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Abstract: *Discrete maximum principles for nonlinear parabolic problems and also associated (geometric) conditions on the meshes and time-steps in the FEM-type schemes are discussed.*

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1 Introduction

The numerical approximations of models described by partial differential equations are naturally required to mirror some basic qualitative properties of the exact solutions. For parabolic equations, such a basic qualitative property is the (continuous) maximum principle (CMP). Several variants of CMPs exist, see e.g. [16, 26]. Its discrete analogues, the so-called discrete maximum principles (DMPs) for parabolic problems were first presented and analysed in the papers [17, 22]. If the finite element method (FEM) is employed for the spatial discretization, then the corresponding DMPs are normally ensured by imposing certain geometrical restrictions on the spatial meshes used, see, e.g., [10, 12, 17, 19] and the references therein. In addition, the time-steps have to be often chosen between certain lower and upper bounds. A related important discrete qualitative property of the numerical solutions is the so-called nonnegativity preservation, investigated e.g. in [8, 9]. The connection of nonnegativity preservation to DMPs is analysed e.g. in [7, 9, 10, 12].

In this paper, we prove discrete maximum principles for nonlinear parabolic problems, which has never been considered so far according to the authors' knowledge. The results are natural extensions of those in [20] (for nonlinear elliptic problems) and [13] (for linear parabolic problems).

The paper is organized as follows. In Section 2, we formulate the nonlinear parabolic problem. The discretization scheme is given in detail in Section 3. Some preliminaries on linear problems and the maximum principle are given in Section 4. The DMP and related nonnegativity preservation, and the conditions for their validity are presented in Section 5: we consider two types of growth conditions for the reaction terms, then we also discuss sufficient geometric conditions on the FE meshes used and finally give two relevant real-life examples.

2 The problem

In the sequel, we consider the following mixed nonlinear parabolic problem. Find a function $u = u(x,t)$ such that

$$\frac{\partial u}{\partial t} - \operatorname{div}\Big(k(x,t,u,\nabla u)\nabla u\Big) + q(x,t,u) = f(x,t) \quad \text{in } Q_T := \Omega \times (0,T), \tag{1}$$

where Ω is a bounded domain in $\mathbf{R}^d$ and $T > 0$. The boundary and initial conditions are given as

$$u(x,t) = g(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T], \tag{2}$$

$$k(x,t,u,\nabla u)\tfrac{\partial u}{\partial \nu} + s(x,t,u) = \gamma(x,t) \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T], \tag{3}$$

$$u(x,0) = u_0(x) \quad \text{for} \quad x \in \Omega, \tag{4}$$

respectively. We impose the following

Assumptions 2.1.

(A1) Ω is a bounded polytopic domain in $\mathbf{R}^d$ with a Lipschitz continuous boundary $\partial\Omega$; $\Gamma_N, \Gamma_D \subset \partial\Omega$ are open sets, such that $\Gamma_N \cap \Gamma_D = \emptyset$ and $\overline{\Gamma}_N \cup \overline{\Gamma}_D = \partial\Omega$.

(A2) The scalar functions $k : \overline{Q}_T \times \mathbf{R}^{d+1} \to \mathbf{R}$, $q : \overline{Q}_T \times \mathbf{R} \to \mathbf{R}$ and $s : \overline{\Gamma}_N \times [0, T] \times \mathbf{R} \to \mathbf{R}$ are measurable and bounded, further, q and s are continuously differentiable w.r.t. t, on their domains of definition. Further, $f \in L^\infty(Q_T)$, $\gamma \in L^2(\Gamma_N \times [0, T])$, $g \in L^\infty(\Gamma_D \times [0, T])$ and $u_0 \in L^\infty(\Omega)$.

(A3) There exist positive constants μ_0 and μ_1 such that

$$0 < \mu_0 \le k(x, t, \xi, \eta) \le \mu_1 \tag{5}$$

for all $(x, t, \xi, \eta) \in \Omega \times (0, T) \times \mathbf{R} \times \mathbf{R}^d$.

(A4) Let $2 \le p_1$ if $d = 2$, or $2 \le p_1 < \frac{2d}{d-2}$ if $d > 2$, further, let $2 \le p_2 < 2.5$ if $d = 2$ or 3 and $p_2 = 2$ if $d > 3$. There exist constants $\alpha_1, \alpha_2, \beta_1, \beta_2 \ge 0$ such that for any $x \in \Omega$ (or $x \in \Gamma_N$, resp.), $t \in (0, T)$ and $\xi \in \mathbf{R}$,

$$0 \le \frac{\partial q(x, t, \xi)}{\partial \xi} \le \alpha_1 + \beta_1 |\xi|^{p_1 - 2}, \qquad 0 \le \frac{\partial s(x, t, \xi)}{\partial \xi} \le \alpha_2 + \beta_2 |\xi|^{p_2 - 2}. \tag{6}$$

We define weak solutions in the usual way as follows. Let $H^1_D(\Omega) := \{u \in H^1(\Omega) : u_{|\Gamma_D} = 0\}$. A function $u : Q_T \to \mathbf{R}$ is called the weak solution of the problem (1)–(4) if u is continuously differentiable with respect to t and $u(., t) \in H^1_D(\Omega)$ for all $t \in (0, T)$ and satisfies the relation

$$\int_\Omega \frac{\partial u}{\partial t} v \, dx + \int_\Omega \Big(k(x, t, u, \nabla u) \nabla u \cdot \nabla v + q(x, t, u) v \Big) \, dx + \int_{\Gamma_N} s(x, t, u) v \, d\sigma \tag{7}$$

$$= \int_\Omega f v \, dx + \int_{\Gamma_N} \gamma v \, d\sigma \qquad (\forall v \in H^1_D(\Omega), \quad t \in (0, T)),$$

further,

$$u = g \quad \text{on} \quad [0, T] \times \Gamma_D, \qquad u|_{t=0} = u_0 \quad \text{in} \quad \Omega, \tag{8}$$

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

3 Discretization scheme

The discretization of problem (1)–(4) is built up in a standard way. The presentation below is the modification of that in [12] to the nonlinear case.

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 $\phi_1, ..., \phi_{\bar{m}}$, assumed to be continuous and to satisfy

$$\phi_i \geq 0 \quad (i = 1, \dots, \bar{m}), \qquad \sum_{i=1}^{\bar{m}} \phi_i \equiv 1, \tag{9}$$

further, that there exist node points $P_i \in \overline{\Omega}$ $(i = 1, \dots, \bar{m})$ such that

$$\phi_i(P_j) = \delta_{ij}, \tag{10}$$

where δ_{ij} is the Kronecker symbol. (These conditions hold e.g. for standard linear, bilinear or prismatic FEM.) Let V_h denote the finite element subspace spanned by the above basis functions:

$$V_h = \text{span}\{\phi_1, ..., \phi_{\bar{m}}\} \ \subset H^1(\Omega).$$

Now, let $m < \bar{m}$ be such that

$$P_1, ..., P_m \tag{11}$$

are the vertices that lie in Ω or on Γ_N, and let

$$P_{m+1}, ..., P_{\bar{m}} \tag{12}$$

be the vertices that lie on $\overline{\Gamma}_D$. Then the basis functions $\phi_1, ..., \phi_m$ satisfy the homogeneous Dirichlet boundary condition on Γ_D, i.e., $\phi_i \in H^1_D(\Omega)$. We define

$$V_h^0 = \text{span}\{\phi_1, ..., \phi_m\} \ \subset H^1_D(\Omega).$$

Then the semidiscrete problem for (7) with initial-boundary conditions (8) reads as follows: find a function $u_h = u_h(x,t)$ such that

$$u_h(x,0) = u_0^h(x), \quad x \in \Omega,$$

$$u_h(.,t) - g_h(.,t) \in V_0^h, \quad t \in (0,T),$$

and

$$\int_\Omega \frac{\partial u_h}{\partial t} v_h \, dx + \int_\Omega \Big(k(x,t,u_h,\nabla u_h) \nabla u_h \cdot \nabla v_h + q(x,t,u_h) v_h \Big) \, dx + \int_{\Gamma_N} s(x,t,u_h) v_h \, d\sigma$$

$$= \int_\Omega f v_h \, dx + \int_{\Gamma_N} \gamma v \, d\sigma \qquad (\forall v_h \in V_0^h, \quad t \in (0,T).) \tag{13}$$

In the above formulae, the functions u_0^h and $g_h(.,t)$ (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 g_h:

$$g_h(x,t) = \sum_{i=1}^{m_\partial} g_i^h(t) \phi_{m+i}(x), \tag{14}$$

where

$$m_\partial := \bar{m} - m.$$

We note that, based on the consistency of the initial and boundary conditions ($g(s, 0) = u_0(s), s \in \partial\Omega$), we obtain

$$g(P_{m+i}, 0) = u_0(P_{m+i}), \quad i = 1, \ldots, m_\partial.$$

We seek the numerical solution in the form

$$u_h(x,t) = \sum_{i=1}^{m} u_i^h(t)\phi_i(x) + g_h(x,t) \tag{15}$$

and notice that it is sufficient that u_h satisfies (13) for $v_h = \phi_i$, $i = 1, 2, \ldots, m$, only. Then, introducing the notation

$$\mathbf{u}^h(t) = [u_1^h(t), \ldots, u_m^h(t), g_1^h(t), \ldots, g_{m_\partial}^h(t)]^T, \tag{16}$$

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

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{G}(\mathbf{u}^h(t)) = \mathbf{f}(t), \tag{17}$$

$$\mathbf{u}^h(0) = \mathbf{u}_0^h = [u_0(P_1), \ldots, u_0(P_m), g_1^h(0), \ldots, g_{m_\partial}^h(0)]^T, \tag{18}$$

where

$$\mathbf{M} = [M_{ij}]_{m\times\bar{m}}, \quad M_{ij} = \int_\Omega \phi_j(x)\phi_i(x)\,dx, \tag{19}$$

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

$$G(\mathbf{u}^h(t))_i = \int\limits_\Omega \Big(k(x,t,u_h,\nabla u_h)\nabla u_h\cdot\nabla\phi_i + q(x,t,u_h)\phi_i\Big)\,dx + \int_{\Gamma_N} s(x,t,u_h)\phi_i\,d\sigma(x)\,,$$

$$\mathbf{f}(t) = [f_i(t)]_{i=1,\ldots,m}, \quad f_i(t) = \int_\Omega f(x,t)\phi_i(x)\,dx + \int_{\Gamma_N} \gamma(x,t)\phi_i(x)\,d\sigma(x).$$

The solution $\mathbf{u}^h = \mathbf{u}^h(t)$ of problem (17)–(18) is called the semidiscrete solution. Its existence and uniqueness 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 $\mathbf{u}^h(n\Delta t)$ and $\mathbf{f}(n\Delta t)$ by $\mathbf{u}^n$ and $\mathbf{f}^n$ (for $n = 0, 1, 2, \ldots, n_T$, where $n_T\Delta t = T$), respectively. To discretize (17) in time, we apply the so-called θ-method 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 (53). This gives no strong difference, since the presence of $\mathbf{M}$ makes the scheme not explicit even for $\theta = 0$.

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

$$\mathbf{M}\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \theta\mathbf{G}(\mathbf{u}^{n+1}) + (1-\theta)\mathbf{G}(\mathbf{u}^n) = \mathbf{f}^{(n,\theta)} := \theta\mathbf{f}^{n+1} + (1-\theta)\mathbf{f}^n, \quad (20)$$

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

$$\mathbf{M}\mathbf{u}^{n+1} + \theta\Delta t\mathbf{G}(\mathbf{u}^{n+1}) = \mathbf{M}\mathbf{u}^n - (1-\theta)\Delta t\mathbf{G}(\mathbf{u}^n) + \Delta t\, \mathbf{f}^{(n,\theta)} \quad (21)$$

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

$$\mathbf{P}(\mathbf{u}^{n+1}) := \mathbf{M}\mathbf{u}^{n+1} + \theta\Delta t\mathbf{G}(\mathbf{u}^{n+1}), \qquad \mathbf{Q}(\mathbf{u}^n) := \mathbf{M}\mathbf{u}^n - (1-\theta)\Delta t\mathbf{G}(\mathbf{u}^n), \quad (22)$$

respectively. Then, the iteration procedure (21) can be also written as

$$\mathbf{P}(\mathbf{u}^{n+1}) = \mathbf{Q}(\mathbf{u}^n) + \Delta t\, \mathbf{f}^{(n,\theta)}. \quad (23)$$

We note that finding $\mathbf{u}^{n+1}$ in (23) requires the solution of a nonlinear algebraic system. The mass matrix $\mathbf{M}$ is positive definite, and it follows from Assumptions 2.1 that $\mathbf{u} \mapsto \mathbf{G}(\mathbf{u})$ has positive semidefinite derivatives. Therefore, by the definition in (22), the function $\mathbf{u} \mapsto \mathbf{P}(\mathbf{u})$ has regular derivatives. This ensures the unique solvability of (23) and, under standard local Lipschitz conditions on the coefficients, also the convergence of the damped Newton iteration, see e.g. [14].

4 Preliminaries: linear problems and the maximum principle

An important and widely studied special case of (1)–(4) is the linear problem with Dirichlet boundary conditions

$$\frac{\partial u}{\partial t} - k\Delta u + c(x,t)u = f(x,t), \quad (24)$$

$$u = g \quad \text{on} \quad [0,T] \times \partial\Omega, \qquad u|_{t=0} = u_0 \quad \text{in} \quad \Omega \quad (25)$$

where $k > 0$ is constant and $c \geq 0$. If the data and solution are assumed to be sufficiently smooth, then problem (24)–(25) is known to satisfy the *continuous maximum principle*, which important property is a starting point for our study:

$$\begin{aligned}&\min\{0; \min_{\Gamma_{t_1}} u\} + t_1 \min\{0; \min_{Q_{t_1}} f\} \leq u(x,t_1) \leq \\ &\leq \max\{0; \max_{\Gamma_{t_1}} u\} + t_1 \max\{0; \max_{Q_{t_1}} f\}\end{aligned} \quad (26)$$

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 [11], is the *continuous non-negativity preservation principle*: relations $f \geq 0$, $g \geq 0$ and $u_0 \geq 0$ imply

$$u(x, t) \geq 0 \tag{27}$$

for all $(x, t) \in Q_T$.

In the discrete case, the ODE system (17) now becomes a linear system

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{K}\mathbf{u}^h(t) = \mathbf{f}, \tag{28}$$

where $\mathbf{K} = \int\limits_{\Omega} \Big(k\, \nabla\phi_i \cdot \nabla\phi_j + c\phi_i\phi_j\Big)$. The full discretization is

$$\mathbf{M}\frac{\mathbf{u}^{n+1} - \mathbf{u}^n}{\Delta t} + \theta\mathbf{K}\mathbf{u}^{n+1} + (1-\theta)\mathbf{K}\mathbf{u}^n = \mathbf{f}^{(n,\theta)} := \theta\mathbf{f}^{n+1} + (1-\theta)\mathbf{f}^n. \tag{29}$$

Then (22)–(23) can be simplified: introducing the matrices

$$\mathbf{A} := \mathbf{M} + \theta\Delta t\mathbf{K}, \qquad \mathbf{B} := \mathbf{M} - (1-\theta)\Delta t\mathbf{K}, \tag{30}$$

equation (29) can now be rewritten as

$$\mathbf{A}\mathbf{u}^{n+1} = \mathbf{B}\mathbf{u}^n + \Delta t\, \mathbf{f}^{(n,\theta)}. \tag{31}$$

To formulate the discrete maximum principle, let us define the following values:

$$g^n_{min} = \min\{0, g^n_1, \ldots, g^n_{m_\partial}\}, \quad g^n_{max} = \max\{0, g^n_1, \ldots, g^n_{m_\partial}\}, \tag{32}$$

$$u^n_{min} = \min\{0, g^n_{min}, u^n_1, \ldots, u^n_m\}, \quad u^n_{max} = \max\{0, g^n_{max}, u^n_1, \ldots, u^n_m\}, \tag{33}$$

for $n = 0, 1, \ldots, n_T$, and

$$f^{(n,n+1)}_{min} := \inf_{\substack{x\in\Omega,\\ \tau\in(n\Delta t,(n+1)\Delta t)}} f(x,\tau), \qquad f^{(n,n+1)}_{max} := \sup_{\substack{x\in\Omega,\\ \tau\in(n\Delta t,(n+1)\Delta t)}} f(x,\tau), \tag{34}$$

for $n = 0, 1, \ldots, n_T - 1$. If f is only in $L^\infty(\Omega)$, then the above infima and suprema will mean essential infima and suprema, respectively. Then the discrete analogue of the continuous maximum principle (26) can be formulated as follows:

$$\begin{aligned} &\min\{0, g^{(n+1)}_{min}, u^{(n)}_{min}\} + \Delta t \min\{0, f^{(n,n+1)}_{min}\} \leq \\ &u^{n+1}_i \leq \max\{0, g^{(n+1)}_{max}, u^{(n)}_{max}\} + \Delta t \max\{0, f^{(n,n+1)}_{max}\}. \end{aligned} \tag{35}$$

This will be denoted by DMP and it corresponds to the continuous maximum principle for one time-level, i.e., when $t_1 \in [n\Delta t, (n+1)\Delta t]$.

It has been proved that the full discretization of the linear problem satisfies the DMP (35) in the following case:

Theorem 4.1 [17, 12]. *Let the basis functions satisfy (9)–(10), and let the following conditions hold for the matrices (30):*

(i) $A_{ij} \le 0 \quad (i \ne j, \;\; i = 1, ..., m, \; j = 1, ..., \bar{m})$*;*

(ii) $B_{ii} \ge 0 \quad (i = 1, ..., m)$*.*

Then the Galerkin solution of the problem (24)–(25), combined with the θ*-method in the time discretization, satisfies the discrete maximum principle (35).*

We note that in the original form, see e.g. [12, Thm. 6], it is also assumed that $K_{ij} \le 0 \;\; (i \ne j, \;\; i = 1, ..., m, \; j = 1, ..., \bar{m})$. However, now by our assumption $\theta > 0$, using (9) and (19) we have $M_{ij} \ge 0$, hence it follows from assumption (i) and (30) that $K_{ij} = (1/\theta\Delta t)(A_{ij} - M_{ij}) \le 0$.

The above result has been extended recently to mixed boundary value problems [13]. Let the boundary conditions in (25) be replaced by

$$u = g \quad \text{on} \quad [0,T] \times \Gamma_D, \qquad k\, \nabla u \cdot \nu = q \quad \text{on} \quad [0,T] \times \Gamma_N^0, \tag{36}$$
$$k\, \nabla u \cdot \nu + \sigma u = \varrho \quad \text{on} \quad [0,T] \times \Gamma_N^1,$$

where $\sigma > 0$ is constant. If the conditions of Theorem 4.1 hold and $q \le 0$, then

$$u_i^{n+1} \le \; \max\{0, g_{max}^{(n+1)}, u_{max}^{(n)}\} + \Delta t \max\{0, f_{max}^{(n,n+1)}\} + \frac{1}{\theta} \max\{0, \Big(\frac{\varrho}{\sigma}\Big)_{max}^{(n,n+1)}\}. \tag{37}$$

In [13] a constant σ is considered for simplicity, in which case σ is simply a constant factor above and $\varrho_{max}^{(n,n+1)}$ is defined analogously to (34). However, their proof can be rewritten exactly in the same way for a variable coefficient $\sigma = \sigma(x, \tau)$, simply estimating ϱ/σ by its suprema, in which case we have the DMP (37) with

$$\Big(\frac{\varrho}{\sigma}\Big)_{max}^{(n,n+1)} := \sup_{\substack{x \in \Gamma_N^1, \\ \tau \in (n\Delta t, (n+1)\Delta t)}} \frac{\varrho(x,\tau)}{\sigma(x,\tau)}. \tag{38}$$

Remark 4.1 The indices $1, ..., m$ that arise in (33) now correspond to node points in the interior of Ω or on Γ_N, as in (11), and accordingly, the other m_∂ indices involved in $g_{max}^{(n+1)}$ in (37) correspond to the values on Γ_D. That is, whereas the DMP (35) involves the values of g on $\partial\Omega$, the DMP (37) involves the values of g on Γ_D only.

5 The discrete maximum principle for the nonlinear problem

5.1 Reformulation of the problem

We can rewrite problem (7) as follows. Let

$$r(x,t,\xi) := \int_0^1 \frac{\partial q}{\partial \xi}(x,t,\alpha\xi)\, d\alpha, \quad z(x,t,\xi) := \int_0^1 \frac{\partial s}{\partial \xi}(x,t,\alpha\xi)\, d\alpha \tag{39}$$

(for any $x \in \Omega$, $t > 0$, $\xi \in \mathbf{R}$),

$$\hat{f}(x,t) := f(x,t) - q(x,t,0), \qquad \hat{\gamma}(x,t) := \gamma(x,t) - s(x,t,0) \qquad (x \in \Omega,\ t > 0).$$

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

$$q(x,t,\xi) - q(x,t,0) = r(x,t,\xi)\,\xi, \qquad s(x,t,\xi) - s(x,t,0) = z(x,t,\xi)\,\xi.$$

Subtracting $q(x,t,0)$ and $s(x,t,0)$ from (1) and (3), respectively, we thus obtain that problem (7) is equivalent to

$$\int_\Omega \frac{\partial u}{\partial t} v\,dx + B(u;u,v) = \int_\Omega \hat{f} v\,dx + \int_{\Gamma_N} \hat{\gamma} v\,d\sigma \qquad (\forall v \in H^1_D(\Omega), \quad t \in (0,T)), \tag{40}$$

where

$$B(w;u,v) := \int_\Omega \Big(k(x,t,w,\nabla w)\nabla u \cdot \nabla v + r(x,t,w)uv\Big)\,dx + \int_{\Gamma_N} z(x,t,w)uv\,d\sigma \tag{41}$$

$(w, u, v \in H^1_D(\Omega))$.

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

$$u_h(x,0) = u^h_0(x), \quad x \in \Omega,$$

$$u_h(.,t) - g_h(.,t) \in V^h_0, \quad t \in (0,T),$$

and

$$\int_\Omega \frac{\partial u_h}{\partial t} v_h\,dx + B(u_h;u_h,v_h) = \int_\Omega \hat{f} v_h\,dx + \int_{\Gamma_N} \hat{\gamma} v_h\,d\sigma \quad (\forall v_h \in V^h_0, \quad t \in (0,T)).$$

Proceeding as in (15)–(17), the Cauchy problem for the system of ordinary differential equations (17) takes the following form:

$$\mathbf{M}\frac{\mathrm{d}\mathbf{u}^h}{\mathrm{d}t} + \mathbf{K}(\mathbf{u}^h)\mathbf{u}^h = \hat{\mathbf{f}}, \tag{42}$$

$$\mathbf{u}^h(0) = \mathbf{u}^h_0 = [u_0(P_1), \ldots, u_0(P_m), g^h_1(0), \ldots, g^h_{m_\partial}(0)]^T, \tag{43}$$

where $\mathbf{M}$ is as in (17),

$$\mathbf{K}(\mathbf{u}^h) = [K(\mathbf{u}^h)_{ij}]_{m\times\bar{m}}\ , \quad K(\mathbf{u}^h)_{ij} = B(u_h;\phi_j,\phi_i),$$

$$\hat{\mathbf{f}}(t) = [\hat{f}_i(t)]_{i=1,\ldots,m}, \quad \hat{f}_i(t) = \int_\Omega \hat{f}(x,t)\phi_i(x)\,dx + \int_{\Gamma_N} \hat{\gamma}(x,t)\phi_i(x)\,d\sigma(x). \tag{44}$$

The full discretization reads as

$$\mathbf{M}\mathbf{u}^{n+1} + \theta\Delta t\mathbf{K}(\mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^n - (1-\theta)\Delta t\mathbf{K}(\mathbf{u}^n)\mathbf{u}^n + \Delta t\,\hat{\mathbf{f}}^{(n,\theta)}. \tag{45}$$

Since we have set $\mathbf{G}(\mathbf{u}^h) = \mathbf{K}(\mathbf{u}^h)\mathbf{u}^h$ in (17), the expressions (22)–(23) become

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

respectively. Then, letting

$$\mathbf{A}(\mathbf{u}^h) := \mathbf{M}+\theta\Delta t\mathbf{K}(\mathbf{u}^h), \qquad \mathbf{B}(\mathbf{u}^h) := \mathbf{M}-(1-\theta)\Delta t\mathbf{K}(\mathbf{u}^h) \qquad (\mathbf{u}^h \in \mathbf{R}^{\bar{m}}), \tag{46}$$

the iteration procedure (45) takes the form

$$\mathbf{A}(\mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{B}(\mathbf{u}^n)\mathbf{u}^n + \Delta t\,\hat{\mathbf{f}}^{(n,\theta)}, \tag{47}$$

which is similar to (31), 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 (A4), i.e. we have

Assumption (A4'): there exist constants $\alpha_1, \alpha_2 \geq 0$ such that for any $x \in \Omega$ (or $x \in \Gamma_N$, resp.), $t \in (0,T)$ and $\xi \in \mathbf{R}$,

$$0 \leq \frac{\partial q(x,t,\xi)}{\partial \xi} \leq \alpha_1, \qquad 0 \leq \frac{\partial s(x,t,\xi)}{\partial \xi} \leq \alpha_2. \tag{48}$$

In what follows, we will need the standard notion of (patch-)regularity of the considered meshes (cf. [3]).

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 *regular* if there exist constants $c_0, c_1 > 0$ such that for any $h > 0$ and basis function ϕ_p,

$$c_1 h^d \leq meas(\operatorname{supp}\phi_p), \quad diam(\operatorname{supp}\phi_p) \leq c_0 h \tag{49}$$

(where *meas* denotes d-dimensional measure and *supp* denotes the support, i.e. the closure of the set where the function does not vanish).

Note that the upper bound in (49) implies the following estimates for the corresponding supports and their boundaries:

$$meas(\operatorname{supp}\phi_p) \leq c_2 h^d \quad \text{and} \quad meas\big(\partial\big(\operatorname{supp}\phi_p\big)\big) \leq c_2 h^{d-1}. \tag{50}$$

Theorem 5.1 *Let problem (1)–(4) satisfy Assumptions 2.1, such that we let $p_1 = p_2 = 2$ in (6), i.e. (A4) reduces to assumption (A4') above. us consider a family of finite element subspaces $\mathcal{V} = \{V_h\}_{h\to 0}$ such that the basis functions satisfy (9)–(10), and the family of associated FE meshes is regular as in Definition 5.1. Let the following assumptions hold:*

(i) for any $i = 1, ..., m,\ j = 1, ..., \bar{m}\ (i \neq j),$ if $meas(\operatorname{supp}\phi_i \cap \operatorname{supp}\phi_j) > 0$ then

$$\nabla\phi_i \cdot \nabla\phi_j \leq 0 \quad on\ \Omega \quad and \quad \int_\Omega \nabla\phi_i \cdot \nabla\phi_j \leq -K_0\, h^{d-2} \tag{51}$$

with some constant $K_0 > 0$ independent of i, j and h;

(ii) the mesh parameter h satisfies

$$h < h_0 := \frac{2\mu_0 K_0}{c_2\alpha_2 + \sqrt{c_2^2\alpha_2^2 + 4\mu_0 K_0 c_2 \alpha_1}}; \tag{52}$$

(iii) we have

$$\Delta t \geq \frac{c_2 h^2}{\theta\big(\mu_0 K_0 - \alpha_1 c_2 h^2 - \alpha_2 c_2 h\big)}\,; \tag{53}$$

(iv) if $\theta < 1$ then

$$\Delta t \leq \frac{1}{(1-\theta)\, R(h)}, \tag{54}$$

where

$$R(h) := \max_{i=1,\ldots,m} \frac{\left[\int\limits_\Omega \Big(\mu_1|\nabla\phi_i|^2 + \alpha_1\phi_i^2\Big) + \int\limits_{\Gamma_N} \alpha_2\,\phi_i^2\right]}{\int_\Omega \phi_i^2}\,. \tag{55}$$

Then for all $\mathbf{u}^h \in \mathbf{R}^{\bar{m}}$, the matrices $\mathbf{A}(\mathbf{u}^h)$ and $\mathbf{B}(\mathbf{u}^h)$, defined in (46), have the following properties:

(1) $A(\mathbf{u}^h)_{ij} \leq 0 \quad (i \neq j,\ \ i = 1, ..., m,\ j = 1, ..., \bar{m})$;

(2) $B(\mathbf{u}^h)_{ii} \geq 0 \quad (i = 1, ..., m)$.

Proof. (1) We have

$$A(\mathbf{u}^h)_{ij} := M_{ij} + \theta\Delta t K(\mathbf{u}^h)_{ij} = \int_\Omega \phi_j\phi_i \ +\ \theta\Delta t B(u_h;\phi_j,\phi_i) \tag{56}$$

$$= \int_\Omega \phi_j\phi_i + \theta\Delta t\left[\int\limits_\Omega \Big(k(x,t,u_h,\nabla u_h)\nabla\phi_j\cdot\nabla\phi_i + r(x,t,u_h)\phi_j\phi_i\Big) + \int\limits_{\Gamma_N} z(x,t,u_h)\phi_j\phi_i\right].$$

Let $\Omega_{ij} := \operatorname{supp}\phi_i \cap \operatorname{supp}\phi_j$ and $\Gamma_{ij} := \partial\Omega_{ij}$. Here, by (9) and (50),

$$\int_\Omega \phi_j\phi_i \leq meas(\Omega_{ij}) \leq c_2 h^d \quad \text{and} \quad \int_{\Gamma_N} \phi_j\phi_i \leq meas(\Gamma_{ij}) \leq c_2 h^{d-1}, \tag{57}$$

and similarly,

$$\int_\Omega r(x,t,u_h)\phi_j\phi_i \leq \alpha_1 c_2 h^d, \qquad \int\limits_{\Gamma_N} z(x,t,u_h)\phi_j\phi_i \leq \alpha_2 c_2 h^{d-1} \tag{58}$$

since by (39), r and z inherit (48). By (5) and (51),

$$\int_\Omega k(x,t,u_h,\nabla u_h)\nabla\phi_j\cdot\nabla\phi_i \le -\mu_0 K_0\, h^{d-2}\,. \tag{59}$$

Altogether, we obtain

$$A(\mathbf{u}^h)_{ij} \le c_2 h^d \left[1+\ \theta\Delta t\left(-\frac{\mu_0 K_0}{c_2}\,\frac{1}{h^2}\ +\alpha_1+\frac{\alpha_2}{h}\right)\right]\,.$$

Since $h<h_0$ for h_0 defined in (52), it readily follows that we have a negative coefficient of $\theta\Delta t$ above, and from (53) we obtain that the expression in the large brackets is nonpositive, hence $A(\mathbf{u}^h)_{ij}\le 0$.

(2) Analogously to (56), we have

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

if and only if

$$\int_\Omega \phi_i^2 \ge\ (1{-}\theta)\Delta t\left[\int_\Omega\Big(k(x,t,u_h,\nabla u_h)|\nabla\phi_i|^2 + r(x,t,u_h)\phi_i^2\Big) + \int_{\Gamma_N} z(x,t,u_h)\,\phi_i^2\right]\,.$$

The latter holds for all Δt if

$$\theta = 1$$

(i.e. the scheme is implicit), and for all Δt that satisfies (55) if $\theta<1$. ■

Now we can derive the corresponding *discrete maximum principle:*

Corollary 5.1 *Let the conditions of Theorem 5.1 hold, and let* $\hat\gamma(x,t) := \gamma(x,t)-s(x,t,0)\le 0$. *Then*

$$u_i^{n+1} \le\ \max\{0, g_{max}^{(n+1)}, u_{max}^{(n)}\} + \Delta t\max\{0,\hat f_{max}^{(n,n+1)}\}. \tag{60}$$

PROOF. Our reformulated problem has the right-hand side $\hat f(x,t) := f(x,t)-q(x,t,0)$, which is in $L^\infty(Q_T)$ by Assumption 2.1 (A2). Further, by (40)–(41), we have the Neumann boundary condition

$$k(x,t,u,\nabla u)\,\nabla u\cdot\nu + z(x,t,u)u = \hat\gamma(x,t) \qquad \text{on}\ \ \Gamma_N,$$

where $z\ge 0$ and $\hat\gamma\le 0$. We can rewrite our boundary conditions to match (36): let Γ_N^0 and Γ_N^1 be the portions where $z\equiv 0$ and $z>0$, respectively. Then, by assumption, $q := \hat\gamma_{|\Gamma_N^0}\le 0$ and $\varrho := \hat\gamma_{|\Gamma_N^1}\le 0$. Therefore (37) can be applied (with $\hat f$) and its last term can be dropped, whence we obtain (60). ■

Remark 5.1 Note that the DMP (60) involves the values of g on Γ_D, see also Remark 4.1. Besides that, (60) is formally identical to the upper part of (35), and could in fact be derived from it directly as an alternate proof. Namely, one can apply Theorem 4.1 as an algebraic result for the ODE system (42). Here $\mathbf{f}$ is replaced by $\hat{\mathbf{f}}$ that also involves the values of $\hat{\gamma}$, see (44). However, by our assumption $\hat{\gamma} \leq 0$, we obtain a further upper bound by dropping the integrals with $\hat{\gamma}$, and we are thus led to (60).

Remark 5.2 *(Discussion of the assumptions in Theorem 5.1.)*

(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 contains given or computable constants from the assumptions on the coefficients, the mesh regularity and geometry.

(iii) The lower bound in (53) is asymptotically

$$\Delta t \geq O(h^2) \tag{61}$$

as $h \longrightarrow 0$, and the constants are similarly computable.

(iv) If $\theta = 1$, i.e. the scheme is implicit, then there is no upper restriction on Δt. If $\theta < 1$, then it can be often proved (e.g. for popular simplicial, bilinear and prismatic elements) that $R(h) = O(h^{-2})$ in (55), hence $\Delta t \geq O(h^2)$ as $h \longrightarrow 0$, which yields with (61) the usual condition

$$\Delta t = O(h^2) \tag{62}$$

(as $h \longrightarrow 0$) for the space and time discretizations. In addition, the lower bound in (53) must be smaller than the upper bound in (54): in view of the factor $1-\theta$ in the latter, this gives a restriction on θ to be close enough to 1.

Remark 5.3 Let us consider problem (1)–(4) with principal parts only, i.e. when $q \equiv s \equiv 0$:

$$\frac{\partial u}{\partial t} - \operatorname{div}\Big(k(x,t,u,\nabla u)\nabla u\Big) = f(x,t) \quad \text{in} \quad Q_T := \Omega \times (0,T),$$

$$u(x,t) = g(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T],$$

$$k(x,t,u,\nabla u)\tfrac{\partial u}{\partial \nu} = \gamma(x,t) \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T],$$

$$u(x,0) = u_0(x) \quad \text{for} \quad x \in \Omega,$$

Then Assumptions (ii)-(iv) of Theorem 5.1 become much simplified, since $\alpha_1 = \alpha_2 = 0$. Namely, assumption (ii) is dropped since formally $h_0 = \infty$, i.e. there is no upper bound on h. Assumptions (iii)-(iv) read as follows:

$$\Delta t \geq \frac{c_2}{\theta \mu_0 K_0} h^2; \qquad \text{if} \ \ \theta < 1 \ \ \text{then} \quad \Delta t \leq \frac{1}{\mu_1 (1-\theta)} \min_{i=1,\dots,m} \frac{\int_\Omega \phi_i^2}{\int\limits_\Omega |\nabla \phi_i|^2} \,. \tag{63}$$

Let us now return to the statement (60). By reversing signs in Corollary 5.1, we obtain the corresponding discrete minimum principle:

Corollary 5.2 *Let the conditions of Theorem 5.1 hold, and let* $\hat{\gamma}(x,t) := \gamma(x,t) - s(x,t,0) \geq 0$. *Then*

$$u_i^{n+1} \geq \min\{0, g_{min}^{(n+1)}, u_{min}^{(n)}\} + \Delta t \min\{0, \hat{f}_{min}^{(n,n+1)}\}. \tag{64}$$

An important special case is the discrete *nonnegativity preservation principle*, the discrete analogue of (27):

Theorem 5.2 *Let the conditions of Theorem 5.1 hold, and let* $\hat{f} \geq 0$, $g \geq 0$, $\hat{\gamma} \geq 0$ *and* $u_0 \geq 0$. *Then the discrete solution satisfies*

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

Proof. Assumptions $\hat{f} \geq 0$, $g \geq 0$ and $\hat{\gamma} \geq 0$ imply $g_{min}^{(n+1)} \geq 0$ and $\hat{f}_{min}^{(n,n+1)}$ for all n and i, hence (64) becomes

$$u_i^{n+1} \geq \min\{0, u_{min}^{(n)}\}.$$

Here assumption $u_0 \geq 0$ implies $u_{min}^{(0)} \geq 0$, hence we obtain by induction that $u_{min}^{(n)} \geq 0$ for all n. ■

By Theorem 5.2, u^h is nonnegative in each node point. Properties (9)–(10) of the basis functions imply that the FEM solution $u^h(., n\Delta t)$ is also nonnegative for all time levels $n\Delta t$. 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 discrete solution satisfies

$$u^h \geq 0 \quad \text{on} \quad Q_T.$$

5.3 The DMP: problems with superlinear growth

In this subsection we allow stronger growth of the nonlinearities q and s than in the above, i.e. we return to Assumption 2.1 (A4). For this we need some extra technical assumptions and results.

Let us first summarize the additional conditions.

Assumptions 5.3.

(B1) We restrict ourselves to the case of implicit scheme:

$$\theta = 1.$$

(B2) V_h is made by linear , bilinear or prismatic elements.

(B3) The coefficient on Γ_N satisfies $\hat{\gamma}(x,t) := \gamma(x,t) - s(x,t,0) \equiv 0$, further, $\Gamma_D \neq \emptyset$.

(B4) The exact solution satisfies $u(.,t) \in W^{1,q}(\Omega)$ for some $q > 2$ (if $d = 2$) or some $q \geq 2d/(d-(d-2)(p_1-2))$ (if $d \geq 3$) for all $t \in [0,T]$.

(B5) The discretization satisfies $M_{p_1} := \sup_{t\in[0,T]} \|u(.,t) - u_h(.,t)\|_{L^{p_1}(\Omega)} < \infty$.

Now, by [1], under Assumption 2.1 (A4), we recall the Sobolev embedding estimates

$$\|v\|_{L^{p_1}(\Omega)} \leq C_{\Omega,p_1}\|v\|_{H^1_D}, \quad \|v\|_{L^{p_2}(\Gamma_N)} \leq C_{\Gamma_N,p_2}\|v\|_{H^1_D} \quad (\forall v \in H^1_D(\Omega)) \tag{65}$$

with some constants $C_{\Omega,p_1}, C_{\Gamma_N,p_2} > 0$ independent of v.

Lemma 5.1 *Let V_h be made by linear , bilinear or prismatic elements. Then there exists a constant $c_{p_2} > 0$ such that*

$$\|v\|_{L^{p_2}(\Gamma_N)} \leq c_{p_2} h^{-1}\|v\|_{L^2(\Omega)} \qquad (v \in V_h). \tag{66}$$

Proof. We have

$$\|v\|^2_{H^1_D} := \int_\Omega |\nabla v|^2 \leq \int_\Omega v^2 \max_{v\in V_h} \frac{\int_\Omega |\nabla v|^2}{\int_\Omega v^2} \leq const. \cdot R(h) \int_\Omega v^2 \,,$$

where $R(h)$ comes from (55) and, as seen before, satisfies $R(h) = O(h^{-2})$. This, combined with (65), yields the required estimate. ■

Now we consider the full discretization (45) for $\theta = 1$:

$$\mathbf{M}\mathbf{u}^{n+1} + \Delta t\mathbf{K}(\mathbf{u}^{n+1})\mathbf{u}^{n+1} = \mathbf{M}\mathbf{u}^n + \Delta t\, \hat{\mathbf{f}}^{(n)}. \tag{67}$$

Let $u^{n+1} \in V_h$ denote the function with coefficient vector $\mathbf{u}^{n+1}$, and let $f^n(x) := f(x, n\Delta t)$. Then, by the definition of the mass and stiffness matrices, (67) implies

$$\int_\Omega u^{n+1}v + \Delta t\, B(u^{n+1}; u^{n+1}, v) = \int_\Omega u^n v + \Delta t\Big(\int_\Omega \hat{f}^n v + \int_{\Gamma_N} \hat{\gamma}^n v\Big) \qquad (v \in V_h). \tag{68}$$

Here, by assumption (B3), the integral on Γ_N vanishes, further, recall that $\hat{f} \in L^\infty(Q_T)$ by Assumption 2.1 (A2).

Lemma 5.2 *If Assumptions 5.3 hold, then for all $t \in [0,T]$*

$$\|u(.,t)\|_{L^{p_1}(\Omega)} \leq \|u^0\|_{L^{p_1}(\Omega)} + T(meas(\Omega))^{\frac{1}{p_1}}\|\hat{f}\|_{L^\infty(Q_T)} \,,$$

wherein the r.h.s. is independent of t.

Proof. Let $v = |u|^{p_1-2}u$, which satisfies $\nabla v = (p_1-1)|u|^{p_1-2}\nabla u$. By assumption (B4), $|\nabla u| \in L^q(\Omega)$, and it is easy to see from the condition on q that $|u|^{p_1-2} \in L^{q'}(\Omega)$ where $(1/q)+(1/q') = 1/2$; these imply by Hölder's inequality that $|\nabla v| \in L^2(\Omega)$. That is, for all fixed t we have $v(.,t) \in H^1_D(\Omega)$, hence we can set it in (40):

$$\int_\Omega \frac{\partial u}{\partial t}\Big(|u|^{p_1-2}u\Big)\,dx + B(u;u,|u|^{p_1-2}u) = \int_\Omega \hat{f}|u|^{p_1-2}u\,dx \qquad (\forall v \in H^1_D(\Omega), \quad t\in(0,T)), \tag{69}$$

where we have used $\hat{\gamma} \equiv 0$. Let

$$N(t) := \|u(.,t)\|^{p_1}_{L^{p_1}(\Omega)} = \int_\Omega |u(x,t)|^{p_1}\,dx\,,$$

then $N'(t) = \int_\Omega p_1\,|u|^{p_1-2}u\,\frac{\partial u}{\partial t}\,dx$. Further, using (41) and that $\nabla v = (p_1 - 1)|u|^{p_1-2}\nabla u$, we obtain

$$B(u;u,|u|^{p_1-2}u) = \int_\Omega \Big(k(x,t,u,\nabla u)(p_1-1)|u|^{p_1-2}|\nabla u|^2$$

$$+r(x,t,u)|u|^{p_1}\Big)\,dx + \int_{\Gamma_N} z(x,t,u)|u|^{p_1}\,d\sigma \geq 0$$

hence the left-hand side of (69) is estimated below by $N'(t)/p_1$. Using Hölder's inequality for the right-hand side of (69), we then obtain

$$\frac{1}{p_1}N'(t) \leq \|\hat{f}(.,t)\|_{L^{p_1}(\Omega)}\|u(.,t)\|^{p_1-1}_{L^{p_1}(\Omega)} \leq (meas(\Omega))^{\frac{1}{p_1}}\|\hat{f}\|_{L^\infty(Q_T)}\,N(t)^{\frac{p_1-1}{p_1}}\,.$$

Excluding the trivial case $u \equiv 0$, we can divide by $N(t)^{\frac{p_1-1}{p_1}}$ and integrate from 0 to t to obtain

$$N(t)^{\frac{1}{p_1}} - N(0)^{\frac{1}{p_1}} \leq T(meas(\Omega))^{\frac{1}{p_1}}\|\hat{f}\|_{L^\infty(Q_T)},$$

which is the desired estimate. ■

Lemma 5.3 *(1) If Assumptions 5.3 (B1) and (B3) hold, then the norms $\|u^n\|_{L^2(\Omega)}$ are bounded, independently of n and V_h, by the constant $K_{L_2} := \|u^0\|_{L^2(\Omega)} + T(meas(\Omega))^{\frac{1}{2}}\|\hat{f}\|_{L^\infty(Q_T)}$.*

(2) If all Assumptions 5.3 hold, then the norms $\|u^n\|_{L^{p_1}(\Omega)}$ are bounded, independently of n and V_h, by the constant $K_{p_1,\Omega} := M_{p_1} + \|u^0\|_{L^{p_1}(\Omega)} + T(meas(\Omega))^{\frac{1}{p_1}}\|\hat{f}\|_{L^\infty(Q_T)}$.

PROOF. (1) Setting $v = u^{n+1}$ in (68), we obtain

$$\int_\Omega (u^{n+1})^2 + \Delta t\, B(u^{n+1}; u^{n+1}, u^{n+1}) = \int_\Omega u^n u^{n+1} + \Delta t \int_\Omega \hat{f}^n u^{n+1}. \tag{70}$$

To estimate below, the bilinear form can be dropped from the l.h.s. since it is coercive, and also using Cauchy-Schwarz inequalities, we have

$$\|u^{n+1}\|^2_{L^2(\Omega)} \le \|u^n\|_{L^2(\Omega)} \|u^{n+1}\|_{L^2(\Omega)} + \Delta t \|\hat{f}^n\|_{L^2(\Omega)} \|u^{n+1}\|_{L^2(\Omega)}.$$

Dividing by $\|u^{n+1}\|_{L^2(\Omega)}$ and repeating the argument n times, we obtain

$$\|u^{n+1}\|_{L^2(\Omega)} \le \|u^0\|_{L^2(\Omega)} + (n+1)\Delta t \|\hat{f}^n\|_{L^2(\Omega)},$$

where the r.h.s. is bounded since $(n+1)\Delta t \le T$ and $\|\hat{f}^n\|_{L^2(\Omega)} \le (meas(\Omega))^{\frac{1}{2}} \|\hat{f}\|_{L^\infty(Q_T)}$.

(2) It follows directly from Lemma 5.2 and assumption (B5). ■

Lemmas 5.1 and 5.3 imply

Corollary 5.3 *We have*

$$\|u^n\|_{L^{p_2}(\Gamma_N)} \le K_{p_2,\Gamma_N} h^{-1}$$

where the constant $K_{p_2,\Gamma_N} > 0$ is bounded independently of n and V_h.

Theorem 5.3 *Let problem (1)–(4) 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 family of associated FE meshes is regular as in Definition 5.1. Let the following assumptions hold:*

(i) for any $i = 1, ..., m,\ j = 1, ..., \bar{m}\ (i \ne j)$, if $meas(\operatorname{supp}\phi_i \cap \operatorname{supp}\phi_j) > 0$ then

$$\nabla\phi_i \cdot \nabla\phi_j \le 0 \quad on\ \Omega \quad and \quad \int_\Omega \nabla\phi_i \cdot \nabla\phi_j \le -K_0\, h^{d-2} \tag{71}$$

with some constant $K_0 > 0$ independent of i, j and h;

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

$$-\frac{\mu_0 K_0}{c_2}\frac{1}{h^2} + \alpha_1 + \frac{\alpha_2}{h} + \frac{\beta_1 K_{p_1,\Omega}^{p_1-2}}{h^{\gamma_1}} + \frac{\beta_2 K_{p_2,\Gamma_N}^{p_2-2}}{h^{\gamma_2}} = 0, \tag{72}$$

where the numbers $0 < \gamma_1, \gamma_2 < 2$ are defined below in (74), (75), respectively;

(iii) we have

$$\Delta t \ge \frac{c_2 h^2}{\theta\big(\mu_0 K_0 2 - c_2\alpha_1 h^2 + c_2\alpha_2 h - c_2\beta_1 K_{p_1,\Omega}^{p_1-2} h^{2-\gamma_1} - c_2\beta_2 K_{p_2,\Gamma_N}^{p_2-2} h^{2-\gamma_2}\big)}. \tag{73}$$

Then the matrices $\mathbf{A}(\mathbf{u}^{n+1})$ *and* $\mathbf{B}(\mathbf{u}^n)$*, defined in (46)–(47), have the following properties:*

(1) $A(\mathbf{u}^{n+1})_{ij} \le 0 \qquad (i \ne j,\;\; i = 1, ..., m,\; j = 1, ..., \bar{m})$*;*

(2) $B(\mathbf{u}^n)_{ii} \ge 0 \qquad (i = 1, ..., m)$*.*

PROOF. We follow the proof of Theorem 5.1. As a first difference, 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.

(1) Since we now have (6) instead of (48), the first estimate in (58) is replaced by

$$\int_\Omega r(x,t,u^{n+1})\phi_j\phi_i \le \int_\Omega \big(\alpha_1 + \beta_1 |u^{n+1}|^{p_1-2}\big)\phi_j\phi_i \le \alpha_1 meas(\Omega_{ij}) + \beta_1 \int_{\Omega_{ij}} |u^{n+1}|^{p_1-2}\,.$$

Here the first term is bounded by $\alpha_1 c_2 h^d$ as before. To estimate the second term, we use Hölder's inequality:

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

For the first factor, we use Lemma 5.3 (2) to find that

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

The second factor satisfies, by (57),

$$\|1\|^2_{L^{p_1}(\Omega_{ij})} = \big(meas(\Omega_{ij})\big)^{2/p_1} \le c_2 h^{\frac{2d}{p_1}} \equiv c_2 h^{d-\gamma_1}$$

with

$$\gamma_1 := d - \frac{2d}{p_1} < 2, \tag{74}$$

since from Assumption 2.1 (A4) we have $\frac{2d}{p_1} > d - 2$. Hence

$$\int_{\Omega_{ij}} |u^{n+1}|^{p_1-2} \le K^{p_1-2}_{p_1,\Omega} c_2 h^{d-\gamma_1}$$

and altogether,

$$\int_\Omega r(x,t,u^{n+1})\phi_j\phi_i \le \alpha_1 c_2 h^d + \beta_1 K^{p_1-2}_{p_1,\Omega} c_2 h^{d-\gamma_1}\,.$$

Similarly,

$$\int_{\Gamma_N} z(x,t,u^{n+1})\phi_j\phi_i \le \alpha_2 c_2 h^{d-1} + \beta_2 \int_{\Gamma_{ij}} |u^{n+1}|^{p_2-2}$$

and here, for $d = 2, 3$ we use Corollary 5.3 and (50) to have

$$\int_{\Gamma_{ij}} |u^{n+1}|^{p_2-2} \leq \|u^{n+1}\|^{p_2-2}_{L^{p_2}(\Gamma_{ij})} \|1\|^2_{L^{p_2}(\Gamma_{ij})} \leq \|u^{n+1}\|^{p_2-2}_{L^{p_2}(\Gamma_N)} \big(meas(\Gamma_{ij})\big)^{2/p_2}$$

$$\leq K^{p_2-2}_{p_2,\Gamma_N} c_2 h^{2-p_2+\frac{2(d-1)}{p_2}} \equiv K^{p_2-2}_{p_2,\Gamma_N} c_2 h^{d-\gamma_2},$$

where

$$\gamma_2 := d - 2 + p_2 - \frac{2(d-1)}{p_2} < 2 \tag{75}$$

from assumption $p_2 \leq 2.5$. Summing up, using the above and (59), we obtain

$$A(\mathbf{u}^h)_{ij} \leq c_2 h^d \left[1 + \ \theta \Delta t \left(-\frac{\mu_0 K_0}{c_2} \frac{1}{h^2} + \alpha_1 + \frac{\alpha_2}{h} + \frac{\beta_1 K^{p_1-2}_{p_1,\Omega}}{h^{\gamma_1}} + \frac{\beta_2 K^{p_2-2}_{p_2,\Gamma_N}}{h^{\gamma_2}} \right) \right].$$

Since $h < h_0$ for h_0 defined in (72), it follows that we have a negative coefficient of $\theta\Delta t$ above, and from (73) we obtain that the expression in the large brackets is nonpositive, hence $A(\mathbf{u}^h)_{ij} \leq 0$.

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

Similarly to the sublinear case, we can derive the corresponding discrete maximum, minimum and nonnegativity preservation principles. We only formulate here the latter:

Corollary 5.4 *Let the conditions of Theorem 5.3 hold, and let $\hat{f} \geq 0$, $g \geq 0$, $\hat{\gamma} \geq 0$ and $u_0 \geq 0$. Then the discrete solution satisfies*

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

5.4 Geometric properties of the space mesh

In order to satisfy condition (71), the most direct way is to require

$$\nabla\phi_i \cdot \nabla\phi_j \leq -K_0\, h^{-2} \tag{76}$$

pointwise on the common support of these basis functions. In view of well-known formulae (see e.g. [2, 5, 25, 27]), the above condition has a nice geometric interpretation: in the case of simplicial meshes, it is sufficient if the employed mesh is uniformly acute [4, 25]. In the case of bilinear elements, condition (76) is equivalent to the so-called strict non-narrowness of the meshes, see [12, 19]. The case of prismatic finite elements is treated in [18].

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. [24]), or one can require (76) only on a proper subpart of each intersection of supports with asymptotically nonvanishing measure, see more details in [21]. These weaker conditions may allow in general easier refinement procedures.

5.5 Examples

We give two real-life examples where discrete nonnegativity can be derived for suitable discretizations.

(a) Nonlinear heat conduction.

Heat conduction in a body $\Omega \subset \mathbf{R}^3$ with nonlinear diffusion coefficient is often described by the model

$$\frac{\partial u}{\partial t} - \operatorname{div}\Big(k(x,t,u)\nabla u\Big) = f(x,t) \tag{77}$$

in $Q_T := \Omega \times (0,T)$, where $T > 0$ is the time interval considered; see, e.g., [15]. The usual boundary and initial conditions are

$$u(x,t) = g(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T], \tag{78}$$

$$k(x,t,u)\tfrac{\partial u}{\partial \nu} = \gamma(x,t) \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T], \tag{79}$$

$$u(x,0) = u_0(x) \quad \text{for} \quad x \in \Omega, \tag{80}$$

where all coefficients are bounded nonnegative measurable functions and k has a positive lower bound. The function u describes the temperature, hence $u \geq 0$.

(b) Reaction-diffusion problems.

A reaction-diffusion process in a body $\Omega \subset \mathbf{R}^d$, $d = 2$ or 3, is often described by the model

$$\frac{\partial u}{\partial t} - \operatorname{div}\Big(k(x,t)\nabla u\Big) + q(x,u) = f(x,t) \tag{81}$$

in $Q_T := \Omega \times (0,T)$. The boundary and initial conditions are

$$u(x,t) = g(x,t) \quad \text{for} \quad (x,t) \in \Gamma_D \times [0,T], \tag{82}$$

$$k(x,t)\tfrac{\partial u}{\partial \nu} + s(x,u) = \gamma(x,t) \quad \text{for} \quad (x,t) \in \Gamma_N \times [0,T], \tag{83}$$

$$u(x,0) = u_0(x) \quad \text{for} \quad x \in \Omega, \tag{84}$$

The function u describes the temperature, hence

$$u \geq 0.$$

Here the coefficients k, f, g, γ and u_0 are bounded nonnegative measurable functions and k has a positive lower bound. Further, q and s desribe the rate of reaction in the body and on the transmission boundary, respectively, hence $q(x,0) = s(x,0) = 0$ for all x. In various examples the reaction process is such that q and s grow along with u, further, the rate is at most polynomial, i.e. we may assume that the growth conditions (6) are satisfied. For instance, $q(x,u) = u^\sigma$ for some $\sigma > 1$ in some autocatalytic chemical reactions, or

$q(x,u) = \frac{1}{\varepsilon}\frac{u}{u+\kappa}$ describes the Michaelis-Menten reaction in enzyme kynetics [6, 23].

In both examples, we have $\hat{f} = f \geq 0, \quad g \geq 0, \quad \hat{\gamma} = \gamma \geq 0$ and $u_0 \geq 0$. Therefore we can use Theorem 5.2 and Corollary 5.4, respectively, to derive the discrete nonnegativity principle:

Theorem 5.4 *Let the full discretization satisfy the conditions of Theorem 5.1 for problem (77)–(80), or the conditions of Theorem 5.3 for problem (81)–(84). Then the discrete solution satisfies*

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

In particular, for problem (77)–(80) we can use the simplified assumptions (63) for Theorem 5.1, as given in Remark 5.3.

Consequently, as pointed out after Theorem 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 the discrete solution satisfies

$$u^h \geq 0 \quad \text{on} \quad Q_T.$$

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