u_k^{(0)}$, g_k and f_k to be continuous on the closure of their domains, then the above inequalities hold if the corresponding max *and* min *are replaced by* ess sup *and* ess inf. *Finally, $n\Delta t$ can be further bounded uniformly by T in all the estimates.*

PROOF. It readily follows from Lemma 5.1. ■

Finally, using statement (2) above, one can readily derive the frequently relevant *discrete nonnegativity principle*:

Corollary 5.2 *Let problem (1)–(5) and its FE discretization satisfy the conditions of Theorem 5.1.*

If $\hat{f}_k \geq 0$, $g_k^h \geq 0$, $\hat{\gamma}_k \geq 0$ and $u_k^{(0),h} \geq 0$ for all $k = 1, \ldots, s$, then the fully discrete solution, obtained from (68), satisfies

$$u_i^n \geq 0 \qquad (n = 0, 1, ..., n_T, \ i = 1, ..., N_0).$$

Remark 5.2 Corollary 5.2 means that the coordinates u_k^h of the semidiscrete solution are nonnegative in each node point. Properties (13)–(14) of the basis functions imply that the coordinates $u^h(., n\Delta t)$ of the FEM solution for all time levels $n\Delta t$ are also nonnegative . If, in addition, we extend the solutions to Q_T with values between those on the neighbouring time levels, e.g. with the method of lines, then we obtain that the coordinates of the discrete solution satisfy

$$u_k^h \geq 0 \quad \text{on } Q_T \quad (k = 1, \ldots, s).$$

5.3 The DMP: problems with superlinear growth

In this subsection we allow stronger growth (of power order) of the nonlinearities q_k and s_k than in the above, i.e. we return to Assumption 2.1 (A5), and extend our DMP results from the previous section to this case. For this we need some extra technical assumptions and results. The discussion of this modification is similar to the scalar case [13], and we may rely on many of the technical results therein.

Let us first summarize the additional conditions.

Assumptions 5.3.

(B1) We restrict ourselves to the case of implicit scheme: $\theta = 1$.

(B2) The coefficients on Γ_N satisfy $\hat{\gamma}_k(x,t) := \gamma_k(x,t) - s_k(x,t,0) \equiv 0$ for all $k = 1, \ldots, s$, further, $\Gamma_D \neq \emptyset$.

(B3) The coordinates of the exact solution satisfy $u_k(.,t) \in W^{1,q}(\Omega)$ for some $q > 2$ (if $d = 2$) or some $q \geq 2d/(d-(d-2)(p_1-2))$ (if $d \geq 3$) for all $t \in [0,T]$.

(B4) The discretization satisfies $M_{p_1} := \sup_{t\in[0,T]} \|u(.,t) - u_h(.,t)\|_{L^{p_1}(\Omega)} < \infty$, further, if $\beta_2 \neq 0$ in (7) then $M_{p_2} := \sup_{t\in[0,T]} \|u_h(.,t)\|_{L^{p_2}(\Gamma_N)} < \infty$.

(B5) The diagonal row-dominance (9) is completed with diagonal dominance w.r.t. columns: for all $k = 1,\dots,s$, $x \in \Omega$ (or $x \in \Gamma_N \cup \Gamma_{int}$, resp.), $t \in (0,T)$, $\xi \in \mathbf{R}^s$,

$$\sum_{l=1}^{s} \frac{\partial q_l}{\partial \xi_k}(x,t,\xi) \geq 0. \qquad \sum_{l=1}^{s} \frac{\partial s_l}{\partial \xi_k}(x,t,\xi) \geq 0. \tag{90}$$

The full discretization (66) for $\theta = 1$ reads as

$$\mathbf{M}\mathbf{u}^{n+1} + \Delta t \mathbf{K}(t_{n+1},\, \mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^{n} + \Delta t\, \hat{\mathbf{f}}^{(n)}. \tag{91}$$

Let $u^{n+1} \in V_h$ denote the function with coefficient vector $\mathbf{u}^{n+1}$, and let $\hat{f}^n(x) := \hat{f}(x, n\Delta t)$. Then, by the definition of the mass and stiffness matrices, (91) implies

$$\int_\Omega \sum_{k=1}^{s} u_k^{n+1} v_k \, dx \; + \Delta t\, B(t_{n+1}, u^{n+1}; u^{n+1}, v) = \int_\Omega \sum_{k=1}^{s} u_k^{n} v_k \, dx \; + \Delta t\, \langle \psi^n, v\rangle \tag{92}$$

(for all $v \in V_h$), where $\langle \psi^n, v\rangle = \int_\Omega \sum\limits_{k=1}^{s} \hat{f}_k^n v_k \, dx \; + \int_{\Gamma_N} \sum\limits_{k=1}^{s} \hat{\gamma}_k^n v_k \, d\sigma$. Here, by assumption (B2), the integral on Γ_N vanishes, further, $\hat{f} \in L^\infty(Q_T)$ by Assumption 2.1 (A2).

Then the following technical results hold.

Lemma 5.2 *Let Assumptions 5.3 hold. Then*

(1) the norms $\|u^n\|_{L^2(\Omega)}$ *are bounded independently of* n *and* V_h *by some constant* $K_{L_2} > 0$.

(2) the norms $\|u^n\|_{L^{p_1}(\Omega)}$ *are bounded independently of* n *and* V_h *by some constant* $K_{p_1,\Omega} > 0$.

Proof. It goes in the same way as in Lemmata 5.2-5.3 in [13], if those proofs are now applied to the coordinate functions of the solution. The additional coercive nonsymmetric terms in the equations do not change the derivation in which the bilinear form is dropped due to coercivity. Any of the equivalent finite-dimensional norms can be chosen for the vector function u^n using the L^2 resp. L^{p_1} norms of its coordinate functions. ∎

Now we can prove the main result on the discretization matrices:

Theorem 5.3 *Let problem (1)–(5) satisfy Assumptions 2.1 and Assumptions 5.3. Let us consider a family of finite element subspaces* $\mathcal{V} = \{V_h\}_{h\to 0}$ *such that the basis functions satisfy (13)–(14), and the family of associated FE meshes is quasi-regular as in Definition 5.1. Let the following assumptions hold:*

(i) for any $p = 1, ..., n_0,\ q = 1, ..., n\ (p \neq q)$, if $meas_d(\operatorname{supp}\varphi_p \cap \operatorname{supp}\varphi_q) > 0$ then

$$\nabla\varphi_p \cdot \nabla\varphi_q \leq 0 \quad on\ \Omega \quad and \quad \int_\Omega \nabla\varphi_p \cdot \nabla\varphi_q \leq -K_0\, h^{d-2} \tag{93}$$

with some constant $K_0 > 0$ independent of p, q and h;

(ii) the mesh parameter h satisfies $h < h_0$, where $h_0 > 0$ is the first positive root of the equation

$$-\frac{\mu_0 K_0}{c_3}\,\frac{1}{h^2} + \alpha_1 + \frac{\omega}{c_3 h^{\varrho\sigma}} + \frac{\beta_1 c_3^{\frac{2-p_1}{p_1}} K_{p_1,\Omega}^{p_1-2}}{h^{\gamma_1}} + \frac{\beta_2 c_2^{\frac{2}{p_2}} M_{p_2}^{p_2-2}}{c_3 h^{\gamma_2}} = 0, \tag{94}$$

where the numbers $0 < \gamma_1, \gamma_2 < 2$ are defined below in (96), (97), respectively, and $\omega := c_2\alpha_2 + c_{grad}\|\mathbf{w}\|_\infty$ as in (74);

(iii) we have

$$\Delta t \geq \frac{c_3 h^2}{\theta\big(\mu_0 K_0 - \alpha_1 c_3 h^2 - \omega h^{2-\varrho\sigma} - \beta_1 c_3^{\frac{2}{p_1}} K_{p_1,\Omega}^{p_1-2} h^{2-\gamma_1} - \beta_2 c_2^{\frac{2}{p_2}} M_{p_2}^{p_2-2} h^{2-\gamma_2}\big)}\,. \tag{95}$$

Then the matrices $\mathbf{M}$, $\mathbf{K}(\mathbf{u}^{n+1})$, $\mathbf{A}(\mathbf{u}^{n+1})$ and $\mathbf{B}(\mathbf{u}^n)$, defined via (25), (64) and (67)–(68), respectively, have the following properties:

(1) $\sum\limits_{j=1}^{N} K(\mathbf{u}^{n+1})_{ij} \geq 0$ for all $i = 1, \ldots, N_0$;

(2) $M_{ij} \geq 0$ for all $i = 1, \ldots, N_0,\ j = 1, \ldots, N$;

(3) $\sum\limits_{j=1}^{N} M_{ij} =: m_i > 0$ for all $i = 1, \ldots, N_0$;

(4) $\mathbf{A}(\mathbf{u}^{n+1})_{ij} \leq 0$ $(i \neq j,\ i = 1, ..., N_0,\ j = 1, ..., N)$;

(5) $\mathbf{B}(\mathbf{u}^n)_{ii} \geq 0$ $(i = 1, ..., N_0)$.

PROOF. We follow the proof of Theorem 5.1. Statements (1)-(3) follow from it immediately, since (as seen obviously from its proof) the new growth conditions only affect the last two properties.

To prove properties (4)-(5), instead of u_h in the arguments, we must consider the functions u^{n+1} (for $\mathbf{A}$) and u^n (for $\mathbf{B}$) that have the coefficient vectors $\mathbf{u}^{n+1}$ and $\mathbf{u}^n$, respectively. The derivations below then follow the proof of the scalar case [13] with a proper adaptation.

(4) Since we now have (7) instead of (69), the first estimate in (86) is replaced by

$$\int_\Omega r_{k_0 k_0}(x, t, u^{n+1})\, \varphi_p\, \varphi_q \leq \int_\Omega \big(\alpha_1 + \beta_1 |u^{n+1}|^{p_1-2}\big)\, \varphi_p\, \varphi_q \leq \alpha_1 meas_d(\Omega_{pq}) + \beta_1 \int_{\Omega_{pq}} |u^{n+1}|^{p_1-2}\,.$$

Here the first term is bounded by $\alpha_1 c_3 h^d$ as before. To estimate the second term, we use Hölder's inequality:

$$\int_{\Omega_{pq}} |u^{n+1}|^{p_1-2} \le \|u^{n+1}\|^{p_1-2}_{L^{p_1}(\Omega_{pq})} \|1\|^2_{L^{p_1}(\Omega_{pq})},$$

where $\|u^{n+1}\|_{L^{p_1}(\Omega_{pq})} := (\int_{\Omega_{pq}} |u^{n+1}|^{p_1})^{(1/p_1)}$ and $|u^{n+1}|$ stands for the Euclidean length of the values of vector function u^{n+1}. For the first factor, we use Lemma 5.2 (2) to find that

$$\|u^{n+1}\|^{p_1-2}_{L^{p_1}(\Omega_{pq})} \le \|u^{n+1}\|^{p_1-2}_{L^{p_1}(\Omega)} \le K^{p_1-2}_{p_1,\Omega}\,.$$

The second factor satisfies, by (85), $\|1\|^2_{L^{p_1}(\Omega_{pq})} = \big(meas_d(\Omega_{pq})\big)^{2/p_1} \le c_3^{\frac{2}{p_1}} h^{\frac{2d}{p_1}} \equiv c_3^{\frac{2}{p_1}} h^{d-\gamma_1}$ with

$$\gamma_1 := d - \frac{2d}{p_1} < 2, \tag{96}$$

since from Assumption 2.1 (A5) we have $\frac{2d}{p_1} > d-2$. Hence $\displaystyle\int_{\Omega_{pq}} |u^{n+1}|^{p_1-2} \le K^{p_1-2}_{p_1,\Omega} c_3^{\frac{2}{p_1}} h^{d-\gamma_1}$ and altogether,

$$\int_\Omega r_{k_0\,k_0}(x,t,u^{n+1})\,\varphi_p\,\varphi_q \le \alpha_1 c_3 h^d + \beta_1 K^{p_1-2}_{p_1,\Omega} c_3^{\frac{2}{p_1}} h^{d-\gamma_1}\,.$$

Similarly,

$$\int_{\Gamma_N} z_{k_0\,k_0}(x,t,u^{n+1})\,\varphi_p\,\varphi_q \le \alpha_2 c_2 h^{d-1} + \beta_2 \int_{\Gamma_{pq}} |u^{n+1}|^{p_2-2}$$

and here we can use Assumption 5.3 (B4) and (72) to have

$$\int_{\Gamma_{pq}} |u^{n+1}|^{p_2-2} \le \|u^{n+1}\|^{p_2-2}_{L^{p_2}(\Gamma_{pq})} \|1\|^2_{L^{p_2}(\Gamma_{pq})} \le \|u^{n+1}\|^{p_2-2}_{L^{p_2}(\Gamma_N)} \big(meas_{d-1}(\Gamma_{pq})\big)^{2/p_2}$$

$$\le M^{p_2-2}_{p_2} c_2^{\frac{2}{p_2}} h^{\frac{2(d-1)}{p_2}} \equiv M^{p_2-2}_{p_2} c_2^{\frac{2}{p_2}} h^{d-\gamma_2},$$

where $\Gamma_{pq} := \partial\Omega_{pq} \cap \Gamma$ and

$$\gamma_2 := d - \frac{2(d-1)}{p_2} < 2 \tag{97}$$

since from Assumption 2.1 (A5) we have $\frac{2d-2}{p_2} > d-2$. Summing up, using the above and (87), we obtain that $A(\mathbf{u}^{n+1})_{ij}$ is bounded by

$$c_3 h^d \left[1 + \;\theta\Delta t\; \left(-\frac{\mu_0 K_0}{c_3}\,\frac{1}{h^2} + \alpha_1 + \frac{c_2\alpha_2 + c_{grad}\|\mathbf{w}\|_{L^\infty(\Omega)^s}}{c_3 h^{\varrho\sigma}} + \frac{\beta_1 K^{p_1-2}_{p_1,\Omega}}{c_3^{\frac{p_1-2}{p_1}}\, h^{\gamma_1}} + \frac{\beta_2 c_2^{\frac{2}{p_2}} M^{p_2-2}_{p_2}}{c_3 h^{\gamma_2}} \right) \right].$$

Since $h < h_0$ for h_0 defined in assumption (ii), it follows that we have a negative coefficient of $\theta\Delta t$ above, and from (95) we obtain that the expression in $[\ldots]$ is nonpositive, hence $A(\mathbf{u}^h)_{ij} \le 0$.

(5) For the considered implicit scheme, $\mathbf{B}(\mathbf{u}^n)$ coincides with the block mass matrix $\mathbf{M}$, whose diagonal entries are positive. ∎

From Theorem 5.3, one can derive the corresponding discrete maximum, minimum and nonnegativity preservation principles, similarly as in Lemma 5.1 and Theorem 5.2 in the sublinear case. Here we only formulate the discrete nonnegativity principle:

Corollary 5.3 *Let the conditions of Theorem 5.3 hold, further, let $\hat{f}_k \geq 0$, $g_k^h \geq 0$ and $u_k^{(0),h} \geq 0$ for all $k = 1, \ldots, s$. Then the fully discrete solution, obtained from (68), satisfies*

$$u_i^n \geq 0 \qquad (n = 0, 1, ..., n_T, \ i = 1, ..., N_0).$$

In addition, similarly to Remark 5.2, if we extend the solutions to Q_T with values between those on the neighbouring time levels, e.g. with the method of lines, then we obtain that the coordinates of the discrete solution satisfy

$$u_k^h \geq 0 \quad \text{on } Q_T \quad (k = 1, \ldots, s).$$

Remark 5.3 In view of Corollary 5.3, it makes sense to pose problem (1)–(5) if its coefficients q_k and/or s_k are a priori defined only for nonnegative arguments for $u_1, \ldots, u_s$, since the described numerical solution only uses these values. This is the case for various real-life models with nonnegative unknown quantities, such as concentration etc. (If an actual inner numerical method still requires arbitrary values of $u_1, \ldots, u_s$, than one may define suitable extensions of q_k and/or s_k.)

Remark 5.4 Similar comments are valid for the assumptions of Theorem 5.3 as in Remark 5.1. In particular, the lower bound in (95) for the space and time discretization steps is asymptotically of the form

$$\Delta t \geq O(h^2)$$

as $h \to 0$, and all the constants involved are easily computable. On the other hand, since we have considered the implicit scheme $\theta = 1$ here, there is no corresponding upper bound as in Remark 5.1.

5.4 Geometric properties of the space mesh

In the above results, the condition on the space mesh to achieve the DMP has been property (93). We briefly summarize some geometric aspects of this condition.

The most direct way to satisfy (93) is to require the stricter property

$$\nabla\varphi_p \cdot \nabla\varphi_q \leq -K_0 \, h^{-2} \tag{98}$$

pointwise on the common support of these basis functions. In view of well-known formulae (see e.g. [2, 5, 27, 41]), the above condition has a nice geometric interpretation: in the case of simplicial meshes, it is sufficient if the employed mesh is uniformly acute [3, 27]. For practical constructions of such meshes see [3, 6, 36] and references therein. In the case of bilinear elements, condition (98) is equivalent to the so-called strict non-narrowness of the meshes, see [19]. The case of prismatic finite elements in this context is treated in [16].

These conditions are sufficient but not necessary. For instance, for linear elements, some obtuse interior angles may occur in the simplices of the meshes, just as for linear problems (see e.g. [26]). Alternatively, one can require (98) only on a proper subpart of each intersection of supports [24]: let there exist subsets $\Omega_{pq}^+ \subset \Omega_{pq}$ for all p, q such that the basis functions satisfy

$$\nabla\varphi_p \cdot \nabla\varphi_q \le -\frac{c}{h^2} < 0 \quad \text{on } \ \Omega_{pq}^+, \qquad \nabla\varphi_q \cdot \nabla\varphi_p \le 0 \quad \text{on } \ \Omega_{pq} \setminus \Omega_{pq}^+,$$

in which case the Ω_{pq}^+ must have asymptotically nonvanishing measure: $\frac{meas_d(\Omega_{pq}^+)}{meas_d(\Omega_{pq})} \ge c_3 > 0$ for some constant c_3 independent of p, q. Clearly, these conditions ensure (93). These weaker conditions may allow in general easier refinement procedures (e.g. allow also right dihedral angles).

6 Examples

We give some examples of problems where the above DMP theorems yield new results. Let us recall here that the main conditions of the applied theorems are the relation $\Delta t = O(h^2)$ for the space and time mesh and the "acuteness" property (93) for the space mesh.

In all these examples, similarly as before, Ω stands for a bounded domain in $\mathbf{R}^d$ and $T > 0$ is a given number, Γ_{int} is a piecewise C^1 surface lying in Ω, we denote $Q_T := (\Omega \setminus \Gamma_{int})$, and $[\,.\,]_{\Gamma_{int}}$ denotes the jump (i.e., the difference of the limits from the two sides of the interface Γ_{int}) of a function.

6.1 A single equation

As a first trivial example, we mention that even for a single equation our results generalize those in [13] in two respects: first, one may now have nonsymmetric terms and interface conditions as well, second, the obtained DMP is now in a form directly analogous to the corresponding CMP.

Let us consider the equation

$$\frac{\partial u}{\partial t} - \operatorname{div}\Big(a(x,t,u,\nabla u)\nabla u\Big) + \mathbf{w}(x,t)\cdot\nabla u + q(x,t,u) = f(x,t) \quad \text{in } \ Q_T, \tag{99}$$

with boundary, interface and initial conditions analogous to (2)–(5) (in fact, one must simply drop the subscript k therein). We impose Assumptions 2.1, which now reduce to the following simpler requirements. The domain and smoothness conditions (A1)-(A2) remain similar, just as the ellipticity condition $0 < \mu_0 \le a(x,t,\xi,\eta) \le \mu_1$ for the principal space term in (A3) and the coercivity conditions $\operatorname{div}\mathbf{w} \le 0$ on Ω, $\mathbf{w}\cdot\nu \ge 0$ on Γ_N, $\big[\mathbf{w}\big]_{\Gamma_{int}} = 0$ and $\big[\mathbf{w}\cdot\nu\big]_{\Gamma_{int}} \ge 0$ in (A4). Conditions (A5)-(A7) become much simpler: cooperativity has no meaning in this case, and the growth and diagonal dominance conditions together become

$$0 \le \frac{\partial q}{\partial \xi}(x,t,\xi) \le \alpha_1 + \beta_1 |\xi|^{p_1-2}, \qquad 0 \le \frac{\partial s}{\partial \xi}(x,t,\xi) \le \alpha_2 + \beta_2 |\xi|^{p_2-2}. \tag{100}$$

Altogether, we just obtain a generalization of the problem in [13].

Then Lemma 5.1 holds together with its consequences. It is worth formulating what Theorem 5.2 yields for this case, as an analogue to (33):

Corollary 6.1 *Let problem (99) and its FE discretization satisfy the conditions of Theorem 5.1. If the functions $u^{(0)}$, g and f are also continuous on the closure of their domains, then the discrete solution, obtained from (68), satisfies the following inequalities, where the notations of Lemma 5.1 are used:*

(1) If $\hat{\gamma} \le 0$, then $u_i^{n+1} \le \max\{0, \max_{\overline{\Gamma}^D_{(n+1)\Delta t}} g^h, \max_{\overline{\Omega}} u^{(0),h}\} + (n+1)\Delta t \max\{0, \max_{\overline{Q}_{(n+1)\Delta t}} \hat{f}\}$.

(2) If $\hat{\gamma} \ge 0$, then $u_i^{n+1} \ge \min\{0, \min_{\overline{\Gamma}^D_{(n+1)\Delta t}} g^h, \min_{\overline{\Omega}} u^{(0),h}\} + (n+1)\Delta t \min\{0, \min_{\overline{Q}_{(n+1)\Delta t}} \hat{f}\}$.

(3) If $\hat{\gamma} \equiv 0$ or $\Gamma_N \cup \Gamma_{int} = \emptyset$, then both of the above inequalities are valid.

6.2 Reaction-diffusion systems in chemistry

6.2.1 Reactions in a domain

Certain reaction-diffusion processes in chemistry in a domain $\Omega \subset \mathbf{R}^d$, $d = 2$ or 3, are described by systems of the following form:

$$\frac{\partial u_k}{\partial t} - b_k \Delta u_k + P_k(x, u_1, \dots, u_s) = f_k(x,t) \quad \text{in } Q_T, \tag{101}$$

with boundary and initial conditions

$$u_k(x,t) = g_k(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T], \tag{102}$$

$$b_k \tfrac{\partial u_k}{\partial \nu} = 0 \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T], \qquad u_k(x,0) = u_k^{(0)}(x) \quad \text{for} \quad x \in \Omega, \tag{103}$$

for all $k = 1, \dots, s$. The DMP for steady-states of such systems has been discussed in [24], now we consider the time-dependent case.

Here, for all k, the quantity u_k describes the concentration of the kth species, and P_k is a polynomial which characterizes the rate of the reactions involving the k-th species. A common way to describe such reactions is the so-called mass action type kinetics [17, 18], which implies that P_k has no constant term for any k, in other words, $P_k(x,0) \equiv 0$ on Ω for all k. The function $f_k \ge 0$ describes a source independent of concentrations.

We consider system (101)–(103) under the following conditions, such that it becomes a special case of system (1)–(5). As pointed out later, such chemical models describe processes with cross-catalysis and strong autoinhibiton.

Assumptions 6.2.1.

(i) Ω is a bounded polytopic domain in $\mathbf{R}^d$, where $d = 2$ or 3, and $\Gamma_N, \Gamma_D \subset \partial\Omega$ are are disjoint open measurable subsets of $\partial\Omega$ such that $\partial\Omega = \overline{\Gamma}_D \cup \overline{\Gamma}_N$.

(ii) (Smoothness and growth.) For all $k, l = 1, \dots, s$, the functions P_k are polynomials of arbitrary degree if $d = 2$ or of degree at most 4 if $d = 3$, and we have $P_k(x, 0) \equiv 0$ on Ω. Further, $f_k \in L^\infty(Q_T)$, $g_k \in L^\infty(\Gamma_D \times [0, T])$ and $u_k^{(0)} \in L^\infty(\Omega)$.

(iii) (Ellipticity for the principal space term.) $b_k > 0$ $(k = 1, \dots, s)$ are given numbers.

(iv) (Cooperativity.) We have

$$\frac{\partial P_k}{\partial \xi_l}(x, \xi) \le 0 \qquad (k, l = 1, \dots, s,\ k \ne l;\ x \in \Omega,\ \xi \in \mathbf{R}^s). \tag{104}$$

(v) (Weak diagonal dominance w.r.t. rows and columns.) We have

$$\sum_{l=1}^{s} \frac{\partial P_k}{\partial \xi_l}(x, \xi) \ge 0, \qquad \sum_{l=1}^{s} \frac{\partial P_l}{\partial \xi_k}(x, \xi) \ge 0 \qquad (k = 1, \dots, s;\ x \in \Omega,\ \xi \in \mathbf{R}^s). \tag{105}$$

Similarly as in Remark 2.1, assumptions (104)–(105) now imply

$$\frac{\partial P_k}{\partial \xi_k}(x, \xi) \ge 0 \qquad (k = 1, \dots, s;\ x \in \Omega,\ \xi \in \mathbf{R}^s). \tag{106}$$

Returning to the model described by system (101)–(103), the chemical meaning of the cooperativity (104) is cross-catalysis, whereas (106) means autoinhibiton. Cross-catalysis arises e.g. in gradient systems [35]. Condition (105) means that autoinhibition is strong enough to ensure both weak diagonal dominances.

By definition, the concentrations u_k are nonnegative, therefore a proper numerical model must produce such numerical solutions. We can use Corollary 5.3 to obtain the required property:

Corollary 6.2 *Let system (101)–(103) satisfy Assumptions 6.2.1, and assume that* $u_k(., t) \in W^{1,q}(\Omega)$ *for some* $q > 2$ *as in Assumptions 5.3 (B3). Let the FE discretization of the system satisfy the conditions of Theorem 5.3.*

If $f_k \ge 0$, $g_k^h \ge 0$ *and* $u_k^{(0),h} \ge 0$ *for all* $k = 1, \dots, s$, *then the discrete solution, obtained from (68), satisfies*

$$u_i^n \ge 0 \qquad (n = 0, 1, ..., n_T,\ i = 1, ..., N_0).$$

In addition, as mentioned after Corollary 5.3, if we extend the solutions to Q_T with values between those on the neighbouring time levels, e.g. with the method of lines, then we obtain that the coordinates of the discrete solution satisfy

$$u_k^h \ge 0 \quad \text{on } Q_T \quad (k = 1, \dots, s).$$

Remark 6.1 For such systems with only Dirichlet boundary conditions, more specific results on the preservation of invariant rectangles under FEM have been obtained in [8].

6.2.2 Reactions localized on an interface

A different type of reaction-diffusion process arises in some cases when the chemical reactions are localized on an interface, i.e. on a subsurface of the domain in 3D or on a curve in 2D, see [20, 21] and the references therein. If one consideres such time-dependent systems, then the problem can be described as follows, where $\Omega \subset \mathbf{R}^d$ is a domain in $d = 2$ or 3:

$$\frac{\partial u_k}{\partial t} - b_k \Delta u_k = f_k(x,t) \quad \text{in} \quad Q_T, \tag{107}$$

with boundary, interface and initial conditions

$$u_k(x,t) = g_k(x,t) \qquad \text{for} \quad (x,t) \in \partial\Omega \times [0,T], \tag{108}$$

$$[u_k]_{\Gamma_{int}} = 0 \quad \text{and} \quad \Big[b_k \tfrac{\partial u_k}{\partial \nu} + S_k(x, u_1, \ldots, u_s) \Big]_{\Gamma_{int}} = 0 \quad \text{for } (x,t) \in \Gamma_{int} \times [0,T], \tag{109}$$

$$u_k(x,0) = u_k^{(0)}(x) \quad \text{for} \quad x \in \Omega, \tag{110}$$

for all $k = 1, \ldots, s$.

Analogously to Assumptions 6.2.1, we now impose

Assumptions 6.2.2.

(i) Ω is a bounded polytopic domain in $\mathbf{R}^d$, where $d = 2$ or 3, and Γ_{int} is a piecewise C^1 surface lying in Ω.

(ii) (Smoothness and growth.) For all $k, l = 1, \ldots, s$, the functions S_k are polynomials of arbitrary degree if $d = 2$ or of degree at most 2 if $d = 3$, and we have $S_k(x, 0) \equiv 0$ on Ω. Further, $f_k \in L^\infty(Q_T)$, $g_k \in L^\infty(\partial\Omega \times [0,T])$ and $u_k^{(0)} \in L^\infty(\Omega)$.

(iii) (Ellipticity for the principal space term.) $b_k > 0$ $(k = 1, \ldots, s)$ are given numbers.

(iv) (Cooperativity.) We have $\dfrac{\partial S_k}{\partial \xi_l}(x,\xi) \le 0 \quad (k, l = 1, \ldots, s, \ k \ne l; \ x \in \Gamma_{int}, \ \xi \in \mathbf{R}^s)$.

(v) (Weak diagonal dominance w.r.t. rows and columns.) We have

$$\sum_{l=1}^{s} \frac{\partial S_k}{\partial \xi_l}(x,\xi) \ge 0, \qquad \sum_{l=1}^{s} \frac{\partial S_l}{\partial \xi_k}(x,\xi) \ge 0 \qquad (k = 1, \ldots, s; \ x \in \Gamma_{int}, \ \xi \in \mathbf{R}^s).$$

Similarly to the previous subsection, assumptions (iv)-(v) imply the analogue of (106), and the chemical meaning for the localized reactions is cross-catalysis and autoinhibition, the latter being strong enough to ensure both weak diagonal dominances.

We can repeat Corollary 6.2, by replacing Assumptions 6.2.1 by Assumptions 6.2.2, to obtain that $u_i^n \ge 0$ $(n = 0, 1, ..., n_T, \ i = 1, ..., N_0)$, and, by a proper extension of u^h to Q_T, that $u_k^h \ge 0$ on Q_T $(k = 1, \ldots, s)$.

6.3 Transport problems

Systems describing transport processes generally involve reaction, diffusion and convection (advection) terms. (Some other possible terms can be mathematically included in the last, zeroth-order reaction terms.) Let us first consider the case of reactions in the whole domain, see, e.g., [42].

The mathematical model of such processes is a modification of (101) if a first order term is added to describe convection. Let us therefore consider the system of equations

$$\frac{\partial u_k}{\partial t} - b_k \Delta u_k + \mathbf{w}_k(x,t) \cdot \nabla u_k + \ P_k(x, u_1, \ldots, u_s) = f_k(x,t) \quad \text{in} \ \ Q_T \tag{111}$$

$(k = 1, \ldots, s)$ with the boundary and initial conditions (102)–(103). We study this system under conditions such that it becomes a special case of system (1)–(5). For this, we only need to add the corresponding part of Assumption 2.1 (A4) to the previously studied properties:

Assumptions 6.3.1. Let Assumptions 6.2.1 hold, and let $\operatorname{div} \mathbf{w}_k \le 0$ on Ω and $\mathbf{w}_k \cdot \nu \ge 0$ on Γ_N $(k = 1, \ldots, s)$.

As pointed out above, Assumptions 6.2.1 mean that the described chemical process is cross-catalyc with suitably strong autoinhibiton. Further, in many cases the convective terms are divergence-free (e.g. if they arise from a related Stokes system): $\operatorname{div} \mathbf{w}_k = 0$, i.e. the first property of $\mathbf{w}_k$ holds. The inequality $\mathbf{w}_k \cdot \nu \ge 0$ on Γ_N means that Neumann conditions are prescribed on the outflow boundary.

Similarly as before, the concentrations u_k are nonnegative, therefore the numerical model must produce such numerical solutions. We can repeat Corollary 6.2, by replacing Assumptions 6.2.1 by Assumptions 6.3.1, to obtain that $u_i^n \ge 0$ $(n = 0, 1, ..., n_T,\ i = 1, ..., N_0)$, and, by a proper extension of u^h to Q_T, that $u_k^h \ge 0$ on Q_T $(k = 1, \ldots, s)$.

Second, for transport processes we can also consider the case when the chemical reactions are localized on an interface. Then we only have uncoupled nonsymmetric equations such that the reactions $P_k(x, u_1, \ldots, u_s)$ are missing from (111), and they instead appear in the interface conditions as in subsection 6.2.2, i.e. the side conditions are (108)–(110). In this case Assumptions 6.2.2 are completed with the conditions $[\mathbf{w}_k]_{\Gamma_{int}} = 0$ and $[\mathbf{w}_k \cdot \nu]_{\Gamma_{int}} \ge 0$ $(k = 1, \ldots, s)$, and provide the desired nonnegativity if these assumptions replace Assumptions 6.2.1 in Corollary 6.2.

6.4 Population systems and reactions proportional to species

Certain systems in population dynamics can be written in the form

$$\begin{cases} \dfrac{\partial u_1}{\partial t} - b_1 \Delta u_1 = u_1 \, M_1(u_1, u_2) \\[2ex] \dfrac{\partial u_2}{\partial t} - b_2 \Delta u_2 = u_2 \, M_2(u_1, u_2), \end{cases} \tag{112}$$

where u_1, u_2 denote the amounts of two species distributed continuously in a plane region Ω, see e.g. [8]. The simple boundary and initial conditions

$$u_k = g_k \quad \text{on } \partial\Omega \times [0,T], \qquad u_k(.,0) = u_k^{(0)} \quad \text{on } \Omega \qquad (k=1,2) \tag{113}$$

are imposed. Such a system can also describe a chemical reaction as in subsection 6.2 if the reaction rates are proportional to the quantity of the species. Here we will use the population terminology. If the species live in symbiosis, then

$$\partial_2 M_1 \geq 0 \qquad \text{and} \qquad \partial_1 M_2 \geq 0. \tag{114}$$

System (112) falls into the type (1) where

$$q_1(\xi_1,\xi_2) = -\xi_1\, M_1(\xi_1,\xi_2) \qquad \text{and} \qquad q_2(\xi_1,\xi_2) = -\xi_2\, M_2(\xi_1,\xi_2)\,, \tag{115}$$

and $f_1 \equiv f_2 \equiv 0$. Most of Assumptions 2.1 are trivially satisfied in a natural way. Namely, let us impose

Assumptions 6.4.1. Ω is a bounded polygonal domain in $\mathbf{R}^2$ and $b_1, b_2 > 0$ are given numbers. Further, $g_1, g_2 \in C(\partial\Omega \times [0,T])$, $u_1^{(0)}, u_2^{(0)} \in C(\overline{\Omega})$, $M_1, M_2 \in C^1(\mathbf{R}^2)$ and they can grow at most with polynomial rate with ξ_1, ξ_2.

These assumptions imply that (A1)-(A5) of Assumptions 2.1 are satisfied. The cooperativity (A6) follows from (114), since by Remark 5.3 we may only consider nonnegative values of ξ_k. In view of Theorem 5.3 that we want to use, it suffices to fulfil the weak diagonal dominances (90). Before giving a condition, we recall the property in Remark 2.1, necessary for diagonal dominance. This expresses that the q_k grow along with their quantity, and for (115), it amounts to $\partial_i\big(\xi_i\; M_i(\xi_1,\xi_2)\big) \leq 0$ $(i=1,2)$ for all ξ_1, ξ_2, where $\partial_i := \frac{\partial}{\partial \xi_i}$. The exact condition for diagonal dominance is a strengthened version of this:

Proposition 6.1 *The functions* (115) *satisfy* (90) *if and only if for all* $i,j,k = 1,2$ *and* $\xi_1, \xi_2 > 0$*,*

$$\partial_i\Big(\xi_i\; M_i(\xi_1,\xi_2)\Big) \leq -\xi_j\; \partial_k M_j(\xi_1,\xi_2) \qquad (j \neq k). \tag{116}$$

PROOF. For brevity, we omit the variables (ξ_1,ξ_2) after M_i. The result follows by checking four elementary relations for (115):

$$\begin{aligned}
\partial_1 q_1 + \partial_2 q_1 \geq 0 \;&\Leftrightarrow\; \partial_1(\xi_1 M_1) \leq -\xi_1\; \partial_2 M_1,\\
\partial_1 q_2 + \partial_2 q_2 \geq 0 \;&\Leftrightarrow\; \partial_2(\xi_2 M_2) \leq -\xi_2\; \partial_1 M_2,\\
\partial_1 q_1 + \partial_1 q_2 \geq 0 \;&\Leftrightarrow\; \partial_1(\xi_1 M_1) \leq -\xi_2\; \partial_1 M_2,\\
\partial_2 q_1 + \partial_2 q_2 \geq 0 \;&\Leftrightarrow\; \partial_2(\xi_2 M_2) \leq -\xi_1\; \partial_2 M_1. \qquad \blacksquare
\end{aligned}$$

Remark 6.2 For instance, the functions (115) sometimes have the form

$$q_i(\xi_1,\xi_2) = G_i\xi_i - \xi_i\xi_j\, h_i(\xi_1,\xi_2), \quad \text{then} \quad M_i(\xi_1,\xi_2) = -G_i + \xi_j\, h_i(\xi_1,\xi_2)$$

$(i = 1,2,\ i \neq j)$, where $G_i > 0$ is the birth-death rate and h_i is a factor for the co-existence of the species. For instance, some Lotka-Volterra type systems can fall into this type. Assume that the rates h_i are small for large populations, in particular, that $|\partial_k h_i(\xi_1,\xi_2)| \leq \frac{c_1}{1+\xi_1^2+\xi_2^2}$. In this case an elementary calculation shows that if c_1 is so small that $c_1(1+2\sqrt{2}) \leq \min(G_1,G_2)$, then M_i satisfy (116).

Now we can use Corollary 5.3 to obtain the required nonnegativity for the numerically computed populations:

Corollary 6.3 *Let system* (112)–(113) *satisfy* (114)*, Assumptions 6.4.1 and* (116)*. Assume further that* $u_k(.,t) \in W^{1,q}(\Omega)$ *(*$k = 1,2$*) for some* $q > 2$ *as in Assumptions 5.3 (B3). Let the FE discretization of the system satisfy the conditions of Theorem 5.3.*

If $g_1^h, g_2^h \geq 0$ *and* $u_1^{(0),h}, u_2^{(0),h} \geq 0$*, then the discrete solution, obtained from (68), satisfies*

$$u_i^n \geq 0 \qquad (n = 0,1,\dots,n_T,\ i = 1,\dots,N_0).$$

Further, by a proper extension of u^h to Q_T, we have $u_1^h, u_2^h \geq 0$ on Q_T.

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