MAXIMUM NORM A POSTERIORI ERROR ESTIMATE FOR A 3D SINGULARLY PERTURBED SEMILINEAR REACTION-DIFFUSION PROBLEM*

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Abstract. A singularly perturbed semilinear reaction-diffusion problem in the unit cube, is discretized on arbitrary nonuniform tensor-product meshes. We establish a second-order maximum norm a posteriori error estimate that holds true uniformly in the small diffusion parameter. No mesh aspect ratio condition is imposed. This result is obtained by combining (i) sharp bounds on the Green's function of the continuous differential operator in the Sobolev $W^{1,1}$ and $W^{2,1}$ norms and (ii) a special representation of the residual in terms of an arbitrary current mesh and the current computed solution. Numerical results on a priori chosen meshes are presented that support our theoretical estimate.

Key words. Semilinear reaction-diffusion, singular perturbation, a posteriori error estimate, maximum norm, no mesh aspect ratio condition, finite differences, layer-adapted mesh.

AMS subject classifications. 65N06, 65N15, 65N50

1. Introduction

We focus on the following singularly perturbed semilinear reaction-diffusion problem posed in the unit cube:

$$\begin{aligned} Tu := -\varepsilon^2 \triangle u + b(x,u) &= 0, \qquad x = (x_1, x_2, x_3) \in \Omega = (0,1)^3, \\ u(x) &= 0, \qquad x \in \partial\Omega. \end{aligned} \tag{1.1}$$

Here ε is a small positive parameter, $\triangle = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2 + \partial^2/\partial x_3^2$ is the standard Laplace operator, the function b is sufficiently smooth and satisfies

$$0 < \beta < b_u(x,u) \le \bar\beta \qquad \text{for all } (x,u) \in [0,1]^3 \times \mathbb{R}. \tag{1.2}$$

Under condition (1.2), problem (1.1) has a unique solution, which exhibits sharp boundary layers of width $O(\varepsilon|\ln\varepsilon|)$ along the boundary $\partial\Omega$.

The aim of the present paper is to extend the two-dimensional a posteriori error estimate of [19] to three dimensions. This result is obtained by combining a special representation of the residual and sharp bounds on the Green's function of the linearized continuous differential operator in the Sobolev $W^{1,1}$ and $W^{2,1}$ norms. Compared to [19], the main difficulties in the present paper lie in the analysis of the Green's function. First, we use the explicit fundamental solution for the constant-coefficient operator $-\varepsilon^2\triangle + \gamma^2$, and it is different in two and three dimensions. Furthermore, some parts of the analysis [19] for the variable-coefficient case, e.g., [19, §3.2], do not yield the desired estimates in three dimensions (one gets additional negative powers of ε in the right-hand sides of the asserted bounds). Other parts

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of [19] were in some ways simplified in the current paper. We refer the reader to Remark 3.2 for a more detailed comparison. In a more general context, we note that sharp estimates for continuous Green's functions (or their generalized versions) frequently play a crucial role in a priori and a posteriori error analyses [12, 14, 27].

Our error estimate will be in the *maximum norm*, which is sufficiently strong to capture layers and hence seems most appropriate for layer solutions. (The few known a posteriori error estimates for anisotropic meshes are in a weaker energy norm; see, e.g., [21, 22].) We also refer the reader to related papers on maximum norm a posteriori error estimation in one dimension [16, 17, 20, 24].

Another essential feature of our error estimate, is that we assume *no mesh aspect ratio condition*. It is crucial in the context of layer solutions, as for problems of type (1.1), a priori error analyses [26, 25, 8, 18] show that ε-uniform numerical approximations of layer solutions can be obtained using relatively small ε-independent numbers of mesh nodes. But this is attained by using a priori meshes that are anisotropic in layer regions, i.e. include extremely thin mesh cells that have extremely high aspect ratios (typically $O(\varepsilon^{-1})$). Note that a posteriori error estimates are typically obtained under the shape-regularity condition (equivalent to bounded-mesh-aspect-ratio condition) [1, 3, 12, 27], so such estimates do not seem very suitable for constructing efficient layer-adapted meshes.

We make no attempt to suggest or analyze any particular adaptive mesh generation algorithm. But we note that many successful algorithms are based on interpolation error estimates such as presented in [10, 9, 7], roughly speaking, the criterion on the generated mesh being a small interpolation error. Thus the generated, possibly, anisotropic mesh is supposed to be (quasi-)uniform under the metric induced by the positive definite Hessian matrix of the solution (or its scaled majorant); see, e.g., [6, 11, 15, 29]. It should be noted that such algorithms are not completely theoretically justified. E.g., the relation of the actual error of a numerical method to the interpolation error under no mesh aspect ratio condition is still to be established for many problems, in particular, in the maximum norm. Furthermore, linear interpolation error bounds involve the Hessian matrix of the unknown exact solution, which is replaced in the adaptive algorithm by its computed-solution analogue. To theoretically justify this replacement, one still needs to establish Hessian-matrix recovery formulas under no mesh aspect ratio condition, which are not available in the literature.

An alternative theoretical justification, to which this paper aims to contribute, might be given by a posteriori error estimates that hold true under no mesh aspect ratio condition and directly relate the actual error to a certain discrete linear-interpolation-error-bound analogue, which involves the local mesh sizes and certain computed-solution approximations of the second-order derivatives. Indeed, roughly speaking, our a posteriori error estimate (1.3), (1.4) below is of this type, i.e. might be viewed as a discrete analogue of the linear interpolation error estimates.

Our problem (1.1) will be discretized using the standard second-order seven-point difference scheme (see (2.2) below) on an arbitrary tensor-product mesh $\{x_{ij\,l}\}$ in $[0,1]^3$, where $x_{ij\,l} = (x_1^{[i]}, x_2^{[j]}, x_3^{[l]})$ with $0 = x_s^{[0]} < x_s^{[1]} < \cdots < x_s^{[N_s]} = 1$ for $s = 1,2,3$, while $h_i = x_1^{[i]} - x_1^{[i-1]}$, $\tau_j = x_2^{[j]} - x_2^{[j-1]}$ and $k_l = x_3^{[l]} - x_3^{[l-1]}$ are the local mesh sizes.

Note that such tensor-product meshes present an idealized situation, as practical a posteriori mesh construction algorithms use either irregular meshes or curvilinear tensor-product meshes. Therefore we consider our error estimate more interesting from a theoretical point of view since it shows that the bounded-mesh-aspect-ratio condition is not essential for a posteriori errors (as well as for interpolation errors). Also, if (possibly-curvilinear) tensor-product meshes are used in layer regions, where the mesh adaptation is most needed, one might conjecture that a local version of our a posteriori error estimate would apply there.

Our main result is the following maximum norm *a posteriori error estimate*, in which the error is understood as the difference between the exact solution and the trilinear interpolant of the computed solution:

$$\|U^{\mathrm{I}}-u\|_\infty \le C_0\Big[\max_{\substack{i=1,\ldots,N_1\\ j=0,\ldots,N_2\\ l=0,\ldots,N_3}}\big\{h_i^2 M_{1,ij\,l}\big\}+\max_{\substack{i=0,\ldots,N_1\\ j=1,\ldots,N_2\\ l=0,\ldots,N_3}}\big\{\tau_j^2 M_{2,ij\,l}\big\}+\max_{\substack{i=0,\ldots,N_1\\ j=0,\ldots,N_2\\ l=1,\ldots,N_3}}\big\{k_l^2 M_{3,ij\,l}\big\}\Big]; \tag{1.3}$$

see Theorem 2.2. Here, roughly speaking,

$$M_{s,ij\,l} \approx |D_s^2 U_{ij\,l}|\ln\big(2+\varepsilon/\kappa\big)+1, \qquad s=1,2,3, \tag{1.4}$$

with $\kappa = \min\{\min_i\{h_i\}, \min_j\{\tau_j\}, \min_l\{k_l\}\}$. By U^{I} we denote the trilinear interpolant of the computed solution U (the finite difference computed solution is originally defined at the mesh nodes only; hence to measure the error in the entire domain, one first has to interpolate the computed solution there). The quantities $D_s^2 U_{ij\,l}$ for $s=1,2,3$ are the standard discrete approximations of $\partial^2 u/\partial x_s^2$ defined in (2.3). In (1.4), a few terms are skipped, for which the one-dimensional analysis [17] and the numerical results of [19] and §6 suggest that they are less important; see Theorem 2.2 for the precise definitions of $M_{s,ij\,l}$. The error constant C_0 in (1.3) is independent of ε, the mesh and aspect ratios of its elements, but we do not specify its value. (Note that for singularly perturbed problems, the error constant may grow as ε becomes small; hence that it is ε-uniform is more important than its precise value.)

The paper is organized as follows. In §2, we describe the numerical method, present our a posteriori error estimate in Theorem 2.2, and outline its proof. Next, in §3, we establish some sharp bounds on the Green's function of a linearized version of (1.1) in the Sobolev $W^{1,1}$ and $W^{2,1}$ norms. They imply certain stability properties of the differential operator T from (1.1), which are presented in §4. Then in §5, we obtain a special representation of the residual in terms of an arbitrary current mesh and the current computed solution, and therefore complete the proof of Theorem 2.2. Finally, in §6, numerical results on a priori chosen meshes are given that support our theoretical estimate.

Notation. Let $\|\cdot\|_{p\,;\tilde\Omega}$, where $1 \le p \le \infty$, denote the standard $L_p(\tilde\Omega)$ norm of scalar or vector functions defined in any domain $\tilde\Omega \subset \mathbb{R}^3$. Furthermore, the standard notation $W^{k,p}(\tilde\Omega)$ is used for the Sobolev spaces with the norm $\|\cdot\|_{k,p\,;\tilde\Omega}$ defined, for any scalar function $v(x)$ in a domain $\tilde\Omega$, by

$$\|v\|_{k,p\,;\tilde\Omega} = \|v\|_{p\,;\tilde\Omega} + \textstyle\sum_{l=1}^k |v|_{l,p\,;\tilde\Omega}, \qquad k=1,2,$$
$$|v|_{1,p\,;\tilde\Omega} = \textstyle\sum_{s=1}^3 \|\frac{\partial}{\partial x_s}v\|_{p\,;\tilde\Omega}\,, \qquad |v|_{2,p\,;\tilde\Omega} = \textstyle\sum_{s,t=1}^3 \|\frac{\partial^2}{\partial x_s\partial x_t}v\|_{p\,;\tilde\Omega}\,;$$

see, e.g., [13]. We shall use the notation $\|\cdot\|_p$ and $\|\cdot\|_{k,p}$ for $\|\cdot\|_{p\,;\Omega}$ and $\|\cdot\|_{k,p\,;\Omega}$ when there is no ambiguity. Sometimes the domain of interest will be an open ball $B(a\,;\rho) = B(a_1,a_2,a_3\,;\rho) = \{x : \sum_{s=1}^3 (x_s-a_s)^2 < \rho^2\}$ centered at a of radius ρ.

Throughout the paper we let C denote a generic positive constant that may take different values in different formulas, but is always independent of the mesh and ε. A subscripted C (e.g., C_1) denotes a positive constant that is independent of the mesh and ε and takes a fixed value. For any two quantities w_1 and w_2, the notation $w_1 = O(w_2)$ means $|w_1| \le C w_2$.

Remark 1.1. The assumption $b_u(x,u) \le \bar\beta$ in (1.2) can be omitted as it follows, for some constant $\bar\beta$, from $0 < \beta < b_u(x,u)$ and u being a unique and bounded solution of (1.1), (to be more precise, $|u| \le \beta^{-1}\|b(\cdot,0)\|_\infty$); see, e.g., [30, §12]. Note that assumption (1.2) enables us to linearize (1.1) and then invoke the Green's function in our analysis.

2. Numerical method. Main result

We consider problem (1.1) under the standard compatibility conditions at the corners of the domain Ω:

$$b(x,0) = 0 \qquad \text{for } x = (x_1,x_2,x_3): \; x_1,x_2,x_3 \in \{0,1\}, \tag{2.1}$$

which guarantee that $u \in C^3(\bar\Omega)$.

Numerical method. The computed solution U is required to satisfy the standard seven-point finite difference discretization of (1.1)

$$-\varepsilon^2[D_1^2 U_{ij\,l} + D_2^2 U_{ij\,l} + D_3^2 U_{ij\,l}] + b(x_{ij\,l}, U_{ij\,l}) = 0, \tag{2.2}$$

where $i = 1,\dots N_1 - 1$, $j = 1,\dots,N_2-1$, $l = 1,\dots,N_3-1$, subject to $U_{ij\,l} = 0$ on the boundary, i.e. if $i = 0, N_1$ or $j = 0, N_2$ or $l = 0, N_3$. Here, as usual, $U_{ij\,l}$ is associated with the mesh node $x_{ij\,l} = (x_1^{[i]}, x_2^{[j]}, x_3^{[l]})$, and we use the standard finite difference operators, defined for any discrete function $V_{ij\,l}$ by

$$\begin{aligned} D_1^- V_{ij\,l} &= \frac{V_{ij\,l} - V_{i-1,j,l}}{h_i}, & D_1^2 V_{ij\,l} &= \frac{D_1^- V_{i+1,j,l} - D_1^- V_{ij\,l}}{(h_i + h_{i+1})/2},\\ D_2^- V_{ij\,l} &= \frac{V_{ij\,l} - V_{i,j-1,l}}{\tau_j}, & D_2^2 V_{ij\,l} &= \frac{D_2^- V_{i,j+1,l} - D_2^- V_{ij\,l}}{(\tau_j + \tau_{j+1})/2},\\ D_3^- V_{ij\,l} &= \frac{V_{ij\,l} - V_{i,j,l-1}}{k_l}, & D_3^2 V_{ij\,l} &= \frac{D_3^- V_{i,j,l+1} - D_3^- V_{ij\,l}}{(k_l + k_{l+1})/2}. \end{aligned} \tag{2.3}$$

By (1.2), there exists a unique solution of the discrete problem (2.2) on an arbitrary mesh $\{x_{ij\,l}\}$; see, e.g., [5].

At this stage, $D_1^2 U_{ij\,l}$ is defined for $i = 1,\dots,N_1-1$, $j = 0,\dots,N_2$, $l = 0,\dots,N_3$. Similarly $D_2^2 U_{ij\,l}$ and $D_3^2 U_{ij\,l}$ are defined for $j = 1,\dots,N_2-1$, $\forall\, i, l$, and $l = 1,\dots,N_3-1$, $\forall\, i,j$, respectively. We now extend $D_1^2 U_{ij\,l}$ to the mesh nodes $i = 0, N_1$ as follows. The zero boundary conditions imply that $D_s^2 U_{0,j,l} = D_s^2 U_{N_1,j,l} = 0$ for $s = 2,3$. In view of this, the discrete equation (2.2) formally extended to $i = 0$ and $i = N_1$, becomes

$$D_1^2 U_{ij\,l} := \varepsilon^{-2} b(x_{ij\,l}, 0) \quad \text{for} \quad i = 0, N_1, \quad j = 0,\dots,N_2,\; l = 0,\dots,N_3. \tag{2.4a}$$

Similarly, we extend $D_2^2 U_{ij\,l}$ to $j = 0, N_2$ and $D_3^2 U_{ij\,l}$ to $l = 0, N_3$ by

$$D_2^2 U_{ij\,l} := \varepsilon^{-2} b(x_{ij\,l}, 0) \quad \text{for} \quad j = 0, N_2, \quad i = 0,\dots,N_1,\; l = 0,\dots,N_3. \tag{2.4b}$$

$$D_3^2 U_{ij\,l} := \varepsilon^{-2} b(x_{ij\,l}, 0) \quad \text{for} \quad l = 0, N_3, \quad i = 0,\dots,N_1,\; j = 0,\dots,N_2. \tag{2.4c}$$

Note that, by (2.1), the above relations (2.4) imply that $D_1^2 U_{ij\,l} = D_2^2 U_{ij\,l} = D_3^2 U_{ij\,l} = 0$ at the corners of our domain, which is consistent with the boundary condition in (1.1).

Remark 2.1. Now that $D_s^2 U_{ij\,l}$, where $s=1,2,3$, are extended by (2.4) to all i, j, l, our discrete equation (2.2) holds true for all $i=0,\dots,N_1$, $j=0,\dots,N_2$ and $l=0,\dots,N_3$.

Trilinear interpolation notation. Let $U^{\rm I}=U^{\rm I}(x)$ be the standard trilinear interpolant of the computed solution $U_{ij\,l}$, i.e. $U^{\rm I}$ is continuous in $\bar\Omega$, trilinear on each $(x_1^{[i-1]},x_1^{[i]})\times(x_2^{[j-1]},x_2^{[j]})\times(x_3^{[l-1]},x_3^{[l]})$, and equal to $U_{ij\,l}$ at the mesh nodes:

$$U^{\rm I}(x_{ij\,l})=U_{ij\,l}\quad\text{for}\quad i=0,\dots,N_1,\ j=0,\dots,N_2,\ l=0,\dots,N_3. \tag{2.5}$$

Similarly, we define the trilinear interpolant $v^{\rm I}(x)$ for any discrete function $v_{ij\,l}$ or any continuous function $v(x)$.

Furthermore, we shall use the standard one-dimensional linear interpolants $v^{{\rm I}_s}$ with respect to x_s for $s=1,2,3$, that are defined, for any function v, as follows. For each fixed x_2,x_3 in the domain of v, we have $v^{{\rm I}_1}(x_1^{[i]},x_2,x_3)=v(x_1^{[i]},x_2,x_3)$, and $v^{{\rm I}_1}(x)$ is linear on each $(x_1^{[i-1]},x_1^{[i]})$. Similarly, $v^{{\rm I}_2}(x_1,x_2^{[j]},x_3)=v(x_1,x_2^{[j]},x_3)$, $v^{{\rm I}_3}(x_1,x_2,x_3^{[l]})=v(x_1,x_2,x_3^{[l]})$ and, furthermore, $v^{{\rm I}_2}$ and $v^{{\rm I}_3}$ are linear on each $(x_2^{[j-1]},x_2^{[j]})$ and $(x_3^{[l-1]},x_3^{[l]})$, respectively.

Note that the trilinear interpolation can be represented as a product of the three one-dimensional interpolation operators independently of the order of the interpolation steps. In particular, for the trilinear interpolant $U^{\rm I}$ of $U_{ij\,l}$ we have

$$U^{\rm I}(x)=[\,U^{{\rm I}_1}]^{{\rm I}_2{\rm I}_3}=[\,U^{{\rm I}_2}]^{{\rm I}_1{\rm I}_3}=[\,U^{{\rm I}_3}]^{{\rm I}_1{\rm I}_2}. \tag{2.6}$$

The next theorem gives a maximum norm a posteriori error estimate, which is the main result of the present paper. Note that this is an extension to three dimensions of [19, Theorem 2.1].

Theorem 2.2. *Let $u(x)$ be a solution of problem (1.1), (1.2), (2.1), $U_{ij\,l}$ a solution of discrete problem (2.2) on an arbitrary mesh $\{x_{ij\,l}\}$, and $U^{\rm I}(x)$ its trilinear interpolant (2.5). Then*

$$\|U^{\rm I}-u\|_\infty\le C_0\Big[\max_{\substack{i=1,\dots,N_1\\ j=0,\dots,N_2\\ l=0,\dots,N_3}}\big\{h_i^2M_{1,ij\,l}\big\}+\max_{\substack{i=0,\dots,N_1\\ j=1,\dots,N_2\\ l=0,\dots,N_3}}\big\{\tau_j^2M_{2,ij\,l}\big\}+\max_{\substack{i=0,\dots,N_1\\ j=0,\dots,N_2\\ l=1,\dots,N_3}}\big\{k_l^2M_{3,ij\,l}\big\}\Big],$$

where

$$M_{1,ij\,l}:=\min\big\{|D_1^2U_{i-1,j,l}|,|D_1^2U_{ij\,l}|\big\}\ln\big(2+\varepsilon/\kappa\big)+\varepsilon|D_1^-D_1^2U_{ij\,l}|+|D_1^-U_{ij\,l}|^2+1,$$
$$M_{2,ij\,l}:=\min\big\{|D_2^2U_{i,j-1,l}|,|D_2^2U_{ij\,l}|\big\}\ln\big(2+\varepsilon/\kappa\big)+\varepsilon|D_2^-D_2^2U_{ij\,l}|+|D_2^-U_{ij\,l}|^2+1,$$
$$M_{3,ij\,l}:=\min\big\{|D_3^2U_{i,j,l-1}|,|D_3^2U_{ij\,l}|\big\}\ln\big(2+\varepsilon/\kappa\big)+\varepsilon|D_3^-D_3^2U_{ij\,l}|+|D_3^-U_{ij\,l}|^2+1,$$

with $\kappa:=\min\{\min_i\{h_i\},\min_j\{\tau_j\},\min_l\{k_l\}\}$, and the constant C_0 is independent of ε and the mesh.

Proof outline. To simplify the presentation, here and throughout §§4-5, in which this proof is continued, we assume that $N_1=N_2=N_3=N$.

In view of (1.1), one gets

$$TU^{\rm I}-Tu=-\varepsilon^2\left[\partial^2/\partial x_1^2+\partial^2/\partial x_2^2+\partial^2/\partial x_3^2\right]U^{\rm I}+b(x,U^{\rm I}).$$

Note that here $\partial^2U^{\rm I}/\partial x_s^2$, for $s=1,2,3$, are understood in the sense of distributions. Next, we introduce an auxiliary function

$$q(x):=b(x,U^{\rm I}(x))$$

and its trilinear interpolant $q^{\rm I}$ on the mesh $\{(x_{ij\,l})\}$. Now one has

$$TU^{\rm I}-Tu=-\varepsilon^2\left[\partial^2/\partial x_1^2+\partial^2/\partial x_2^2+\partial^2/\partial x_3^2\right]U^{\rm I}+q^{\rm I}+\left[q-q^{\rm I}\right].$$

As $q_{ij\,l}:=q(x_{ij\,l})=b(x_{ij\,l},U_{ij\,l})$, in view of Remark 2.1, the discrete equation (2.2) yields $q_{ij\,l}=\varepsilon^2[D_1^2U_{ij\,l}+D_2^2U_{ij\,l}+D_3^2U_{ij\,l}]$ for $i,\ j,\ l=0,\dots,N$. This observation leads to the decomposition $q_{ij\,l}=q_{1,ij\,l}+q_{2,ij\,l}+q_{3,ij\,l}$, where

$$q_{s,ij\,l}:=\varepsilon^2D_s^2U_{ij\,l}\qquad\text{for}\quad s=1,2,3,\quad i,j,l=0,\dots,N, \tag{2.7}$$

and then to

$$q^{\rm I}(x)=q_1^{\rm I}(x)+q_2^{\rm I}(x)+q_3^{\rm I}(x)=[\,q_1^{{\rm I}_1}]^{{\rm I}_2{\rm I}_3}+[\,q_2^{{\rm I}_2}]^{{\rm I}_1{\rm I}_3}+[\,q_3^{{\rm I}_3}]^{{\rm I}_1{\rm I}_2},\qquad x\in\bar\Omega.$$

Here we also used a version of (2.6) for functions q_s with $s=1,2,3$. We now get

$$TU^{\rm I}-Tu=\left[-\varepsilon^2\tfrac{\partial^2}{\partial x_1^2}U^{{\rm I}_1}+q_1^{{\rm I}_1}\right]^{{\rm I}_2{\rm I}_3}+\left[-\varepsilon^2\tfrac{\partial^2}{\partial x_2^2}U^{{\rm I}_2}+q_2^{{\rm I}_2}\right]^{{\rm I}_1{\rm I}_3}+\left[-\varepsilon^2\tfrac{\partial^2}{\partial x_3^2}U^{{\rm I}_3}+q_3^{{\rm I}_3}\right]^{{\rm I}_1{\rm I}_2}+\left[q-q^{\rm I}\right].$$

To obtain this equation, we also used the following relations:

$$\tfrac{\partial^2}{\partial x_1^2}U^{\rm I}=\left[\tfrac{\partial^2}{\partial x_1^2}U^{{\rm I}_1}\right]^{{\rm I}_2{\rm I}_3},\qquad \tfrac{\partial^2}{\partial x_2^2}U^{\rm I}=\left[\tfrac{\partial^2}{\partial x_2^2}U^{{\rm I}_2}\right]^{{\rm I}_1{\rm I}_3},\qquad \tfrac{\partial^2}{\partial x_3^2}U^{\rm I}=\left[\tfrac{\partial^2}{\partial x_3^2}U^{{\rm I}_3}\right]^{{\rm I}_1{\rm I}_2}. \tag{2.8}$$

The above three relations follow from (2.6) as any operator ∂^2/∂^2x_s is commutative with ${\rm I}_t$ for $t\neq s$ (but not with ${\rm I}_s$); see also Remark 2.3.

The proof will be completed in §5 by representing the residual $TU^{\rm I}-Tu$ as

$$TU^{\rm I}-Tu=\tfrac{\partial}{\partial x_1}F_1(x)+\tfrac{\partial}{\partial x_2}F_2(x)+\tfrac{\partial}{\partial x_3}F_3(x)+\left[q-q^{\rm I}\right], \tag{2.9}$$

where F_1, F_2 and F_3 are some functions of the current mesh and computed solution. In view of (2.9), the error $U^{\rm I}-u$ will be estimated in the maximum norm by linearizing the operator T and invoking its stability properties. Stability of T will be addressed in §4 using certain bounds for the Green's function of §3.

Remark 2.3. We understand $\partial^2U^{\rm I}/\partial x_s^2$, for $s=1,2,3$, in the sense of distributions. To be more precise, in (2.8) we use

$$\tfrac{\partial^2}{\partial x_1^2}U^{{\rm I}_1}=\textstyle\sum_{i=1}^{N-1}\left[\hbar_i\,D_1^2U_{ij\,l}\right]\delta(x_1-x_1^{[i]}),$$

$$\left[\tfrac{\partial^2}{\partial x_1^2}U^{{\rm I}_1}\right]^{{\rm I}_2{\rm I}_3}=\textstyle\sum_{i=1}^{N-1}\hbar_i\left[D_1^2U_{ij\,l}\right]^{{\rm I}_2{\rm I}_3}\delta(x_1-x_1^{[i]}),$$

where $\hbar_i:=(h_i+h_{i+1})/2$ and $\delta(\cdot)$ is the Dirac δ-distribution.

3. Green's function

To investigate the error U^I-u, we shall linearize (2.9) and then invoke certain estimates of the Green's function of the resulting linear equation. These estimates are the main result of this section. Thus, throughout the section, we focus on a linear case of (1.1), where we set $b(x,u):=p(x)u-f(x)$ and thus arrive at

$$Lu:=-\varepsilon^2\Delta u+p(x)u=f(x)\quad\text{in }\Omega,\qquad u=0\quad\text{on }\partial\Omega. \tag{3.1}$$

Here $p\in L_\infty(\Omega)$, and, in agreement with (1.2), it also satisfies

$$0<\beta\le p(x)\le\bar\beta. \tag{3.2}$$

Let $G(x;\xi)$ be the Green's function of the linear self-adjoint operator L. For each $x=(x_1,x_2,x_3)\in\Omega$, it satisfies

$$\begin{aligned} L_\xi G=-\varepsilon^2\,\Delta_\xi G+p(\xi)G&=\delta(x-\xi), &&\xi\in\Omega,\\ G(x;\xi)&=0, &&\xi\in\partial\Omega, \end{aligned} \tag{3.3}$$

where $\xi = (\xi_1, \xi_2, \xi_3)$ and $\Delta_\xi = \partial^2/\partial\xi_1^2 + \partial^2/\partial\xi_2^2 + \partial^2/\partial\xi_2^2$, while $\delta(\cdot)$ is the three-dimensional Dirac δ-distribution. We now have an explicit formula for the unique solution u of problem (3.1):

$$u(x) = \int_\Omega G(x;\xi)\, f(\xi)\, d\xi, \tag{3.4}$$

where we used the notation $d\xi = d\xi_1\, d\xi_2\, d\xi_3$.

Theorem 3.1. *The Green's function $G(x;\xi)$ from (3.3) satisfies*

$$\|G(x;\cdot)\|_{1\,;\Omega} + \varepsilon\, |G(x;\cdot)|_{1,1\,;\Omega} \le C. \tag{3.5a}$$

Furthermore, for any ball $B(\tilde{x}\,;\rho)$ of radius ρ centered at any $\tilde{x} \in \Omega$ we have

$$|G(x;\cdot)|_{1,1\,;B(\tilde{x}\,;\rho)\cap\Omega} \le C\,\varepsilon^{-2}\rho; \tag{3.5b}$$

while for the ball $B(x\,;\rho)$ of radius ρ centered at x, we have

$$|G(x;\cdot)|_{2,1\,;\Omega\setminus B(x\,;\rho)} \le C\,\varepsilon^{-2}\ln(2+\varepsilon/\rho). \tag{3.5c}$$

This entire section is devoted to the proof of this theorem, which is the main result of the section. The proof is in two steps. First, in §3.1 we shall estimate the auxiliary Green's function $\bar{G}$ in the constant-coefficient case in the positive octant space using the explicit fundamental solution. The remaining part of the proof (§3.2-§3.3) will, roughly speaking, deal with $G - \bar{G}$.

Remark 3.2. Note that the statement of Theorem 3.1 is precisely as in the two-dimensional case [19, Theorem 3.1]. The proof, however, is different in a few ways. First, we note that the fundamental solutions for the constant-coefficient operator $-\varepsilon^2\triangle + \gamma^2$, which are used in both analyses, are different in two and three dimensions. Furthermore, the argument of [19, §3.2] for a variable-coefficient case does not yield the desired estimates in three dimensions (it leads to additional negative powers of ε in the right-hand sides of our asserted bounds). For this case, we therefore give a completely different proof and even weaken the assumption $|\frac{\partial}{\partial x_i}p| \le C$ of [19, §3.2] to $\varepsilon|\frac{\partial}{\partial x_i}p| \le C$ in §3.2. The final part of the proof for the most general case of p (see §3.3) has evolved from [19, §3.3], and is simpler in the sense that now we avoid using any cut-off functions and deal either with $G - \bar{G}$ or sometimes directly with G.

3.1. **Constant-coefficient case.** The first step in the proof of Theorem 3.1 consists in establishing it for a particular constant-coefficient case. Set $p := \gamma^2$ for some $\gamma = \text{const} > 0$, and let Ω be the positive octant space $\mathbb{R}^3_+ = \{x_1, x_2, x_3 > 0\}$. We denote the differential operator in this particular case by $\bar{L}$, and the Green's function by $\bar{G}$. Thus for each x we have

$$\bar{L}_\xi \bar{G}(x;\xi) := -\varepsilon^2\,\Delta_\xi \bar{G} + \gamma^2 \bar{G} = \delta(x-\xi), \qquad \xi_1, \xi_2, \xi_3 > 0. \tag{3.6}$$

The fundamental solution for the operator $-\Delta_\xi + \nu^2$ in $\mathbb{R}^3$ is $e^{-\nu r}/(4\pi r)$; see, e.g., [28, §8.3]. This readily provides the fundamental solution for our differential operator $\bar{L}$, which is

$$g(x;\xi) := \frac{1}{4\pi\varepsilon^2}\frac{e^{-\gamma r/\varepsilon}}{r}, \quad r := \sqrt{(\xi_1-x_1)^2 + (\xi_2-x_2)^2 + (\xi_3-x_3)^2}. \tag{3.7}$$

Now the Green's function for $\bar{L}$ over the octant is easily obtained by the method of images and involves eight terms of the type $\pm g(\pm x_1, \pm x_2, \pm x_3; \xi)$; to be more precise we have

$$\bar{G}(x;\xi) = \sum_{\sigma_1,\sigma_2,\sigma_3=-1,1} (\sigma_1\sigma_2\sigma_3)\, g\big(x^{[\sigma_1,\sigma_2,\sigma_3]};\xi\big), \quad x^{[\sigma_1,\sigma_2,\sigma_3]} := (\sigma_1 x_1, \sigma_2 x_2, \sigma_3 x_3). \tag{3.8}$$

Lemma 3.3. (i) *For $\bar{G}(x;\xi)$ of (3.8), estimates (3.5) of Theorem 3.1 hold true, in which G is replaced by $\bar{G}$.*
(ii) *Furthermore, we have*

$$\|\bar{G}(x;\cdot)\|_{2\,;\Omega} \le C\,\varepsilon^{-3/2}, \qquad \|\bar{G}(x;\cdot)\|_{2\,;\Omega\setminus B(x\,;\rho)} \le C\,\varepsilon^{-3/2} e^{-\gamma\rho/\varepsilon}. \tag{3.9}$$

Proof. It suffices to prove estimates (3.5) and (3.9) with G and $\bar{G}$, respectively, replaced by the term $g(x;\xi)$ of the representation (3.8) of $\bar{G}$, as the estimates for the other seven terms are similar.

Let the stretching transformation from $\xi = (\xi_1, \xi_2, \xi_3)$ to the new coordinates $\hat{\xi} = (\hat{\xi}_1, \hat{\xi}_2, \hat{\xi}_3) := (\xi - x)/\varepsilon$ map any domain $\Omega' \subset \mathbb{R}^3$ into $\hat{\Omega}'$. Furthermore, consider a scaled version $\hat{g}(\hat{\xi})$ of $g(x;\xi)$ from (3.7) defined by

$$\hat{g}(\hat{\xi}) := \varepsilon^3 g(x;\xi) = \frac{1}{4\pi}\frac{e^{-\gamma\hat{r}}}{\hat{r}}, \qquad \text{where} \quad \hat{r} := \sqrt{\hat{\xi}_1^2 + \hat{\xi}_2^2 + \hat{\xi}_3^2}\,, \tag{3.10}$$

so that $g\,d\xi = \hat{g}\,d\hat{\xi}$, where $d\hat{\xi} = d\hat{\xi}_1\,d\hat{\xi}_2\,d\hat{\xi}_2 = \varepsilon^{-3}d\xi$. Therefore for any domain Ω' we have

$$|g(x;\cdot)|_{k,1\,;\Omega'} = \varepsilon^{-k}\,|\hat{g}|_{k,1\,;\hat{\Omega}'}\,, \qquad \|g(x;\cdot)\|_{2\,;\Omega'} = \varepsilon^{-3/2}\,\|\hat{g}\|_{2\,;\hat{\Omega}'}\,. \tag{3.11}$$

Now we shall establish parts (i) and (ii) of our lemma.
(i) A calculation using the standard differentiation formulas

$$\frac{\partial\hat{g}}{\partial\hat{\xi}_i} = \frac{\partial\hat{g}}{\partial\hat{r}}\cdot\frac{\partial\hat{r}}{\partial\hat{\xi}_i}, \qquad \frac{\partial^2\hat{g}}{\partial\hat{\xi}_i\,\partial\hat{\xi}_j} = \frac{\partial^2\hat{g}}{\partial\hat{r}^2}\cdot\frac{\partial\hat{r}}{\partial\hat{\xi}_i}\cdot\frac{\partial\hat{r}}{\partial\hat{\xi}_j} + \frac{\partial\hat{g}}{\partial\hat{r}}\cdot\frac{\partial^2\hat{r}}{\partial\hat{\xi}_i\,\partial\hat{\xi}_j},$$

where

$$\frac{\partial\hat{g}}{\partial\hat{r}} = -\frac{1}{4\pi}\frac{\gamma\hat{r}+1}{\hat{r}^2}e^{-\gamma\hat{r}}, \qquad \frac{\partial^2\hat{g}}{\partial\hat{r}^2} = \frac{1}{4\pi}\frac{\gamma^2\hat{r}^2 + 2\gamma\hat{r} + 2}{\hat{r}^3}e^{-\gamma\hat{r}}$$

and also $|\partial\hat{r}/\partial\hat{\xi}_i| = |\hat{\xi}_i/\hat{r}| \le 1$ and $|\partial^2\hat{r}/(\partial\hat{\xi}_i\,\partial\hat{\xi}_j)| \le 1/\hat{r}$, yields

$$\hat{r}^2\Big|\frac{\partial\hat{g}}{\partial\hat{\xi}_i}\Big| \le C(\gamma\hat{r}+1)e^{-\gamma\hat{r}}, \qquad \hat{r}^2\Big|\frac{\partial^2\hat{g}}{\partial\hat{\xi}_i\,\partial\hat{\xi}_j}\Big| \le C\,\frac{\hat{r}^2+1}{\hat{r}}e^{-\gamma\hat{r}}.$$

Combining this with the first relation in (3.11), we obtain the required analogues of (3.5) for g as follows. First, note that

$$\|g(x;\cdot)\|_{1\,;\Omega} + \varepsilon|g(x;\cdot)|_{1,1\,;\Omega} = \|\hat{g}\|_{1,1\,;\hat{\Omega}} \le C\int_0^\infty (\gamma\hat{r}+1)e^{-\gamma\hat{r}}\,d\hat{r} \le C.$$

Similarly, we obtain

$$|g(x;\cdot)|_{1,1\,;B(\tilde{x}\,;\rho)} \le |g(x;\cdot)|_{1,1\,;B(x\,;\rho)} \le C\varepsilon^{-1}\int_0^{\rho/\varepsilon}(\gamma\hat{r}+1)e^{-\gamma\hat{r}}\,d\hat{r} \le C\varepsilon^{-1}(\rho/\varepsilon);$$

here replacing the integral over $B(\tilde{x}\,;\rho)$ by the integral over $B(x\,;\rho)$ yields an upper bound, since $(\gamma\hat{r}+1)e^{-\gamma\hat{r}}$ is a positive decreasing function. Finally, we get

$$|g(x;\cdot)|_{2,1\,;\Omega\setminus B(x\,;\rho)} \le C\varepsilon^{-2}\int_{\rho/\varepsilon}^\infty \frac{\hat{r}^2+1}{\hat{r}}e^{-\gamma\hat{r}}\,d\hat{r} \le \varepsilon^{-2}\ln(2+\varepsilon/\rho).$$

(ii) A straightforward calculation using (3.10) shows that

$$\|\hat g\|^2_{2\,;\hat\Omega} \le C\int_0^\infty e^{-2\gamma\hat r}\,d\hat r \le C, \qquad \|\hat g\|^2_{2\,;\hat\Omega\setminus\hat B(x\,;\rho)} \le C\int_{\rho/\varepsilon}^\infty e^{-2\gamma\hat r}\,d\hat r \le Ce^{-2\gamma\rho/\varepsilon}.$$

Combining these with the second relation in (3.11), we immediately get the required analogues of (3.9) for g. □

Remark 3.4. An inspection of the proof of Lemma 3.3, in which we used the explicit representation (3.8),(3.7) of the Green's function in the constant-coefficient case, shows that the estimates of the Green's function in Theorem 3.1 are sharp.

3.2. **Smooth-coefficient case.** In this subsection, we shall use the estimates for the constant-coefficient Green's function $\bar G$ to establish a variable-coefficient case of Theorem 3.1 under the additional assumption that the coefficient p is differentiable and

$$\varepsilon\left|\tfrac{\partial}{\partial x_i}p\right| \le C \qquad \text{for } \ i = 1,2,3. \tag{3.12}$$

Lemma 3.5. *If the coefficient p satisfies (3.2) and (3.12), then the Green's function $G(x;\xi)$ from (3.3) satisfies estimates (3.5).*

Proof. Set $\gamma^2 := \beta$ in the definition (3.6) of $\bar G$. Note that in addition to (3.3), G satisfies $L_xG(x;\xi) = -\varepsilon^2\,\Delta_xG+p(x)G = \delta(x-\xi)$ subject to $G(x;\xi)=0$ for $x\in\partial\Omega$. Similarly, $\bar G$ satisfies $\bar L_x\bar G(x;\xi) = -\varepsilon^2\,\Delta_x\bar G+\gamma^2\bar G = \delta(x-\xi)$ subject to $\bar G(x;\xi)=0$ if $x_1=0$ or $x_2=0$ or $x_3=0$. Hence we have $L_x(\bar G-G) = [p-\gamma^2]\bar G = [p-\beta]\bar G \ge 0$, while $\bar G - G = \bar G \ge 0$ for $x\in\partial\Omega$. Now, applying the maximum principle, one gets $\bar G - G \ge 0$, or $0\le G\le \bar G$, so $\|G(x;\cdot)\|_{1\,;\Omega} \le \|\bar G(x;\cdot)\|_{1\,;\Omega}\le C$, where the bound for $\bar G$ is given by Lemma 3.3.

Next, let $\xi\in[0,\frac12]^3$ and construct a function

$$v(x;\xi) := G(x;\xi) - \omega(x)\,\bar G(x;\xi), \tag{3.13}$$

where $\omega(x)$ is a smooth cut-off function that equals 1 for $x\in[0,\frac34]^3$ and vanishes on the boundaries $x_1=1$, $x_2=1$ and $x_3=1$. Thus $v=0$ for $x\in\partial\Omega$. A calculation using $L_xG=\bar L_x\bar G$ yields $L_xv = (\gamma^2-p)\bar G + L_x[(1-\omega)\bar G]$, or

$$L_xv(x;\xi) = [-\varepsilon^2\triangle_x + p(x)]\,v(x;\xi) = \phi(x;\xi),$$

where $\phi=\phi_1+\phi_2$ with

$$\phi_1(x;\xi) := \big[\gamma^2 - p(x)\big]\bar G(x;\xi), \qquad \phi_2(x;\xi) := L_x\big[(1-\omega(x))\bar G(x;\xi)\big].$$

Comparing the problem for v with problem (3.1) and recalling (3.4), we arrive at

$$v(x,\xi) = \int_\Omega G(x;\eta)\,\phi(\eta;\xi)\,d\eta. \tag{3.14}$$

Applying $\frac{\partial}{\partial\xi_i}$, $i=1,2,3$, to this formula, one gets

$$|v(x;\cdot)|_{1,1\,;\Omega'} \le \|G(x;\cdot)\|_{1,\Omega}\cdot\max_{\eta\in\Omega}|\phi(\eta;\cdot)|_{1,1\,;\Omega'}. \tag{3.15}$$

We have already proved that $\|G(x;\cdot)\|_{1,\Omega}\le C$. Note also that $|\phi_1(\eta;\cdot)|_{1,1\,;\Omega'} \le C|\bar G(\eta;\cdot)|_{1,1\,;\Omega'}$. Furthermore, if $\Omega'\subset[0,\frac12]^3$ then $|\phi_2(\eta;\cdot)|_{1,1\,;\Omega'}\le C$ (the latter estimate holds as $\phi_2(\eta;\xi)=0$ for $\eta\in[0,\frac34]^3$; otherwise, $|\xi-\eta|\ge\frac14$ so any derivative of ϕ_2 is bounded by some C). Combining these observations with (3.15) and then noting that (3.13) implies $|G(x;\cdot)|_{1,1\,;\Omega'} \le |v(x;\cdot)|_{1,1\,;\Omega'} + |\bar G(x;\cdot)|_{1,1\,;\Omega'}$, we arrive at

$$|G(x;\cdot)|_{1,1\,;\Omega'} \le C\,\big(\max_{\eta\in\Omega} |\bar G(\eta;\cdot)|_{1,1\,;\Omega'} + 1\big),$$

where $\Omega' \subset [0,\frac12]^3$. Setting $\Omega' = [0,\frac12]^3$ and $\Omega' = B(\tilde x;\rho)\cap[0,\frac12]^3$ yields (3.5a), (3.5b) with Ω replaced by its subdomain $[0,\frac12]^3$. Dealing with the remaining seven cubic subdomains of Ω in a similar manner, one finally gets (3.5a), (3.5b).

To establish the remaining estimate (3.5c), it suffices, by (3.13), to obtain $|v(x;\cdot)|_{2,1\,;\Omega'} \le C\varepsilon^{-2}$. Let $v = v_1 + v_2$, where v_k, for $k = 1,2$, is defined by (3.15) with v and ϕ respectively replaced by v_k and ϕ_k. Imitating our above argument, we get $|v_2(x;\cdot)|_{2,1\,;\Omega'} \le C\max_{\eta\in\Omega} |\phi_2(\eta;\cdot)|_{2,1\,;\Omega'} \le C$. We have, however, to modify our approach to estimate $|v_1(x;\cdot)|_{2,1\,;\Omega'}$. First, examining (3.7) and (3.8), we note that $\frac{\partial}{\partial\xi_1} g(x;\xi) = -\frac{\partial}{\partial x_1} g(x;\xi)$, so $\frac{\partial}{\partial\xi_1} g(\pm x_1, \sigma_2 x_2, \sigma_3 x_3;\xi) = \mp\frac{\partial}{\partial x_1} g(\pm x_1, \sigma_2 x_2, \sigma_3 x_3;\xi)$, so $\frac{\partial}{\partial\xi_1} \bar G(x;\xi) = -\frac{\partial}{\partial x_1} \tilde G(x;\xi)$, where $\tilde G$ involve the same eight terms as $\bar G$ in (3.8), only with possibly different signs. Furthermore, $\tilde G$ satisfies (3.5) (imitate the proof of Lemma 3.3). In view of this, one gets

$$\frac{\partial}{\partial\xi_1} v_1(x,\xi) = \int_\Omega G(x;\eta)\{\gamma^2 - p(\eta)\}\,\frac{\partial}{\partial\xi_1}\bar G(\eta;\xi)d\eta = \int_\Omega \frac{\partial}{\partial\eta_1}[G(x;\eta)\{\gamma^2 - p(\eta)\}]\tilde G(\eta;\xi)d\eta.$$

Next, applying $\frac{\partial}{\partial\xi_i}$, $i = 1,2,3$, to this formula yields

$$\|\tfrac{\partial^2}{\partial\xi_1\partial\xi_i} v_1(x;\cdot)\|_{1\,;\Omega'} \le |G(x;\cdot)\{\gamma^2 - p(\cdot)\}|_{1,1\,;\Omega}\cdot \max_{\eta\in\Omega} |\tilde G(\eta;\cdot)|_{1,1\,;\Omega'} \le C\varepsilon^{-2},$$

where we used (3.2), (3.12) and (3.5a) that we already have for both G and $\tilde G$. As all second-order derivatives of v_1 can be estimated in a similar manner, we get $|v_1(x;\cdot)|_{2,1\,;\Omega'} \le C\varepsilon^{-2}$ and thus complete the proof of (3.5c). □

We have now proved Theorem 3.1 under condition (3.12). This condition is suitable for the particular linear case L of T. When we linearize (2.9) in the general semilinear case, the coefficient p depends on u and U. It may satisfy (3.12), but it is more convenient to avoid this assumption in our error analysis. Thus in the next subsection, we prove the general case of Theorem 3.1 under assumption (3.2) only.

Remark 3.6. One beneficial feature of the argument used in §3.2 is that it does not require a pointwise barrier for G (readily provided by $\bar G$ in §3.3). Instead, it suffices to have a sharp bound on $\|G(x;\cdot)\|_{1\,;\Omega}$. This feature is significant, when the above argument is extended in a future paper to more complicated singularly perturbed convection-diffusion equations.

3.3. **General case. Proof of Theorem 3.1.** Fix $x = (x_1, x_2, x_3) \in \Omega$; without loss of generality, we shall consider only the case of $x \in [0,\,1/2]^3$, as the other cases are similar.

Set $\gamma^2 := \beta$ in the definition (3.6) of $\bar G$. Since, by Lemma 3.3(i), estimates (3.5) hold true for $\bar G$, to get the desired estimates (3.5) for G, it suffices to show that

$$\varepsilon^2|(\bar G - G)(x;\cdot)|_{2,1\,;B(x\,;\varepsilon)\cap\Omega} + \varepsilon|(\bar G - G)(x;\cdot)|_{1,1\,;B(x\,;\varepsilon)\cap\Omega} \le C, \tag{3.16a}$$

$$\varepsilon|(\bar G - G)(x;\cdot)|_{1,1\,;B(\tilde x\,;\rho)\cap\Omega} \le C\,\rho/\varepsilon \quad \text{for } \rho \le \varepsilon, \tag{3.16b}$$

$$\varepsilon^2|G(x;\cdot)|_{2,1\,;\Omega\setminus B(x\,;\varepsilon)} + \varepsilon|G(x;\cdot)|_{1,1\,;\Omega\setminus B(x\,;\varepsilon)} \le C. \tag{3.16c}$$

Indeed, (3.5a) follows from its analogue for $\bar G$ combined with (3.16a) and (3.16c). The next estimate (3.5b) follows from (3.5a) if $\rho > \varepsilon$, and from its analogue for $\bar G$ combined with (3.16b) otherwise. Finally, estimate (3.5c) follows from (3.16c) for $\rho \ge \varepsilon$, and is obtained combining its analogue for $\bar G$ with (3.16a) and (3.16c) otherwise.

Now, to complete the proof, we shall establish each of the estimates in (3.16).

(a) Note that, by (3.3) and (3.6), we get

$$L_\xi(\bar G - G) = [-\varepsilon^2\triangle_\xi + p(\xi)\,]\,(\bar G - G) = [p(\xi) - \beta]\,\bar G. \tag{3.17}$$

Therefore, by (3.2), we have $L_\xi(\bar G - G) \ge 0$. Combining this with $\bar G - G \ge 0$ on $\partial\Omega$ and then applying the maximum/comparison principle yields $0 \le G \le \bar G$.

Next, using the variable $\hat\xi = (\xi - x)/\varepsilon$ and the notation $\hat w(\hat\xi) := w(\xi)$ for any function w, rewrite (3.17) in terms of the variable $\hat\xi$ as $[-\triangle + \hat p\,](\hat{\bar G} - \hat G) = [\hat p - \beta]\hat{\bar G}$, or $\triangle(\hat{\bar G} - \hat G) = \hat p\hat{\bar G} - \beta\hat G$. Now, an application of [23, Lemma 8.2 (Chap. 3, p. 181)] yields

$$\|\hat{\bar G} - \hat G\|_{2,2\,;\hat B(x\,;\varepsilon)\cap\hat\Omega} \le C_2\Big[\|\triangle(\hat{\bar G} - \hat G)\|_{2\,;\hat B(x\,;2\varepsilon)\cap\hat\Omega} + \|\hat{\bar G} - \hat G\|_{2\,;\hat B(x\,;2\varepsilon)\cap\hat\Omega}\Big], \tag{3.18}$$

where the constant C_2 is independent of ε since $\operatorname{dist}(\partial\hat B(x\,;\varepsilon), \partial\hat B(x\,;2\varepsilon)) = 1$. Note that the condition of [23, Lemma 8.2] that $\hat{\bar G} - \hat G = 0$ for $\hat\xi \in \partial\hat\Omega \cap \hat B(x\,;2\varepsilon)$, or, equivalently, $\bar G - G = 0$ for $\xi \in \partial\Omega \cap B(x\,;2\varepsilon)$, is immediately satisfied for $\varepsilon < 1/4$ since $x \in [0,\,1/2]^3$ (otherwise, if $\varepsilon \in [1/4,\,1]$, one gets a version of (3.18) for $\hat B(x\,;\varepsilon')$ and $\hat B(x\,;2\varepsilon')$ with $\varepsilon' := \varepsilon/5 < 1/4$; then an obvious modification of our further argument will again yield (3.5)).

To estimate the right-hand side in (3.18), recall that $0 \le G \le \bar G$, thus $0 \le \hat G \le \hat{\bar G}$, so $|\hat{\bar G} - \hat G| \le \hat{\bar G}$ and $|\triangle(\hat{\bar G} - \hat G)| = |\hat p\hat{\bar G} - \beta\hat G| \le C\hat{\bar G}$. These observations lead to

$$\|\hat{\bar G} - \hat G\|_{2,2\,;\hat B(x\,;\varepsilon)\cap\hat\Omega} \le C\|\hat{\bar G}\|_{2\,;\hat B(x\,;2\varepsilon)\cap\hat\Omega}\,. \tag{3.19}$$

Rewriting this in terms of the original variable ξ, we get

$$\varepsilon^2|(\bar G - G)(x;\cdot)|_{2,2\,;B(x\,;\varepsilon)\cap\Omega} + \varepsilon|(\bar G - G)(x;\cdot)|_{1,2\,;B(x\,;\varepsilon)\cap\Omega} \le C\|\bar G(x;\cdot)\|_{2\,;B(x\,;2\varepsilon)\cap\Omega},$$

where $\|\bar G(x;\cdot)\|_{2\,;B(x\,;2\varepsilon)\cap\Omega} \le C\,\varepsilon^{-3/2}$, by the first estimate in (3.9). Combining this with $|\bar G - G|_{k,1\,;B(x\,;\varepsilon)\cap\Omega} \le C\varepsilon^{3/2}|\bar G - G|_{k,2\,;B(x\,;\varepsilon)\cap\Omega}$, for $k = 1, 2$, yields (3.16a).

(b) Let x be an arbitrary point in Ω and $\tilde x \in [0,\,1/2]^3$ (as the other cases are similar). To show (3.16b), imitate the argument used to prove (3.16a) with $B(x\,;\varepsilon)$ and $B(x\,;2\varepsilon)$ replaced by $B(\tilde x\,;\rho)$ and $B(\tilde x\,;\rho+\varepsilon)$, invoking $|\bar G - G|_{k,1\,;B(\tilde x\,;\rho)} \le C\rho^{3/2}|\bar G - G|_{k,2\,;B(\tilde x\,;\rho)}$ and $\sqrt{\rho/\varepsilon} \le 1$.

(c) Let $\rho_j := 2^j\varepsilon$ and divide the domain $\Omega\backslash B(x\,;\varepsilon)$ into the non-overlapping subdomains $\mathcal D_j := \{\xi \in \Omega\,:\,\rho_j < r < \rho_{j+1}\}$ where $j = 0, 1, \ldots$. Furthermore, $\mathcal D_j \subset \mathcal D'_j := \mathcal D_{j-1} \cup \bar{\mathcal D}_j \cup \mathcal D_{j+1}$, so that $\operatorname{dist}(\partial\mathcal D'_j\backslash\partial\Omega, \partial\mathcal D_j\backslash\partial\Omega) \ge \varepsilon/2$.

Let the stretching transformation from ξ to $\hat\xi = (\xi - x)/\varepsilon$ map $\mathcal D_j$ into $\hat{\mathcal D}_j$. Rewriting the equation from (3.3) for $\xi \ne x$ in terms of the stretched variable $\hat\xi$ as $-\Delta\hat G + \hat p\,\hat G = 0$ yields

$$\|\hat G\|_{2,2\,;\hat{\mathcal D}_j} \le C_2\|\hat G\|_{2\,;\hat{\mathcal D}'_j}\,; \tag{3.20}$$

see [23, Lemma 8.2 (Chap. 3, p. 181)]; here the constant C_2 is independent of ε since $\mathrm{dist}(\partial\hat{\mathcal{D}}_j\backslash\partial\hat{\Omega}, \partial\hat{\mathcal{D}}'_j\backslash\partial\hat{\Omega}) \geq 1/2$. Note that the condition of [23, Lemma 8.2] that $\hat{G} = 0$ on $\partial\hat{\mathcal{D}}'_j \cap \partial\hat{\Omega}$ is satisfied due to the boundary condition in (3.3).

Rewritten in terms of the original variable ξ, estimate (3.20) implies that

$$\varepsilon^2 |G(x;\cdot)|_{2,2\,;\mathcal{D}_j} + \varepsilon |G(x;\cdot)|_{1,2\,;\mathcal{D}_j} \leq C\|G(x;\cdot)\|_{2\,;\mathcal{D}'_j} \leq C\|\bar{G}(x;\cdot)\|_{2\,;\mathcal{D}'_j}. \tag{3.21}$$

where we also used $G \leq \bar{G}$. Noting that $\mathcal{D}'_j \subset \Omega\backslash B(x\,;\rho_{j-1})$ and recalling the second estimate in (3.9), we get $\|\bar{G}(x;\cdot)\|_{2\,;\mathcal{D}'_j} \leq C\varepsilon^{-3/2} e^{-\gamma\rho_{j-1}/\varepsilon}$. Combining this with (3.21) and $|G|_{k,1\,;\mathcal{D}_j} \leq C\rho_j^{3/2} |G|_{k,2\,;\mathcal{D}_j}$, for $k = 1, 2$, we arrive at

$$\varepsilon^2 |G(x;\cdot)|_{2,1\,;\mathcal{D}_j} + \varepsilon |G(x;\cdot)|_{1,1\,;\mathcal{D}_j} \leq C\rho_j^{3/2} \varepsilon^{-3/2} e^{-\gamma\rho_{j-1}/\varepsilon}.$$

Now, the required estimate (3.16c) is obtained recalling that $\Omega\backslash B(x\,;\varepsilon) = \cup_{j=0}^{\infty}\mathcal{D}_j$ and noting that we have

$$\sum_{j=0}^{\infty} \Big(\frac{\gamma\rho_j}{\varepsilon}\Big)^{3/2} e^{-\gamma\rho_{j-1}/\varepsilon} \leq C \sum_{j=0}^{\infty} \frac{\gamma(\rho_j - \rho_{j-1})}{4\varepsilon} e^{-\gamma\rho_j/(4\varepsilon)} \leq C \int_{\gamma/8}^{\infty} e^{-s} ds,$$

since $s^{1/2}e^{-2s} \leq Ce^{-s}$ and $\rho_j = 2(\rho_j - \rho_{j-1})$, and for the decreasing function e^{-s} the right Riemann sum gives a lower estimate of the corresponding integral. □

4. Stability properties of differential operators

In this section, we are concerned with subtle stability properties of the semilinear differential operator T from (1.1). The main result of this section, Theorem 4.1, will be applied in §5 to equation (2.9), which relates the exact solution and the computed solution.

Suppose the right-hand side f is of the special form

$$f(x) = -\nabla \cdot \big[F(x) + \bar{F}(x)\big] + \bar{f}(x), \tag{4.1a}$$

where $F = (F_1, F_2, F_3)$ and $\bar{F} = (\bar{F}_1, \bar{F}_2, \bar{F}_3)$ are vector functions, whose components together with $\bar{f}$ are in $L_\infty(\Omega)$, and $\nabla \cdot F = \partial F_1/\partial x_1 + \partial F_2/\partial x_2 + \partial F_3/\partial x_3$. Furthermore, we assume that

$$F_1(x) = A_i(x_2, x_3)\,(x_1 - x_1^{[i-1/2]}) \quad \text{for } x \in (x_1^{[i-1]}, x_1^{[i]}) \times [0,1] \times [0,1], \tag{4.1b}$$

$$F_2(x) = B_j(x_1, x_3)\,(x_2 - x_2^{[j-1/2]}) \quad \text{for } x \in [0,1] \times (x_2^{[j-1]}, x_2^{[j]}) \times [0,1], \tag{4.1c}$$

$$F_3(x) = Q_l(x_1, x_2)\,(x_3 - x_3^{[l-1/2]}) \quad \text{for } x \in [0,1] \times [0,1] \times (x_3^{[l-1]}, x_3^{[l]}), \tag{4.1d}$$

where $i, j, l = 1, \ldots, N$, respectively, and the notation $x_s^{[i-1/2]} := (x_s^{[i-1]} + x_s^{[i]})/2$ is used with $s = 1, 2, 3$.

Theorem 4.1. *Suppose the function b in the definition (1.1) of T satisfies (1.2), and f is defined by (4.1). Then, for any functions $v, w \in W^{1,2}(\Omega)$ such that $Tv(x) - Tw(x) = f(x)$, and $v = w$ on $\partial\Omega$, we have*

$$\|v - w\|_\infty \leq C\varepsilon^{-2}\big[E_1 + E_2 + E_3\big]\, \ln\!\big(2 + \varepsilon/\kappa\big) + C\varepsilon^{-1}\|\bar{F}\|_\infty + \beta^{-1}\|\bar{f}\|_\infty,$$

where $\kappa = \min\{\min_i\{h_i\}, \min_j\{\tau_j\}, \min_l\{k_l\}\}$ and

$$E_1 := \max_{i=1,\ldots,N}\big\{h_i^2 \max_{x_2,x_3\in[0,1]} |A_i(x_2,x_3)|\big\},\quad E_2 := \max_{j=1,\ldots,N}\big\{\tau_j^2 \max_{x_1,x_3\in[0,1]} |B_j(x_1,x_3)|\big\},$$

$$E_3 := \max_{l=1,\ldots,N}\big\{k_l^2 \max_{x_1,x_2\in[0,1]} |Q_l(x_1,x_2)|\big\}.$$

The above theorem is a three-dimensional version of [19, Theorem 4.1]. The proof is in lines with the one in [19], so we only sketch it below for completeness.

Proof. Using the standard linearization technique, one gets $Tv - Tw = L\big[v - w\big]$, where the linear operator L is defined by (3.1), in which, by (1.2), the coefficient $p(x)$ satisfies (3.2). As we now have the linear equation $L[u - v] = f$, we shall deal with various components of f separately and, in particular, invoke the Green's function G of the operator L in our analysis.

First we note that if $F = (F_1, F_2, F_3) := 0$ in (4.1a), then

$$\|u - v\|_\infty \le C\varepsilon^{-1}\|\bar{F}\|_\infty + \beta^{-1}\|\bar{f}\|_\infty. \tag{4.2}$$

This is easily shown by imitating the proof of [19, Lemma 4.2], more specifically, by combining (3.4) with estimate (3.5a).

Next, we claim that if $\bar{F} := 0$ and $\bar{f} := 0$ in (4.1), then

$$\|u - v\|_\infty \le C\varepsilon^{-2}\big[E_1 + E_2 + E_3\big]\,\ln\big(2 + \varepsilon/\kappa\big). \tag{4.3}$$

Combining this with the observation (4.2) yields the assertion of the theorem. Thus it remains to prove (4.3).

We get (4.3) by extending the proof from [19, Lemma 4.3] to three dimensions as briefly described below. Note that it suffices to get (4.3) only in the case of $f := -\partial F_1/\partial x_1$, i.e. $F_2 = F_3 := 0$, as the cases of $f := -\partial F_s/\partial x_s$, for $s = 2, 3$, are similar. Fix x and denote $v(\xi) := G(x;\xi)$. Then, using (3.4), one gets

$$(u-v)(x) = \int_\Omega F_1(\xi)\, v_{\xi_1}(\xi)\, d\xi = \sum_{i=1}^{N}\int_0^1 d\xi_2 \int_0^1 d\xi_3\, A_i(\xi_2,\xi_3) \int_{x_1^{[i-1]}}^{x_1^{[i]}} (\xi_1 - x_1^{[i-1/2]})\, v_{\xi_1}(\xi)\, d\xi_1.$$

For the integral in ξ_1, a calculation shows that

$$\Big|\int_{x_1^{[i-1]}}^{x_1^{[i]}} (\xi_1 - x_1^{[i-1/2]})\, v_{\xi_1}(\xi)\, d\xi_1\Big| \le \frac{h_i^2}{4}\int_{x_1^{[i-1]}}^{x_1^{[i]}} |v_{\xi_1\xi_1}(\xi)| d\xi_1. \tag{4.4}$$

However, we have to be careful when integrating $v_{\xi_1\xi_1} = G_{\xi_1\xi_1}$ as this function has such a singularity at $\xi = x$ that it is not in $L_1(\Omega)$. Thus we form a rectangular-box neighbourhood Ω' of $\xi = x$ (of diameter not exceeding $O(\kappa)$). Outside this neighbourhood the integral $\int F_1\, v_{\xi_1}\, d\xi$ is estimated using (4.4) and then (3.5c). Over this neighbourhood, the integral $\int F_1\, v_{\xi_1}\, d\xi$ is estimated using (3.5b). This completes the proof of (4.3) in the case of $f := -\partial F_1/\partial x_1$. □

5. Analysis of the numerical method. Proof of Theorem 2.2

To complete the proof of our main result, Theorem 2.2, which we started in §2, we shall invoke the following lemma.

Lemma 5.1. [17, 19] *We have*

$$-\varepsilon^2 \tfrac{\partial^2}{\partial x_s^2} U^{\mathrm{I}_s} + q_s^{\mathrm{I}_s} = \tfrac{\partial}{\partial x_s} F_s, \qquad s = 1, 2, 3,$$

where the semi-discrete functions $F_1 = F_1(x_1, x_2^{[j]}, x_3^{[l]})$, $F_2 = F_2(x_1^{[i]}, x_2, x_3^{[l]})$ *and* $F_3 = F_3(x_1^{[i]}, x_2^{[j]}, x_3)$ *are defined by*

$$F_1 := q_{1,ij\,l}\,(x_1 - x_1^{[i-1/2]}) + \tfrac12 D_1^- q_{1,ij\,l}\,(x_1^{[i]} - x_1)^2, \quad x_1 \in (x_1^{[i-1]}, x_1^{[i]}), \tag{5.1a}$$

for $i = 1, \ldots, N$ *and* $j,\, l = 0, \ldots, N$,

$$(5.1b)\qquad F_2 := q_{2,ij\,l}\,(x_2 - x_2^{[j-1/2]}) + \tfrac{1}{2} D_2^- q_{2,ij\,l}\,(x_2^{[j]} - x_2)^2, \quad x_2 \in (x_2^{[j-1]}, x_2^{[j]}),$$

for $j = 1, \dots, N$ *and* $i,\, l = 0, \dots, N$,

$$(5.1c)\qquad F_3 := q_{3,ij\,l}\,(x_3 - x_3^{[l-1/2]}) + \tfrac{1}{2} D_3^- q_{3,ij\,l}\,(x_3^{[l]} - x_3)^2, \quad x_3 \in (x_3^{[l-1]}, x_3^{[l]}),$$

for $l = 1, \dots, N$ *and* $i,\, j = 0, \dots, N$.

Proof. Imitate the proofs of [17, Theorem 3.3] and [19, Lemma 5.1]. □

Remark 5.2. One can easily check that F_s, for $s = 1, 2, 3$, of (5.1) allow an alternative representation:

$$\begin{aligned}
F_1 &= [q_1]_{i-1,j,l}\,(x_1 - x_1^{[i-1/2]}) + [D_1^- q_{1,ij\,l}]\, O(h_i^2), \qquad x_1 \in (x_1^{[i-1]}, x_1^{[i]}),\\
F_2 &= [q_2]_{i,j-1,l}\,(x_2 - x_2^{[j-1/2]}) + [D_2^- q_{2,ij\,l}]\, O(\tau_j^2), \qquad x_2 \in (x_2^{[j-1]}, x_2^{[j]}),\\
F_3 &= [q_3]_{i,j,l-1}\,(x_3 - x_3^{[l-1/2]}) + [D_3^- q_{3,ij\,l}]\, O(k_l^2), \qquad x_3 \in (x_3^{[l-1]}, x_3^{[l]}).
\end{aligned}$$

Here, e.g., the new representation of F_1 follows from $q_{1,ij\,l} = [q_1]_{i-1,j,l} + h_i\,[D_1^- q_{1,ij\,l}]$.

Proof of Theorem 2.2 (continued from §2). Extend F_s, $s = 1, 2, 3$, of Lemma 5.1 onto the whole domain $\bar\Omega$ by the trilinear interpolation

$$F_1(x) := \bigl[F_1(x_1, x_2^{[j]}, x_3^{[l]})\bigr]^{\mathrm{I}_2\mathrm{I}_3}, \qquad F_2(x) := \bigl[F_2(x_1^{[i]}, x_2, x_3^{[l]})\bigr]^{\mathrm{I}_1\mathrm{I}_3},$$
$$F_3(x) := \bigl[F_3(x_1^{[i]}, x_2^{[j]}, x_3)\bigr]^{\mathrm{I}_1\mathrm{I}_2}.$$

Now, noting that any operator $\partial/\partial x_s$ is commutative with I_t for $t \neq s$, we obtain the representation (2.9) for the residual $TU^{\mathrm{I}} - Tu$. So, by Theorem 4.1, one gets

$$(5.2)\quad \|U^{\mathrm{I}} - u\|_\infty \le C\varepsilon^{-2}\bigl[E_1 + E_2 + E_3\bigr]\,\ln\bigl(2 + \varepsilon/\kappa\bigr) + C\varepsilon^{-1}\bar E + \beta^{-1}\|q - q^{\mathrm{I}}\|_\infty,$$

where

$$(5.3a)\qquad E_1 = \max_{i=1,\dots,N}\bigl\{h_i^2 \max_{x_2,x_3\in[0,1]} |(q_{1,ij\,l})^{\mathrm{I}_2\mathrm{I}_3}|\bigr\} = \max_{\substack{i=1,\dots,N\\ j,l=0,\dots,N}} \bigl\{h_i^2 |q_{1,ij\,l}|\bigr\},$$

and similarly

$$(5.3b)\qquad E_2 = \max_{\substack{j=1,\dots,N\\ i,l=0,\dots,N}} \bigl\{\tau_j^2 |q_{2,ij\,l}|\bigr\}, \qquad E_3 = \max_{\substack{l=1,\dots,N\\ i,j=0,\dots,N}} \bigl\{k_l^2 |q_{3,ij\,l}|\bigr\},$$

while

$$\bar E = \max_{\substack{i=1,\dots,N\\ j,l=0,\dots,N}} \bigl\{h_i^2 |D_1^- q_{1,ij\,l}|\bigr\} + \max_{\substack{j=1,\dots,N\\ i,l=0,\dots,N}} \bigl\{\tau_j^2 |D_2^- q_{2,ij\,l}|\bigr\} + \max_{\substack{l=1,\dots,N\\ i,j=0,\dots,N}} \bigl\{k_l^2 |D_3^- q_{3,ij\,l}|\bigr\}.$$

Furthermore, in view of Remark 5.2 (compare it with (5.1)), we observe that the quantities $|q_{s,ij\,l}|$, $s = 1, 2, 3$, in (5.3) can be replaced by $\min\{|q_{1,i-1,j,l}|, |q_{1,ij\,l}|\}$, $\min\{|q_{2,i,j-1,l}|, |q_{2,ij\,l}|\}$ and $\min\{|q_{3,i,j,l-1}|, |q_{3,ij\,l}|\}$, respectively. This yields a sharper version of (5.2), (5.3), which is then combined with (2.7). Now, to get the desired a posteriori error estimate of Theorem 2.2, it remains to show the trilinear interpolation estimate

$$\begin{aligned}
\|q - q^{\mathrm{I}}\|_\infty \le C\Bigl[&\max_{\substack{i=1,\dots,N\\ j,l=0,\dots,N}} \bigl\{h_i^2(1 + |D_1^- U_{ij\,l}|^2)\bigr\}\\
&+ \max_{\substack{j=1,\dots,N\\ i,l=0,\dots,N}} \bigl\{\tau_j^2(1 + |D_2^- U_{ij\,l}|^2)\bigr\} + \max_{\substack{j=1,\dots,N\\ i,l=0,\dots,N}} \bigl\{k_l^2(1 + |D_3^- U_{ij\,l}|^2)\bigr\}\Bigr].
\end{aligned}$$

This estimate follows from $q - q^{\mathrm{I}} = [q - q^{\mathrm{I}_1}] + [q^{\mathrm{I}_1} - (q^{\mathrm{I}_1})^{\mathrm{I}_2}] + [q^{\mathrm{I}_1\mathrm{I}_2} - (q^{\mathrm{I}_1\mathrm{I}_2})^{\mathrm{I}_3}]$ combined with the observation that $|\partial^2 q/\partial x_s^2| \le C(1 + |D_s^- U_{ij\,l}|^2)$ in each mesh

Table 6.1. Bakhvalov mesh, $\lambda = 3$: maximum norm error e and the efficiency constant e/η for the upper error estimator η.

	$\varepsilon = 10^{-1}$		$\varepsilon = 10^{-2}$		$\varepsilon = 10^{-3}$		$\varepsilon = 10^{-k}$, $k = 4, \dots, 10$	
N	e	e/η	e	e/η	e	e/η	e	e/η
16	1.74e-2	1.80e-1	1.71e-2	1.31e-1	1.73e-2	1.31e-1	1.73e-2	1.31e-1
32	4.51e-3	1.82e-1	4.31e-3	1.28e-1	4.36e-3	1.28e-1	4.38e-3	1.28e-1
64	1.17e-3	1.86e-1	1.08e-3	1.26e-1	1.09e-3	1.26e-1	1.10e-3	1.27e-1
128	2.96e-4	1.87e-1	2.70e-4	1.26e-1	2.74e-4	1.26e-1	2.75e-4	1.26e-1

Table 6.2. Bakhvalov mesh, $\lambda = 3$: upper maximum norm error estimator η, its components η_1, η_2, η_3, and its efficiency constant e/η.

	$\varepsilon = 10^{-1}$				$\varepsilon = 10^{-k}$, $k = 4, \dots, 10$			
N	η_1	η_2	$\eta_3 = \eta$	e/η	η_1	η_2	$\eta_3 = \eta$	e/η
16	4.43e-2	7.79e-2	9.64e-2	1.80e-1	1.10e-1	1.07e-1	1.33e-1	1.31e-1
32	1.29e-2	2.24e-2	2.48e-2	1.82e-1	3.10e-2	3.09e-2	3.41e-2	1.28e-1
64	3.50e-3	6.00e-3	6.29e-3	1.86e-1	8.26e-3	8.25e-3	8.65e-3	1.27e-1
128	9.07e-4	1.55e-3	1.58e-3	1.87e-1	2.13e-3	2.13e-3	2.18e-3	1.26e-1

cell $(x_1^{[i-1]}, x_1^{[i]}) \times (x_2^{[j-1]}, x_2^{[j]}) \times (x_3^{[l-1]}, x_3^{[l]})$; see [2, Comment 2.15] for a similar argument. $\square$

6. Numerical results

Our main result, the maximum norm a posteriori error estimate of Theorem 2.2, can be rewritten as

$$e := \|U^{\mathrm{I}} - u\|_\infty \le \tilde{C}\eta, \qquad \eta := \max\{\eta_0, \eta_1, \eta_2, \eta_3\}, \tag{6.1}$$

$$\eta_n := \max\Big\{ \max_{\substack{i=1,\dots,N_1\\ j=0,\dots,N_2\\ l=0,\dots,N_3}} \big\{h_i^2 M_{1,ij\,l}^{(n)}\big\}\ ;\ \max_{\substack{i=0,\dots,N_1\\ j=1,\dots,N_2\\ l=0,\dots,N_3}} \big\{\tau_j^2 M_{2,ij\,l}^{(n)}\big\}\ ;\ \max_{\substack{i=0,\dots,N_1\\ j=0,\dots,N_2\\ l=1,\dots,N_3}} \big\{k_l^2 M_{3,ij\,l}^{(n)}\big\}\ \Big\},$$

for $n = 0, 1, 2, 3$. Here we use $\tilde{C} = C \ln\big(2 + \varepsilon/\kappa\big)$,

$$M_{1,ij\,l}^{(2)} := \min\big\{|D_1^2 U_{i-1,j,l}|, |D_1^2 U_{ij\,l}|\big\}, \quad M_{2,ij\,l}^{(2)} := \min\big\{|D_2^2 U_{i,j-1,l}|, |D_2^2 U_{ij\,l}|\big\},$$

$$M_{3,ij\,l}^{(2)} := \min\big\{|D_3^2 U_{i,j,l-1}|, |D_3^2 U_{ij\,l}|\big\},$$

and for $s = 1, 2, 3$, we also use

$$M_{s,ij\,l}^{(0)} = 1, \qquad M_{s,ij\,l}^{(1)} := |D_s^- U_{ij\,l}|^2, \qquad M_{s,ij\,l}^{(3)} := \varepsilon |D_s^- D_s^2 U_{ij\,l}|.$$

Note that the quantities η_n involve $M^{(n)}$, $n = 1, 2, 3$, which can be viewed as discrete analogues of (possibly scaled) nth-order derivatives.

We give numerical results on a priori chosen meshes to illustrate the efficiency of the upper maximum norm error estimator η in (6.1) and its particular components η_n, $n = 0, 1, 2, 3$. We are also interested in which of η_n is the principal component in η if any. We shall compute the errors e and, more importantly, the quantities η, e/η, η_n, e/η_n and then examine their dependence on ε, numbers of mesh nodes and particular meshes.

TABLE 6.3. Uniform mesh: maximum norm error e and the efficiency constant e/η_2 for the component η_2 of the upper maximum norm error estimator η.

	$\varepsilon = 10^{-2}$		$\varepsilon = 10^{-3}$		$\varepsilon = 10^{-4}$		$\varepsilon = 10^{-k}$, $k = 5, \dots, 10$	
N	e	e/η_2	e	e/η_2	e	e/η_2	e	e/η_2
16	7.36e-1	8.02e-1	9.90e-1	9.99e-1	9.99e-1	1.01e+0	1.00e+0	1.01e+0
32	4.35e-1	5.31e-1	9.80e-1	9.87e-1	9.99e-1	1.00e+0	1.00e+0	1.00e+0
64	1.64e-1	2.86e-1	9.43e-1	9.53e-1	9.99e-1	9.99e-1	1.00e+0	1.00e+0
128	5.61e-2	2.00e-1	8.24e-1	8.52e-1	9.97e-1	9.98e-1	1.00e+0	1.00e+0

TABLE 6.4. Uniform mesh: the components η_2 and η_3 of the upper maximum norm error estimator η and the efficiency constant e/η_2 for η_2.

	$\varepsilon = 10^{-4}$			$\varepsilon = 10^{-7}$			$\varepsilon = 10^{-10}$		
N	η_2	$\eta_3 = \eta$	e/η_2	η_2	$\eta_3 = \eta$	e/η_2	η_2	$\eta_3 = \eta$	e/η_2
16	9.91e-1	6.20e+2	1.01e+0	9.91e-1	6.20e+5	1.01e+0	9.91e-1	6.20e+8	1.01e+0
32	9.98e-1	3.12e+2	1.00e+0	9.98e-1	3.12e+5	1.00e+0	9.98e-1	3.12e+8	1.00e+0
64	9.99e-1	1.56e+2	9.99e-1	9.99e-1	1.56e+5	1.00e+0	9.99e-1	1.56e+8	1.00e+0
128	9.99e-1	7.81e+1	9.98e-1	1.00e+0	7.81e+4	1.00e+0	1.00e+0	7.81e+7	1.00e+0

We let $\varepsilon = 10^{-k}$, $k = 1, \dots, 10$ and $N = \{2^k\}_{k=5}^{9}$, with $N_1 = N_2 = N_3 = N$. Two tensor-product meshes are considered: a variant of the layer-adapted mesh by Bakhvalov [4] and a simple uniform mesh; see Tables 6.1–6.5.

For $\varepsilon \le \bar\varepsilon$, our Bakhvalov-type mesh is defined by $x_1^{[i]} = x_2^{[i]} = x_3^{[i]} := \varphi(i/N)$, $i = 0, 1, \dots, N$, where $\varphi(t) := \varepsilon\lambda \ln[b/(b-t)]$ for $t \in [0, \theta]$, $\varphi(1) := 1$, and $\varphi(t)$ is continuous on $[0, 1]$ and linear on $[\theta, 1]$. We use the constants $b = 1/2$, $\bar\varepsilon = b/\lambda$, and $\theta = b - \varepsilon\lambda$. The constant λ will be specified later. For $\varepsilon > \bar\varepsilon$, the Bakhvalov mesh is defined to be a simple uniform mesh. Note that a suitable Bakhvalov-type layer-adapted mesh yields ε-uniform second-order accuracy [4, 18]. Besides, we expect efficient adaptive algorithms to generate meshes that are similar, in some sense, to a Bakhvalov mesh, as in [20, §6 and Figure 2].

As a test problem, we use linear problem (3.1) with $p(x) := 1$ and $f(x)$ such that the exact solution is given by

$$u(x) = \big(\cos(\tfrac{1}{2}\pi x_1) - \mu(x_1)\big)\big(1 - x_2 - \mu(x_2)\big)\big(1 - x_3^2 - \mu(x_3)\big), \; \mu(t) = \frac{e^{-t/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}}.$$

Note that this $u(x)$ exhibits boundary and corner layers.

In Tables 6.1 and 6.2, we give numerical results for the Bakhvalov mesh with $\lambda = 3$. Under this choice of λ, the mesh yields ε-uniform second-order accuracy in the maximum norm, so, roughly speaking, one would like to be able to construct similar adaptive meshes. Examining Table 6.1, we observe agreement with our theoretical estimate (6.1). Not only does e/η stabilize, but it becomes close to the linear interpolation error constant $1/8 = 1.25e-1$. The components η_n of η can be compared when examining Table 6.2. For $\varepsilon = 10^{-k}$, $k = 1, \dots, 10$, we observe that $\eta_2 \approx \eta_3 = \eta$. Furthermore, for $\varepsilon \le 10^{-2}$ we have $\eta_1 \approx \eta_2 \approx \eta_3$, while for $\varepsilon = 10^{-1}$ the quantity η_1 is dominated by η_2 and η_3. The quantity η_0 is not given, as it is negligible (and known a priori).

TABLE 6.5. Bakhvalov mesh, $\lambda = 1$: maximum norm error e, upper maximum norm error estimator η, its components η_1, η_2, η_3, and its efficiency constant e/η.

	$\varepsilon = 10^{-5}$					$\varepsilon = 10^{-10}$				
N	e	η_1	η_2	$\eta_3 = \eta$	e/η	e	η_1	η_2	$\eta_3 = \eta$	e/η
16	1.75e-1	5.49e-2	3.77e-2	4.36e-1	4.02e-1	2.24e-1	5.49e-2	3.77e-2	4.83e-1	4.64e-1
32	1.02e-1	1.47e-2	1.67e-2	2.13e-1	4.81e-1	1.31e-1	1.47e-2	1.58e-2	2.43e-1	5.40e-1
64	5.44e-2	3.78e-3	8.37e-3	1.05e-1	5.19e-1	7.06e-2	3.79e-3	7.94e-3	1.21e-1	5.82e-1
128	2.75e-2	9.61e-4	4.22e-3	5.16e-2	5.34e-1	3.65e-2	9.61e-4	4.00e-3	6.00e-2	6.08e-1

Numerical results for uniform meshes are given in Tables 6.3 and 6.4. On these meshes, the boundary layers are not resolved and $e = O(1)$. This is correctly identified by $\eta = \eta_3$ blowing up even more significantly than e. Note that the component η_2 also correctly indicates that the method is inaccurate, but, unlike η_3, it remains bounded. Furthermore, η_2 better reflects the actual errors since $e/\eta_2 \approx \text{const} = 1.0$ in Table 6.4.

Table 6.5 gives numerical results for the Bakhvalov mesh, but now with $\lambda = 1$. Thus the condition $\lambda > 2$, which implies ε-uniform second-order accuracy for our test problem [4, 18], is violated. Hence the errors slightly increase as $\varepsilon \to 0$. In this case, we observe that η_1 is too small compared to η and e.

In summary, our numerical results suggest that the error estimator η correctly indicates whether or not the method is ε-uniformly accurate. We also note that the quantity $\eta = \eta_3$ may blow up (see Table 6.4), while the component η_1 is sometimes too optimistic (see Table 6.5). The component η_2 seems the most relevant estimator for the actual error e. In particular, η_2 does not blow up, like η_3, and hence seems a more suitable error indicator in possible adaptive mesh construction. We finally note that our conclusions agree with the numerical results in two dimensions [19].

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