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MAXIMUM NORM A POSTERIORI ERROR ESTIMATION FOR A TIME-DEPENDENT REACTION-DIFFUSION PROBLEM

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Dedicated to Professor Martin Stynes on occasion of his 60th birthday

Abstract — A semilinear second-order singularly perturbed parabolic equation in one space dimension is considered. For this equation, we give computable a posteriori error estimates in the maximum norm for a difference scheme that uses Backward-Euler in time and central differencing in space. Sharp L_1-norm bounds for the Green's function of the parabolic operator and its derivatives are derived that form the basis of the a posteriori error analysis. Numerical results are presented.

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1. Introduction

Consider the singularly perturbed second-order semilinear parabolic problem of finding $u : [0,1] \times [0,T] \to \mathbb{R}$ such that

$$\mathcal{M}u := \partial_t u - \varepsilon^2 \partial_x^2 u + \varphi(\cdot,\cdot,u) = 0 \quad \text{in } (0,1)\times(0,T], \tag{1a}$$

with a small parameter $\varepsilon \in (0,1]$, subject to the initial and homogeneous Dirichlet boundary conditions

$$u(\cdot,0) = u_0 \quad \text{on } [0,1], \tag{1b}$$

$$u(0,\cdot) = u(1,\cdot) = 0 \quad \text{on } [0,T]. \tag{1c}$$

We assume that $\varphi : [0,1]\times[0,T]\times\mathbb{R} \to \mathbb{R}$ is differentiable in the third argument and, for some constants ϱ and $\bar{\varrho}$, satisfies

$$0 \leqslant \varrho^2 \leqslant \partial_z \varphi(x,t,z) \leqslant \bar{\varrho}^2 \quad \text{for} \quad (x,t,z) \in [0,1]\times[0,T]\times\mathbb{R}. \tag{2}$$

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Note that when $\varepsilon \ll 1$, solutions of (1) may exhibit sharp boundary layers; furthermore, sharp interior layers may form in the solution if the initial data u_0 is discontinuous.

The purpose of this paper is to obtain computable error bounds in the maximum norm for a difference scheme applied to problem (1). The method combines a Backward-Euler discretisation in time with a central three-point discretisation in space on an arbitrary mesh.

Relation to earlier results. Novelty.

(i) We shall give a posteriori error estimates in the *maximum norm*, which is sufficiently strong to capture the layers. As we consider a singularly perturbed equation, we are interested in error estimates that work for all values of the *singular perturbation parameter* ε so any dependence on this parameter will be shown explicitly.

Note that earlier pointwise/maximum-norm a posteriori error estimates for parabolic problems are typically given for regular (i.e. non-singularly perturbed) equations [1, 4, 5, 7]. The only such estimates for singularly perturbed equations that we are aware of are by the authors [14, 15], for FEMs applied to a higher-dimensional version of (1). Three discretisations in time were considered in [14, 15]: the first-order implicit Euler method, the second-order Crank-Nicolson method, and the third-order discontinuous Galerkin method dG(1); the relation of the present paper to [14] is discussed in item (iv) below.

(ii) 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 $p = 1$ is the discretisation order of the Backward-Euler method and τ_j is the local step size in time. For this, similarly to [14], we use computed-solution interpolants that are *piecewise-constant* in time. Consequently, we allow the residuals of computed solutions to be understood as *distributions* [9]; this inclusion plays a crucial role in our analysis and simplifies the arguments.

The Backward-Euler method for the equation $u_t - \triangle u = f$ was considered in [7, 4] and $u_t - \triangle u + u = f$ in [5]. The a posteriori error estimate of Theorem 3.1 below resembles (but is not identical with) the one of [7, (1.13)] in that it involves terms such as $|U^j - U^{j-1}|$, where U^j is the computed solution at time t_j, that may be interpreted as approximating $\tau_j|\partial_t u|$. (Note also that [7, (1.13)] is given without proof, and does not appear to be proved elsewhere).

By contrast, the a posteriori error estimates of [4, 5] include terms (denoted there by $\tau_j|g^j - g^{j-1}|$) that may be interpreted as approximating the quantity $\tau_j|\partial_t^2 u + \dots|$, which seems less suitable for a first-order method in time.

(iii) Similarly to [4, 5, 14, 15], the a posteriori error analysis in this paper considerably relies on certain bounds for the *Green's function* of the continuous parabolic operator. To be more specific, we estimate the Green's function and its spatial and temporal derivatives in the spatial L_1 norm (which is dual to the maximum norm L_∞ in which we estimate the solution errors). Crucially, any dependence on the small perturbation parameter ε is shown explicitly. These bounds are of independent interest. For example, they may be used in [14, 15] in the singularly perturbed regime. In a more general numerical-analysis context, we note that sharp estimates for continuous Green's functions (or their generalised versions) frequently play a crucial role in a priori and a posteriori error analyses [6, 10, 17, 13].

(iv) One distinctive feature of [4, 5], as well as [14, 15], is the use of an elliptic reconstruction technique, which was recently introduced as a counterpart of the Ritz-projection in the a posteriori error estimation for parabolic problems. By contrast, in this paper we use a *direct analysis*. In comparison, this approach typically requires a more intricate analysis, and for this reason may be less general, but it yields *sharper* error estimates, or, to be more precise, similar estimates but with sharper error constants. (As a posteriori error

estimates are derived to be used in adaptive algorithms, less sharp error constants result in mesh overrefinement and consequently, make the algorithm less efficient.)

Our interest in considering a direct analysis, even in a simpler one space dimension, is partly motivated by a comparison of the resulting error estimates with a similar, but supposedly less sharp estimate of [14], obtained using elliptic reconstructions. Indeed, here we get a similar, but sharper error estimate; furthermore, a comparison suggests that the results of [14] are reasonably sharp; see Remark 3.2.

Note that the bounds for the parabolic Green's function of this paper may be extended to higher space dimensions for cubic or smooth spatial domains (along the lines of [13]), the main difficulty lying in estimating spatial derivatives. Consequently, in some cases, the direct-analysis error estimates of §3 may be extended to higher dimensions as well, but this would require considerably more tedious calculations.

Outline. The paper is organised as follows. In Section 2, we derive estimates for the Green's function associated with the differential operator $\mathcal{M}$ in (1). We shall distinguish between the special linear case of $\varphi(x,t,z) = r(x)z - f(x,t)$, for which our Green's function bounds are sharp, and the general semilinear case, for which they are sharp only up to an ε-independent multiplier. These Green's-function bounds are used in Section 3 to obtain a posteriori error estimates for our finite difference scheme applied to (1). Results of numerical experiments are presented in Section 4.

2. The Green's function

Estimates for the Green's function for the linear version of problem (1) with $\varphi(x,t,z) = r(x)z - f(x,t)$ will be derived in three steps by considering: *(i)* constant coefficient $r \equiv \gamma^2$, infinite spatial domain, *(ii)* constant coefficient $r \equiv \gamma^2$, bounded spatial domain $(0,1)$, and *(iii)* variable coefficient r, bounded spatial domain $(0,1)$. In §2.4 the general case of a semilinear problem will be briefly discussed.

Notation. Subsequently, C denotes a generic positive constant that may take different values in different formulae, but is *independent of the diffusion coefficient* ε.

2.1. Constant-coefficient problem in an infinite spatial domain

For the constant-coefficient operator $\bar{\mathcal{M}} := \partial_t - \varepsilon^2\partial_x^2 + \gamma^2$ in $\mathbb{R}\times\mathbb{R}_+$, we denote the associated Green's function by $\bar{\mathcal{G}} = \bar{\mathcal{G}}(x,t;\xi,s)$. For fixed (x,t), this function $\bar{\mathcal{G}}(x,t;\xi,s) =: \bar{\Gamma}^*(\xi,s)$ solves the adjoint terminal-value problem

$$\bar{\mathcal{M}}^*\bar{\Gamma}^* := [-\partial_s - \varepsilon^2\partial_\xi^2 + \gamma^2]\,\bar{\Gamma}^*(\xi,s) = 0 \qquad \text{for } (\xi,s) \in \mathbb{R}\times[0,t), \tag{3a}$$

$$\bar{\Gamma}^*(\xi,t) = \delta(\xi - x) \qquad \text{for } \xi \in \mathbb{R}. \tag{3b}$$

The Green's function $\bar{\mathcal{G}}$ can be easily obtained from the fundamental solution of the heat equation. The latter can be found, e.g., in [18, §III.3], [8, §2.3.1]. So one gets

$$\bar{\mathcal{G}}(x,t;\xi,s) = \frac{\mathrm{e}^{-\gamma^2(t-s)}}{2\varepsilon\sqrt{\pi(t-s)}}\exp\left(-\frac{(\xi-x)^2}{4\varepsilon^2(t-s)}\right). \tag{4}$$

Lemma 2.1. *The Green's function $\bar{\mathcal{G}}$ associated with the operator $\bar{\mathcal{M}}$ on an infinite domain satisfies, for $k = 0,1,2,$ the bounds*

$$\int_{-\infty}^{\infty}\left|\partial_\xi^k\bar{\mathcal{G}}(x,t;\xi,s)\right|\,\mathrm{d}\xi = \kappa_k\,\frac{\mathrm{e}^{-\gamma^2(t-s)}}{\varepsilon^k(t-s)^{k/2}}, \tag{5}$$

with $\kappa_0 = 1$, $\kappa_1 = 1/\sqrt{\pi}$ *and* $\kappa_2 = \sqrt{2/(\pi \mathrm{e})}$.

Proof. First note that, for $x, \xi, t, s \in \mathbb{R}$, $t > s$, the Green's function $\bar{\mathcal{G}}$ of (4) is positive and piecewise monotone, i.e., $\bar{\mathcal{G}}(x, t; \xi, s) > 0$,

$$\partial_\xi \bar{\mathcal{G}}(x, t; \xi, s) > 0 \quad \text{if } \xi < x, \quad \text{and} \quad \partial_\xi \bar{\mathcal{G}}(x, t; \xi, s) < 0 \quad \text{if } x < \xi.$$

Furthermore,

$$\bar{\mathcal{G}}(x, t; \xi, s)\, \mathrm{d}\xi = \mathrm{e}^{-\gamma^2(t-s)}\, \psi(\zeta)\, \mathrm{d}\zeta, \quad \text{where} \quad \psi(\zeta) := \frac{\mathrm{e}^{-\zeta^2}}{\sqrt{\pi}}, \quad \zeta := \frac{\xi - x}{2\varepsilon\sqrt{t-s}}. \tag{6}$$

Here ψ is the density function of the normalised Gaussian distribution with the property $\int_{-\infty}^{\infty} \psi(\zeta)\, \mathrm{d}\zeta = 1$. This observation immediately yields (5) for $k = 0$.

Next, because of the sign and the symmetry property of $\partial_\xi \bar{\mathcal{G}}$ we have

$$\int_{-\infty}^{\infty} \left|\partial_\xi \bar{\mathcal{G}}(x, t; \xi, s)\right| \mathrm{d}\xi = 2 \int_{-\infty}^{x} \partial_\xi \bar{\mathcal{G}}(x, t; \xi, s)\, \mathrm{d}\xi = 2\bar{\mathcal{G}}(x, t; x, s),$$

which, combined with (4), implies (5) for $k = 1$.

It remains to establish (5) for $k = 2$. Using (6) and noting that $\partial_\xi \zeta = 1/(2\varepsilon\sqrt{t-s})$ and $\partial_\xi^2 \zeta = 0$, one gets

$$\partial_\xi^2 \bar{\mathcal{G}}(x, t; \xi, s) = 2(\partial_\xi^2 \zeta)^2\, (2\zeta^2 - 1)\, \bar{\mathcal{G}}(x, t; \xi, s) = \frac{2\zeta^2 - 1}{2\varepsilon^2(t-s)} \bar{\mathcal{G}}(x, t; \xi, s). \tag{7}$$

Consequently,

$$\int_{-\infty}^{\infty} \left|\partial_\xi^2 \bar{\mathcal{G}}(x, t; \xi, s)\right| \mathrm{d}\xi = \frac{\mathrm{e}^{-\gamma^2(t-s)}}{2\varepsilon^2(t-s)} \int_{-\infty}^{\infty} \left|2\zeta^2 - 1\right| \psi(\zeta)\, \mathrm{d}\zeta,$$

which yields (5) for $k = 2$. □

Next, we consider two related auxiliary functions that will be used when estimating the Green's functions in the finite spatial domain $[0, 1]$. Let

$$\tilde{\mathcal{G}}_0(x, t; \xi, s) := \bar{\mathcal{G}}(x, t; \xi, s) - \bar{\mathcal{G}}(x, t; -\xi, s) - \bar{\mathcal{G}}(x, t; 2 - \xi, s), \tag{8a}$$

$$\tilde{\mathcal{G}}_1(x, t; \xi, s) := \bar{\mathcal{G}}(x, t; \xi, s) + \bar{\mathcal{G}}(x, t; -\xi, s) + \bar{\mathcal{G}}(x, t; 2 - \xi, s). \tag{8b}$$

Note that, in view of (4),

$$\partial_\xi \tilde{\mathcal{G}}_0(x, t; \xi, s) = -\partial_x \tilde{\mathcal{G}}_1(x, t; \xi, s). \tag{9}$$

Furthermore,

$$\int_0^1 |\partial_\xi^k \tilde{\mathcal{G}}_m(x, t; \xi, s)|\, \mathrm{d}\xi \leqslant \int_{-\infty}^{\infty} |\partial_\xi^k \bar{\mathcal{G}}(x, t; \xi, s)|\, \mathrm{d}\xi \quad \text{for } m = 0, 1,\ k = 0, 1, 2. \tag{10}$$

The assertion (10) is easily checked setting $v(\xi) := \partial_\xi^k \bar{\mathcal{G}}(x, t; \xi, s)$ and then noting that $\int_0^1 |v(-\xi)|\, \mathrm{d}\xi = \int_{-1}^0 |v(\xi)|\, \mathrm{d}\xi$ and $\int_0^1 |v(2 - \xi)|\, \mathrm{d}\xi = \int_1^2 |v(\xi)|\, \mathrm{d}\xi$.

Finally, when studying the variable coefficient case, we shall also use

$$\int_{-\infty}^{\infty} |\xi - x|\ \bar{\mathcal{G}}(x, t; \xi, s)\, \mathrm{d}\xi = \frac{2\varepsilon}{\sqrt{\pi}} \sqrt{t-s}\, \mathrm{e}^{-\gamma^2(t-s)}, \tag{11}$$

which immediately follows from (6), and

$$\int_0^1 |\xi - x|\, \big|\partial_\xi \tilde{\mathcal{G}}_0(x,t;\xi,s)\big|\, \mathrm{d}\xi \leqslant \int_{-\infty}^{\infty} |x-\xi|\, \big|\partial_\xi \bar{\mathcal{G}}(x,t;\xi,s)\big|\, \mathrm{d}\xi = \kappa_0 \mathrm{e}^{-\gamma^2(t-s)}. \tag{12}$$

Here the first relation is obtained similarly to (10) using $v(\xi) := \partial_\xi \bar{\mathcal{G}}(x,t;\xi,s)$. Clearly, $\int_0^1 |\xi - x|\,|v(-\xi)|\,\mathrm{d}\xi = \int_{-1}^0 |\xi + x|\,|v(\xi)|\,\mathrm{d}\xi$, $\int_0^1 |\xi - x|\,|v(2-\xi)|\,\mathrm{d}\xi = \int_1^2 |\xi + x - 2|\,|v(\xi)|\,\mathrm{d}\xi$. Next, we observe that $x \in (0,1)$ so for $\xi \in (-1,0)$ one has $|\xi - x| = |\xi| + |x| \geqslant |\xi + x|$, while for $\xi \in (1,2)$ one has $|\xi - x| = |\xi - 1| + |1 - x| \geqslant |\xi + x - 2|$. The second line in (12) follows from (4).

2.2. Constant-coefficient problem in a bounded spatial domain

Let us again consider the constant-coefficient operator $\bar{\mathcal{M}}$, introduced in §2.1, but now in the bounded spatial domain $[0,1]$. The associated Green's function is denoted by $\hat{\mathcal{G}}(x,t;\xi,s)$. For fixed (x,t), the function $\hat{\mathcal{G}}(x,t;\xi,s) =: \hat{\Gamma}^*(\xi,s)$ solves the terminal-value problem

$$\bar{\mathcal{M}}^*\hat{\Gamma}^* = [-\partial_s - \varepsilon^2\partial_\xi^2 + \gamma^2]\,\hat{\Gamma}^*(\xi,s) = 0 \quad \text{for} \quad (\xi,s) \in (0,1)\times[0,t), \tag{13a}$$

$$\hat{\Gamma}^*(\xi,t) = \delta(\xi - x) \text{ for } \xi \in (0,1), \tag{13b}$$

$$\hat{\Gamma}^*(0,s) = \hat{\Gamma}^*(1,s) = 0 \quad \text{for} \quad s \in [0,t]. \tag{13c}$$

Shortly, we shall see that the function $\tilde{\mathcal{G}}_0$ of (8a) gives an approximation to $\hat{\mathcal{G}}$. Indeed, in view of (3), $\tilde{\mathcal{G}}_0$ satisfies (13a) and (13b), but not (13c). Consequently, for fixed (x,t), the function $g(\xi,s) := \hat{\mathcal{G}}(x,t;\xi,s) - \tilde{\mathcal{G}}_0(x,t;\xi,s)$ satisfies the terminal-value problem

$$\bar{\mathcal{M}}^* g(\xi,s) = 0 \quad \text{for } (\xi,s) \in (0,1)\times[0,t), \tag{14a}$$

$$g(\xi,t) = 0 \quad \text{for } \xi \in (0,1), \tag{14b}$$

$$g(0,s) = \bar{\mathcal{G}}(x,t;2,s) \quad \text{for } s \in [0,t], \tag{14c}$$

$$g(1,s) = \bar{\mathcal{G}}(x,t;-1,s) \quad \text{for } s \in [0,t]. \tag{14d}$$

Here the boundary conditions follow from (8a) and (13c).

Furthermore, for $\partial_\xi^2 g$ one has a similar terminal-value problem:

$$\bar{\mathcal{M}}^*\, \partial_\xi^2 g(\xi,s) = 0 \quad \text{for } (\xi,s) \in (0,1)\times[0,t), \tag{15a}$$

$$\partial_\xi^2 g(\xi,t) = 0 \quad \text{for } \xi \in (0,1), \tag{15b}$$

$$\partial_\xi^2 g(0,s) = \partial_\xi^2 \bar{\mathcal{G}}(x,t;2,s) \quad \text{for } s \in [0,t], \tag{15c}$$

$$\partial_\xi^2 g(1,s) = \partial_\xi^2 \bar{\mathcal{G}}(x,t;-1,s) \quad \text{for } s \in [0,t]. \tag{15d}$$

Here the boundary conditions are obtained noting that (13a) and (13c) imply that $\partial_\xi^2\hat{\Gamma}^*\big|_{\xi=0,1} = 0$ and hence $\partial_\xi^2 g\big|_{\xi=0,1} = -\partial_\xi^2\tilde{\mathcal{G}}_0\big|_{\xi=0,1}$, and then employing (8a) to evaluate $\partial_\xi^2\tilde{\mathcal{G}}_0$ at $\xi = 0, 1$.

Next, we estimate the boundary data in problems (14) and (15). Let $p > 0$ be arbitrary, but fixed. Note that for ψ of (6), there exists a constant $C = C(p) > 0$ such that

$$|\zeta|\,\psi(\zeta) \leqslant C|\zeta|^{-p} \quad \text{and} \quad 2|\zeta|^3(2\zeta^2 - 1)\,\psi(\zeta) \leqslant C|\zeta|^{-p}. \tag{16}$$

Using (6) and (7), one gets

$$\bar{\mathcal{G}}(x,t;\xi,s) = \mathrm{e}^{-\gamma^2(t-s)}\,\frac{\zeta\,\psi(\zeta)}{\xi - x}, \quad \partial_\xi^2 \bar{\mathcal{G}}(x,t;\xi,s) = \mathrm{e}^{-\gamma^2(t-s)}\,\frac{2\zeta^3(2\zeta^2-1)\,\psi(\zeta)}{(\xi-x)^3}.$$

Combine this with (16). Then note that for $\xi = -1, 2$ and $x \in [0,1]$ we have $|\xi - x| \geqslant 1$ so $|\zeta| \geqslant 1/(2\varepsilon\sqrt{t-s})$. Consequently,

$$\left|\partial_\xi^k \bar{\mathcal{G}}(x,t;\xi,s)\right| \leqslant C\varepsilon^p\,(t-s)^{p/2}\,\mathrm{e}^{-\gamma^2(t-s)} \qquad \text{for}\ \ k=0,2,\ \ \xi=-1,2,\ \ x\in[0,1].$$

Now an application of the maximum/comparison principle to problems (14) and (15) yields

$$\left|\partial_\xi^k g(\xi,s)\right| \leqslant C\varepsilon^p\,(t-s)^{p/2}\,\mathrm{e}^{-\gamma^2(t-s)} \tag{17}$$

for $k = 0, 2$. For $k = 1$, the bound (17) follows in view of [2, Lemma 1].

Finally, recalling that $\hat{\mathcal{G}} = \tilde{\mathcal{G}}_0 + g$ and then combining (17) with (10) and (5), we arrive at a version of Lemma 2.1 for $\hat{\mathcal{G}}$.

Lemma 2.2. *Let $p > 0$ be fixed. Then there exists a constant $C = C(p)$ such that for the Green's function $\hat{\mathcal{G}}$ of (13) one has*

$$\int_0^1 \left|\partial_\xi^k \hat{\mathcal{G}}(x,t;\xi,s)\right|\,\mathrm{d}\xi \leqslant \left(\frac{\kappa_k}{\varepsilon^k(t-s)^{k/2}} + C\varepsilon^p\,(t-s)^{p/2}\right)\mathrm{e}^{-\gamma^2(t-s)}, \tag{18}$$

for $k = 0, 1, 2$, where the constants κ_k are defined in (5).

Remark 2.1. For $k = 0$, one has a sharper version of (18) with $C = 0$. This observation follows from an application of the maximum/comparison principle to problem (13), which, in view of (3), yields $0 \leqslant \hat{\mathcal{G}} \leqslant \bar{\mathcal{G}}$. It remains to employ the bound (5) for $\bar{\mathcal{G}}$ in the case of $k = 0$.

2.3. Variable-coefficient problem in a bounded spatial domain

We are now prepared to estimate the Green's function $\mathcal{G}$ associated with the operator $\mathcal{M} := \partial_t - \varepsilon^2\partial_x^2 + r$ with a variable reaction coefficient $r = r(x)$. I.e., we restrict ourselves to the case when r does not vary in time. For fixed (x,t), the Green's function $\mathcal{G}(x,t;\xi,s) =: \Gamma^*(\xi,s)$ solves the terminal-value problem

$$\mathcal{M}^*\Gamma^* := [-\partial_s - \varepsilon^2\partial_\xi^2 + r]\,\Gamma^* = 0 \qquad \text{in}\ \ (0,1)\times[0,t), \tag{19a}$$

$$\Gamma^*(\xi,t) = \delta(\xi - x)\ \text{for}\ \ \xi \in (0,1), \tag{19b}$$

$$\Gamma^*(0,s) = \Gamma^*(1,s) = 0 \qquad \text{for}\ \ s \in [0,t]. \tag{19c}$$

Theorem 2.1. *Let $r \in C^1[0,1]$. Assume $\varrho^2 \leqslant r$ on $[0,1]$ with some constant $\varrho > 0$. Then, for the Green's function $\mathcal{G}$ there holds*

$$\int_0^1 |\mathcal{G}(x,t;\xi,s)|\,\mathrm{d}\xi \leqslant \kappa_0\,\mathrm{e}^{-\varrho^2(t-s)}, \tag{20a}$$

$$\int_0^1 \left|\partial_\xi^k \mathcal{G}(x,t;\xi,s)\right|\,\mathrm{d}\xi \leqslant \frac{\kappa_k\,\mathrm{e}^{-\varrho^2(t-s)}}{\varepsilon^k(t-s)^{k/2}} + \mathcal{O}\left(\varepsilon^{k-1}\right), \quad \textit{for}\ \ k = 1,2, \tag{20b}$$

and

$$\int_0^1 |\partial_s \mathcal{G}(x,t;\xi,s)|\,\mathrm{d}\xi \leqslant \left(\frac{\kappa_2}{t-s} + \kappa_0\|r\|_\infty\right)\mathrm{e}^{-\varrho^2(t-s)} + \mathcal{O}\left(\varepsilon\right). \tag{20c}$$

The constants κ_k are defined in (5).

Proof of Theorem 2.1. Let (x,t) be fixed. Let $\gamma \geqslant \varrho$ be defined by $\gamma^2 := r(x)$.

(i) Applying the maximum principle, as in Remark 2.1, one easily gets $0 \leqslant \mathcal{G} \leqslant \bar{\mathcal{G}}$ and hence (20a).

(ii) Set $\gamma^2 = r(x)$ in (13) (then x will appear in this problem as a parameter and all the results of §2.2 remain valid with $\gamma^2 \geqslant \varrho^2$). Next, comparing problems (19) and (13), we conclude that for fixed (x,t), the difference $v := \hat{\Gamma}^* - \Gamma^*$ satisfies

$$\begin{aligned} \big(\bar{\mathcal{M}}^* v\big)(\xi,s) &= (r(\xi) - r(x))\, \Gamma^*(\xi,s) && \text{for } (\xi,s) \in (0,1)\times[0,t),\\ v(\xi,t) &= 0 && \text{for } \xi \in (0,1),\\ v(0,s) = v(1,s) &= 0 && \text{for } s \in [0,t]. \end{aligned}$$

Hence, v can be represented via the solution $\hat{\mathcal{G}}$ of (13) as

$$v(\xi,s) = \int_s^t \int_0^1 \hat{\mathcal{G}}(\eta,\sigma;\xi,s)\,\big(r(\eta) - r(x)\big)\,\Gamma^*(\eta,\sigma)\,\mathrm{d}\eta\,\mathrm{d}\sigma. \tag{21}$$

Applying ∂_ξ to this representation, one gets

$$\int_0^1 |\partial_\xi v(\xi,s)|\,\mathrm{d}\xi \leqslant \|r'\|_\infty \int_s^t \int_0^1 \left(\int_0^1 \big|\partial_\xi \hat{\mathcal{G}}(\eta,\sigma;\xi,s)\big|\,\mathrm{d}\xi\right) |\eta - x|\,\Gamma^*(\eta,\sigma)\,\mathrm{d}\eta\,\mathrm{d}\sigma.$$

Now, apply Lemma 2.2 with $k = p = 1$; then recall from part (i) that $\Gamma^* = \mathcal{G} \leqslant \bar{\mathcal{G}}$, so apply (11). Consequently, we get

$$\int_0^1 |\partial_\xi v(\xi,s)|\,\mathrm{d}\xi \leqslant C. \tag{22}$$

Finally, the bound of Lemma 2.2 with $k = p = 1$, combined with (22), and a triangle inequality yield (20b) for $k = 1$.

(iii) Next, we estimate $\partial_\xi^2 v$. Note, if ∂_ξ^2 were applied to (21), a similar calculation would lead to a diverging integral. Instead we recall that $\hat{\mathcal{G}} = \tilde{\mathcal{G}}_0 + g$ from §2.2, so split v as $v = \tilde{v} + v_g$, where $\tilde{v}$ and v_g are represented by (21) with $\hat{\mathcal{G}}$ respectively replaced by $\tilde{\mathcal{G}}_0$ and g.

Now, applying ∂_ξ^2 to v_g, one gets

$$\begin{aligned} \int_0^1 \big|\partial_\xi^2 v_g(\xi,s)\big|\,\mathrm{d}\xi &\leqslant \|r\|_\infty \int_s^t \int_0^1 \left(\int_0^1 \big|\partial_\xi^2 g(\eta,\sigma;\xi,s)\big|\,\mathrm{d}\xi\right) \Gamma^*(\eta,\sigma)\,\mathrm{d}\eta\,\mathrm{d}\sigma \\ &\leqslant C\varepsilon^p\,\mathrm{e}^{-\varrho^2(t-s)} \int_s^t (\sigma - s)^{p/2}\,\mathrm{d}\sigma = \mathcal{O}\left(\varepsilon^p\right), \end{aligned} \tag{23}$$

where we have used (17) with $k = 2$ and (20a).

It remains to estimate $\partial_\xi^2 \tilde{v}$, which requires a more elaborate argument. First, an application of ∂_ξ to the representation of $\tilde{v}$ of type (21) gives

$$\partial_\xi \tilde{v}(\xi,s) = \int_s^t \int_0^1 \partial_\xi \tilde{G}_0(\eta,\sigma;\xi,s)\,\big(r(\eta) - r(x)\big)\,\Gamma^*(\eta,\sigma)\,\mathrm{d}\eta\,\mathrm{d}\sigma.$$

In view of (9), an integration by parts yields

$$\partial_\xi \tilde{v}(\xi,s) = \int_s^t \int_0^1 \tilde{\mathcal{G}}_1(\eta,\sigma;\xi,s)\,\partial_\eta\Big[\big(r(\eta) - r(x)\big)\Gamma^*(\eta,\sigma)\Big]\,\mathrm{d}\eta\,\mathrm{d}\sigma.$$

Apply ∂_ξ and integrate for $\xi \in [0,1]$ in order to obtain

$$\int_0^1 \left|\partial_\xi^2 \tilde{v}(\xi,s)\right| \,\mathrm{d}\xi \leqslant \int_s^t \int_0^1 \Psi(\eta,\sigma;s) \left|\partial_\eta \Big[\big(r(\eta)-r(x)\big)\Gamma^*(\eta,\sigma)\Big]\right| \mathrm{d}\eta\,\mathrm{d}\sigma,$$

with

$$\Psi(\eta,\sigma;s) := \int_0^1 \left|\partial_\xi \tilde{\mathcal{G}}_1(\eta,\sigma;\xi,s)\right| \,\mathrm{d}\xi \leqslant \kappa_1 \frac{\mathrm{e}^{-\gamma^2(\sigma-s)}}{\varepsilon\sqrt{\sigma-s}}, \tag{24}$$

by (10) and (5).

Thus

$$\int_0^1 \left|\partial_\xi^2 \tilde{v}(\xi,s)\right| \,\mathrm{d}\xi \leqslant \frac{\kappa_1 \|r'\|_\infty}{\varepsilon} \int_s^t \frac{\mathrm{e}^{-\gamma^2(\sigma-s)}}{\sqrt{\sigma-s}} \int_0^1 \left[|\eta-x| \left|\partial_\eta \Gamma^*(\eta,\sigma)\right| + \Gamma^*(\eta,\sigma)\right] \,\mathrm{d}\eta\,\mathrm{d}\sigma.$$

Note that here $\Gamma^* = \mathcal{G}(x,t;\cdot,\cdot) = \tilde{\mathcal{G}}_0(x,t;\cdot,\cdot) + v + g$, where

$$\int_0^1 |\partial_\eta v(\eta,s)| \,\mathrm{d}\eta \leqslant C \quad \text{and} \quad \int_0^1 |\partial_\eta g(\eta,s)| \,\mathrm{d}\eta \leqslant C\varepsilon^P,$$

because of (17) and (22). Then, by (12) and (20a),

$$\int_0^1 \left|\partial_\xi^2 \tilde{v}(\xi,s)\right| \,\mathrm{d}\xi \leqslant C\varepsilon^{-1}.$$

To finish the proof of (20b) for $k=2$, use Lemma 2.2 with $k=p=1$ and a triangle inequality.

(iv) Finally, (20c) follows from (19) and (20b). □

2.4. Semilinear problem in a bounded spatial domain

In this section we sketch how bounds for the Green's function can be obtained for the general semilinear problem (1). Given any pair of bounded functions v and w whose difference vanishes at the boundary of the spatial domain, we have

$$\big(v-w\big)(x,t) = \int_0^1 \Gamma^*(\xi,0)\,\big(v-w\big)(\xi,0)\,\mathrm{d}\xi + \int_0^t\int_0^1 \Gamma^*(\xi,s)\,\big(\mathcal{M}v-\mathcal{M}w\big)(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s, \tag{25}$$

where $\Gamma^*(\xi,s) = \mathcal{G}_{[v,w]}(x,t;\xi,s)$, the Green's function of the linearised problem, solves the terminal-value problem

$$\mathcal{M}^*_{[v,w]}\Gamma^* := \left[-\partial_s - \varepsilon^2\partial_\xi^2 + a\right]\Gamma^* = 0 \qquad \text{in } (0,1)\times[0,t), \tag{26a}$$

$$\Gamma^*(\xi,t) = \delta(\xi-x) \text{ for } \xi\in(0,1), \tag{26b}$$

$$\Gamma^*(0,s) = \Gamma^*(1,s) = 0 \qquad \text{for } s\in[0,t], \tag{26c}$$

with $a(\xi,s) := \int_0^1 \partial_z\varphi\big(\xi,s,w+z(v-w)\big)\,\mathrm{d}z$. Clearly $\varrho^2 \leqslant a(\xi,s) \leqslant \bar{\varrho}^2$, by (2). Note that when (1) is linear, i.e., $\varphi(x,t,z) = r(x,t)z - f(x,t)$, then $a \equiv r$.

(i) Applying the maximum principle to the linearised problem (26), as in Remark 2.1, one easily gets $0 \leqslant \mathcal{G}_{[v,w]} \leqslant \bar{\mathcal{G}}$, with $\bar{\mathcal{G}}$ defined in (4), but γ replaced by ϱ.

(ii) When studying $\partial_\xi \Gamma$, our argument is similar to that of §2.3. Let $\hat{\Gamma}^* = \hat{\mathcal{G}}(x,t;\cdot,\cdot)$ be the Green's function of §2.2 with $\gamma = \varrho$. The difference $v := \hat{\Gamma}^* - \Gamma^*$ satisfies

$$\Gamma^* := \big(\mathcal{M}^*_{[v,w]} v\big)(\xi,s) = \big(a(\xi,s) - \varrho^2\big)\,\Gamma^*(\xi,s) \quad \text{for} \quad (\xi,s) \in (0,1)\times[0,t),$$
$$v(\xi,t) = 0 \quad \text{for} \quad \xi \in (0,1), \qquad v(0,s) = v(1,s) = 0 \quad \text{for} \quad s \in [0,t].$$

Hence, v can be represented via $\hat{\mathcal{G}}$ as

$$v(\xi,s) = \int_s^t \int_0^1 \hat{\mathcal{G}}(\eta,\sigma;\xi,s)\,\big(a(\eta,\sigma) - \varrho^2\big)\,\Gamma^*(\eta,\sigma)\; \mathrm{d}\eta\, \mathrm{d}\sigma.$$

Apply ∂_ξ and integrate for $\xi \in [0,1]$ to obtain

$$\int_0^1 |\partial_\xi v(\xi,s)|\; \mathrm{d}\xi \leqslant \int_s^t \int_0^1 \left(\int_0^1 \big|\partial_\xi \hat{\mathcal{G}}(\eta,\sigma;\xi,s)\big|\, \mathrm{d}\xi\right) \big(\bar{\varrho}^2 - \varrho^2\big)\Gamma^*(\eta,\sigma)\, \mathrm{d}\eta\, \mathrm{d}\sigma.$$

Using Lemma 2.2 with $k=1$, we get

$$\begin{aligned}\int_0^1 |\partial_\xi v(\xi,s)|\, \mathrm{d}\xi &\leqslant \big(\bar{\varrho}^2 - \varrho^2\big)\; \mathrm{e}^{-\varrho^2(t-s)} \int_s^t \left(\frac{\kappa_1}{\varepsilon\sqrt{\sigma - s}} + C\varepsilon^p\,(\sigma - s)^{p/2}\right) \mathrm{d}\sigma \\ &\leqslant \left(\frac{\kappa_1}{\varepsilon\sqrt{t-s}} + C\varepsilon^[\,(t-s)^{p/2}\right)\Big[2(\bar{\varrho}^2 - \varrho^2)\,(t-s)\Big]\, \mathrm{e}^{-\varrho^2(t-s)}.\end{aligned}$$

Next, Lemma 2.2 and a triangle inequality give

$$\int_0^1 |\partial_\xi \Gamma^*(\xi,s)|\; \mathrm{d}\xi \leqslant \left(\frac{\kappa_1}{\varepsilon\sqrt{t-s}} + C\varepsilon^p\,(t-s)^{p/2}\right)\; \Big[1 + 2(\bar{\varrho}^2 - \varrho^2)\,(t-s)\Big]\, \mathrm{e}^{-\varrho^2(t-s)}.$$

(iii) As a bound for $\partial_s \Gamma^*$ we quote Lemma 2.2 from [14]:

$$\int_0^{t-\tau} \int_0^1 \big|\partial_s \mathcal{G}(x,t;\xi,s)\big|\, \mathrm{d}\xi\, \mathrm{d}s \leqslant \frac{3\,\ell(\tau,t)}{2^{3/2}} + \mu, \quad \ell(\tau,t) := \int_\tau^t s^{-1}\mathrm{e}^{-\frac{1}{2}\varrho^2 s}\, \mathrm{d}s \leqslant \ln\frac{t}{\tau}.$$

Here $\mu \geqslant 0$ is an ε-independent constant with $\mu = (\bar{\varrho}^2 - \varrho^2)\,\hat{\mu}$, where $\hat{\mu} = \hat{\kappa}_2(\varrho)$ if $\varrho > 0$, and $\hat{\mu} = \hat{\mu}(T)$ if $\varrho = 0$.

(iv) Finally, $\partial_\xi^2 \Gamma^*$ is bounded using (26a).

Remark 2.2. If condition (2) is replaced with $|\partial_z \varphi(x,t,z)| \leqslant \bar{\varrho}^2$, then $|a| \leqslant \bar{\varrho}^2$ in (26a), so one can obtain similar bounds for Γ^* replaced by $\tilde{\Gamma}^* := \Gamma^*\,\mathrm{e}^{-\bar{\varrho}^2(t-s)}$ (as the version of (26a) for $\tilde{\Gamma}^*$ will involve $a \geqslant 0$). Consequently, one can extend the results of §3 to this case, only the error estimate will involve additional factors of type $\mathrm{e}^{\bar{\varrho}^2 t_m}$ (which remain bounded unless long-term computations are required).

3. A posteriori error bounds for a difference scheme

In this section we introduce a finite difference scheme for (1) using backward Euler in time and central differencing in space. A posteriori error estimates will be derived for this scheme.

3.1. Discretisation

Let the mesh in time be $0 = t_0 < t_1 < \cdots < t_M = T$ with mesh intervals $J_j = (t_{j-1}, t_j]$ and step sizes $\tau_j := t_j - t_{j-1}$. At each time t_j, $j = 1, \ldots, M$, the spatial mesh is $\omega^j : 0 = x_0^j < x_1^j < \cdots < x_{N_j}^j = 1$ with mesh sizes $h_i^j := x_i^j - x_{i-1}^j$. The numerical approximation on this mesh is: Find U such that

$$\Delta_t U_i^j - \varepsilon^2 \Delta_x^2 U_i^j + \varphi\left(x_i, t_j, U_i^j\right) = 0 \quad \text{for } i = 1, \ldots N_j - 1,\ j = 1, \ldots, M, \tag{27a}$$

$$U_0^j = U_{N_j}^j = 0 \quad \text{for } \ j = 1, \ldots, M, \tag{27b}$$

where

$$\Delta_t U_i^j := \frac{U_i^j - \hat{U}_i^{j-1}}{\tau_j}, \quad \Delta_x^2 v_i^j := \frac{1}{\hbar_i^j}\left(\frac{v_{i+1}^j - v_i^j}{h_{i+1}^j} - \frac{v_i^j - v_{i-1}^j}{h_i^j}\right), \quad \hbar_i^j := \frac{h_i^j + h_{i+1}^j}{2}.$$

Furthermore, for $j = 2, \ldots, M$, $\hat{U}^{j-1}$ is a projection of U^{j-1} onto the mesh ω^j, while $\hat{U}^0$ is an approximation of the initial value u_0 on the mesh ω^1. For example, $\hat{U}^j$ can be obtained by interpolation, L_2 projection or by Ritz projection.

The approximation U of u is defined at mesh points only. In order to represent the error by means of the Green's function, U has to be extended to a function defined on $[0,1] \times [0,T]$. For any mesh function ψ, we define an interpolant ψ^I that is piecewise Π_0 in time and piecewise Π_1 in space, i.e.,

$$\psi^I(x,t) := \frac{x - x_{i-1}}{h_i}\psi_i^j + \frac{x_i - x}{h_i}\psi_{i-1}^j \quad \text{for } \ x \in [x_{i-1}, x_i], \quad t \in \begin{cases} \bar{J}_1, \\ J_j,\ j = 2, \ldots, M. \end{cases}$$

We shall identify the numerical solution defined in the mesh points with its interpolant U^I, and write U instead of U^I for the sake of simplicity. Similarly, $\hat{U}^{j-1}$ is defined on the mesh ω_j only. However, we shall identify it with its piecewise linear interpolant on ω_j.

3.2. A posteriori error analysis

Set $q := \varphi(\cdot, \cdot, U)$ on $[0,1] \times [0,T]$ and

$$\Psi_k^j := \Delta_t U_k^j - q_k^j \quad \text{for } \ k = 0, \ldots, N_j,\ j = 1, \ldots, M. \tag{28}$$

By (27), we have $\Psi_k^j = \varepsilon^2 \Delta_x^2 U_k^j$ for $k = 1, \ldots, N_j - 1$, $j = 1, \ldots, M$. Thus, Ψ is an extension of $\varepsilon^2 \Delta_x^2 U$ onto mesh points on the boundary of the domain.

Theorem 3.1. *Let u be the solution of* (1) *and U its approximation by* (27)*. Then the error at time level t_m satisfies*

$$\left|\big(u - U\big)(x, t_m)\right| \leqslant \eta := \eta_{osc} + \eta_{init} + \eta_{proj} + \eta_t + \eta_t^* + \eta_d + \eta_d^* + \eta_d^\dagger,$$

where

$$\eta_{osc} := \sum_{j=1}^{m} K_j \tau_j \left\| q - q^I \right\|_{L^\infty((0,1)\times J_j)}, \quad \eta_{init} := T_0 \left\| u_0 - \hat{U}^0 \right\|_{L^\infty(0,1)},$$

$$\eta_{proj} := \sum_{j=1}^{m-1} T_j \left\| U^j - \hat{U}^j \right\|_{L^\infty(0,1)}, \quad \eta_t := \Theta \max_{\substack{j=1,\dots,m-1\\ k=0,\dots,N_j}} \left| U_k^j - \hat{U}_k^{j-1} \right|,$$

$$\eta_t^* := \bar{\Theta} \max_{k=0,\dots,N_m} \left| U_k^m - \hat{U}_k^{m-1} \right|, \quad \eta_d := \Xi_1 \max_{\substack{j=1,\dots,m-1\\ k=1,\dots,N_j}} \frac{\left(h_k^j\right)^2}{6\varepsilon} \left| \Psi_k^j - \Psi_{k-1}^j \right|,$$

$$\eta_d^* := \bar{\Xi}_1 \sqrt{\tau_m} \max_{k=1,\dots,N_m} h_k^m \frac{\left|\Psi_k^m\right| + \left|\Psi_{k-1}^m\right|}{2\varepsilon}, \quad \eta_d^\dagger := \Xi_2 \max_{\substack{j=1,\dots,m-1\\ k=1,\dots,N_j}} \left[\frac{\left(h_k^j\right)^2}{8\varepsilon^2} \max\left\{ \left|\Psi_k^j\right|, \left|\Psi_{k-1}^j\right| \right\} \right],$$

and

$$K_j := \frac{1}{\tau_j} \int_{t_{j-1}}^{t_j} \int_0^1 \Gamma^*(\xi,s) \,\mathrm{d}\xi \,\mathrm{d}s, \quad T_j := \int_0^1 \Gamma^*(\xi,t_j) \,\mathrm{d}\xi, \quad \Theta := \int_0^{t_{m-1}} \int_0^1 \left| \partial_s \Gamma^*(\xi,s) \right| \,\mathrm{d}\xi \,\mathrm{d}s,$$

$$\bar{\Theta} := \int_{t_{m-1}}^{t_m} \frac{t_m - s}{\tau_m} \int_0^1 \left| \partial_s \Gamma^*(\xi,s) \right| \mathrm{d}\xi \,\mathrm{d}s, \quad \Xi_1 := \varepsilon \int_0^{t_{m-1}} \int_0^1 \left| \partial_\xi \Gamma^*(\xi,s) \right| \mathrm{d}\xi \,\mathrm{d}s,$$

$$\Xi_2 := \varepsilon^2 \int_0^{t_{m-1}} \int_0^1 \left| \partial_\xi^2 \Gamma^*(\xi,s) \right| \mathrm{d}\xi \,\mathrm{d}s, \quad \bar{\Xi}_1 := \frac{\varepsilon}{\sqrt{\tau_m}} \int_{t_{m-1}}^{t_m} \int_0^1 \left| \partial_\xi \Gamma^*(\xi,s) \right| \mathrm{d}\xi \,\mathrm{d}s.$$

Here $\Gamma^* := \mathcal{G}_{[u,U]}(x,t_m;\cdot,\cdot)$ *is the Green's function associated with* $\mathcal{M}$*.*

Remark 3.1. The constants in the error estimate can be bounded using the results from Section 2. For example, in the linear case with $r = r(x)$, Theorem 3.1 holds with

$$K_j := T_j := \mathrm{e}^{-\varrho^2(t_m - t_j)}, \quad \Xi_1 := \varrho^{-1} + \mathcal{O}(\varepsilon), \quad \bar{\Xi}_1 = \frac{2}{\sqrt{\pi}} + \mathcal{O}(\varepsilon),$$

$$\Xi_2 := \sqrt{\frac{2}{\pi \mathrm{e}}} \ln \frac{t_m}{\tau_m} + \mathcal{O}(\varepsilon), \quad \Theta = \Xi_2 + \varrho^{-2} \left\| r \right\|_{L^\infty}, \quad \bar{\Theta} = \sqrt{\frac{2}{\pi \mathrm{e}}} + \mathcal{O}(\tau_m + \varepsilon).$$

Remark 3.2. The result of Theorem 3.1 combined with Remark 3.1 is similar to the one of [14, Cor. 6.6 combined with Rem. 2.3], but involves sharper constants. Nevertheless, the latter estimate appears reasonably sharp in comparison. For example, it involves a term (which appears as $\kappa_1 \, \ell_m \max_{j=1,\dots,m-1} \eta^j$ in [14, (6.5)]) similar to the dominating term $\eta_{\mathrm{d}}^\dagger$ of our present estimator (see Table 1 below), but with the constant Ξ_2 replaced by $2\,\Xi_2$.

Proof of Theorem 3.1. First, we derive a representation of the error by means of the Green's function of the continuous operator $\mathcal{M}$. Fix $x \in [0,1]$ and the time level t_m. Then the error can be written as

$$\begin{aligned} \big(u - U\big)(x,t_m) = &\int_0^1 \big(u_0 - U^1\big)(\xi)\, \Gamma^*(\xi,0) \,\mathrm{d}\xi \\ &+ \int_0^{t_m} \int_0^1 \big(q - \partial_s U + \varepsilon^2 \partial_\xi^2 U\big)(\xi,s)\, \Gamma^*(\xi,s) \,\mathrm{d}\xi \,\mathrm{d}s. \end{aligned} \tag{29}$$

The second integral in (29) involves distributions. These are dealt with as follows:

$$\left(\partial_s U\right)(\xi,s) = \sum_{j=1}^{m-1} \big(U^{j+1} - U^j\big)(\xi)\ \delta(s - t_j)$$

because the numerical solution U is piecewise constant in time. Therefore,

$$\int_0^{t_m}\int_0^1 \big(\partial_s U\,\Gamma^*\big)(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s = \sum_{j=1}^{m-1}\int_0^1 \big(U^{j+1}-U^j\big)(\xi)\ \Gamma^*(\xi,t_j)\,\mathrm{d}\xi. \tag{30}$$

Similarly, because U is piecewise linear in space, we have

$$\big(\partial_\xi^2 U\big)(\xi,s) = \sum_{k=1}^{N_j-1}\left(\frac{U_{k+1}^j-U_k^j}{h_{k+1}^j}-\frac{U_k^j-U_{k-1}^j}{h_k^j}\right)\delta(\xi-x_k^j)\quad \text{for}\quad s\in(t_{j-1},t_j].$$

Consequently,

$$\int_0^{t_m}\int_0^1 \big(\partial_\xi^2 U\,\Gamma^*\big)(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s = \sum_{j=1}^{m-1}\sum_{k=1}^{N_j-1}\hbar_k^j\Delta_x^2 U_k^j\int_{t_{j-1}}^{t_j}\Gamma^*(x_k^j,s)\,\mathrm{d}s. \tag{31}$$

Furthermore, (28) implies

$$\int_{t_{j-1}}^{t_j}\int_0^1\big(\Delta_t U^j-\Psi^I-q^I\big)(\xi,s)\ \Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s = 0.$$

Adding this to (29) and using (30) and (31), we obtain the error representation

$$\big(u-U\big)(x,t_m) = E_{\text{time}}+E_{\text{reac}}+E_{\text{diff}} \tag{32}$$

with

$$E_{\text{time}} := \int_0^1\big(u_0-U^1\big)(\xi)\,\Gamma^*(\xi,0)\,\mathrm{d}\xi-\sum_{j=1}^{m-1}\int_0^1\big(U^{j+1}-U^j\big)(\xi)\,\Gamma^*(\xi,t_j)\,\mathrm{d}\xi$$
$$\qquad +\sum_{j=1}^{m}\int_{t_{j-1}}^{t_j}\int_0^1\Delta_t U^j\,\Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s,$$
$$E_{\text{reac}} := \int_0^{t_m}\int_0^1\big(q-q^I\big)(\xi,s)\,\Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s$$

and

$$E_{\text{diff}} := \sum_{j=1}^m E_{\text{diff}}^j\,,\quad E_{\text{diff}}^j := \sum_{k=1}^{N_j-1}\hbar_k^j\Psi_k^j\int_{t_{j-1}}^{t_j}\Gamma^*(x_k^j,s)\,\mathrm{d}s-\int_{t_{j-1}}^{t_j}\int_0^1\big(\Psi^I\Gamma^*\big)(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s.$$

These three terms will be estimated separately.
Reaction/source term. Use the Hölder inequality to estimate as follows.

$$\left|\int_0^{t_m}\int_0^1\big(q-q^I\big)(\xi,s)\,\Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s\right|\leqslant\sum_{j=1}^m K_j\tau_j\left\|q-q^I\right\|_{L^\infty((0,1)\times J_j)}\,. \tag{33}$$

Time discretisation. Using the identity

$$\int_{t_{j-1}}^{t_j}\Gamma^*(\xi,s)\,\mathrm{d}s = \int_{t_{j-1}}^{t_j}(t_j-s)\partial_s\Gamma^*(\xi,s)\,\mathrm{d}s+\tau_j\Gamma^*(\xi,t_{j-1}),$$

we get

$$E_{\text{time}} = \int_0^1 \big(u_0 - \hat{U}^0\big)(\xi)\,\Gamma^*(\xi,0)\,\mathrm{d}\xi + \sum_{j=1}^{m-1} \int_0^1 \big(U^j - \hat{U}^j\big)(\xi)\,\Gamma^*(\xi,t_j)\,\mathrm{d}\xi$$
$$+ \sum_{j=1}^{m} \int_0^1 \Delta_t U^j \int_{t_{j-1}}^{t_j} (t_j - s)\,\partial_s \Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s.$$

For the first two terms, we have

$$\left| \int_0^1 \big(u_0 - \hat{U}^0\big)(\xi)\,\Gamma^*(\xi,0)\,\mathrm{d}\xi \right| \leqslant T_0 \big\| u_0 - \hat{U}^0 \big\|_{L^\infty(0,1)} \tag{34a}$$

and

$$\left| \sum_{j=1}^{m-1} \int_0^1 \big(U^j - \hat{U}^j\big)(\xi)\,\Gamma^*(\xi,t_j)\,\mathrm{d}\xi \right| \leqslant \sum_{j=1}^{m-1} T_j \big\| U^j - \hat{U}^j \big\|_{L^\infty(0,1)}, \tag{34b}$$

while for the third term the argument splits because the integral $\int_0^1 \int_0^{t_m} |\partial_s \Gamma^*(\xi,s)|\,\mathrm{d}\xi\,\mathrm{d}s$ does not exist. We treat the last time level differently from all previous ones.

$$\begin{aligned} &\left| \sum_{j=1}^{m} \int_0^1 \Delta_t U^j \int_{t_{j-1}}^{t_j} (t_j - s)\,\partial_s \Gamma^*(\xi,s)\,\mathrm{d}\xi\,\mathrm{d}s \right| \\ &\qquad \leqslant \Theta \max_{k=0,\dots,N_m} \big| U_k^m - \hat{U}_k^{m-1} \big| + \bar{\Theta} \max_{j=1,\dots,m-1} \max_{k=0,\dots,N_j} \big| U_k^j - \hat{U}_k^{j-1} \big| \end{aligned} \tag{34c}$$

Diffusion term. The Green's function vanishes at the boundary of the domain. Thus, for $s \in (t_{j-1}, t_j]$,

$$\sum_{k=1}^{N_j-1} \hbar_k^j \Psi_k^j \Gamma^*(x_k^j, s) - \int_0^1 \big(\Psi^I \Gamma^*\big)(\xi,s)\,\mathrm{d}\xi = \sum_{k=1}^{N_j} \chi_k(s)$$

with

$$\chi_k(s) = \frac{h_k^j}{2}\Big[\Psi_k^j \Gamma^*(x_j^k, s) + \Psi_{k-1}^j \Gamma^*(x_{j-1}^k, s)\Big] - \int_{x_{k-1}^j}^{x_k^j} \big(\Psi^I \Gamma^*\big)(\xi,s)\,\mathrm{d}\xi.$$

On each spatial mesh interval, Ψ^I is linear. Therefore,

$$\begin{aligned} \chi_k(s) = \Psi_k^j &\int_{x_{k-1}^j}^{x_k^j} \big(\Gamma^*(x_k^j, s) - \Gamma^*(\xi,s)\big) \frac{\xi - x_{k-1}^j}{h_k^j}\,\mathrm{d}\xi \\ &+ \Psi_{k-1}^j \int_{x_{k-1}^j}^{x_k^j} \big(\Gamma^*(x_{k-1}^j, s) - \Gamma^*(\xi,s)\big) \frac{x_k^j - \xi}{h_k^j}\,\mathrm{d}\xi \end{aligned}$$

and

$$\chi_k(s) = \Psi_k^j \int_{x_{k-1}^j}^{x_k^j} \partial_\xi \Gamma^*(\xi,s) \frac{(\xi - x_{k-1}^j)^2}{2h_k^j}\,\mathrm{d}\xi - \Psi_{k-1}^j \int_{x_{k-1}^j}^{x_k^j} \partial_\xi \Gamma^*(\xi,s) \frac{(x_k^j - \xi)^2}{2h_k^j}\,\mathrm{d}\xi. \tag{35}$$

This yields the first bound for $\chi_k(s)$:

$$|\chi_k(s)| \leqslant h_k^j \frac{\left|\Psi_k^j\right| + \left|\Psi_{k-1}^j\right|}{2} \int_{x_{k-1}^j}^{x_k^j} \left|\partial_\xi \Gamma^*(\xi, s)\right| \,\mathrm{d}\xi. \tag{36}$$

Furthermore, continuing with (35), we have

$$\begin{aligned}\chi_k(s) &= h_k^j \frac{\Psi_k^j - \Psi_{k-1}^j}{6} \int_{x_{k-1}^j}^{x_k^j} \partial_\xi \Gamma^*(\xi, s) \,\mathrm{d}\xi \\ &\quad + \int_{x_{k-1}^j}^{x_k^j} \partial_\xi \Gamma^*(\xi, s) \left[\Psi_k^j \left(\frac{(\xi - x_{k-1}^j)^2}{2h_k^j} - \frac{h_k^j}{6}\right) - \Psi_{k-1}^j \left(\frac{(x_k^j - \xi)^2}{2h_k^j} - \frac{h_k^j}{6}\right)\right] \mathrm{d}\xi.\end{aligned}$$

Integrate the second term by parts. Then

$$\begin{aligned}\chi_k(s) &= h_k^j \frac{\Psi_k^j - \Psi_{k-1}^j}{6} \int_{x_{k-1}^j}^{x_k^j} \partial_\xi \Gamma^*(\xi, s) \,\mathrm{d}\xi \\ &\quad - \int_{x_{k-1}^j}^{x_k^j} \partial_\xi^2 \Gamma^*(\xi, s) \frac{(\xi - x_{k-1}^j)(\xi - x_k^j)}{6h_k^j} \left[\Psi_k^j \left(\xi - x_{k-1}^j + h_k^j\right) + \Psi_{k-1}^j \left(\xi - x_k^j - h_k^j\right)\right] \mathrm{d}\xi.\end{aligned}$$

We get a second bound for χ_k^j:

$$\begin{aligned}|\chi_k(s)| &\leqslant \frac{\left(h_k^j\right)^2}{8} \max\left\{\left|\Psi_k^j\right|, \left|\Psi_{k-1}^j\right|\right\} \int_0^1 \left|\partial_\xi^2 \Gamma^*(\xi, t)\right| \,\mathrm{d}\xi \\ &\quad + \frac{1}{6}\left(h_k^j\right)^2 \left|\Psi_k^j - \Psi_{k-1}^j\right| \int_0^1 \left|\partial_\xi \Gamma^*(\xi, t)\right| \,\mathrm{d}\xi.\end{aligned} \tag{37}$$

When estimating E_{diff}, the argument splits again because the integral $\int_0^1 \int_0^{t_m} \left|\partial_\xi^2 \Gamma^*(\xi, s)\right| \mathrm{d}\xi \,\mathrm{d}s$ does not exist. Summing (37) for $k = 1, \ldots, N_j$ and then integrating for $s \in [0, t_{m-1}]$, we get

$$\begin{aligned}\left|\sum_{j=1}^{m-1} E_{\mathrm{diff},j}\right| &\leqslant \Xi_1 \max_{j=1,\ldots,M-1} \max_{k=1,\ldots,N_j} \frac{\left(h_k^j\right)^2}{6\varepsilon} \left|\Psi_k^j - \Psi_{k-1}^j\right| \\ &\quad + \Xi_2 \max_{j=1,\ldots,M-1} \max_{k=1,\ldots,N_j} \left[\frac{\left(h_k^j\right)^2}{8\varepsilon^2} \max\left\{\left|\Psi_k^j\right|, \left|\Psi_{k-1}^j\right|\right\}\right].\end{aligned} \tag{38a}$$

On the last time slab we use (36) to estimate as follows:

$$\left|E_{\mathrm{diff},m}\right| \leqslant \bar{\Xi}_1 \max_{k=1,\ldots,N_m} h_k^m \frac{\left|\Psi_k^m\right| + \left|\Psi_{k-1}^m\right|}{2\varepsilon}. \tag{38b}$$

Finally, combine (32), (33), (34) and (38) to complete the proof. □

4. Numerical results

Consider the test problem

$$\begin{aligned}\partial_t u - \varepsilon^2 \partial_x^2 u + (1 + x)u = 1 + \sin 10xt, \quad \text{in } (0, 1) \times (0, T], \\ u(x, 0) = (1 - x)(1 - e^x), \quad x \in [0, 1], \quad u(0, t) = u(1, t) = 0, \quad t \in (0, T].\end{aligned} \tag{39}$$

K	$\|u-U\|_\infty$	rate	η_{init}	rate	η_{t}	rate	η_{t}^*	rate		
	η	$\frac{C_{\text{eff}}}{\ln(1/\tau)}$	η_{osc}	rate	η_{d}	rate	$\eta_{\text{d}}^\dagger$	rate	η_{d}^*	rate
2^{10}	2.915e-2	0.93	9.937e-4	1.04	8.208e-3	0.89	1.719e-3	1.01		
	2.730e-1	1.352	9.183e-3	0.99	8.370e-8	0.94	**2.392e-1**	**0.90**	1.469e-2	0.92
2^{11}	1.534e-2	0.98	4.844e-4	0.93	4.423e-3	0.90	8.549e-4	0.99		
	1.456e-1	1.245	4.639e-3	1.00	4.356e-8	0.98	**1.279e-1**	**0.93**	7.756e-3	0.95
2^{12}	7.805e-3	0.99	2.543e-4	1.02	2.369e-3	0.91	4.298e-4	1.00		
	7.619e-2	1.173	2.317e-3	1.01	2.205e-8	0.99	**6.707e-2**	**0.93**	4.004e-3	0.97
2^{13}	3.938e-3	0.97	1.256e-4	0.97	1.264e-3	0.91	2.153e-4	1.00		
	3.992e-2	1.125	1.149e-3	0.98	1.110e-8	0.97	**3.525e-2**	**0.90**	2.047e-3	0.96
2^{14}	2.017e-3	0.99	6.433e-5	1.01	6.716e-4	0.92	1.077e-4	1.00		
	2.134e-2	1.090	5.809e-4	1.00	5.685e-9	0.99	**1.893e-2**	**0.91**	1.049e-3	0.98
2^{15}	1.018e-3	0.99	3.188e-5	0.98	3.556e-4	0.92	5.393e-5	1.00		
	1.128e-2	1.066	2.904e-4	1.00	2.870e-9	0.99	**1.005e-2**	**0.92**	5.321e-4	0.99
2^{16}	5.125e-4	0.99	1.618e-5	1.00	1.877e-4	0.93	2.696e-5	1.00		
	5.953e-3	1.048	1.454e-4	1.00	1.445e-9	0.99	**5.324e-3**	**0.92**	2.687e-4	0.99
2^{17}	2.575e-4	1.00	8.070e-6	0.99	9.878e-5	0.93	1.348e-5	1.00		
	3.136e-3	1.034	7.270e-5	1.00	7.260e-10	1.00	**2.816e-3**	**0.92**	1.354e-4	0.99
2^{18}	1.292e-4	1.00	4.056e-6	1.00	5.186e-5	0.93	6.740e-6	1.00		
	1.649e-3	1.023	3.637e-5	1.00	3.642e-10	1.00	**1.486e-3**	**0.93**	6.802e-5	0.99
2^{19}	6.475e-5	1.00	2.030e-6	1.00	2.717e-5	0.94	3.371e-6	1.00		
	8.654e-4	1.014	1.819e-5	1.00	1.826e-10	1.00	**7.825e-4**	**0.93**	3.414e-5	1.00
2^{20}	3.242e-5	—	1.015e-6	—	1.420e-5	—	1.685e-6	—		
	4.532e-4	1.008	9.094e-6	—	9.144e-11	—	**4.111e-4**	—	1.711e-5	—

Table 1. Actual and estimated errors on a Bakhvalov mesh

We study the numerical error at final time $T = 1$ and compare it to the a posteriori error estimator η of Theorem 3.1. The diffusion parameter is taken to be $\varepsilon = 10^{-6}$. Almost identical results are obtained for other small values of ε, which illustrates that our estimator applies and remains realistic independently of how small the perturbation parameter is.

In space we employ a layer resolving Bakhvalov mesh [2] with N mesh intervals. This spatial mesh is fixed in time: $x_i^j = x_i = \mu(i/N)$ with the mesh generating function

$$\mu(\zeta) = \begin{cases} \vartheta(\zeta) := \dfrac{\sigma\varepsilon}{\varrho} \ln \dfrac{\alpha}{\alpha - \zeta} & \zeta \in [0, \zeta^*], \\ \vartheta(\zeta^*) + \vartheta'(\zeta^*)(\zeta - \zeta^*) & \zeta \in [\zeta^*, 1/2], \\ 1 - \mu(1-\zeta) & \zeta \in [1/2, 1]. \end{cases}$$

The transition point ζ^* satisfies $(1 - 2\zeta^*)\vartheta'(\zeta^*) = 1 - 2\vartheta(\zeta^*)$ which implies $\mu \in C^1[0,1]$. For the mesh parameters are chosen we take $\sigma = 4$ and $\alpha = 1/4$. In time a uniform mesh with K mesh intervals of length $\tau = 1/K$ is used.

The difference scheme is of second order in space, but only of first order in time. In order to balance the scheme we take $N = \lceil \sqrt{K} \rfloor$, i.e., $\sqrt{K}$ rounded to the nearest integer.

The exact solution of (39) is unknown. Therefore, the errors are approximated by comparison with the numerical solution obtained on a mesh that is 4 times as fine in space and 16 times as fine in time.

The a posteriori error estimator contains two terms that involve the data of problem:

$\eta_{\rm init}$ and $\eta_{\rm osc}$. Both require sampling. This is done as follows

$$\left\|q - q^I\right\|_{L^\infty([x_{i-1},x_i]\times[t_{j-1},t_j])} \approx \max_{k,\ell=0,\dots,4} \left|\left(q - q^I\right)(x_{i-1} + kh_i/4, t_{j-1} + \ell\tau_j/4)\right|$$
$$\left\|u_0 - \hat{U}^0\right\|_{L^\infty(0,1)} \approx \max_{k=0,\dots,4} \left|\left(u_0 - \hat{U}^0\right)(x_{i-1} + kh_i/4)\right|.$$

For the test problem, the constants in the error estimator are given in Remark 3.1. Terms of order τ and ε are neglected.

The results for our test computations are presented in Table 1. The first column displays the number of time steps K. The second column contains the actual errors and the estimated error, while in the third column the rate of convergence and the effectivity of the error estimator can be found. The remaining columns display the various components of the error estimator. Note that $\eta_{\rm proj} = 0$ because the spatial mesh is constant in time.

For a quantity $\pi = \pi^K$ converging to zero, we estimate the rate of convergence by computing $\log_2(\pi^K/\pi^{2K})$. The effectivity of the estimator is computed using the formula $C_{\rm eff} = \|(u-U)(T)\|_\infty/\eta$. Clearly $C_{\rm eff} \geqslant 1$, because η is an upper bound on the error. The effectivity is the better the closer $C_{\rm eff}$ to 1.

The dominant term $\eta_{\rm d}^\dagger$ in the estimator is highlighted in the table. It does not converge with first order because of the presence of the $\ln(1/\tau)$ term (which also appears in [1, 4, 5, 7]). Also, note that the efficiency slightly deteriorates with increasing K. $C_{\rm eff}$ is approximately proportional to $\ln K$ (or $\ln(1/\tau)$). We conjecture that the factors $\ln(1/\tau)$ appearing in $\eta_{\rm d}^\dagger$ and $\eta_{\rm t}$ are merely an artifact of the analysis. Apart from this the estimator is quite effective with $C_{\rm eff} \approx 10\dots14$ and $\frac{C_{\rm eff}}{\ln(1/\tau)} \approx 1$.

It has to be noted that these are results for a single test problem with a particular a priori chosen layer-resolving mesh that does not change in time. At least, in this important case, we observe that our a posteriori estimate is rather satisfactory in serving one of the purposes of such estimates: to correctly judge the quality of a given approximation. (Note also that for steady-state singularly perturbed equations, a priori chosen layer-resolving meshes were used in [11, 12] to test error estimators that subsequently were proved to yield robust adaptive methods [16, 3].) More extensive experiments are required for other test problems and meshes. In particular, mesh adaptation and movement in time will be investigated in a future paper.

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