A POSTERIORI ERROR ESTIMATION FOR PARABOLIC PROBLEMS USING ELLIPTIC RECONSTRUCTIONS. I: BACKWARD-EULER AND CRANK-NICOLSON METHODS*

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Abstract. A semilinear second-order parabolic equation is considered in a regular and a singularly-perturbed regime. For this equation, we give computable a posteriori error estimates in the maximum norm. Fully discrete Bakward-Euler and Crank-Nicolson methods are addressed, for which we employ elliptic reconstructions that are, respectively, piecewise-constant and piecewise-linear in time. We also use certain bounds for the Green's function of the parabolic operator.

Key words. a posteriori error estimate, maximum norm, singular perturbation, elliptic reconstruction, Backward-Euler, Crank-Nicolson, parabolic equations, reaction-diffusion.

AMS subject classifications. 65M15 , 65M60.

1. Introduction. Consider a semilinear parabolic equation in the form

$$\mathcal{M}u := \partial_t u + \mathcal{L}u + f(x,t,u) = 0 \qquad \text{for} \quad (x,t) \in Q := \Omega \times (0,T], \tag{1.1a}$$

with a second-order linear elliptic operator $\mathcal{L} = \mathcal{L}(t)$ in a spatial domain $\Omega \subset \mathbb{R}^n$ with Lipschitz boundary, subject to the initial and Dirichlet boundary conditions

$$u(x,0) = \varphi(x) \quad \text{for} \quad x \in \bar{\Omega}, \qquad u(x,t) = 0 \quad \text{for} \quad (x,t) \in \partial\Omega \times [0,T]. \tag{1.1b}$$

We assume that f is differentiable in the third argument and, for some positive constants γ and $\bar{\gamma}$, satisfies

$$0 \le \gamma^2 \le \partial_z f(x,t,z) \le \bar{\gamma}^2 \qquad \text{for} \quad (x,t,z) \in \bar{\Omega} \times [0,T] \times \mathbb{R}. \tag{1.2}$$

The purpose of this paper is to obtain computable a posteriori error estimates for fully discrete methods applied to problem (1.1). We consider the first-order Backward-Euler and the second-order Crank-Nicolson discretizations in time. Furthermore, in a forthcoming paper [9], a similar approach will be used to analyze the third-order Discontinuous Galerkin method dG(1).

These results are applied to the model equation with $\mathcal{L} := -\varepsilon^2\triangle = -\varepsilon^2\sum_{i=1}^n \partial_{x_i}^2$:

$$\mathcal{M}u := \partial_t u - \varepsilon^2\triangle u + f(x,t,u) = 0 \tag{1.3}$$

posed in a bounded polyhedral spatial domain $\Omega \subset \mathbb{R}^n$, with $n = 1,2,3$. This equation will be considered in the two regimes:

$$\text{(i)} \quad \varepsilon = 1, \ \ \gamma \ge 0; \qquad\qquad \text{(ii)} \quad \varepsilon \ll 1, \ \ \gamma > 0.$$

Note that regime (ii) yields a singularly perturbed reaction-diffusion equation, whose solutions may exhibit sharp layer phenomena. So it is important in this regime that a posteriori error estimates are robust in the sense that any dependence on the small perturbation parameter ε should be shown explicitly [13, 16].

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We will give error estimates in the *maximum norm*, which is sufficiently strong to capture sharp layers and singularities that may occur, in particular, if problem (1.1) is of singularly-perturbed type. Our estimates will be of *interpolation type* in the sense that they will include certain terms that may be interpreted as approximating $\tau_j^p|\partial_t^p u|$, where p and τ_j are the discretization order and local step size in time, respectively.

We employ the *elliptic reconstruction* technique, which was introduced in the recent papers [14, 11, 3] as a counterpart of the Ritz-projection in the a posteriori error estimation for parabolic problems. We also use certain bounds for the *Green's function* of the continuous parabolic operator in a manner similar to [3], only for a more general semilinear parabolic operator of (1.3) (compared to $\partial_t - \triangle$ in [3]).

One distinctive feature of our analysis in this paper (compared, e.g., to [1, 3]) is that we use computed solutions and elliptic reconstructions that are *piecewise-constant* in time when dealing with the Backward-Euler method, and *piecewise-linear* in time when dealing with the Crank-Nicolson method. Consequently, we allow the residuals of computed solutions, as well as other functions, to be understood as *distributions*; this inclusion plays a crucial role in our analysis.

The paper is organized as follows. In Section 2, we introduce the Green's function and obtain a certain stability lemma, which is then used in Sections 3–4 to obtain a posteriori error estimates for semidiscrete Backward-Euler and Crank-Nicolson methods (with no spatial discretization). Next, in Section 5 we cite some elliptic a posteriori error estimates, which are used in Sections 6–7 to derive a posteriori error estimates for fully discrete Backward-Euler and Crank-Nicolson methods. The final Section 8 gives a proof of certain Green's function bounds deferred from Section 2.

Notation. Throughout the paper, C, as well as c, denotes a generic positive constant that may take different values in different formulas, but is *independent of the diffusion coefficient* ε *and any mesh sizes.* We use $|x|$ for the Euclidian norm of $x \in \mathbb{R}^n$. The usual spaces $C(\bar\Omega)$ and $H_0^1(\Omega)$ are used, as well as the spaces L_p, $1 \le p \le \infty$, with the norm $\|\cdot\|_{p,\Omega}$, while $\langle \phi, \psi \rangle = \int_\Omega \phi(x)\psi(x)\,\mathrm{d}x$ denotes the inner product in $L_2(\Omega)$.

Distributions and left-continuity convention. Certain functions will be understood as distributions [7], which will in most cases be indicated. By contrast, if a certain function is Lebesgue-integrable in $\Omega \times (0,T)$, we shall refer to it as a regular function. Whenever we deal with a regular function, it will be understood right-continuous at $t = 0$ and *left-continuous* for all $t \in (0,T]$. In particular, this convention will be applied to all piecewise-continuous temporal derivatives.

2. The Green's function of the parabolic operator. In this section we consider the Green's function $\mathcal{G}$ associated with the operator $\mathcal{M}$ of (1.1). Our interest in the Green's function is in that it will be used to express the error of a numerical approximation in terms of its residual.

For definitions and properties of fundamental solutions and Green's functions of parabolic operators with variable coefficients, we refer the reader to [6, Chap. 1 and §7 of Chap. 3]. In particular, for fixed $(x,t) \in Q$, the Green's function $\mathcal{G}(x,t;\xi,s) =: \Gamma(\xi,s)$ solves the adjoint terminal-value problem

$$[-\partial_s - \mathcal{L}^* + a(\xi,s)]\,\Gamma(\xi,s) = 0 \qquad \text{for} \quad (\xi,s) \in \Omega \times [0,t), \tag{2.1a}$$

$$\Gamma(\xi,t) = \delta(\xi - x) \quad \text{for} \quad \xi \in \Omega, \tag{2.1b}$$

$$\Gamma(\xi,s) = 0 \qquad \text{for} \quad (\xi,s) \in \partial\Omega \times [0,t]. \tag{2.1c}$$

Here $\delta(\cdot)$ is the Dirac δ-distribution in $\mathbb{R}^n$ [7], and $\mathcal{L}^*$ is the adjoint operator to the linear operator $\mathcal{L}$. We set $a(x,t) := \partial_z f(x,t,z)$ if f is linear in the third argument, i.e.

$f(x,t,z) = a(x,t)z + b(x,t)$. If f is nonlinear, we associate $a(x,t) := \int_0^1 \partial_z f(x,t,w + z[v-w])\,\mathrm{d}z$ with a pair of bounded functions v and w that vanish on $\partial\Omega$. As the standard linearization now yields $\mathcal{M}v - \mathcal{M}w = [\partial_t + \mathcal{L} + a(x,t)](v-w)$, so with the help of this Green's function, the difference $v - w$ is represented as

$$[v-w](x,t) = \int_\Omega \mathcal{G}(x,t;\xi,0)\,[v-w](\xi,0)\,\mathrm{d}\xi + \int_0^t \int_\Omega \mathcal{G}(x,t;\xi,s)\,[\mathcal{M}v - \mathcal{M}w](\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s. \tag{2.2}$$

The analysis in this paper will be carried out under the following condition.

CONDITION 2.1. *There are constants κ_0, $\kappa_1 > 0$ and $\kappa_2 \geq 0$ such that the Green's function $\mathcal{G}$ of (2.1), (1.2) satisfies*

$$\|\mathcal{G}(x,t;\cdot,s)\|_{1,\Omega} \leq \kappa_0\,\mathrm{e}^{-\gamma^2(t-s)}, \qquad \int_0^{t-\tau} \|\partial_s \mathcal{G}(x,t;\cdot,s)\|_{1,\Omega}\,\mathrm{d}s \leq \kappa_1\,\ell(\tau,t) + \kappa_2,$$

where $x \in \Omega$, $\tau \in (0,t]$, $t \in (0,T]$, and $\ell(\tau,t) := \int_\tau^t s^{-1}\mathrm{e}^{-\frac{1}{2}\gamma^2 s}\,\mathrm{d}s \leq \ln(t/\tau)$.

Note that our model problem satisfies this condition as follows.

LEMMA 2.2. *Let $\varepsilon \in (0,1]$ and $\gamma \geq 0$. Under assumption (1.2), the model problem (1.3) satisfies Condition 2.1 with $\kappa_0 := 1$, $\kappa_1 := \frac{3^n}{2^{n/2+1}}$ and an ε-independent constant $\kappa_2 \geq 0$. If $f(x,t,z) = a(x)z + b(x,t)$, then $\kappa_2 = 0$. In general, $\kappa_2 = (\bar\gamma^2 - \gamma^2)\,\hat\kappa_2$, where $\hat\kappa_2 = \hat\kappa_2(\gamma)$ if $\gamma > 0$, and $\hat\kappa_2 = \hat\kappa_2(T)$ if $\gamma = 0$.*

Proof. We defer the proof to Section 8. □

REMARK 2.3. *The constants κ_0 and κ_1 given by Lemma 2.2 are reasonably sharp. E.g., for the constant-coefficient version $\partial_t u - \varepsilon^2\partial_x^2 u + \gamma^2 u = b(x,t)$ of (1.3) in the spatial domain $\Omega := \mathbb{R}$, a calculation yields $\|\mathcal{G}(x,t;\cdot,s)\|_{1,\Omega} = 1$ and $\|\partial_s\mathcal{G}(x,t;\cdot,s)\|_{1,\Omega} \leq \big(\sqrt{\frac{2}{\pi\,\mathrm{e}}}(t-s)^{-1} + \gamma^2\big)\,\mathrm{e}^{-\gamma^2(t-s)}$ so Condition 2.1 is satisfied with $\kappa_0 = 1$ (as in Lemma 2.2), $\kappa_1 = \sqrt{\frac{2}{\pi\,\mathrm{e}}} \approx 0.48$, $\kappa_2 = 1$, while Lemma 2.2 gives $\kappa_1 = \frac{3}{2^{3/2}} \approx 1.06$.*

The above Condition 2.1 will be employed by means of the following lemma, which plays a crucial role in our analysis here and in the forthcoming paper [9]. The lemma is formulated in the context of an arbitrary nonuniform mesh in the time direction

$$0 = t_0 < t_1 < t_2 < \ldots < t_M = T, \quad \text{with } \tau_j = t_j - t_{j-1} \quad \text{for } j = 1,\ldots,M. \tag{2.3}$$

LEMMA 2.4. *Suppose the parabolic operator $\mathcal{M}$ of (1.1) satisfies (1.2) and Condition 2.1, and v, w are bounded in $\bar\Omega \times [0,T]$. Furthermore, let $v(\cdot,t), w(\cdot,t) \in H_0^1(\Omega) \cap C(\bar\Omega)$ for $t \in [0,T]$, and*

$$\mathcal{M}v - \mathcal{M}w = \partial_t \mu + \vartheta \quad \textit{in } Q, \tag{2.4}$$

where the function μ is continuous and bounded on $[t_0,t_1]$ and each $(t_{j-1},t_j]$, while $\partial_t\mu$ is continuous and bounded on $(t_{m-1},t_m]$ for some $1 \leq m \leq M$, and $\|\vartheta(\cdot,s)\|_{\infty,\Omega}$ is integrable on $(0,t_m)$ (possibly, in the sense of distributions). Then

$$\begin{aligned}
&\big\|[v-w](\cdot,t_m)\big\|_{\infty,\Omega} \\
&\quad\leq \kappa_0\mathrm{e}^{-\gamma^2 t_m}\big\|[v-w-\mu](\cdot,0)\big\|_{\infty,\Omega} + (\kappa_1\,\ell_m + \kappa_2)\sup_{s\in[0,t_{m-1}]}\big\|\mu(\cdot,s)\big\|_{\infty,\Omega} \\
&\qquad + \kappa_0 \sup_{s\in(t_{m-1},t_m]}\big\|\mu(\cdot,s)\big\|_{\infty,\Omega} + \kappa_0\,\tau_m \sup_{s\in(t_{m-1},t_m]}\big\|\partial_s\mu(\cdot,s)\big\|_{\infty,\Omega} \\
&\qquad + \kappa_0 \int_0^{t_m} \mathrm{e}^{-\gamma^2(t_m-s)}\,\big\|\vartheta(\cdot,s)\big\|_{\infty,\Omega}\,\mathrm{d}s,
\end{aligned}$$

where $\ell_m = \ell_m(\gamma) := \int_{\tau_m}^{t_m} s^{-1}e^{-\frac{1}{2}\gamma^2 s}\,ds \le \ln(t_m/\tau_m)$.

REMARK 2.5. *The term $\partial_t\mu$ in the right-hand side of (2.4) is understood in the sense of distributions.*

REMARK 2.6. *One can easily check that if $\gamma = 0$, then $\ell_m = \ln(t_m/\tau_m)$. Otherwise, if $\gamma > 0$, one has $\ell_m(\gamma) = E_1(\frac{1}{2}\gamma^2\tau_m) - E_1(\frac{1}{2}\gamma^2 t_m)$, where $E_1(t) = \int_t^\infty s^{-1}e^{-s}\,ds$; so $\ell_m(\gamma) \le |\ln(\frac{1}{2}\gamma^2\tau_m)|$ provided that $\frac{1}{2}\gamma^2\tau_m \le 0.67$ (this is easily checked by finding the only root ≈ 0.67 of the equation $E_1(s) = |\ln s|$ on $(0,1)$). Note also that $\ell_1 = 0$ for any $\gamma \ge 0$.*

Proof. Combining representation (2.2) with the notation $\Gamma(\xi,s) := \mathcal{G}(x,t_m;\xi,s)$ for the Green's function of (2.1), one gets

$$[v-w](x,t_m) = \big\langle [v-w](\cdot,0),\, \Gamma(\cdot,0)\big\rangle + \int_0^{t_m} \big\langle [\mathcal{M}v - \mathcal{M}w](\cdot,s),\, \Gamma(\cdot,s)\big\rangle\,ds.$$

Here, in view of (2.4), the integral on the right-hand side involves μ and ϑ, so can be represented as a sum $J_\mu + J_\vartheta$ of the corresponding integrals, which we consider separately. We use the notation $\int^{b^+} := \lim_{\beta\to 0^+}\int^{b+\beta}$ and so split J_μ as

$$J_\mu = J_\mu^{(1)} + J_\mu^{(2)} := \int_0^{t_{m-1}^+} \big\langle \partial_s\mu, \Gamma(\cdot,s)\big\rangle\,ds + \int_{t_{m-1}^+}^{t_m} \big\langle \partial_s\mu, \Gamma(\cdot,s)\big\rangle\,ds.$$

Here, for $J_\mu^{(1)}$, an integration by parts yields

$$J_\mu^{(1)} = \big\langle \mu(\cdot,t_{m-1}^+), \Gamma(\cdot,t_{m-1})\big\rangle - \big\langle \mu(\cdot,0), \Gamma(\cdot,0)\big\rangle - \int_0^{t_{m-1}} \big\langle \mu(\cdot,s), \partial_s\Gamma(\cdot,s)\big\rangle\,ds.$$

Consequently, we arrive at

$$\begin{aligned}[v-w](x,t_m) = \big\langle [v-w-\mu](\cdot,0),\, \Gamma(\cdot,0)\big\rangle &- \int_0^{t_{m-1}} \big\langle \mu(\cdot,s),\, \partial_s\Gamma(\cdot,s)\big\rangle\,ds\\
&+ \big\langle \mu(\cdot,t_{m-1}^+), \Gamma(\cdot,t_{m-1})\big\rangle + \int_{t_{m-1}^+}^{t_m} \big\langle \partial_s\mu, \Gamma(\cdot,s)\big\rangle\,ds\\
&+ \int_0^{t_m} \big\langle \vartheta(\cdot,s),\, \Gamma(\cdot,s)\big\rangle\,ds,\end{aligned}$$

where the last term represents J_ϑ. Finally, Condition 2.1 implies that

$$\|\Gamma(\cdot,s)\|_{1,\Omega} \le \kappa_0\, e^{-\gamma^2(t_m-s)} \le \kappa_0, \qquad \int_0^{t_{m-1}} \|\partial_s\Gamma(\cdot,s)\|_{1,\Omega}\,ds \le \kappa_1\,\ell_m + \kappa_2,$$

so we get the desired result. ∎

3. Semidiscrete Backward Euler method (no spatial discretization). Consider an arbitrary nonuniform mesh (2.3) in the time direction and discretize the abstract parabolic problem (1.1) in time using the first-order Backward Euler method (also referred to as the implicit Euler method or the Discontinuous Galerkin method dG(0)) as follows. We associate an approximate solution $U^j \in H_0^1(\Omega)\cap C(\bar\Omega)$ with the time level t_j and require it to satisfy

$$\delta_t U^j + \mathcal{L}^j U^j + f^j = 0 \quad \text{in } \Omega, \quad j = 1,\dots,M; \qquad U^0 = \varphi, \tag{3.1a}$$

where

$$\delta_t U^j := \frac{U^j - U^{j-1}}{\tau_j}, \quad \mathcal{L}^j := \mathcal{L}(t_j) \quad \text{and} \quad f^j := f(\cdot, t_j, U^j). \tag{3.1b}$$

For this discretization, we give the following a posteriori error estimate.

THEOREM 3.1. *Let u solve the problem (1.1) with the parabolic operator $\mathcal{M}$ satisfying (1.2) and Condition 2.1, and U^j solve the corresponding semidiscrete problem (3.1). Then, for $m = 1, \dots, M$, one has*

$$\begin{aligned} &\left\| U^m - u(\cdot, t_m) \right\|_{\infty,\Omega} \\ &\quad \le (\kappa_1 \, \ell_m + \kappa_2) \max_{j=1,\dots,m-1} \left\| U^j - U^{j-1} \right\|_{\infty,\Omega} + 2\kappa_0 \left\| U^m - U^{m-1} \right\|_{\infty,\Omega} \\ &\qquad + \kappa_0 \sum_{j=1}^{m} \int_{t_{j-1}}^{t_j} \mathrm{e}^{-\gamma^2 (t_m - s)} \left\| [\vartheta_{\mathcal{L}} + \vartheta_f](\cdot, s) \right\|_{\infty,\Omega} \mathrm{d}s \,, \end{aligned} \tag{3.2}$$

where $\vartheta_{\mathcal{L}}$ and ϑ_f are regular functions defined, for $t \in (t_{j-1}, t_j]$, $j = 1, \dots, M$, by

$$\vartheta_{\mathcal{L}}(\cdot, t) := [\mathcal{L}(t) - \mathcal{L}^j] \, U^j, \qquad \vartheta_f(\cdot, t) := f(\cdot, t, U^j) - f(\cdot, t_j, U^j). \tag{3.3}$$

Proof. Let $I_t U$ be the standard piecewise-linear interpolant of U^j in time:

$$I_t U(\cdot, t) := \tfrac{t_j - t}{\tau_j} \, U^{j-1} + \tfrac{t - t_{j-1}}{\tau_j} \, U^j \qquad \text{for } t \in [t_{j-1}, t_j], \quad j = 1, \dots, M. \tag{3.4}$$

Furthermore, we define a ***piecewise-constant*** interpolant $\tilde{U}$ of U^j by

$$\tilde{U}(\cdot, t) := U^j \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1 \dots, M; \qquad \tilde{U}(\cdot, 0) := U^1, \tag{3.5}$$

(so $\tilde{U}$ is continuous on $[t_0, t_1]$). Note that the temporal derivative $\partial_t \tilde{U}$ is understood as a distribution, while $\partial_t(I_t U)$ is a regular function, equal to $\delta_t U^j$ for $t \in (t_{j-1}, t_j]$ (in agreement with our left-continuity convention). Consequently, (3.1a) implies that

$$\partial_t(I_t U) + \mathcal{L}(t)\tilde{U} + f(x, t, \tilde{U}) = \vartheta_{\mathcal{L}} + \vartheta_f \qquad \text{for } (x, t) \in \Omega \times (0, T]. \tag{3.6}$$

Here we also used the observation that, by (3.5), the regular functions $\vartheta_{\mathcal{L}}$ and ϑ_f of (3.3) can be rewritten for $t \in (t_{j-1}, t_j]$ as $\vartheta_{\mathcal{L}} = \mathcal{L}(t)\tilde{U} - \mathcal{L}^j U^j$ and $\vartheta_f = f(\cdot, t, \tilde{U}) - f^j$.

Next, combining (3.6) with (1.1a) yields

$$\mathcal{M}\tilde{U} - \mathcal{M}u = \partial_t \tilde{U} + \mathcal{L}(t)\tilde{U} + f(x, t, \tilde{U}) = \partial_t[\tilde{U} - I_t U] + [\vartheta_{\mathcal{L}} + \vartheta_f] \quad \text{in } Q.$$

Now the desired bound for $U^m - u(\cdot, t_m) = [\tilde{U} - u](\cdot, t_m)$ is obtained by an application of Lemma 2.4 with $\mu := \tilde{U} - I_t U$ and $\vartheta := \vartheta_{\mathcal{L}} + \vartheta_f$, using the following two observations. First, we note that $[\tilde{U} - u - \mu](\cdot, 0) = U^1 - \varphi - (U^1 - \varphi) = 0$. Second, for $t \in (t_{j-1}, t_j]$, one has

$$\mu = \tfrac{t_j - t}{\tau_j} \, (U^j - U^{j-1}) \qquad \Longrightarrow \qquad |\mu| \le \left| U^j - U^{j-1} \right|, \quad \tau_j \, |\partial_t \mu| = \left| U^j - U^{j-1} \right|.$$

This completes the proof. □

COROLLARY 3.2. *Under assumption (1.2), the a posteriori error estimate (3.2) applies to the model problem (1.3) with ϑ_f from (3.3), $\vartheta_{\mathcal{L}} = 0$, and the constants κ_0, κ_1, κ_2 from Lemma 2.2.*

4. Semidiscrete Crank-Nicolson method (no spatial discretization). Consider an arbitrary nonuniform mesh (2.3) in the time direction and discretize the abstract parabolic problem (1.1) in time using the second-order Crank-Nicolson method as follows. We associate an approximate solution $U^j \in H_0^1(\Omega) \cap C(\bar{\Omega})$ with the time level t_j and require it to satisfy

$$\delta_t U^j + \tfrac{1}{2}\big(\mathcal{L}^{j-1}U^{j-1} + \mathcal{L}^j U^j\big) + \tfrac{1}{2}(f^{j-1} + f^j) = 0 \quad \text{in } \Omega, \quad j = 1, \dots, M, \tag{4.1a}$$

where we again let

$$U^0 = \varphi, \quad \delta_t U^j := \frac{U^j - U^{j-1}}{\tau_j}, \quad \mathcal{L}^j := \mathcal{L}(t_j) \quad \text{and} \quad f^j := f(\cdot, t_j, U^j). \tag{4.1b}$$

To give an a posteriori error estimate for this discretization, we will use the standard piecewise linear interpolation I_t, which, for any continuous function $w = w(t)$, is defined by

$$I_t w(t) := \tfrac{t_j - t}{\tau_j}\, w(t_{j-1}) + \tfrac{t - t_{j-1}}{\tau_j}\, w(t_j) \quad \text{for } t \in [t_{j-1}, t_j], \quad j = 1, \dots, M, \tag{4.2}$$

(this definition is almost identical with (3.4)).

THEOREM 4.1. *Let u solve the problem (1.1) with the parabolic operator $\mathcal{M}$ satisfying (1.2) and Condition 2.1, and U^j solve the corresponding semidiscrete problem (4.1). Then for $m = 1, \dots, M$, one has*

$$\begin{aligned}\big\|U^m - u(\cdot, t_m)\big\|_{\infty,\Omega} \le \tfrac{1}{8}\,(\kappa_1\,\ell_m + \kappa_2) \max_{j=1,\dots,m-1} \tau_j^2 \,\big\|\delta_t(\mathcal{L}^j U^j + f^j)\big\|_{\infty,\Omega} \\ + \tfrac{5}{8}\,\kappa_0\,\tau_m^2 \,\big\|\delta_t(\mathcal{L}^m U^m + f^m)\big\|_{\infty,\Omega} \\ + \kappa_0 \sum_{j=1}^{m} \int_{t_{j-1}}^{t_j} \mathrm{e}^{-\gamma^2(t_m - s)} \,\big\|[\vartheta_{\mathcal{L}} + \vartheta_f](\cdot, s)\big\|_{\infty,\Omega}\, \mathrm{d}s\,. \end{aligned} \tag{4.3}$$

Here $\vartheta_{\mathcal{L}}$ and ϑ_f are regular functions defined, for $t \in (t_{j-1}, t_j]$, $j = 1, \dots, M$, by

$$\vartheta_{\mathcal{L}} := \mathcal{L}(t)\,U - I_t[\mathcal{L}(t)\,U], \qquad \vartheta_f := f(\cdot, t, U) - I_t[f(\cdot, t, U)], \tag{4.4}$$

where we use $U(\cdot, t) := I_t U(\cdot, t)$ of (3.4) and I_t of (4.2).

REMARK 4.2. *As the exact solution u of (1.1) satisfies $\partial_t^2 u = -\partial_t(\mathcal{L}u + f(x,t,u))$, so the terms $\tau_j^2\, \|\delta_t(\mathcal{L}^j U^j + f^j)\|_{\infty,\Omega}$ in (4.3) can be considered discrete analogues of $\tau_j^2\, \|\partial_t^2 u\|_{\infty,\Omega}$. We also note that these terms can be bounded using $\tau_j^2\, \|\delta_t w^j\|_{\infty,\Omega} \le \tau_j\, (\|w^{j-1}\|_{\infty,\Omega} + \|w^j\|_{\infty,\Omega})$ with $w^j := \mathcal{L}^j U^j + f^j$.*

Proof. Consider $t \in [t_{j-1}, t_j]$. In view of (4.2), for any function $w = w(t)$ with the notation $w^j := w(t_j)$, one has $I_t w(t) = \frac{1}{2}(w^{j-1} + w^j) + (t - t_{j-1/2})\,\delta_t w^j$. So using (4.4) and then this property, for $t \in [t_{j-1}, t_j]$, one easily gets

$$\begin{aligned} f(\cdot, t, U) - \tfrac{1}{2}\big(f^{j-1} + f^j\big) &= \big\{I_t[f(\cdot, t, U)] - \tfrac{1}{2}\big(f^{j-1} + f^j\big)\big\} + \vartheta_f \\ &= (t - t_{j-1/2})\,\delta_t f^j + \vartheta_f, \end{aligned}$$

and a similar relation

$$\begin{aligned} \mathcal{L}(t)\,U - \tfrac{1}{2}\big(\mathcal{L}^{j-1}U^{j-1} + \mathcal{L}^j U^j\big) &= \big\{I_t[\mathcal{L}(t)\,U] - \tfrac{1}{2}\big(\mathcal{L}^{j-1}U^{j-1} + \mathcal{L}^j U^j\big)\big\} + \vartheta_{\mathcal{L}} \\ &= (t - t_{j-1/2})\,\delta_t[\mathcal{L}^j U^j] + \vartheta_{\mathcal{L}}. \end{aligned}$$

Note also that $U(\cdot,t) = I_t U(\cdot,t)$ implies that $\delta_t U^j = \partial_t U$ for $t \in (t_{j-1}, t_j]$.

Combining these three observations with (4.1a), one deduces that

$$\partial_t U + \mathcal{L}(t)\, U + f(\cdot, t, U) = (t - t_{j-1/2})\, \delta_t[\mathcal{L}^j U^j + f^j] + [\vartheta_{\mathcal{L}} + \vartheta_f], \qquad (4.5)$$

for $t \in (t_{j-1}, t_j]$ (here the left-hand side is a regular function). Next, combining (4.5) with (1.1a) yields

$$\mathcal{M}U - \mathcal{M}u = \partial_t U + \mathcal{L}(t)\, U + f(x, t, U) = \partial_t \mu + [\vartheta_{\mathcal{L}} + \vartheta_f] \quad \text{in } Q, \qquad (4.6)$$

where $\mu = \mu(x,t)$ is a continuous function defined by

$$\mu(\cdot, t) := -\tfrac{1}{2}(t_j - t)(t - t_{j-1}) \cdot \delta_t[\mathcal{L}^j U^j + f^j] \qquad \text{for } t \in [t_{j-1}, t_j]. \qquad (4.7)$$

This is easily checked by using the relation $\frac{d}{dt}[-\frac{1}{2}(t_j - t)(t - t_{j-1})] = t - t_{j-1/2}$ to evaluate $\partial_t \mu$.

Now the desired bound (4.3) for $U^m - u(\cdot, t_m)$ is obtained by an application of Lemma 2.4 to the equation (4.6) with μ defined by (4.7), and $\vartheta := \vartheta_{\mathcal{L}} + \vartheta_f$, using the following two observations. First, note that $[U - u - \mu](\cdot, 0) = U^1 - \varphi - 0 = 0$. Second, for $t \in (t_{j-1}, t_j]$, one has

$$|\mu| \le \tfrac{1}{8}\tau_j^2 \left|\delta_t(\mathcal{L}^j U^j + f^j)\right| \quad \text{and} \quad \tau_j\, |\partial_t \mu| \le \tfrac{1}{2}\tau_j^2 \left|\delta_t(\mathcal{L}^j U^j + f^j)\right|.$$

This completes the proof. ☐

COROLLARY 4.3. *Under assumption (1.2), the a posteriori error estimate (4.3) applies to the model problem (1.3) with* ϑ_f *from (4.4),* $\vartheta_{\mathcal{L}} = 0$*, and the constants* κ_0*,* κ_1*,* κ_2 *from Lemma 2.2.*

REMARK 4.4. *If the term* $\frac{1}{2}(f^{j-1} + f^j)$ *in the Crank-Nicolson discretization (4.1) is replaced by* $f_h^j := \tau_j^{-1} \int_{t_{j-1}}^{t_j} f(\cdot, t, U)\, dt$*, then the proof of Theorem 4.1 remains applicable with the only modification that the right-hand side in (4.6) involves, for* $t \in (t_{j-1}, t_j]$*, an additional term* $-\bar\vartheta_f := \frac{1}{2}(f^{j-1} + f^j) - f_h^j$*. Consequently, the statement of Theorem 4.1 remains valid with* $[\vartheta_{\mathcal{L}} + \vartheta_f]$ *in the final line of (4.3) replaced by* $[\vartheta_{\mathcal{L}} + \vartheta_f - \bar\vartheta_f]$*, where, as one can easily deduce,* $\bar\vartheta_f = \tau_j^{-1} \int_{t_{j-1}}^{t_j} \vartheta_f\, dt$ *is the average value of* ϑ_f *on* $[t_{j-1}, t_j]$*.*

REMARK 4.5. *The a posteriori error estimates given by Theorem 4.1 and Remark 4.4 resemble (but are not identical with) error estimates of [1]. Our analysis of the semidiscrete Crank-Nicolson method seems more straightforward as we work with the standard piecewise linear interpolant of the computed solution, while the analysis in [1] involves a construction of a certain piecewise-quadratic polynomial of the computed solution in time. Furthermore, in Section 7, we derive a posteriori error estimates for fully discrete Crank-Nicolson methods, which were not considered in [1].*

5. Elliptic a posteriori error estimators. In this section, we consider a steady-state version of the abstract parabolic problem (1.1):

$$\mathcal{L}v + g(x, v) = 0 \quad \text{for } x \in \Omega, \qquad v = 0 \quad \text{for } x \in \partial\Omega, \qquad (5.1)$$

and its discretizations in the form

$$\text{Find } v_h \in \mathring{V}_h : \quad \mathcal{L}_h v_h + \mathcal{P}_h[g(\cdot, v_h)] = 0, \qquad \text{where } \mathring{V}_h := V_h \cap H_0^1(\Omega). \qquad (5.2a)$$

Here $V_h \subset C(\bar\Omega)$ is some finite-element space, and for the related Lagrange interpolation operator I_h onto V_h, we use some linear operators $\mathcal{L}_h$ and $\mathcal{P}_h$ such that

$$\begin{aligned} &\mathcal{L}_h : \ H_0^1(\Omega) \to \mathring{V}_h - I_h[g(\cdot,0)], \\ &\mathcal{P}_h v \in \mathring{V}_h + I_h v \quad \forall\, v \in C(\bar\Omega), \qquad \mathcal{P}_h v_h = v_h \quad \forall\, v_h \in V_h. \end{aligned} \tag{5.2b}$$

Note that as any $v_h \in \mathring{V}_h$ vanishes on $\partial\Omega$, so $\mathring{V}_h - I_h[g(\cdot,0)] = \mathring{V}_h - I_h[g(\cdot,v_h)]$, so the definition (5.2) is consistent.

Assumptions. We assume, for any admissible g, that

(i) there exist unique solutions v and v_h of problems (5.1) and (5.2), respectively;

(ii) an a posteriori error estimate is available for these solutions in the form

$$\|v - v_h\|_{\infty,\Omega} \le \eta\big(V_h, v_h, g(\cdot, v_h)\big). \tag{5.3}$$

Note that the availability of elliptic a posteriori error estimates, such as (5.3), enables one to employ elliptic reconstructions in the a posteriori error estimation of the related parabolic problems. Moreover, $\mathcal{L}_h$ and $\mathcal{P}_h$ are not necessarily needed to be evaluated explicitly to compute the a posteriori estimator either for the elliptic problem or the parabolic problem.

5.1. Elliptic model problem. Many standard finite element discretizations of elliptic equations (including those with quadrature) allow a representation of type (5.2). For example, consider a steady-state elliptic version of our model problem (1.3) posed in a bounded polyhedral domain $\Omega \subset \mathbb{R}^n$:

$$-\varepsilon^2 \triangle v + g(x,v) = 0 \ \text{ for } x \in \Omega, \quad v = 0 \ \text{ for } x \in \partial\Omega, \quad \partial_z g(x,z) \ge \gamma^2 > 0. \tag{5.4}$$

With a finite-element space $V_h \subset C(\bar\Omega)$ and $\mathring{V}_h := V_h \cap H_0^1(\Omega)$, a standard Galerkin finite element method for this problem can be described by

$$\text{Find } v_h \in \mathring{V}_h : \qquad \varepsilon^2 \langle \nabla v_h, \nabla \chi\rangle + \langle g(\cdot, v_h), \chi\rangle_h = 0 \qquad \forall\, \chi \in \mathring{V}_h, \tag{5.5}$$

where $\langle\cdot,\cdot\rangle_h$ is either exactly the inner product $\langle\cdot,\cdot\rangle$ in $L_2(\Omega)$, or some quadrature formula for $\langle\cdot,\cdot\rangle$.

REMARK 5.1. *The discretization (5.5) is of type (5.2). Suppose, for example, that $\langle\psi,\chi\rangle_h = \langle\psi,\chi\rangle$ for all ψ, $\chi \in V_h$. Then $\langle \mathcal{L}_h\varphi, \chi\rangle = \varepsilon^2\langle\nabla\varphi, \nabla\chi\rangle$ and $\langle \mathcal{P}_h\psi, \chi\rangle = \langle\psi,\chi\rangle_h$, subject to (5.2b), for all $\varphi \in H_0^1(\Omega)$, $\psi \in C(\bar\Omega)$ and $\chi \in \mathring{V}_h$. In particular,*

(i) if $\langle\cdot,\cdot\rangle_h := \langle\cdot,\cdot\rangle$ (i.e. no quadrature is used), then $\mathcal{P}_h$ is the L_2 projection;

(ii) if a quadrature of type $\langle\psi,\chi\rangle_h := \langle I_h\psi, \chi\rangle$ is used, where I_h is the Lagrange interpolation operator associated with V_h, then $\mathcal{P}_h := I_h$.

REMARK 5.2. *Suppose that one employs a quadrature of lumped-mass type defined by $\langle\psi,\chi_i\rangle_h = \langle I_h(\psi\chi_i), 1\rangle = \psi_i\langle\chi_i, 1\rangle$ for all basis functions χ_i of V_h, where $\psi \in C(\bar\Omega)$ and $\sum\psi_i\chi_i = I_h\psi$. Then again $\mathcal{P}_h := I_h$, but $\mathcal{L}_h\varphi := \sum a_i\chi_i$ with $a_i := \varepsilon^2 \frac{\langle\nabla\varphi,\nabla\chi_i\rangle}{\langle\chi_i,1\rangle}$ for interior mesh nodes, and $a_i := -[g(\cdot,0)]_i$ for boundary mesh nodes. Consequently, $\mathcal{L}_h v_h$ is easily computable for any $v_h \in \mathring{V}_h$ by applying the normalized stiffness matrix to the column vector of nodal values $\{v_{h,i}\}$.*

We now cite elliptic estimators of type (5.3) for particular cases of (5.4) and (5.5).

5.2. Elliptic model problem: regular regime. We first consider the steady-state version (5.4) of our model problem (1.3) in the regular regime of $\varepsilon := 1$.

Let v solve the problem (5.4) with $\varepsilon = 1$, $\gamma \geq 0$, posed in a bounded polyhedral domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, and v_h solve the discrete problem (5.5) with V_h and $\langle \cdot, \cdot \rangle_h$ defined as follows. Given a conforming and shape-regular triangulation $\mathcal{T}_h$ of $\bar{\Omega}$ made of elements T, we let V_h be the space of continuous piecewise polynomial finite element functions of degree $l \geq 1$, and $\mathring{V}_h := V_h \cap H_0^1(\Omega)$. We employ $\langle \varphi, \psi \rangle_h := \sum_{T \in \mathcal{T}_h} Q_T(\varphi\psi)$, where Q_T is a quadrature formula for the integral over T with positive weights, and quadrature points contained in T, such that Q_T is exact for the polynomials of degree q with $q \geq \max\{2l - 2, 1\}$.

In [15, Theorem 4.2], an a posteriori error estimate of type (5.3) is given with $\eta = \eta_0$ defined by

$$\eta_0\big(V_h, v_h, g(\cdot, v_h)\big) := \Big[c_0 \max_{T \in \mathcal{T}_h} \Big\{ h_T^2 \big\| (\triangle v_h - g(\cdot, v_h)) \big\|_{\infty, T} + h_T \big\| [\![\partial_n u_h]\!] \big\|_{\infty, \partial T \setminus \partial \Omega} \Big\} + c_1 \big\| \nu_{n/2,T}^{q} \big\|_{l_{n/2}} + c_2 \big\| h_T\, \nu_{n,T}^{q-1} \big\|_{l_n} \Big] \times |\ln h_{\min}|^2, \tag{5.6}$$

where $h_{\min}$ is the smallest mesh size, h_T is the diameter of T, $[\![\partial_n u_h]\!]$ is the jump of the normal derivatives across an inter-element side, $\| \cdot \|_{l_p}$ is the l_p norm, and the quantity

$$\nu_{n',T}^{q'} := |T|^{1/n'} \big\| g(\cdot, v_h) - I_{h,q'}[g(\cdot, v_h)] \big\|_{\infty, T}$$

is defined using the Lagrange interpolation operator $I_{h,q'}$ onto the space of piecewise polynomials of degree $\leq q'$.

5.3. Elliptic model problem: singularly-perturbed regime in one dimension. We now consider the steady-state version (5.4) of our model problem (1.3) in the singularly-perturbed regime of $\varepsilon \ll 1$.

Let v solve the problem (5.4) with $\varepsilon \in (0, 1]$ and $\gamma > 0$, posed in the domain $\Omega := (0, 1)$, and v_h solve the discrete problem (5.5) using the space V_h of continuous ***piecewise-linear*** finite element functions on an arbitrary nonuniform mesh $\{x_i\}_{i=1}^N$ with $0 = x_0 < x_1 < \cdots < x_N = 1$ and $h_i := x_i - x_{i-1}$. Note that here we make absolutely no mesh regularity assumptions (as solutions of our problem typically exhibit sharp layers so a suitable mesh is expected to be highly-nonuniform; see, e.g., [13]).

Consider two choices of $\langle \cdot, \cdot \rangle_h$, which are defined using the standard piecewise-linear Lagrange polynomial I_h onto V_h:

$$\langle \varphi, \psi \rangle_h := \langle I_h \varphi, \psi \rangle, \qquad \text{(quadrature)} \tag{5.7a}$$

$$\langle \varphi, \psi \rangle_h := \langle I_h [\varphi \psi], 1 \rangle. \qquad \text{(lumped-mass quadrature)} \tag{5.7b}$$

Remark 5.3. *To illustrate Remarks 5.1 and 5.2, note that the described two discretizations using either (5.7a) or (5.7b) are of type (5.2). In particular, for (5.7a), we get* $\mathcal{L}_h := -\varepsilon^2 [\partial_x^2]_h$ *and* $\mathcal{P}_h := I_h$. *Here the operator* $[\partial_x^2]_h : H_0^1(\Omega) \to \mathring{V}_h + \varepsilon^{-2} I_h[g(\cdot, 0)]$ *is defined by* $\langle -[\partial_x^2]_h \varphi, \chi \rangle = \langle \varphi', \chi' \rangle$ *for all* $\varphi \in H_0^1(\Omega)$, $\chi \in \mathring{V}_h$. *Consequently, the discrete problem using (5.7a) may be represented as*

$$-\varepsilon^2 \, [\partial_x^2]_h v_h + I_h[g(\cdot, v_h)] = 0. \tag{5.8a}$$

By contrast, (5.7b) can be rewritten as a difference scheme: $-\varepsilon^2 \delta_x^2 v_{h,i} + g(x_i, v_{h,i}) = 0$, *for* $i = 1, \ldots, N-1$, *where* $\delta_x^2 v_{h,i} := \frac{2}{h_i + h_{i+1}} \big[\frac{1}{h_{i+1}} (v_{h,i+1} - v_{h,i}) - \frac{1}{h_i} (v_{h,i} - v_{h,i-1}) \big]$

is the standard finite-difference operator. Letting $\delta_x^2 v_{h,i} := \varepsilon^{-2}\, g(x_i, v_{h,i})$ *for* $i = 0, N$ *and applying the linear interpolation* I_h *to* $\{\delta_x^2 v_{h,i}\}_{i=0}^N$*, we can represent the discrete problem using (5.7b) as*

$$-\varepsilon^2\, I_h[\delta_x^2 v_h] + I_h[g(\cdot, v_h)] = 0, \tag{5.8b}$$

where the values $\delta_x^2 v_{h,i}$ *are easily explicitly computable.*

We cite a posteriori error bounds [8, 12, 13] of type (5.3) with $\eta := \eta_\varepsilon\big(V_h, g(\cdot, v_h)\big)$ for (5.7a) and $\eta := \eta_{\varepsilon;\,\mathrm{l.m.}}\big(V_h, g(\cdot, v_h)\big)$ for (5.7b), respectively, defined by

$$\eta_\varepsilon\big(V_h, g_*\big) := \max_{i=1,\dots,N}\Big\{ \tfrac{h_i^2}{4\varepsilon^2}\, \|I_h g_*\|_{\infty,(x_{i-1},x_i)} \Big\} + \gamma^{-2}\|g_* - I_h g_*\|_{\infty,(0,1)}, \tag{5.9a}$$

$$\eta_{\varepsilon;\,\mathrm{l.m.}}\big(V_h, g_*\big) := \eta_\varepsilon + \max_{i=1,\dots,N}\Big\{ \tfrac{h_i^2}{6\gamma\,\varepsilon}\, \|\partial_x(I_h g_*)\|_{\infty,(x_{i-1},x_i)} \Big\}, \tag{5.9b}$$

where $\qquad g_* := g(\cdot, v_h)$.

Remark 5.4. *The error estimators (5.9a) and (5.9b) are* <u>*robust*</u> *although they involve negative powers of the small parameter* ε*. Indeed, an inspection of representations (5.8a) and (5.8b) for the two considered numerical methods shows that* $\varepsilon^{-2}h_i^2|I_h g_*| = \varepsilon^{-2}h_i^2|I_h[g(\cdot, v_h)]|$ *becomes* $h_i^2|[\partial_x^2]_h v_h|$ *or* $h_i^2|\delta_x^2 v_h|$*, so it approximates* $h_i^2|\partial_x^2 v|$*, where* v *is the exact solution of our equation* $-\varepsilon^2\partial_x^2 v + g(\cdot, v) = 0$*. Similarly, the term* $\varepsilon^{-1}h_i^2|\partial_x(I_h g_*)|$ *approximates* $\varepsilon\,|\partial_x^3 v|$*, which has similar magnitude to* $h_i^2|\partial_x^2 v|$ *in the layer regions.*

By contrast, if $\langle\cdot,\cdot\rangle_h := \langle\cdot,\cdot\rangle$ *(i.e. no quadrature is used), then one can obtain a simpler-looking error estimate of type (5.3) with* $\eta := \max_{i=1,\dots,N}\big\{ \frac{h_i^2}{4\varepsilon^2}\, \|g_*\|_{\infty,(x_{i-1},x_i)} \big\}$*. However, this estimate is not robust. To see this, split* $g_* = P_h g_* + (g_* - P_h g_*)$ *using the standard* L_2 *projection* P_h*. Then, instead of (5.8a), we have the representation* $-\varepsilon^2\,[\partial_x^2]_h v_h + P_h[g_*] = 0$ *for our numerical method. The component* $\varepsilon^{-2}h_i^2|P_h g_*|$ *approximates* $h_i^2|\partial_x^2 v|$ *so it yields a robust part of the estimator. But the other component* $\varepsilon^{-2}h_i^2|g_* - P_h g_*|$ *may be as large as* $\mathcal{O}(\varepsilon^{-2}h_i^4)$*, which may become quite large if* ε *is small compared to the local mesh size. For this numerical method one can, in fact, obtain a robust error estimator, which is almost identical with (5.9a), only* I_h *in* η_ε *should be replaced by* P_h *(but this latter estimator is less practical, as it requires the* L_2 *projection* $P_h g_*$ *to be explicitly computed).*

6. Fully discrete Backward Euler method. To fully discretize the abstract parabolic problem (1.1), we now apply a spatial discretization of type (5.2) to the semidiscrete problem (3.1) as follows. We associate a finite-element space $V_h^j \subset C(\bar\Omega)$ and a computed solution $u_h^j \in \mathring{V}_h^j := V_h^j \cap H_0^1(\Omega)$ with the time level t_j and require, for $j = 1, \dots, M$, that

$$\mathcal{L}_h^j\, u_h^j + \mathcal{P}_h^j\,[f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j] = 0, \tag{6.1a}$$

with some $u_h^0 \approx \varphi$ in $\mathring{V}_h^0$. Here $\mathcal{L}_h^j$ and $\mathcal{P}_h^j$ are also associated with the time level t_j and, in agreement with (5.2b), for the Lagrange interpolation operator I_h^j onto V_h^j, we let

$$\begin{aligned} &\mathcal{L}_h^j:\ H_0^1(\Omega) \to \mathring{V}_h^j - I_h^j[f(\cdot, t_j, 0)],\\ &\mathcal{P}_h^j v \in \mathring{V}_h^j + I_h^j v \quad \forall v \in C(\bar\Omega), \qquad \mathcal{P}_h^j v_h = v_h \quad \forall v_h \in V_h^j. \end{aligned} \tag{6.1b}$$

Note that as both u_h^j and $\delta_t^* u_h^j$ vanish on $\partial\Omega$, so $\mathring{V}_h^j - I_h^j[f(\cdot, t_j, 0)]$ coincides with $\mathring{V}_h^j - I_h^j[f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j]$, so the definition (6.1) is consistent.

The term $\delta_t^* u_h^j$ in (6.1a) approximates $\partial_t u$ and is defined by

$$\delta_t^* u_h^j := \frac{u_h^j - \hat{u}_h^{j-1}}{\tau_j}, \quad \text{where } \hat{u}_h^0 := u_h^0. \tag{6.1c}$$

The operator δ_t^* is identical with δ_t of (3.1b) for $j = 1$, while for $j > 1$ it involves the intermediate computed solution $\hat{u}_h^{j-1} \in H_0^1(\Omega)$ that we associate with the time level t_{j-1}^+ (this is indicated by the hat notation).

We do not presently specify $\hat{u}_h^{j-1}$, but note two particular cases of interest:

$$\text{Case A:} \quad \hat{u}_h^{j-1} := u_h^{j-1} \qquad \Rightarrow \quad \delta_t^* u_h^j \in \operatorname{span}\{\mathring{V}_h^{j-1}, \mathring{V}_h^j\}, \tag{6.2a}$$

$$\text{Case B:} \quad \hat{u}_h^{j-1} := I_*^j u_h^{j-1}, \quad I_*^j : \mathring{V}_h^{j-1} \to \mathring{V}_h^j \quad \Rightarrow \quad \delta_t^* u_h^j \in \mathring{V}_h^j. \tag{6.2b}$$

Here I_*^j is some interpolation operator such that $I_*^j u_h^{j-1} := u_h^{j-1}$ if $V_h^{j-1} \subset V_h^j$.

Note that if $V_h^{j-1} \subset V_h^j$ (which includes the case of $V_h^j = V_h$ being fixed for all $j = 0, \ldots, M$), then Cases A and B are identical. Note also that to define I_*^j in Case B, one may employ, e.g., the standard Lagrange interpolation or the L_2 projection.

6.1. A posteriori error estimate using piecewise-constant elliptic reconstructions. To estimate the error of the fully discrete Backward-Euler method (6.1), we shall employ the *elliptic reconstruction*, which was introduced in the recent papers [14, 11, 3] as a counterpart of the Ritz-projection in the a posteriori error estimation for parabolic problems.

We associate an elliptic reconstruction $R^j \in H_0^1(\Omega) \cap C(\bar{\Omega})$ with the time level t_j and require, for $x \in \Omega$, $j = 1, \ldots, M$, that

$$\mathcal{L}^j R^j + g^j(x, R^j) = 0, \quad \text{where} \quad g^j(x, v) := f(x, t_j, v) + \delta_t^* u_h^j, \tag{6.3}$$

so this relation may be considered somewhat between (3.1a) and (6.1a). On the other hand, (6.3) is a version of the elliptic problem (5.1) with $\mathcal{L} := \mathcal{L}^j$ and $g := g^j$, while the numerical method (5.2) applied to this problem is identical with (6.1) and yields the computed solution u_h^j. Furthermore, applying the elliptic a posteriori error estimate (5.3) to the exact solution R^j and the corresponding computed solution u_h^j, one gets

$$\eta^j := \|R^j - u_h^j\|_{\infty,\Omega} \le \eta\big(V_h^j, u_h^j, g^j(\cdot, u_h^j)\big) \qquad \text{for } j = 1, \ldots, M. \tag{6.4}$$

We now give an a posteriori error estimate for the fully discrete method (6.1).

THEOREM 6.1. *Let u solve the problem (1.1), (1.2) with the parabolic operator $\mathcal{M}$ satisfying Condition 2.1, u_h^j solve the discrete problem (6.1), and R^j be the elliptic reconstruction defined by (6.3) and satisfying (6.4). Then for $m = 1, \ldots, M$, one has*

$$\begin{aligned}
\big\|u_h^m - u(\cdot, t_m)\big\|_{\infty,\Omega} \le \kappa_0\, \mathrm{e}^{-\gamma^2 t_m} \big\|u_h^0 - \varphi\big\|_{\infty,\Omega} \\
+ (\kappa_1\, \ell_m + \kappa_2) \max_{j=1,\ldots,m-1} \Big\{ \big\|u_h^j - u_h^{j-1}\big\|_{\infty,\Omega} + \eta^j \Big\} \\
+ 2\kappa_0 \big\|u_h^m - u_h^{m-1}\big\|_{\infty,\Omega} + (\kappa_0 + 1)\, \eta^m \\
+ \kappa_0 \sum_{j=1}^m \int_{t_{j-1}}^{t_j} \mathrm{e}^{-\gamma^2 (t_m - s)} \big\|[\vartheta_{\mathcal{L},R} + \vartheta_{f,R}](\cdot, s)\big\|_{\infty,\Omega}\, \mathrm{d}s \\
+ \kappa_0 \sum_{j=2}^m \mathrm{e}^{-\gamma^2 (t_m - t_j)} \big\|\hat{u}_h^{j-1} - u_h^{j-1}\big\|_{\infty,\Omega},
\end{aligned} \tag{6.5}$$

where $\vartheta_{\mathcal{L},R}$ and $\vartheta_{f,R}$ are regular functions defined, for $t \in (t_{j-1}, t_j]$, $j = 1, \dots, M$, by

$$\vartheta_{\mathcal{L},R}(\cdot, t) := [\mathcal{L}(t) - \mathcal{L}^j]\, R^j, \quad \vartheta_{f,R}(\cdot, t) := f(\cdot, t, R^j) - f(\cdot, t_j, R^j). \tag{6.6}$$

REMARK 6.2. *The final term in (6.5) vanishes in Case A of (6.2); in particular, when one has $V_h^{j-1} \subset V_h^j$ for all $j = 1, \dots, M$.*

Proof. In view of (6.4), to get the desired bound (6.5) for $u_h^m - u(\cdot, t_m)$, it suffices to obtain a bound of type (6.5) for $R^m - u(\cdot, t_m)$ only with $(\kappa_0 + 1)$ replaced by κ_0, and then apply the triangle inequality. So we focus on estimating $R^m - u(\cdot, t_m)$.

We partially imitate the proof of Theorem 3.1. Let $I_t u_h$ be a standard piecewise-linear interpolant of u_h^j in time:

$$I_t u_h(\cdot, t) := \tfrac{t_j - t}{\tau_j}\, u_h^{j-1} + \tfrac{t - t_{j-1}}{\tau_j}\, u_h^j \quad \text{for } t \in [t_{j-1}, t_j], \quad j = 1, \dots, M. \tag{6.7}$$

Furthermore, we define a ***piecewise-constant*** interpolant $\tilde{R}$ of R^j in time by

$$\tilde{R}(\cdot, t) := R^j \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1 \dots, M; \qquad \tilde{R}(\cdot, 0) := R^1, \tag{6.8}$$

(so $\tilde{R}$ is continuous on $[t_0, t_1]$; compare with $\tilde{U}$ of (3.5)). Note that the temporal derivative $\partial_t \tilde{R}$ is understood in the sense of distributions, while $\partial_t(I_t u_h)$ is a regular function. Now, in view of (6.3), one gets

$$\partial_t(I_t u_h) + \mathcal{L}(t)\tilde{R} + f(\cdot, t, \tilde{R}) = \vartheta_{\mathcal{L},R} + \vartheta_{f,R} + \vartheta_* \qquad \text{in } Q, \tag{6.9}$$

where ϑ_* is a regular function defined by

$$\vartheta_*(\cdot, t) := \partial_t(I_t u_h) - \delta_t^* u_h^j \quad \text{for } t \in (t_{j-1}, t_j]. \tag{6.10}$$

To get (6.9), we also used the observation that, by (6.8), the regular functions $\vartheta_{\mathcal{L},R}$ and $\vartheta_{f,R}$ of (6.6) can be rewritten for $t \in (t_{j-1}, t_j]$ as $\vartheta_{\mathcal{L},R} = \mathcal{L}(t)\tilde{R} - \mathcal{L}^j R^j$ and $\vartheta_{f,R} = f(\cdot, t, \tilde{R}) - f(\cdot, t_j, R^j)$.

Next, combining (6.9) with (1.1a) yields

$$\mathcal{M}\tilde{R} - \mathcal{M}u = \partial_t \tilde{R} + \mathcal{L}(t)\tilde{R} + f(\cdot, t, \tilde{R}) = \partial_t[\tilde{R} - I_t u_h] + [\vartheta_{\mathcal{L},R} + \vartheta_{f,R} + \vartheta_*].$$

Now the desired bound of type (6.5) for $R^m - u(\cdot, t_m) = [\tilde{R} - u](\cdot, t_m)$, only with $(\kappa_0 + 1)$ replaced by κ_0, is obtained by an application of Lemma 2.4 with $\mu := \tilde{R} - I_t u_h$ and $\vartheta := \vartheta_{\mathcal{L},R} + \vartheta_{f,R} + \vartheta_*$, using the following three observations. First, note that

$$[\tilde{R} - u - \mu](\cdot, 0) = R^1 - \varphi - (R^1 - u_h^0) = u_h^0 - \varphi. \tag{6.11}$$

Next, for $t \in (t_{j-1}, t_j]$, we have $\mu = R^j - u_h^j + \frac{t_j - t}{\tau_j}(u_h^j - u_h^{j-1})$. Thus,

$$|\mu| \le |R^j - u_h^j| + |u_h^j - u_h^{j-1}| \quad \text{and} \quad \tau_j\, |\partial_t \mu| = |u_h^j - u_h^{j-1}|, \tag{6.12}$$

where $\|R^j - u_h^j\|_{\infty,\Omega} = \eta^j$. Finally, (6.10) combined with (6.1c), (6.7) implies that $\vartheta_*(\cdot, t) = \frac{1}{\tau_j}(\hat{u}_h^{j-1} - u_h^{j-1})$ for $t \in (t_{j-1}, t_j]$. Therefore,

$$\int_{t_{j-1}}^{t_j} \mathrm{e}^{-\gamma^2(t_m - s)}\, \big\|\vartheta_*(\cdot, s)\big\|_{\infty,\Omega}\, \mathrm{d}s \le \mathrm{e}^{-\gamma^2(t_m - t_j)} \big\|\hat{u}_h^{j-1} - u_h^{j-1}\big\|_{\infty,\Omega}, \tag{6.13}$$

where $\hat u_h^0 - u_h^0 = 0$. The three observations (6.11), (6.12), (6.13) yield the required bound for $\|R^m - u(\cdot, t_m)\|_{\infty,\Omega}$. □

THEOREM 6.1*. *The statement of Theorem 6.1 remains valid with the terms* $\|u_h^j - u_h^{j-1}\|_{\infty,\Omega}$ *and* $\|u_h^m - u_h^{m-1}\|_{\infty,\Omega}$ *in (6.5) respectively replaced by* $\|u_h^j - \hat u_h^{j-1}\|_{\infty,\Omega}$ *and* $\|u_h^m - \hat u_h^{m-1}\|_{\infty,\Omega}$.

Proof. We imitate the proof of Theorem 6.1, but with $I_t u_h$ of (6.7) replaced by the piecewise-continuous interpolant

$$I_t^* u_h(\cdot, t) := \tfrac{t_j - t}{\tau_j}\, \hat u_h^{j-1} + \tfrac{t - t_{j-1}}{\tau_j}\, u_h^j \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1, \ldots, M, \tag{6.14}$$

with $I_t^* u_h(\cdot, 0) := \hat u_h^0 = u_h^0$. Furthermore, ϑ_* is defined not by (6.10), but by

$$\vartheta_*(\cdot, t) := \partial_t (I_t^* u_h) - \delta_t^* u_h^j = [\hat u_h^{j-1} - u_h^{j-1}]\, \delta(t - t_{j-1}^+) \quad \text{for } t \in (t_{j-1}, t_j], \tag{6.15}$$

where $\delta(\cdot)$ is the one-dimensional Dirac δ-distribution. (Note that $\hat u_h^0 = u_h^0$ and the right-continuity convention at $t = 0$ imply that $\vartheta_* = 0$ on $[0, t_1]$.) So instead of (6.13) we get

$$\int_0^{t_m} \mathrm{e}^{-\gamma^2 (t_m - s)}\, \big\|\vartheta_*(\cdot, s)\big\|_{\infty,\Omega}\, \mathrm{d}s \le \sum_{j=2}^{m} \mathrm{e}^{-\gamma^2 (t_m - t_{j-1})} \big\|\hat u_h^{j-1} - u_h^{j-1}\big\|_{\infty,\Omega}\,. \tag{6.16}$$

The required bound for $R^m - u(\cdot, t_m) = [\tilde R - u](\cdot, t_m)$ is again obtained by an application of Lemma 2.4 only with $\mu := \tilde R - I_t^* u_h$, for which we have a version of (6.12) with u_h^{j-1} replaced by $\hat u_h^{j-1}$. □

REMARK 6.3. *The terms* $\vartheta_{\mathcal{L},R}$ *and* $\vartheta_{f,R}$ *in (6.5) involve the elliptic reconstruction* R^j. *In view of the bound (6.4), their discrepancy from* $\vartheta_{\mathcal{L},u_h}$ *and* ϑ_{f,u_h}, *respectively, can be easily estimated. E.g., for* $\vartheta_{f,R}$ *with* $t \in (t_{j-1}, t_j]$, *we have*

$$\begin{aligned}\big\|[\vartheta_{f,R} - \vartheta_{f,u_h}](\cdot, t)\big\|_{\infty,\Omega} &\le \eta^j \sup_{(t_{j-1}, t_j] \times \mathbb{R}} \big\|\partial_z f(\cdot, t, z) - \partial_z f(\cdot, t_j, z)\big\|_{\infty,\Omega} \\ &\le \tau_j\, \eta^j \sup_{(t_{j-1}, t_j] \times \mathbb{R}} \big\|\partial_t \partial_z f(\cdot, t, z)\big\|_{\infty,\Omega},\end{aligned}$$

where η^j *is estimated using (6.4). In fact, if* $|\partial_t \partial_z f| \le C$, *then the discrepancy* $\|[\vartheta_{f,R} - \vartheta_{f,u_h}](\cdot, t)\|_{\infty,\Omega}$ *between* $\vartheta_{f,R}$ *and* ϑ_{f,u_h} *becomes* $\mathcal{O}(\tau_j\, \eta^j)$, *i.e. negligible compared with the terms* η^j *that explicitly appear in (6.5).*

6.2. Applications to the model problem (1.3). Consider a fully discrete Backward-Euler method for (1.3), obtained by applying the spatial discretization (5.5) to a version of the semidiscrete Backward-Euler method (3.1):

$$\text{Find } u_h^j \in \mathring{V}_h^j: \quad \varepsilon^2 \big\langle \nabla u_h^j, \nabla \chi \big\rangle + \big\langle f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j,\, \chi \big\rangle_h = 0 \quad \forall\, \chi \in \mathring{V}_h^j, \tag{6.17}$$

where $\langle \cdot, \cdot \rangle_h$ is either exactly the inner product $\langle \cdot, \cdot \rangle$ in $L_2(\Omega)$, or some quadrature formula for $\langle \cdot, \cdot \rangle$, and $\delta_t^* u_h^j$ is defined by (6.1c), (6.2).

Note that the full discretization (6.17) is of type (6.1). For some particular cases of $\langle \cdot, \cdot \rangle_h$, the operators $\mathcal{L}_h^j$ and $\mathcal{P}_h^j$ are defined as in Remarks 5.1 and 5.2 only using V_h^j instead of V_h.

6.2.1. Model problem (1.3): regular regime. Let u solve the problem (1.3) with $\varepsilon = 1$, $\gamma \geq 0$, posed in a bounded polyhedral spatial domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, and u_h^j solve the discrete problem (6.17) with V_h^j and $\langle \cdot, \cdot \rangle_h$ defined, for each time level t_j, as in §5.2. To be more specific, we let $\mathcal{T}_h^j$ be a conforming and shape-regular triangulation of $\bar{\Omega}$ made of elements T, V_h^j be the space of continuous piecewise polynomial finite element functions of degree $l \geq 1$, and $\mathring{V}_h^j := V_h^j \cap H_0^1(\Omega)$. We then employ a quadrature formula $\langle \varphi, \psi \rangle_h := \sum_{T \in \mathcal{T}_h^j} Q_T(\varphi\psi)$, as described in §5.2.

Corollary 6.4. *Let the above numerical method be applied to problem (1.3) with $\varepsilon = 1$, $\gamma \geq 0$. Then the a posteriori error estimates of Theorems 6.1 and 6.1* are valid with $\vartheta_{\mathcal{L},R} = 0$, $\vartheta_{f,R}$ computed as described in Remark 6.3, and*

$$\eta^j := \eta_0\big(V_h^j, u_h^j, f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j\big) \qquad \textit{for } j = 1, \ldots, M,$$

where η_0 is defined in (5.6).

Remark 6.5. *The Backward-Euler method for a linear version of (1.3) with $\varepsilon = 1$ was considered in [4, 3]. The a posteriori error estimate (6.5) of Corollary 6.4 resembles (but is not identical with) the one of [4, (1.13)] in that it involves terms such as $|u_h^j - u_h^{j-1}|$, that may be interpreted as approximating $\tau_j |\partial_t u|$. (Note also that [4, (1.13)] is given without proof, and does not appear to be proved elsewhere).*

By contrast, the a posteriori error estimates of [3] include terms (denoted there by $\tau_j |g^j - g^{j-1}|$) that may be interpreted as approximating the quantity $\tau_j |\partial_t^2 u + \ldots|$, which seems less suitable for a first-order method in time.

6.2.2. Model problem (1.3): singularly perturbed regime in one dimension. Now, consider $\varepsilon \ll 1$. Let u solve (1.3) with $\varepsilon \in (0, 1]$, $\gamma > 0$, posed in the domain $\Omega := (0, 1)$. Let u_h solve the discrete problem (6.17) with V_h^j and $\langle \cdot, \cdot \rangle_h$ defined, for each time level t_j, as in §5.3. Thus V_h^j is the space of continuous ***piecewise-linear*** finite element functions on an arbitrary nonuniform mesh $\{x_i^j\}_{i=1}^N$ with $0 = x_0^j < x_1^j < \cdots < x_N^j = 1$ under absolutely no mesh regularity assumptions. We consider the two choices (5.7a) and (5.7b) of $\langle \cdot, \cdot \rangle_h$, using the piecewise-linear Lagrange interpolant $I_h := I_h^j$ onto V_h^j.

Corollary 6.6. *Let the above numerical method be applied to problem (1.3) with $\varepsilon \in (0, 1]$, $\gamma > 0$, $\Omega := (0, 1)$. Then the a posteriori error estimates of Theorems 6.1 and 6.1* are valid with $\vartheta_{\mathcal{L},R} = 0$, $\vartheta_{f,R}$ computed as described in Remark 6.3, and*

$$\eta^j := \begin{cases} \eta_\varepsilon\big(V_h^j, f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j\big) & \textit{for (5.7a)}, \\ \eta_{\varepsilon;\,\mathrm{l.m.}}\big(V_h^j, f(\cdot, t_j, u_h^j) + \delta_t^* u_h^j\big) & \textit{for (5.7b)}, \end{cases}$$

for $j = 1, \ldots, M$, where η_ε and $\eta_{\varepsilon;\,\mathrm{l.m.}}$ are defined in (5.9), *with I_h replaced by I_h^j.*

Remark 6.7. *The a posteriori error estimators of Corollary 6.6 are <u>robust</u> as the argument of Remark 5.4 applies to η^j with v replaced by $u(\cdot, t_j)$, so $\varepsilon^{-2} h_i^2 |I_h g_*|$ approximates $h_i^2 |\partial_x^2 u(\cdot, t_j)|$, while the term $\varepsilon^{-1} h_i^2 |\partial_x (I_h g_*)|$ approximates $\varepsilon\, |\partial_x^3 u(\cdot, t_j)|$, which has similar magnitude to $h_i^2 |\partial_x^2 u(\cdot, t_j)|$ in the layer regions.*

Remark 6.8. *Consider the term $\|g_* - I_h^j g_*\|_{\infty,\Omega}$ in the error estimators of Corollary 6.6 for Cases A and B of (6.2). In Case B, one has $\delta_t^* u_h^j - I_h^j[\delta_t^* u_h^j] = 0$, hence $\|g_* - I_h^j g_*\|_{\infty,\Omega}$ simplifies to $\|f(\cdot, t_j, u_h^j) - I_h^j f(\cdot, t_j, u_h^j)\|_{\infty,\Omega}$. In Case A, the final term in (6.5) vanishes (see Remark 6.2). However, $g_* - I_h^j g_*$ again involves $f(\cdot, t_j, u_h^j) - I_h^j f(\cdot, t_j, u_h^j)$ and, furthermore, $\delta_t^* u_h^j - I_h^j[\delta_t^* u_h^j] = -\frac{1}{\tau_j}(u_h^{j-1} - I_h^j[u_h^{j-1}])$.*

Interestingly, Case A and Case B with $I_*^j := I_h^j$ *are identical, but, in view of the above, yield different error estimators. Note that one seems to get a sharper estimator when this method is interpreted as Case B with* $I_*^j := I_h^j$.

7. Fully discrete Crank-Nicolson method. We now describe a full discretization of Crank-Nicolson type for the abstract parabolic problem (1.1). To this end, we apply a spatial discretization of type (5.2) to the semidiscrete problem (4.1) as follows. A finite-element space $V_h^j \subset C(\bar\Omega)$ and a computed solution $u_h^j \in \mathring{V}_h^j := V_h^j \cap H_0^1(\Omega)$ are associated with the time level t_j, while a computed solution $\hat u_h^{j-1} \in \mathring{V}_h^j$ is associated with the time level t_{j-1}^+ (this is indicated by the hat notation). We require, for $j = 1, \dots, M$, that

$$\delta_t^* u_h^j + \tfrac12\big(\hat{\mathcal L}_h^{j-1}\hat u_h^{j-1} + \mathcal L_h^j\, u_h^j\big) + \tfrac12\,\mathcal P_h^j\big[f(\cdot, t_{j-1}, \hat u_h^{j-1}) + f(\cdot, t_j, u_h^j)\big] = 0 \qquad (7.1a)$$

with some $u_h^0 \approx \varphi$ in $\mathring{V}_h^0$. Here $\mathcal L_h^j$ and $\mathcal P_h^j$ are associated with the time level t_j, while $\hat{\mathcal L}_h^{j-1}$ is associated with the time level t_{j-1}^+. In agreement with (5.2b), for the Lagrange interpolation operator I_h^j onto V_h^j, we let

$$\begin{aligned}
&\mathcal L_h^j : H_0^1(\Omega) \to \mathring{V}_h^j - I_h^j[f(\cdot, t_j, 0)], \qquad \hat{\mathcal L}_h^{j-1} : H_0^1(\Omega) \to \mathring{V}_h^j - I_h^j[f(\cdot, t_{j-1}, 0)],\\
&\mathcal P_h^j v \in \mathring{V}_h^j + I_h^j v \quad \forall\, v \in C(\bar\Omega), \qquad\qquad \mathcal P_h^j v_h = v_h \quad \forall\, v_h \in \mathring{V}_h^j.
\end{aligned} \qquad (7.1b)$$

Note that any $v_h \in \mathring{V}_h^j$ vanishes on $\partial\Omega$, so $\mathring{V}_h^j - I_h[f(\cdot, t_k, 0)] = \mathring{V}_h^j - I_h[f(\cdot, t_k, v_h)]$ for $k = j-1, j$, while we also impose that $\delta_t^* u_h^j \in \mathring{V}_h^j$. So the definition (7.1) is consistent.

The term $\delta_t^* u_h^j$ in (7.1a) approximates $\partial_t u$ and is identical with (6.1c):

$$\delta_t^* u_h^j := \frac{u_h^j - \hat u_h^{j-1}}{\tau_j}, \quad \text{where } \hat u_h^0 := u_h^0. \qquad (7.1c)$$

The operator δ_t^* is identical with δ_t of (4.1b) for $j = 1$, while for $j > 1$ it involves $\hat u_h^{j-1}$ defined by

$$\hat u_h^{j-1} := I_*^j\, u_h^{j-1}, \quad I_*^j : \mathring{V}_h^{j-1} \to \mathring{V}_h^j \quad \Longrightarrow \quad \delta_t^* u_h^j \in \mathring{V}_h^j. \qquad (7.1d)$$

Here I_*^j is some linear interpolation operator such that $I_*^j\, u_h^{j-1} = u_h^{j-1}$ if $V_h^{j-1} \subset V_h^j$. Thus, in this section we restrict our analysis to Case B of (6.2b). Note that if $V_h^{j-1} \subset V_h^j$ (which includes the case of $V_h^j = V_h$ being fixed for all j), then $\hat u_h^{j-1} = u_h^{j-1}$. Also, to define I_*^j, one may employ, e.g., the standard Lagrange interpolation or the L_2 projection.

7.1. A posteriori error estimate using piecewise-linear elliptic reconstructions. We associate elliptic reconstructions R^j, $\hat R^{j-1} \in H_0^1(\Omega) \cap C(\bar\Omega)$, respectively, with the time levels t_j and t_{j-1}^+, and require, for $x \in \Omega$, $j = 1, \dots, M$, that

$$\mathcal L^j\, R^j + g^j(x, R^j) = 0, \quad \mathcal L^{j-1}\, \hat R^{j-1} + \hat g^{j-1}(x, \hat R^{j-1}) = 0, \qquad (7.2a)$$

where

$$g^j(\cdot, v) := f(\cdot, t_j, v) - \Big\{\mathcal L_h^j u_h^j + \mathcal P_h^j\,[f(\cdot, t_j, u_h^j)]\Big\}, \qquad (7.2b)$$

$$\hat g^{j-1}(\cdot, v) := f(\cdot, t_{j-1}, v) - \Big\{\hat{\mathcal L}_h^{j-1}\hat u_h^{j-1} + \mathcal P_h^j\,[f(\cdot, t_{j-1}, \hat u_h^{j-1})]\Big\}. \qquad (7.2c)$$

Combining (7.2) with (7.1a) immediately yields

$$\delta_t^* u_h^j + \tfrac12\big[\mathcal L^{j-1}\, \hat R^{j-1} + \mathcal L^j\, R^j\big] + \tfrac12\big[f(\cdot, t_{j-1}, \hat R^{j-1}) + f(\cdot, t_j, R^j)\big] = 0, \qquad (7.3)$$

which may be considered somewhat between (4.1a) and (7.1a).

Note that (7.2a) describes two versions of the elliptic problem (5.1) with $\mathcal{L} := \mathcal{L}^j$, $g := g^j$, and with $\mathcal{L} := \hat{\mathcal{L}}^{j-1}$, $g := \hat{g}^{j-1}$, and exact solutions R^j and $\hat{R}^{j-1}$, respectively. Furthermore, the numerical method (5.2), using the finite element space V_h^j, applied to these two problems yields

$$\mathcal{L}_h^j R_h^j + \mathcal{P}_h^j [g^j(x, R_h^j)] = 0, \qquad \hat{\mathcal{L}}_h^{j-1} \hat{R}_h^{j-1} + \mathcal{P}_h^j \left[\hat{g}^{j-1}(x, \hat{R}_h^{j-1})\right] = 0. \tag{7.4}$$

We have assumed that solutions of these two discrete problems are unique. Thus, $R_h^j = u_h^j$ and $\hat{R}_h^{j-1} = \hat{u}_h^{j-1}$. This is easily checked by combining (7.4) with the definitions of g^j and $\hat{g}^{j-1}$ in (7.2), in which the terms $\{\cdots\} \in \mathring{V}_h^j$. Consequently, applying the elliptic a posteriori error estimate (5.3) to the exact solutions R^j and $\hat{R}^{j-1}$ and the corresponding computed solutions u_h^j and $\hat{u}_h^{j-1}$, one gets, for $j = 1, \ldots, M$,

$$\eta^j := \|R^j - u_h^j\|_{\infty,\Omega} \le \eta\big(V_h^j, u_h^j, g^j(\cdot, u_h^j)\big), \tag{7.5a}$$

$$\hat{\eta}^{j-1} := \|\hat{R}^{j-1} - \hat{u}_h^{j-1}\|_{\infty,\Omega} \le \eta\big(V_h^j, \hat{u}_h^{j-1}, \hat{g}^{j-1}(\cdot, \hat{u}_h^{j-1})\big). \tag{7.5b}$$

To formulate our a posteriori error estimate for $u_h - u$, we generalize the piecewise linear interpolation I_t of (4.2) to any *left-continuous* function $w = w(t)$ by setting

$$I_t^* w(t) := \tfrac{t_j - t}{\tau_j}\, w(t_{j-1}^+) + \tfrac{t - t_{j-1}}{\tau_j}\, w(t_j) \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1, \ldots, M. \tag{7.6}$$

In a similar manner, we apply I_t^* to the elliptic reconstruction (7.2) and define

$$R(\cdot, t) := I_t^* R(\cdot, t) := \tfrac{t_j - t}{\tau_j}\, \hat{R}^{j-1} + \tfrac{t - t_{j-1}}{\tau_j}\, R^j \quad \text{for } t \in (t_{j-1}, t_j], \quad j = 1, \ldots, M. \tag{7.7}$$

(In agreement with the adapted left-/right-continuity convention, both R and $I_t^* w$ are right-continuous at $t = 0$.)

Theorem 7.1. *Let u solve (1.1), (1.2) with a parabolic operator $\mathcal{M}$ satisfying Condition 2.1, u_h^j solve the discrete problem (7.1), and R^j, $\hat{R}^{j-1}$ be the elliptic reconstructions defined by (7.2) and satisfying (7.5). Then, for $m = 1, \ldots, M$, one has*

$$\begin{aligned}
\big\|u_h^m - u(\cdot, t_m)\big\|_{\infty,\Omega} \le{}& \kappa_0\, \mathrm{e}^{-\gamma^2 t_m} \big\|u_h^0 - \varphi\big\|_{\infty,\Omega} \\
&+ (\kappa_1\, \ell_m + \kappa_2) \max_{j=1,\ldots,m-1} \Big\{ \tfrac{1}{8} \tau_j^2 \,\big\|\delta_t^* \Psi^j\big\|_{\infty,\Omega} + \eta^j + \hat{\eta}^{j-1} \Big\} \\
&+ \tfrac{5}{8} \kappa_0\, \tau_m^2 \,\big\|\delta_t^* \Psi^m\big\|_{\infty,\Omega} + (2\kappa_0 + 1)\, \eta^m + 2\kappa_0\, \hat{\eta}^{m-1} \\
&+ \kappa_0 \sum_{j=1}^{m} \int_{t_{j-1}}^{t_j} \mathrm{e}^{-\gamma^2 (t_m - s)} \,\big\|[\vartheta_{\mathcal{L},R} + \vartheta_{f,R}](\cdot, s)\big\|_{\infty,\Omega}\, \mathrm{d}s \\
&+ \kappa_0 \sum_{j=2}^{m} \mathrm{e}^{-\gamma^2 (t_m - t_{j-1})} \,\big\|\hat{u}_h^{j-1} - u_h^{j-1}\big\|_{\infty,\Omega}\, .
\end{aligned} \tag{7.8}$$

Here, for $j = 1, \ldots, M$, we use $\delta_t^* \Psi^j = \frac{1}{\tau_j}(\Psi^j - \hat{\Psi}^{j-1})$ with

$$\Psi^j := \mathcal{L}_h^j u_h^j + \mathcal{P}_h^j [f(\cdot, t_j, u_h^j)], \quad \hat{\Psi}^{j-1} := \hat{\mathcal{L}}_h^{j-1} \hat{u}_h^{j-1} + \mathcal{P}_h^j [f(\cdot, t_{j-1}, \hat{u}_h^{j-1})], \tag{7.9}$$

while $\vartheta_{\mathcal{L}}$ and ϑ_f are regular functions defined, for $t \in (t_{j-1}, t_j]$, $j = 1, \ldots, M$, by

$$\vartheta_{\mathcal{L},R} := \mathcal{L}(t)\, R - I_t^* [\mathcal{L}(t)\, R], \quad \vartheta_{f,R} := f(\cdot, t, R) - I_t^* [f(\cdot, t, R)], \tag{7.10}$$

with I_t^* and R from (7.6) and (7.7).

Proof. In view of (7.5a), to get the desired bound (7.8) for $u_h^m - u(\cdot, t_m)$, it suffices to obtain a bound of type (7.8) for $R^m - u(\cdot, t_m)$, with $(2\kappa_0 + 1)$ replaced by $2\kappa_0$, and then apply the triangle inequality. So we consider $R^m - u(\cdot, t_m)$ only.

We partially imitate the proof of Theorem 4.1. Let $t \in [t_{j-1}, t_j]$. In view of (7.6), for any left-continuous function $w = w(t)$ with the notation $w^j := w(t_j)$ and $\hat{w}^{j-1} := w(t_{j-1}^+)$, one has $I_t^* w(t) = \frac{1}{2}(\hat{w}^{j-1} + w^j) + (t - t_{j-1/2})\, \delta_t^* w^j$. So combining (7.10) and this property, for $t \in (t_{j-1}, t_j]$, one easily gets

$$f(\cdot, t, R) - \tfrac{1}{2}\big(f(\cdot, t_{j-1}, \hat{R}^{j-1}) + f(\cdot, t_j, R^j)\big) = (t - t_{j-1/2})\, \delta_t^* [f(\cdot, t, R)]^j + \vartheta_{f,R},$$

and a similar relation

$$\mathcal{L}(t)\, R - \tfrac{1}{2}\big(\mathcal{L}^{j-1} \hat{R}^{j-1} + \mathcal{L}^j R^j\big) = (t - t_{j-1/2})\, \delta_t^* [\mathcal{L}(t)\, R]^j + \vartheta_{\mathcal{L},R}.$$

Combining these two observations with (7.3), one deduces that

$$\begin{aligned} \delta_t^* u_h^j + \mathcal{L}(t)\, R + f(\cdot, t, R) &= (t - t_{j-1/2})\, \delta_t^* [\mathcal{L}(t)\, R + f(\cdot, t, R)]^j + [\vartheta_{\mathcal{L},R} + \vartheta_{f,R}] \\ &= (t - t_{j-1/2})\, \delta_t^* \Psi^j + [\vartheta_{\mathcal{L},R} + \vartheta_{f,R}], \end{aligned}$$

where $\delta_t^* u_h^j = \frac{1}{\tau_j}(\Psi^j - \hat{\Psi}^{j-1})$ with

$$\Psi^j := \mathcal{L}^j\, R^j + f(\cdot, t_j, R^j) \quad \text{and} \quad \hat{\Psi}^{j-1} := \mathcal{L}^{j-1}\, \hat{R}^{j-1} + f(\cdot, t_{j-1}, \hat{R}^{j-1}).$$

In view of (7.2), these definitions of Ψ^j and $\hat{\Psi}^{j-1}$ are equivalent to (7.9). Finally,

$$\delta_t^* u_h^j + \mathcal{L}(t)\, R + f(\cdot, t, R) = \partial_t \mu_1(\cdot, t) + [\vartheta_{\mathcal{L},R} + \vartheta_{f,R}] \tag{7.11}$$

for $t \in (t_{j-1}, t_j]$, where $\mu_1 = \mu_1(x, t)$ is a continuous function defined by

$$\mu_1(\cdot, t) := -\tfrac{1}{2}(t_j - t)(t - t_{j-1}) \cdot \delta_t^* \Psi^j \qquad \text{for } t \in [t_{j-1}, t_j]. \tag{7.12}$$

This is easily checked by using the relation $\frac{d}{dt}[-\frac{1}{2}(t_j - t)(t - t_{j-1})] = t - t_{j-1/2}$ to evaluate $\partial_t \mu_1$.

Next, we shall invoke $I_t^* u_h$ defined by (6.14), for which we have (6.15) and (6.16). Combining (7.11) with (1.1a) and then (6.15) yields

$$\begin{aligned} \mathcal{M}R - \mathcal{M}u &= \partial_t R + \mathcal{L}(t)\, R + f(\cdot, t, R) \\ &= \partial_t (R - I_t^* u_h) + \partial_t \mu_1(\cdot, t) + [\vartheta_{\mathcal{L},R} + \vartheta_{f,R} + \vartheta_*] \quad \text{in } Q. \end{aligned} \tag{7.13}$$

So the desired bound of type (7.8) for $R^m - u(\cdot, t_m)$, only with $(2\kappa_0 + 1)$ replaced by $2\kappa_0$, is obtained by an application of Lemma 2.4 to (7.13) with $\mu := \mu_0 + \mu_1 := (R - I_t^* u_h) + \mu_1$ and $\vartheta := \vartheta_{\mathcal{L},R} + \vartheta_{f,R} + \vartheta_*$, using (6.16) and the following two observations. First, $[R - u - \mu](\cdot, 0) = \hat{R}^0 - \varphi - [(\hat{R}^0 - u_h^0) + 0] = u_h^0 - \varphi$. Second, for $t \in (t_{j-1}, t_j]$, we have

$$\begin{aligned} |\mu_0| &\le |R^j - u_h^j| + |\hat{R}^{j-1} - \hat{u}_h^{j-1}|, \qquad & \tau_j\, |\partial_t \mu_0| &\le |R^j - u_h^j| + |\hat{R}^{j-1} - \hat{u}_h^{j-1}|, \\ |\mu_1| &\le \tfrac{1}{8} \tau_j^2\, \big|\delta_t^* \Psi^j\big|, & \tau_j\, |\partial_t \mu_1| &\le \tfrac{1}{2} \tau_j^2\, \big|\delta_t^* \Psi^j\big|, \end{aligned}$$

where we used $\mu_0 = R - I_t^* u_h = I_t^*(R - u_h)$ and (7.12). Finally, recall (7.5) to obtain the required bound for $\|R^m - u(\cdot, t_m)\|_{\infty,\Omega}$. □

Remark 7.2. *It is essential for the **computability** of the error estimator (7.8) that some explicitly computable bounds are available for η^j, $\hat\eta^{j-1}$ and $\|\delta_t^*\Psi^j\|_{\infty,\Omega}$. For this, it is sufficient (but not necessary) that one can explicitly compute Ψ^j and $\hat\Psi^{j-1}$. Indeed, (7.5) and (7.9) show that η^j and $\hat\eta^{j-1}$ are computable via the functions g^j and $\hat g^{j-1}$ of (7.2b), (7.2c), while the latter can be represented as*

$$g^j(\cdot,v) = f(\cdot,t_j,v) - \Psi^j, \qquad \hat g^{j-1}(\cdot,v) = f(\cdot,t_{j-1},v) - \hat\Psi^{j-1}. \tag{7.14}$$

The remaining terms $\vartheta_{\mathcal{L},R}$ and $\vartheta_{f,R}$ in (6.5) can be computed using $\vartheta_{\mathcal{L},I_t^* u_h}$ and $\vartheta_{f,I_t^* u_h}$ as described in Remark 6.3. For example, if $|\partial_z\partial_t^2 f| \le C$ for some constant C, then $\vartheta_{f,R}$ can be effectively replaced by $\vartheta_{f,I_t^* u_h}$ as a calculation shows, for $t\in(t_{j-1},t_j]$, that $\|[\vartheta_{f,R} - \vartheta_{f,I_t^* u_h}](\cdot,t)\|_{\infty,\Omega} \le C\tau_j^2(\eta^j + \hat\eta^{j-1})$.

7.2. Applications to the model problem. Estimator computability. Consider a fully discrete Crank-Nicolson method for (1.3), obtained by applying the spatial discretization (5.5) to the semidiscrete problem (4.1): Find $u_h^j \in \mathring{V}_h^j$ such that

$$\varepsilon^2\big\langle \tfrac12\nabla(\hat u_h^{j-1} + u_h^j), \nabla\chi\big\rangle + \big\langle \tfrac12[f(\cdot,t_{j-1},\hat u_h^{j-1}) + f(\cdot,t_j,u_h^j)] + \delta_t^* u_h^j,\, \chi\big\rangle_h = 0, \tag{7.15}$$

$\forall\chi\in\mathring{V}_h^j$, where $\langle\cdot,\cdot\rangle_h$ is either exactly the inner product $\langle\cdot,\cdot\rangle$ in $L_2(\Omega)$, or some quadrature formula for $\langle\cdot,\cdot\rangle$, and $\delta_t^* u_h^j$ is defined by (7.1c), (7.1d).

Note that the full discretization (7.15) is of type (7.1) with $\hat{\mathcal{L}}_h^{j-1} := \mathcal{L}_h^j$. For some particular cases of $\langle\cdot,\cdot\rangle_h$, the operators $\mathcal{L}_h^j$ and $\mathcal{P}_h^j$ are defined as in Remarks 5.1 and 5.2 only using V_h^j instead of V_h.

7.2.1. Model problem (1.3): regular regime. Let u solve problem (1.3) with $\varepsilon=1$, $\gamma\ge0$, posed in a bounded polyhedral spatial domain $\Omega\subset\mathbb{R}^n$, $n=2,3$, and u_h^j solve the discrete problem (7.15) with V_h^j and $\langle\cdot,\cdot\rangle_h$ defined, for each time level t_j, as in §5.2. To be more specific, we let $\mathcal{T}_h^j$ be a conforming and shape-regular triangulation of $\bar\Omega$ made of elements T, V_h^j be the space of continuous piecewise polynomial finite element functions of degree $l\ge1$, and $\mathring{V}_h^j := V_h^j \cap H_0^1(\Omega)$. We then employ a quadrature formula $\langle\varphi,\psi\rangle_h := \sum_{T\in\mathcal{T}_h^j} Q_T(\varphi\psi)$, as described in §5.2.

Corollary 7.3. *Let the above numerical method be applied to problem (1.3) with $\varepsilon=1$, $\gamma\ge0$. Then the a posteriori error estimate of Theorem 7.1 is valid with $\vartheta_{\mathcal{L},R}=0$ and $\vartheta_{f,R}$ computed as described in Remark 7.2. The quantities η^j and $\hat\eta^{j-1}$ satisfy (7.5) combined with (7.14), where $\eta:=\eta_0$ is defined in (5.6).*

7.2.2. Model problem (1.3): singularly perturbed regime in one dimension. Now consider the regime of $\varepsilon\ll1$. Let u solve the problem (1.3) with $\varepsilon\in(0,1]$, $\gamma>0$, posed in the domain $\Omega:=(0,1)$, and u_h solve the discrete problem (7.15) with V_h^j and $\langle\cdot,\cdot\rangle_h$ defined, for each time level t_j, as in §5.3. Thus V_h^j is the space of continuous ***piecewise-linear*** finite element functions on an arbitrary nonuniform mesh $\{x_i^j\}_{i=1}^{N_j}$ with $0=x_0^j<x_1^j<\cdots<x_{N_j}^j=1$ under absolutely no mesh regularity assumptions. We consider the two choices (5.7a) and (5.7b) of $\langle\cdot,\cdot\rangle_h$, using the piecewise-linear Lagrange polynomial $I_h := I_h^j$ onto V_h^j.

Corollary 7.4. *Let the above numerical method be applied to problem (1.3) with $\varepsilon\in(0,1]$, $\gamma>0$, $\Omega:=(0,1)$. Then the a posteriori error estimate of Theorem 7.1 is valid with $\vartheta_{\mathcal{L},R}=0$ and $\vartheta_{f,R}$ computed as described in Remark 7.2. The quantities η^j and $\hat\eta^{j-1}$ satisfy (7.5) combined with (7.14), where $\eta:=\eta_\varepsilon$ for (5.7a), and $\eta:=\eta_{\varepsilon;\mathrm{l.m.}}$ for (5.7b), while η_ε and $\eta_{\varepsilon;\mathrm{l.m.}}$ are defined in (5.9a) and (5.9b), respectively, in which I_h is now replaced by I_h^j.*

7.2.3. Computability. In view of Remark 7.2, we now further discuss the computability of the error estimator (7.8) when applied to the model problem (1.3).

(i) Suppose that in (7.15), one employs a **lumped-mass** quadrature $\langle \psi, \chi_i \rangle_h$. Then $\mathcal{P}_h^j := I_h^j$ is the Lagrange interpolation operator onto V_h^j, and $\mathcal{L}_h^j v_h = \hat{\mathcal{L}}_h^{j-1} v_h$ is easily computable for any $v_h \in \mathring{V}_h^j$ by applying the normalized stiffness matrix to the column vector of nodal values $\{v_{h,i}\}$; see Remark 5.2. Consequently, η^j, $\hat{\eta}^{j-1}$ and $\|\delta_t^* \Psi^j\|_{\infty,\Omega}$ are explicitly computable, as described in Remark 7.2.

(ii) Let $V_h^j \subset V_h^{j-1}$ for all j. In general, (7.1a) combined with (7.9) yields $\delta_t^* u_h^j + \frac{1}{2}\big(\hat{\Psi}_h^{j-1} + \Psi_h^j\big) = 0$. In our case, one has $\hat{\Psi}_h^{j-1} = \Psi_h^{j-1}$ so $\Psi_h^j = -\Psi_h^{j-1} - 2\delta_t^* u_h^j$ is explicitly computable for $j = 1, \dots, M$ provided that Ψ_h^0 is computed (as in (iii)).

(iii) In the general case, the computation of $\mathcal{L}_h^j v_h$, and hence of $\hat{\Psi}_h^{j-1}$ and Ψ_h^j, may be more expensive. Roughly speaking, $\mathcal{L}_h^j v_h$ can be obtained by an application of $M_j^{-1} K_j$ to the column vector of nodal values $\{v_{h,i}\}$, where M_j is the mass matrix and K_j is the stiffness matrix associated with the time level t_j. Note that the computation of u_h^j at each time level by the Crank-Nicolon method already involves an application of M_j^{-1}. Furthermore, in some cases, an inversion of M_j can be entirely avoided by using bounds of the type $\big\|\delta_t^* \Psi^j\big\|_{\infty,\Omega} \le \|M_j^{-1}\|_\infty \cdot \big\|\delta_t^*(M_j \Psi^j)\big\|_{\infty,\Omega}$, where $\|M_j^{-1}\|_\infty$ denotes the associated matrix norm (which may be bounded a priori).

8. Proof of Lemma 2.2. First, note that the Green's function $\mathcal{G}$ associated with our problem (1.3) in the spatial domain Ω and the Green's function $\hat{\mathcal{G}}$ for the related problem $\hat{\mathcal{M}}\hat{u} := \partial_t \hat{u} - \triangle \hat{u} + f(x/\varepsilon, t, \hat{u}) = 0$ in the spatial domain $\hat{\Omega} := \Omega/\varepsilon$ satisfy $\|\partial_s^k \mathcal{G}(x,t;\cdot,s)\|_{1,\Omega} = \|\partial_s^k \hat{\mathcal{G}}(x/\varepsilon,t;\cdot,s)\|_{1,\hat{\Omega}}$ for $k = 0, 1$. Consequently, it suffices to prove Condition 2.1 for the case of $\varepsilon = 1$ with κ_0, κ_1 and κ_2 independent of $|\Omega|$, so throughout the proof we set $\mathcal{L}^* = -\triangle$ in (2.1a).

(i) We start by proving the first bound in Condition 2.1. The Green's function $\bar{\mathcal{G}}$ associated with $\bar{\mathcal{M}} := \partial_t - \triangle + \gamma^2$ in the domain $\bar{\Omega} := \mathbb{R}^n$ can be easily obtained from the fundamental solution of the heat equation (the latter can be found, e.g., in [17, §III.3], [5, §2.3.1]. So one gets

$$\bar{\mathcal{G}}(x,t;\xi,s) = g(x-\xi, t-s), \quad \text{where} \quad g(x,t) := \frac{\mathrm{e}^{-\gamma^2 t}}{(4\pi t)^{n/2}} \exp\Big(-\frac{|x|^2}{4t}\Big). \tag{8.1}$$

Next, note that, by (1.2), the coefficient a in (2.1a) satisfies $a \ge \gamma^2$ so an application of the maximum principle to problem (2.1) yields $0 \le \mathcal{G} \le \bar{\mathcal{G}}$. Finally, note that

$$\bar{\mathcal{G}}(x,t;\xi,s)\,\mathrm{d}\xi = \mathrm{e}^{-\gamma^2(t-s)}\,\psi(\zeta)\,\mathrm{d}\zeta, \quad \text{where} \quad \psi(\zeta) := \frac{\mathrm{e}^{-|\zeta|^2}}{\pi^{n/2}}, \quad \zeta := \frac{\xi - x}{2\sqrt{t-s}}. \tag{8.2}$$

As $\int_{\mathbb{R}^n} \psi(\zeta)\,\mathrm{d}\zeta = 1$, we immediately get $\|\bar{\mathcal{G}}(x,t;\cdot,s)\|_{1,\Omega} \le 1$, which yields the first bound in Condition 2.1 with $\kappa_0 = 1$.

(ii) Next, we prove the second bound in Condition 2.1 in the linear case of $f(x,t,z) = a(x)z + b(x,t)$ with $\kappa_2 = 0$. In this case, the differential operator in (2.1) does not involve s, so one can invoke [2, Corollary 5] (in using this result, we imitate the proof of [3, Lemma 2.1]). In view of the above bound $0 \le \mathcal{G} \le \bar{\mathcal{G}}$, an application of [2, Corollary 5] with $\beta = 2$, $\gamma = 1$, $c_1 = \frac{1}{4}$, $c_2 = \frac{4}{9}c_1$ and $\alpha(t) = \frac{\mathrm{e}^{-\gamma^2 t}}{(4\pi t)^{n/2}}$ yields $|\partial_s \mathcal{G}(x,t;\xi,s)| \le 18 c_1 c_2\,(t-s)^{-1}\,\alpha(\frac{1}{2}[t-s])\,\mathrm{e}^{-(c_2/c_1)|\zeta|^2}$, where ζ is chosen as in part (i) of this proof. Now an observation similar to (8.2) leads to the estimate $\|\partial_s \mathcal{G}(x,t;\cdot,s)\|_{1,\Omega} \le \kappa_1 (t-s)^{-1} \mathrm{e}^{-\frac{1}{2}\gamma^2(t-s)}$, which immediately implies the second bound in Condition 2.1 with $\kappa_2 = 0$.

(iii) It remains to establish the second bound in Condition 2.1 in the general case of $f(x,t,z)$ satisfying (1.2), which implies that for the coefficient a in (2.1a) one has $\gamma^2 \le a(\xi,s) \le \bar\gamma^2$. For any fixed $(x,t)\in\Omega\times(0,T]$, consider the Green's function $\hat{\mathcal{G}}(x,t;\xi,s) =: \hat\Gamma(\xi,s)$ associated with the operator $\partial_t - \triangle + \gamma^2$ in the domain Ω so $\hat\Gamma(\xi,s)$ satisfies a version of (2.1) with a replaced by γ^2. Comparing this problem with the problem (2.1) for Γ and noting that $\mathcal{L}=\mathcal{L}^*=\triangle$, we find that for any fixed (x,t), the function $v(\xi,s) := \hat\Gamma(\xi,s) - \Gamma(\xi,s)$ solves the terminal-value problem

$$[-\partial_s - \triangle + \gamma^2\,]\, v(\xi,s) = F(\xi,s) \quad \text{for} \quad (\xi,s)\in\Omega\times[0,t), \tag{8.3a}$$

$$v(\xi,t) = 0 \qquad \text{for} \quad \xi\in\Omega, \tag{8.3b}$$

$$v(\xi,s) = 0 \qquad \text{for} \quad (\xi,s)\in\partial\Omega\times[0,t], \tag{8.3c}$$

where $F(\xi,s) := [a(\xi,s)-\gamma^2]\,\Gamma(\xi,s)$ so, using $\Gamma\le\bar G$ and (8.1),

$$0 \le F(\xi,s) \le (\bar\gamma^2-\gamma^2)\, g(x-\xi,t-s). \tag{8.3d}$$

Note that in part (ii) we have shown that $\hat\Gamma$ satisfies the second bound in Condition 2.1 with $\kappa_2=0$. So it remains to show that v satisfies the second bound in Condition 2.1 with $\kappa_1=0$ and $\kappa_2=(\bar\gamma^2-\gamma^2)\hat\kappa_2$. This latter bound is immediately obtained by an application of Lemma 8.1 below to the terminal-value problem (8.3). □

The next lemma is applied to the terminal-value problem (8.3), but it is convenient to formulate it in the context of an initial-value problem.

LEMMA 8.1. *Let v satisfy $[\partial_t - \triangle + \gamma^2]\,v = F$ in Q and vanish for $t=0$ and $x\in\partial\Omega$, where $0\le F(x,t)\le g(x-x_0,t)$ with g from (8.1) and some $x_0\in\Omega$. Then $\int_0^T \|\partial_t v(\cdot,t)\|_{1,\Omega}\,\mathrm{d}t \le \hat\kappa_2$, where $\hat\kappa_2$ is independent of $|\Omega|$, and $\hat\kappa_2=\hat\kappa_2(\gamma)$ if $\gamma>0$, while $\hat\kappa_2=\hat\kappa_2(T)$ if $\gamma=0$.*

Proof. Without loss of generality, assume that $x_0=0\in\Omega$ so $F(x,t)\le g(x,t)$. Recall that $\bar{\mathcal{M}}g=0$ with $\bar{\mathcal{M}}=\partial_t-\triangle+\gamma^2$; this implies that $\bar M[tg]=g$, so an application of the maximum principle yields

$$0\le v(x,t)\le t\,g(x,t). \tag{8.4}$$

(i) First we establish the desired estimate with $\hat\kappa_2$ that depends on $|\Omega|$. Let $w(x,t) := \varrho(t)\,v$ with the weight $\varrho := t^{\frac13}\,\mathrm{e}^{\frac12\gamma^2 t}$ so $\varrho' = (\frac13 t^{-1}+\frac12\gamma^2)\,\varrho$. Note that

$$\begin{aligned}\|\partial_t v\|_{1,\Omega\times[0,T]} &\le \|\varrho^{-1}\|_{2,\Omega\times[0,T]}\;\|\varrho\,\partial_t v\|_{2,\Omega\times[0,T]}\\ &\le \hat\kappa_3\,|\Omega|^{\frac12}\Big(\|\partial_t w\|_{2,\Omega\times[0,T]}+\|\varrho'\,v\|_{2,\Omega\times[0,T]}\Big),\end{aligned} \tag{8.5}$$

where we used $\varrho\,\partial_t v = \partial_t w - \varrho'\,v$ and

$$\|\varrho^{-1}\|^2_{2,\Omega\times[0,T]} = |\Omega|\int_0^T t^{-\frac23}\,\mathrm{e}^{-\gamma^2 t}\,\mathrm{d}t =: |\Omega|\,\hat\kappa_3^2$$

(so $\hat\kappa_3^2\le 3T^{1/3}$ for $\gamma\ge0$, and $\int_0^\infty t^{-\frac23}\,\mathrm{e}^{-t}\,\mathrm{d}t\approx 2.7$ implies $\hat\kappa_3^2\lesssim 2.7\gamma^{-2/3}$ for $\gamma>0$). To estimate $\partial_t w$ in (8.5), we note that $\bar{\mathcal{M}}w = \varrho\,F+\varrho'\,v\le\varrho\,g+\varrho'\,v$ and so apply an a priori estimate [10, (6.6) of Chapter III]:

$$\|\partial_t w\|_{2,\Omega\times[0,T]} \le \|\bar{\mathcal{M}}w\|_{2,\Omega\times[0,T]} \tag{8.6}$$

(in fact, the cited estimate is given for a slightly different differential operator, but the argument also applies to $\bar{\mathcal{M}}$). In view of $\varrho' v \le (\frac{1}{3}+\frac{1}{2}\gamma^2 t)\,\varrho\, g$ (which follows from (8.4)), one gets

$$\|\partial_t v\|_{1,\Omega\times[0,T]} \le 2\,\hat\kappa_3\,|\Omega|^{\frac12}\,\|\hat\varrho\, g\|_{2,\Omega\times[0,T]}, \qquad \text{where} \quad \hat\varrho := (\tfrac{4}{3}+\tfrac{1}{2}\gamma^2 t)\,\varrho. \tag{8.7}$$

Finally, a calculation using $\zeta := \frac{x}{\sqrt{2t}}$ and $\psi(\zeta)$ from (8.2) yields

$$\|\hat\varrho\, g\|^2_{2,\Omega\times[0,T]} \le \int_0^T \frac{\hat\varrho^2(t)\,\mathrm{e}^{-2\gamma^2 t}}{(8\pi t)^{n/2}} \int_{\mathbb{R}^n} \psi(\zeta)\,\mathrm{d}\zeta\,\mathrm{d}t = \int_0^T \frac{\big(\frac43+\frac12\gamma^2 t\big)^2\, t^{2/3}\,\mathrm{e}^{-\gamma^2 t}}{(8\pi t)^{n/2}}\,\mathrm{d}t =: \hat\kappa_4^2$$

(this integral is convergent as $\frac{n}{2}-\frac{2}{3}<1$ for $n\le 3$). Combining this with (8.7), we arrive at the desired bound with $\hat\kappa_2 := 2\,\hat\kappa_3\hat\kappa_4\,|\Omega|^{\frac12}$.

(ii) Now we shall show the desired result with $\hat\kappa_2$ independent of $|\Omega|$ (which requires a more subtle estimation). Divide $\mathbb{R}^n$ into the non-overlapping subdomains $\Omega_0 := \{|x|<2\}$ and $\Omega_j := \{2^j<|x|<2^{j+1}\}$ for $j=1,\ldots$; furthermore let $\Omega'_0 := \Omega$ and $\Omega'_j := \{2^{j-1}<|x|<2^{j+2}\}\supset\Omega_j$. Note that

$$|\Omega_j|^{\frac12} \le c_n\, 2^{\frac12 nj}. \tag{8.8}$$

Now we partially imitate the proof in part (i). First, note that one has the bound (8.5) with Ω replaced by Ω_j for $j=0,1,\ldots$. So for $j=0$, using the results of part (i), one immediately gets

$$\|\partial_t v\|_{1,(\Omega\cup\Omega_0)\times[0,T]} \le 2\,\hat\kappa_3\hat\kappa_4\,|\Omega_0|^{\frac12} \tag{8.9}$$

(compare with $\hat\kappa_2$ from part (i)).

For $j\ge 1$, we combine the local version of (8.5) with a local version of the global estimate (8.6) from

$$\|\partial_t w\|_{2,(\Omega\cap\Omega_j)\times[0,T]} \le \bar C\Big\{\|\bar{\mathcal{M}} w\|_{2,(\Omega\cap\Omega'_j)\times[0,T]} + \|w\|_{2,(\Omega\cap\Omega'_j)\times[0,T]}\Big\},$$

with the constant $\bar C$ independent of Ω and T (this estimate is obtained similarly to [10, (6.6), (6.11) of Chapter III]). Here $\bar{\mathcal{M}} w$ is estimated as in part (i), while $w=\varrho\, v\le t\varrho\, g$ by (8.4). This yields a local version of (8.7):

$$\|\partial_t v\|_{1,(\Omega\cup\Omega_j)\times[0,T]} \le 2\,\hat\kappa_3\,|\Omega_j|^{\frac12}\;\bar C\,\|(\hat\varrho+t\varrho)\,g\|_{2,\Omega'_j\times[0,T]} \qquad \text{for } j\ge 1. \tag{8.10}$$

Next, we use $\zeta := \frac{x}{2\sqrt{t}}$ and $\psi(\zeta)$ from (8.2), and also the observation that as $j\ge1$ so $(\exp(-\frac{|x|^2}{4t}))^2 \le \mathrm{e}^{-\frac{4^{j-2}}{t}}\,\mathrm{e}^{-|\zeta|^2} \le c'_n\,(\frac{t}{4^j})^n\,\mathrm{e}^{-|\zeta|^2}$. So for $j\ge1$ a calculation shows that

$$\|(\hat\varrho+t\varrho)\,g\|^2_{2,\Omega'_j\times[0,T]} \le c'_n\,4^{-jn}\int_0^T \frac{(\hat\varrho+t\varrho)^2\,\mathrm{e}^{-2\gamma^2 t}\,t^n}{(4\pi t)^{n/2}}\int_{\mathbb{R}^n}\psi(\zeta)\,\mathrm{d}\zeta\,\mathrm{d}t = c''_n\,4^{-jn}.$$

Combining this with (8.10) and then with (8.9) and (8.8), we arrive at

$$\|\partial_t v\|_{1,(\Omega\cup\Omega_j)\times[0,T]} \le 2\,\hat\kappa_3\,c_n \begin{cases} \hat\kappa_4 & \text{for } j=0,\\ \sqrt{c''_n}\,2^{-\frac12 nj} & \text{for } j\ge 1.\end{cases}$$

This immediately yields the desired bound with $\hat\kappa_2 := 2\,\hat\kappa_3\,c_n[\hat\kappa_4+\sqrt{c''_n}\,(2^{\frac12 n}-1)^{-1}]$ independent of $|\Omega|$. □

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