Pointwise Error Estimates for 2d Singularly Perturbed Semilinear Reaction-Diffusion Problems ⋆

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Abstract. A semilinear reaction-diffusion equation with multiple solutions is considered in a smooth two-dimensional domain. Its diffusion parameter ε^2 is arbitrarily small, which induces boundary layers. We extend the numerical method and its maximum norm error analysis of the paper [N. Kopteva: Maximum norm error analysis of a 2d singularly perturbed semilinear reaction-diffusion problem. Math. Comp., 2007], in which a parametrization of the boundary $\partial\Omega$ is assumed to be known, to a more practical case when the domain is defined by an ordered set of boundary points. It is shown that, using layer-adapted meshes, one gets second-order convergence in the discrete maximum norm, uniformly in ε. Numerical experiments are performed to support the theoretical results.

1 Introduction

Consider the singularly perturbed semilinear reaction-diffusion problem

$$Fu \equiv -\varepsilon^2 \triangle u + b(x,u) = 0, \qquad x = (x_1, x_2) \in \Omega \subset \mathbb{R}^2, \tag{1a}$$

$$u(x) = g(x), \qquad x \in \partial\Omega, \tag{1b}$$

where ε is a small positive parameter, $\triangle = \partial^2/\partial x_1^2 + \partial^2/\partial x_2^2$ is the Laplace operator, and Ω is a bounded two-dimensional domain whose boundary $\partial\Omega$ is sufficiently smooth. Assume also that the functions b and g are sufficiently smooth. We shall examine solutions of (1) that exhibit boundary layer behaviour.

The aim of the present paper is to extend the numerical method and its maximum norm error analysis of the recent paper [7], in which a parametrization of the boundary $\partial\Omega$ is assumed to be known, to a more practical case when the domain is defined by an ordered set of boundary points $\{(\varphi_j, \psi_j)\}_{j=0}^{M}$, where $(\varphi_0, \psi_0) = (\varphi_M, \psi_M)$ and the distance between any two consecutive points $(\varphi_{j-1}, \psi_{j-1})$ and (φ_j, ψ_j) does not exceed Ch for some constant C, while $C^{-1}h \le M \le Ch$.

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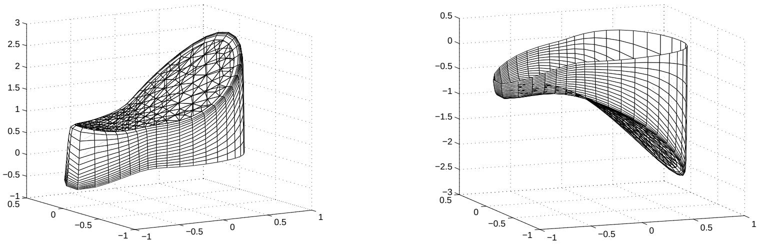

Fig. 1. *Multiple boundary-layer solutions of model problem (33); in the interior subdomain* $u(x) \approx \bar{u}_0(x)$ *(left) or* $u(x) \approx -\bar{u}_0(x)$ *(right), where* $\pm\bar{u}_0(x)$ *are stable solutions of the reduced problem (2).*

The reduced problem of (1) is defined by formally setting $\varepsilon = 0$ in (1a), viz.,

$$b(x, u_0(x)) = 0 \quad \text{for } x \in \Omega. \tag{2}$$

Any solution u_0 of (2) does not in general satisfy the boundary condition (1b).

In the numerical analysis literature it is often assumed—see, e.g., [14, 2]—that $b_u(x, u) > \gamma^2 > 0$ for all $(x, u) \in \Omega \times \mathbb{R}^1$, for some positive constant γ. Under this condition the reduced problem has a unique solution u_0, which is sufficiently smooth in $\bar{\Omega}$. This global condition is nevertheless rather restrictive. E.g., mathematical models of biological and chemical processes frequently involve problems related to (1) with $b(x, u)$ that is *non-monotone* with respect to u [11, §14.7], [6, §2.3]. Hence, following [7], we consider problem (1) under the following weaker *assumptions* from [5, 12]:

- it has a *stable reduced solution*, i.e., there exists a sufficiently smooth solution u_0 of (2) such that

$$b_u(x, u_0) > \gamma^2 > 0 \quad \text{for all } x \in \Omega; \tag{A1}$$

- the boundary condition satisfies

$$\int_{u_0(x)}^{v} b(x, s)\, ds > 0 \qquad \text{for all } \ v \in \big(u_0(x), g(x)\big]', \qquad x \in \partial\Omega. \tag{A2}$$

  Here the notation $(a, b]'$ is defined to be $(a, b]$ when $a < b$ and $[b, a)$ when $a > b$, while $(a, b]' = \emptyset$ when $a = b$.

If $g(x) \approx u_0(x)$, then (A2) follows from (A1) combined with (2); if $g(x) = u_0(x)$ for some $x \in \partial\Omega$, then (A2) does not impose any restriction on g at this point.

Conditions (A1), (A2) intrinsically arise from the asymptotic analysis of problem (1) and guarantee that there exists a boundary-layer solution u of (1) such that $u \approx u_0$ in the interior subdomain of Ω away from the boundary, while the boundary layer is of width $O(\varepsilon|\ln\varepsilon|)$ [5, 12, 7]. Note that assumption (A1) is

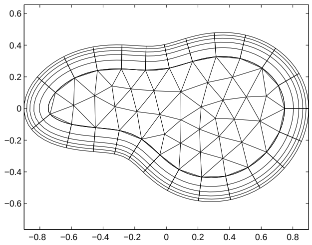

Fig. 2. *Layer-adapted mesh.*

local. Furthermore, if multiple stable solutions of the reduced problem satisfy (A2), problem (1) has *multiple* boundary-layer solutions; see Figure 1.

We discretize the domain as in Figure 2—see §§3.1, 4.1 for details—using layer-adapted meshes of Bakhvalov and Shishkin types whose number of mesh nodes does not exceed Ch^{-2}. Here $h > 0$ is the maximum side length of mesh elements of the layer-adapted meshes that we consider.

Then we discretize equation (1a) combining finite differences on the curvilinear tensor-product part of the mesh and lumped mass linear finite elements on a quasiuniform Delaunay triangulation in the interior region. Constructing discrete sub- and super-solutions and then invoking the theory of Z-fields, we prove existence and investigate the accuracy of multiple discrete solutions of problem (1). Our main result is Theorem 4.5 that states second-order convergence (with, in the case of the Shishkin mesh, a logarithmic factor) in the discrete maximum norm, uniformly in ε.

Throughout our analysis we assume that

$$\varepsilon \leq Ch. \tag{A3}$$

This is not a practical restriction, and from a theoretical viewpoint the analysis of a nonlinear problem such as (1) would be very different if ε were not small.

Note that similar one-dimensional and two-dimensional problems were considered in [2–4, 8, 10, 14, 16]; see [7] for further discussion.

The paper is organized as follows. In §2 we discuss asymptotic properties of solutions of (1) and construct sub- and super-solutions. In §3 we recall the layer-adapted meshes and the numerical method from [7], which explicitly uses a parametrization of the boundary $\partial\Omega$. In §4 the above method is extended to to a more practical case when the domain is defined by an ordered set of boundary points. Precise convergence results for the numerical method are then derived on Bakhvalov and Shishkin meshes. Finally, in §5, numerical results support our error estimates.

Notation. Throughout this paper we let C denote a generic positive constant that may take different values in different formulas, but is always independent of h and ε. A subscripted C (e.g., C_1) denotes a positive constant that is independent of h and ε and takes a fixed value. For any two quantities w_1 and w_2, the notation $w_1 = O(w_2)$ means $|w_1| \leq Cw_2$.

2 Local Curvilinear Coordinates. Asymptotic Expansion. Sub-and Super-Solutions

Given a sufficiently smooth boundary $\partial\Omega$, let its arc-length parametrization with counterclockwise orientation be defined by

$$x_1 = \varphi(l), \qquad x_2 = \psi(l), \qquad 0 \le l \le L, \tag{3}$$

where L is the arc-length of $\partial\Omega$. Hence the tangent vector (φ', ψ') has magnitude $\tau = \sqrt{\varphi'^2 + \psi'^2} = 1$ for all l. Furthermore, $(\varphi(0), \psi(0)) = (\varphi(L), \psi(L))$ and all functions that are defined for l beyond $[0, L]$ are understood as extended L-periodically. We also use the curvature κ of the boundary at $(\varphi(l), \psi(l))$ given by

$$\kappa = \kappa(l) = \varphi'\psi'' - \psi'\varphi''. \tag{4}$$

In a narrow neighbourhood of $\partial\Omega$ that will be specified later, introduce the curvilinear local coordinates (r, l) by

$$x_1 = \varphi(l) - r\psi'(l), \qquad x_2 = \psi(l) + r\varphi'(l), \tag{5}$$

where $(-\psi', \varphi')$ is the inward unit normal to $\partial\Omega$ at $(\varphi(l), \psi(l))$, which is orthogonal to the tangent vector (φ', ψ'). Since $\partial\Omega$ is smooth, there exists a sufficiently small constant C_1 such that in the subdomain $\bar\Omega_{C_1} = \{0 \le r \le C_1\}$ the new coordinates are well-defined. Throughout the paper we shall use a smooth positive cut-off function $\omega(x)$ that equals 1 for $r \le C_1/2$ and vanishes in $\bar\Omega \backslash \bar\Omega_{C_1}$.

Lemma 2.1 ([7, Lemma 2.1]). *For the Laplace operator we have*

$$\triangle u = \eta^{-1}\frac{\partial}{\partial r}\Big(\eta\frac{\partial u}{\partial r}\Big) + \eta^{-1}\frac{\partial}{\partial l}\Big(\eta^{-1}\frac{\partial u}{\partial l}\Big), \quad \textit{where } \eta := 1 - \kappa r. \tag{6}$$

To obtain an asymptotic expansion, introduce the stretched variable $\xi := r/\varepsilon$ and the function $v_0(\xi, l)$ defined by $-\partial^2 v_0/\partial\xi^2 + b(\bar x, u_0(\bar x) + v_0) = 0$ for $\xi > 0$, with the boundary conditions $v_0(0, l) = g(\bar x) - u_0(\bar x)$ and $v_0(\infty, l) = 0$. Here $\bar x = \bar x(l) := (\varphi(l), \psi(l))$. Our conditions (A1),(A2) are precisely what is needed to ensure existence and asymptotic properties of v_0 [5, 12, 8].

Theorem 2.2 ([12, Theorem 3]). *Under hypotheses (A1), (A2), for sufficiently small ε there exists a solution $u(x)$ of (1) in an $O(\varepsilon)$-neighbourhood of the zero-order asymptotic expansion $u_0(x) + v_0(\xi, l)\,\omega(x)$.*

Our sub- and super-solutions will invoke the function $\beta(x; p)$ constructed in [7, §2.3], which is a modified first-order asymptotic expansion such that

$$\beta(x; p) = u(x) + O(\varepsilon^2 + p). \tag{7}$$

The value p in the definition of β is a small real number that will be chosen later and is typically $o(h)$. To be more precise,

$$\beta(x; p) = u_0(x) + \bar v(\xi, l; p)\,\omega(x) + C_0 p, \qquad \Big|\frac{\partial^{k+m}}{\partial\xi^k\,\partial^m l}\,\bar v(\xi, l; p)\Big| \le Ce^{-\gamma_0\xi}, \tag{8}$$

where C_0 and γ_0 are positive constants and $\gamma_0^2 < \min_{x\in\partial\Omega} b_u(x, u_0(x))$.

Lemma 2.3 ([7, Corollaries 2.7, 2.9]). *There exists $p_0 \in (0, \gamma_0^2)$ such that for all $|p| \le p_0$ the function $\beta(x;p)$ is well-defined. Furthermore, there exists $C_0 > 0$ and $C_2 > 0$ such that $C_2\varepsilon^2 \le p \le p_0$ implies $\beta(x;-p) \le \beta(x;p)$ and*

$$F\beta(x;-p) \le -C_0|p|\,\gamma^2/2, \qquad F\beta(x;p) \ge C_0 p\,\gamma^2/2.$$

Such $\beta(x;-p)$ and $\beta(x;p)$ are called sub- and super-solutions of problem (1).

3 Numerical Method from [7]

3.1 Layer-Adapted Meshes

Introduce a small positive parameter σ that will be specified later. Let $\sigma \le C_1$ so that the closed curve $\partial\Omega_\sigma$ that is defined by the equation $r = \sigma$ does not intersect itself. Furthermore, let Ω_σ be the interior of $\partial\Omega_\sigma$. Our problem will be discretized separately in Ω_σ and $\Omega \setminus \Omega_\sigma$, to which we shall refer as the interior region and the layer region respectively; see Figure 2.

The boundary-layer region $\Omega \setminus \Omega_\sigma$ is the rectangle $(0, \sigma) \times [0, L]$ in the coordinates (r, l). Hence in this subdomain introduce the tensor-product mesh $\{(r_i, l_j), i = 0, \ldots, N, j = -1, \ldots M\}$, where, as usual, $r_0 = 0$, $r_N = \sigma$, $l_0 = 0$, and $l_M = L$, while $l_{-1} = l_{M-1} - L$. Furthermore, let $\{l_j\}$ be a quasiuniform mesh on $[0, L]$, i.e., $C^{-1}h \le l_j - l_{j-1} \le Ch$. The choice of the *layer-adapted* mesh $\{r_i\}$ on $[0, \sigma]$ is crucial and will be discussed later; see (a),(b). Now assume only that $r_i - r_{i-1} \le h$ and $C^{-1}h^{-1} \le N \le Ch^{-1}$.

In the interior region Ω_σ introduce a quasiuniform Delaunay triangulation, i.e. the maximum side length of any triangle is at most h, the area of any triangle is bounded below by Ch^2, and the sum of the angles opposite to any edge is less than or equal to π (while any angle opposite to $\partial\Omega_\sigma$ does not exceed $\pi/2$).

Furthermore, let the union of all the triangles define a polygonal domain Ω_σ^h whose boundary vertices lie on $\partial\Omega_\sigma$. Note that we do not replace our original domain Ω by a similar polygonal domain Ω^h, since a significant part of the boundary layer would be lost in $\Omega \setminus \Omega^h$. We also require that both the interior and layer meshes have the same sets of nodes on $\partial\Omega_\sigma$.

We focus on two particular choices of $\{r_i\}$:
3.1(a) Bakhvalov mesh. [1] Set $\sigma := 2\gamma_0^{-1}\varepsilon|\ln\varepsilon|$ and define the mesh $\{r_i\}$ by $r_i := r\big([1-\varepsilon]\,i/N\big),\ i = 0 \ldots, N, \quad r(t) := -2\gamma_0{}^{-1}\varepsilon\ln(1-t)$ for $t \in [0, 1-\varepsilon]$.
3.1(b) Shishkin mesh. [15] Set $\sigma = 2\gamma_0^{-1}\varepsilon\ln N$ and introduce a uniform mesh $\{r_i\}_{i=0}^N$ on $[0, \sigma]$, i.e. $r_i - r_{i-1} = \sigma/N = 2\gamma_0^{-1}\varepsilon N^{-1}\ln N$.

Note that if ε is sufficiently small—recall (A3)—the condition $\sigma \le C_1$ is satisfied and the meshes (a) and (b) are well-defined. If (A3) is not satisfied, but (a) $\sigma \le C_1$ and $\varepsilon \le 1/2$, or (b) $\sigma \le C_1$, the meshes 3.1(a) and 3.1(b) remain well-defined. Otherwise we have $\varepsilon > C$, i.e. our problem is not singularly perturbed.

3.2 Discretization in the Boundary-Layer Region

Recall that $\Omega \setminus \Omega_\sigma$ is the rectangle $(0, \sigma) \times [0, L]$ in the coordinates (r, l). Hence rewrite (1a) in (r, l) coordinates, by (6), and then discretize it using the standard finite differences on the tensor-product mesh $\{(r_i, l_j)\}$ [13]. In the interior of $\Omega \setminus \Omega_\sigma$, i.e. for $i = 1, \ldots, N-1$, $j = 0, \ldots M-1$, set

$$\begin{aligned} F^h U_{ij} := -\varepsilon^2 \eta_{ij}^{-1} D_r[\zeta_{ij} D_r^- U_{ij}] - \varepsilon^2 \eta_{ij}^{-1} D_l[\vartheta_{ij}^{-1} D_l^- U_{ij}] + b(x_{ij}, U_{ij}) = 0, \\ U_{i,M} = U_{i,0}, \qquad U_{i,-1} = U_{i,M-1}, \qquad U_{0,j} = g(x_{0,j}). \end{aligned} \tag{9}$$

Here U_{ij} is the computed solution at the mesh node $x_{ij} = \big(\varphi_j - r_i \psi_j', \psi_j + r_i \varphi_j'\big)$,

$$D_r^- v_{ij} := \frac{v_{ij} - v_{i-1,j}}{r_i - r_{i-1}}, \qquad D_r v_{ij} := \frac{v_{i+1,j} - v_{ij}}{(r_{i+1} - r_{i-1})/2}, \tag{10}$$

$$D_l^- v_{ij} := \frac{v_{ij} - v_{i,j-1}}{H_j}, \qquad D_l v_{ij} := \frac{v_{i,j+1} - v_{ij}}{(H_j + H_{j+1})/2}, \qquad H_j := l_j - l_{j-1},$$

$$\eta_{ij} := 1 - \kappa_j r_i, \qquad \zeta_{ij} := 1 - \kappa_j r_{i-1/2}, \qquad \vartheta_{ij} := 1 - \frac{\kappa_{j-1} + \kappa_j}{2}\, r_i,$$

while $\kappa_j = \kappa(l_j)$, $\varphi_j = \varphi(l_j)$, $\psi_j = \psi(l_j)$, $\varphi_j' = \varphi'(l_j)$, and $\psi_j' = \psi'(l_j)$.

On the *interface boundary* $\partial\Omega_\sigma$ introduce the fictitious Neumann condition

$$\frac{\partial u}{\partial r} = \phi(x) \qquad \text{for } x \in \partial\Omega_\sigma. \tag{11}$$

For $i = N$, $j = 0, \ldots M-1$, following [13], we discretize (1a), (6), (11) as follows:

$$\begin{aligned} F_-^h U_{Nj} := -\varepsilon^2\, \delta_r^2 U_{Nj} - \varepsilon^2 \eta_{Nj}^{-1} D_l[\vartheta_{Nj}^{-1} D_l^- U_{Nj}] + b(x_{Nj}, U_{Nj}) = 0, \\ U_{N,M} = U_{N,0}, \qquad U_{N,-1} = U_{N,M-1}, \end{aligned} \tag{12}$$

where we use $h_N := r_N - r_{N-1}$ and

$$\delta_r^2 U_{Nj} := \eta_{Nj}^{-1} \frac{\eta_{Nj}\, \phi_j - \zeta_{Nj}\, D_r^- U_{Nj}}{h_N/2} = \frac{2}{h_N}\phi_j - \eta_{Nj}^{-1} \frac{2}{h_N} \zeta_{Nj}\, D_r^- U_{Nj}\,. \tag{13}$$

Note that F_-^h involves an unknown function ϕ. The actual discretization on the interface boundary $\partial\Omega_\sigma^h$ is obtained by combining (12) with (16) eliminating ϕ.

3.3 Discretization in the Interior Region. Existence and Accuracy.

Let $S^h \subset W_2^1(\Omega_\sigma^h)$ be the standard finite element space of continuous functions that are linear on each of the triangles of our mesh in Ω_σ^h. In Ω_σ^h define the approximate solution $U \in S^h$ by

$$\varepsilon^2 (\nabla U, \nabla \chi_i) + \varepsilon^2 \phi_i \oint_{\partial\Omega_\sigma^h} \chi_i\, ds + b(X_i, U_i)\,(1, \chi_i) = 0 \qquad \forall\, \chi_i \in S^h, \tag{14}$$

where X_i is a mesh node in $\bar{\Omega}_\sigma^h$, while $U_i = U(X_i)$, $\phi_i = \phi(X_i)$, and $\chi_i \in S^h$ are the nodal basis functions, i.e. $\chi_i(X_j)$ equals 1 if $i = j$ and 0 otherwise. Here we used the *lumped mass* discretization of both the boundary integral and the integral involving b.

At *interior meshnodes* X_i of Ω_σ, our discretization (14) implies

$$F^h U_i := \frac{\varepsilon^2}{(1,\chi_i)}(\nabla U, \nabla\chi_i) + b(X_i, U_i) = 0 \qquad \forall\, X_i \in \Omega_\sigma. \tag{15}$$

Similarly, at mesh nodes X_j on the *interface boundary* $\partial\Omega_\sigma$, we get

$$F^h_+ U_j := \frac{\varepsilon^2}{(1,\chi_j)}(\nabla U, \nabla\chi_j) + \frac{\varepsilon^2 a_j}{h}\phi_j + b(X_j, U_j) = 0 \qquad \forall\, X_j \in \partial\Omega_\sigma, \tag{16}$$

where

$$a_j := \frac{h}{(1,\chi_j)}\oint_{\partial\Omega^h_\sigma} \chi_j\, ds, \qquad 0 < C^{-1} < a_j < C. \tag{17}$$

Finally the discretizations F^h_- (12) and F^h_+ (16) are compiled, eliminating ϕ, as in [7, (3.14)]; see also a similar formula (29).

Theorem 3.1 ([7, Theorem 3.20]). *Let the mesh* $\{r_i\}_{i=0}^N$ *be the Bakhvalov mesh of §3.1(a), or the Shishkin mesh of §3.1(b). There exists a discrete solution* U *of (9),(12),(15),(16) such that for* h *sufficiently small,*

$$\bigl|U(X_i) - u(X_i)\bigr| \le Ch^2|\ln h|^m \qquad \forall \text{ mesh nodes } X_i \in \bar\Omega,$$

where $m = 0$ *for the Bakhvalov mesh (a) and* $m = 2$ *for the Shishkin mesh (b).*

4 Numerical Method Using Approximate Curvature

We cannot implement the numerical method of §3 since no parametrization (3) is available. Instead we are given an ordered set of boundary points $\{(\varphi_j, \psi_j)\}_{j=0}^M$. Using these data, we modify our method as follows.

4.1 Modified Layer-Adapted Meshes. Approximate Curvature

We imitate the layer-adapted meshes of §3.1 that use the arc-length parametrization (3), in which $l = 0$ is associated with (φ_0, ψ_0) and $l = L$ is associated with (φ_M, ψ_M). The mesh $\{l_j\}$ is chosen on $[0, L]$ so that $(\varphi_j, \psi_j) = (\varphi(l_j), \psi(l_j))$. Clearly, this mesh $\{l_j\}$ exists and is unique, but the exact values of l_j will remain unknown. We associate (r_i, l_j) with the point $\tilde x_{ij} \approx x_{ij} = x(r_i, l_j)$ defined by

$$\tilde x_{ij} := \bigl(\varphi_j - r_i\tilde\psi'_j\,,\ \psi_j + r_i\tilde\varphi'_j\bigr). \tag{18}$$

Here we normalize $(\hat\varphi'_j, \hat\psi'_j)$ to get the unit vector $\bigl(\tilde\varphi'_j, \tilde\psi'_j\bigr) := [\hat\varphi'^2_j + \hat\psi'^2_j]^{-1/2}\bigl(\hat\varphi'_j, \hat\psi'_j\bigr)$, which approximates the unit vector $(\varphi'(l_j), \psi'(l_j))$. If $\tilde H_{j+1} - \tilde H_j = O(h^2)$, we simply set $\hat\varphi'_j := \bigl(\tilde D^-_l\varphi_j + \tilde D^-_l\varphi_{j+1}\bigr)/2$ and $\hat\psi'_j := \bigl(\tilde D^-_l\psi_j + \tilde D^-_l\psi_{j+1}\bigr)/2$. Otherwise we modify $\hat\varphi'_j$, $\hat\psi'_j$ to $\hat\varphi'_j := \bigl(\tilde H_{j+1}\tilde D^-_l\varphi_j + \tilde H_j\tilde D^-_l\varphi_{j+1}\bigr)/(\tilde H_j + \tilde H_{j+1})$ and $\hat\psi'_j := \bigl(\tilde H_{j+1}\tilde D^-_l\psi_j + \tilde H_j\tilde D^-_l\psi_{j+1}\bigr)/(\tilde H_j + \tilde H_{j+1})$. Furthermore,

$$\begin{aligned}&\tilde D^-_l v_{ij} := \frac{v_{ij} - v_{i,j-1}}{\tilde H_j}, \qquad \tilde D_l v_{ij} := \frac{v_{i,j+1} - v_{ij}}{(\tilde H_j + \tilde H_{j+1})/2},\\ &\tilde H_j := \sqrt{(\varphi_j - \varphi_{j-1})^2 + (\psi_j - \psi_{j-1})^2}.\end{aligned} \tag{19}$$

Next, let the ordered set of vertices $\{\tilde{x}_{Nj}\}_{j=0}^{M}$ define the polygonal domain Ω_σ^h, in which we introduce a quasiuniform Delaunay triangulation, whose set of the boundary nodes is precisely the set $\{\tilde{x}_{Nj}\}_{j=1}^{M}$. Note that $\tilde{x}_{Nj} \approx x_{Nj} \in \partial\Omega_\sigma$ implies that $\partial\Omega_\sigma^h$ is an $O(h^2)$-perturbation of $\partial\Omega_\sigma$.

Furthermore, our method will invoke the approximate curvature $\tilde{\kappa}_j \approx \kappa(l_j)$:

$$\tilde{\kappa}_j := \frac{\tilde{D}_l^- \varphi_j + \tilde{D}_l^- \varphi_{j+1}}{2} \tilde{D}_l \tilde{D}_l^- \psi_j - \frac{\tilde{D}_l^- \psi_j + \tilde{D}_l^- \psi_{j+1}}{2} \tilde{D}_l \tilde{D}_l^- \varphi_j \tag{20}$$

—compare with (4)—for which a calculation shows that

$$\tilde{\kappa}_j = \frac{(\varphi_j - \varphi_{j-1})(\psi_{j+1} - \psi_j) - (\varphi_{j+1} - \varphi_j)(\psi_j - \psi_{j-1})}{\tilde{H}_j \tilde{H}_{j+1}(\tilde{H}_j + \tilde{H}_{j+1})/2}. \tag{21}$$

Remark 4.1. Note that (20) gives a second-order approximation of $\kappa(l_j)$ only if $\tilde{H}_{j+1} - \tilde{H}_j = O(h^2)$. Otherwise, (20) and hence (21) should be modified to another standard second-order approximation of $\kappa(l_j)$, which involves $\{(\varphi_i, \psi_i)\}_{i=j-2}^{j+2}$.

Lemma 4.2. *For $\tilde{H}_j$, $\tilde{\kappa}_j$ and $\tilde{x}_{ij}$ defined by (18),(19) and (20) combined with Remark 4.1, we have*

$$H_j = \tilde{H}_j[1+O(h^2)], \qquad \tilde{\kappa}_j = \kappa(l_j) + O(h^2), \qquad \tilde{x}_{ij} = x_{ij} + O(r_i h^2) = x_{ij} + O(\sigma h^2).$$

Proof. Since (3) is an arc-length parametrization, i.e. $\sqrt{\varphi'^2(l) + \psi'^2(l)} = 1$ for all l, we have $H_j = H_j\sqrt{\varphi'^2(l_{j-1/2}) + \psi'^2(l_{j-1/2})}$, where

$$\varphi'(l_{i-1/2}) = (\varphi_j - \varphi_{j-1})/H_j + O(H_j^2), \;\; \psi'(l_{i-1/2}) = (\psi_j - \psi_{j-1})/H_j + O(H_j^2).$$

Combining this with $C^{-1}h \le \tilde{H}_j \le Ch$, we get $H_j = \tilde{H}_j[1 + O(h^2)]$.

Since $H_j = \tilde{H}_j[1+O(h^2)]$ implies $\tilde{D}_l^- = [1+O(h^2)]D_l^-$, $\tilde{D}_l = [1+O(h^2)]D_l$, it suffices to prove the desired estimates for $\tilde{\kappa}_j$ and $\tilde{x}_{ij}$ with $\tilde{D}_l^-$ and $\tilde{D}_l$ replaced by D_l^- and D_l in the definitions of $\tilde{\kappa}_j$, $\tilde{\varphi}_j'$ and $\tilde{\psi}_j'$. Such estimates follow immediately from Taylor series expansions. Note that $(\hat{\varphi}_j', \hat{\psi}_j')$ and the corresponding normalized unit vector $(\tilde{\varphi}_j', \tilde{\psi}_j')$ are both $O(h^2)$ approximations of the unit vector $(\varphi'(l_j), \psi'(l_j))$. □

4.2 Modified Discretization in the Boundary-Layer Region

In $\Omega \setminus \Omega_\sigma^h$, i.e. for $i = 1, \dots, N-1$, $j = 0, \dots M-1$, we modify (9) as follows:

$$\begin{gathered} \tilde{F}^h \tilde{U}_{ij} := -\varepsilon^2 \tilde{\eta}_{ij}^{-1} D_r[\tilde{\zeta}_{ij} D_r^- \tilde{U}_{ij}] - \varepsilon^2 \tilde{\eta}_{ij}^{-1} \tilde{D}_l[\tilde{\vartheta}_{ij}^{-1} \tilde{D}_l^- \tilde{U}_{ij}] + b(\tilde{x}_{ij}, \tilde{U}_{ij}) = 0, \\ \tilde{U}_{i,M} = \tilde{U}_{i,0}, \qquad \tilde{U}_{i,-1} = \tilde{U}_{i,M-1}, \qquad \tilde{U}_{0,j} = g(x_{0,j}). \end{gathered} \tag{22}$$

Here $\tilde{U}_{ij}$ is the discrete computed solution at the mesh node $\tilde{x}_{ij}$, the finite difference operators D_r^-, D_r, $\tilde{D}_l^-$, $\tilde{D}_l$ and the quantities $\tilde{x}_{ij}$, $\tilde{\kappa}_j$ are defined by (10),(19),(18) and (20) combined with Remark 4.1, while

$$\tilde{\eta}_{ij} := 1 - \tilde{\kappa}_j r_i\,, \qquad \tilde{\zeta}_{ij} := 1 - \tilde{\kappa}_j r_{i-1/2}\,, \qquad \tilde{\vartheta}_{ij} := 1 - \frac{\tilde{\kappa}_{j-1} + \tilde{\kappa}_j}{2} r_i\,.$$

For $i = N$, $j = 0, \dots M-1$, imitating (12),(13), we discretize (1a),(6) combined with (11) as follows:

$$\begin{aligned} \tilde F^h_- \tilde U_{Nj} := -\varepsilon^2\, \delta_r^2 \tilde U_{Nj} - \varepsilon^2 \tilde\eta_{Nj}^{-1} \tilde D_l [\tilde\vartheta_{Nj}^{-1} \tilde D_l^- \tilde U_{Nj}] + b(\tilde x_{Nj}, \tilde U_{Nj}) = 0,\\ \tilde U_{N,M} = \tilde U_{N,0}, \qquad \tilde U_{N,-1} = \tilde U_{N,M-1}, \end{aligned} \tag{23}$$

where $h_N := r_N - r_{N-1}$ and

$$\delta_r^2 \tilde U_{Nj} := \tilde\eta_{Nj}^{-1} \frac{\tilde\eta_{Nj}\,\phi_j - \tilde\zeta_{Nj}\, D_r^- \tilde U_{Nj}}{h_N/2} = \frac{2}{h_N}\phi_j - \tilde\eta_{Nj}^{-1}\frac{2}{h_N}\tilde\zeta_{Nj}\, D_r^- \tilde U_{Nj}. \tag{24}$$

Lemma 4.3. *Let $\beta(x;p)$ be described by (8), and the mesh $\{r_i\}_{i=0}^N$ be either the Bakhvalov mesh of §3.1(a), or the Shishkin mesh of §3.1(b). Then for all $|p| \le p_0$ at all interior mesh nodes $x_{ij}, i = 1, \dots, N-1, j = 0, \dots, M-1$ we have*

$$\left|\tilde F^h \beta(x_{ij}) - F\beta(x_{ij})\right| \le Ch^2 |\ln h|^m, \tag{25a}$$

while at all interface-boundary mesh nodes $x_{Nj} \in \partial\Omega^h_\sigma$ we have

$$\tilde F^h_- \beta(x_{Nj}) - F\beta(x_{Nj}) = \frac{2\varepsilon^2}{h_N}\Big(\frac{\partial\beta}{\partial r}\Big|_{x_{Nj})} - \phi_j\Big) + O\big(h^2\big), \tag{25b}$$

where $m = 0$ for the Bakhvalov mesh (a) and $m = 2$ for the Shishkin mesh (b).

Proof. [7, Lemma 3.11 and Lemma 3.13] state (25) with $\tilde F^h$ replaced by F^h. Hence it remains to estimate $\tilde F^h\beta(x_{ij}) - F^h\beta(x_{ij})$. Throughout this proof, we use $|\partial^k\beta/\partial r^k| \le C\varepsilon^{-k}$ and $|\partial^k\beta/\partial l^k| \le C$, $k = 1, 2$, which follow from (8).

First, invoking the estimate for $\tilde x_{ij}$ of Lemma 4.2, we get

$$b(\tilde x_{ij}, \beta(x_{ij})) - b(x_{ij}, \beta(x_{ij})) = O(\sigma h^2) = O(h^2). \tag{26}$$

Furthermore, the estimates for $\tilde H_j$ and $\tilde\kappa_j$ of Lemma 4.2 imply that

$$\tilde\vartheta_{ij}^{-1} \tilde D_l^- \beta(x_{ij}) = \vartheta_{ij}^{-1} D_l^- \beta(x_{ij})[1 + O(h^2)] = \vartheta_{ij}^{-1} D_l^- \beta(x_{ij}) + O(h^2).$$

Combining this with a similar estimate

$$\varepsilon^2 \tilde\eta_{ij}^{-1} \tilde D_l [\tilde\vartheta_{ij}^{-1} \tilde D_l^- \beta(x_{ij})] = \varepsilon^2 \eta_{ij}^{-1} D_l [\tilde\vartheta_{ij}^{-1} \tilde D_l^- \beta(x_{ij})][1 + O(h^2)]$$

and $D_l[O(h^2)] = O(h)$, which follows from $H_j = l_j - l_{j-1} \ge Ch$, yields

$$\varepsilon^2 \tilde\eta_{ij}^{-1} \tilde D_l [\tilde\vartheta_{ij}^{-1} \tilde D_l^- \beta(x_{ij})] = \varepsilon^2 \eta_{ij}^{-1} D_l [\vartheta_{ij}^{-1} D_l^- \beta(x_{ij})] + O(\varepsilon^2 h). \tag{27}$$

Next, by the estimate for $\tilde\kappa_j$ of Lemma 4.2, we get

$$D_r[(\tilde\zeta_{ij} - \zeta_{ij}) D_r^- \beta(x_{ij})] = (\kappa_j - \tilde\kappa_j) D_r[r_{i-1/2} D_r^- \beta(x_{ij})] = O(\varepsilon^{-2}h^2).$$

Combining this with $\tilde\eta_{ij}^{-1} = \eta_{ij}^{-1} + O(\sigma h^2)$ and then with (26) and (27), we arrive at $\tilde F^h\beta(x_{ij}) - F^h\beta(x_{ij}) = O(\varepsilon^2 h + h^2) = O(h^2)$, where we also used (A3). Thus (25a) is established. Estimate (25b) is obtained similarly, observing that

$$\frac{(\tilde\eta_{Nj} - \eta_{Nj})\, \frac{\partial\beta}{\partial r}\big|_{x_{Nj}} - (\tilde\zeta_{Nj} - \zeta_{Nj}) D_r^- \beta_{Nj}}{h_N/2} = (\kappa_j - \tilde\kappa_j) \frac{r_N \frac{\partial\beta}{\partial r}\big|_{x_{Nj}} - r_{N-1/2} D_r^- \beta_{Nj}}{h_N/2}.$$

□

4.3 Discretization in the Interior Region

In the interior part of the domain Ω_σ^h we use the lumped-mass finite elements (15),(16),(17); see also [7]:

$$\tilde F^h \tilde U_i := F^h \tilde U_i = 0 \quad \forall\, X_i \in \Omega_\sigma^h; \qquad \tilde F_+^h \tilde U_j := F_+^h \tilde U_j = 0 \quad \forall\, X_j \in \partial\Omega_\sigma^h. \quad (28)$$

Finally, the discretization $\tilde F_-^h$ (23),(24) and the above discretization $\tilde F_+^h$ are compiled as in [7] by eliminating the auxiliary unknown function ϕ:

$$\tilde F^h \tilde U_j := \frac{(h_N/2)\, \tilde F_-^h \tilde U_j + (h/a_j)\, \tilde F_+^h \tilde U_j}{h_N/2 + h/a_j} \qquad \forall\, X_j \in \partial\Omega_\sigma^h. \quad (29)$$

Lemma 4.4 ([7, Lemmas 3.15, 3.16]). *Let $\beta^I \in S^h$ be a non-standard piecewise linear interpolant of $\beta(x;p)$ such that $\beta^I(X_i;p) := \beta(X_i;p)$ at all mesh nodes $X_i \in \Omega_\sigma^h$, while $\beta^I(X_j;p) := \beta(x_{Nj};p)$ at all mesh nodes $X_j = \tilde x_{Nj} \in \partial\Omega_\sigma^h$. Furthermore, let σ be chosen as in either §3.1(a) or §3.1(b). Then for all $|p| \le p_0$ we have*

$$\left|\tilde F^h \beta_i^I - F\beta(X_i)\right| \le Ch^2 \qquad \forall\, X_i \in \Omega_\sigma^h; \quad (30a)$$

at all mesh nodes $X_j = \tilde x_{Nj}$ on $\partial\Omega_\sigma^h$ we have

$$\tilde F_+^h \beta_j^I - F\beta(x_{Nj}) = -a_j \frac{\varepsilon^2}{h}\Big(\frac{\partial\beta}{\partial r}\Big|_{x_{Nj}} - \phi_j\Big) + O(h^2) \qquad \forall\, X_j \in \partial\Omega_\sigma^h; \quad (30b)$$

and for $\tilde F^h$ of (29) at all mesh nodes $X_j = \tilde x_{Nj}$ on $\partial\Omega_\sigma^h$ we have

$$\left|\tilde F^h \beta(x_{Nj}) - F\beta(x_{Nj})\right| \le Ch^2 \qquad \forall\, X_j \in \partial\Omega_\sigma^h. \quad (31)$$

Proof. [7, Lemmas 3.15, 3.16] give the desired estimates (30) in the case of β^I being the standard interpolant of β in $\bar\Omega_\sigma^h$, and x_{Nj} replaced by $X_j = \tilde x_{Nj}$. Note that the proof of [7, Lemma 3.16] is applicable to the domain Ω_σ^h, since $\partial\beta/\partial n = -\partial\beta/\partial r\big|_{X_j} + O(h)$ within $O(h)$-distance from X_j, which follows from $\partial\Omega_\sigma^h$ being an $O(h^2)$-perturbation of $\partial\Omega_\sigma$. Hence to prove (30), it suffices to show that (i) the values of $\tilde F_+^h \beta_j^I$ for the standard interpolant and the interpolant of our Lemma 4.4 differ by $O(h^2)$; (ii) the values of $\tilde F^h \beta_j^I$ enjoy a similar property; (iii) $F\beta(x_{Nj}) - F\beta(\tilde x_{Nj}) = O(h^2)$; (iv) similarly the values of $\partial\beta/\partial r$ at $\tilde x_{Nj}$ and x_{Nj} differ by $O(h^2)$. These assertions (i)-(iv) follow from $\|\beta\|_{C^2(\bar\Omega_\sigma \cup \bar\Omega_\sigma^h)} \le C$ combined with $|\tilde x_{Nj} - x_{Nj}| \le Ch^2$ and (A3).

Estimate (31) (25b) and (30b) combined with (17); see the proof of [7, Lemma 3.18] for more details. □

4.4 Existence and Accuracy. Discrete Sub- and Super-solutions

Theorem 4.5. *Let the mesh $\{r_i\}_{i=0}^N$ be either the Bakhvalov mesh of §3.1(a), or the Shishkin mesh of §3.1(b). There exists a discrete solution $\tilde U$ of (22),(28),(29) such that for h sufficiently small,*

$$\left|\tilde U(X_i) - u(X_i)\right| \le Ch^2 |\ln h|^m \qquad \forall \text{ mesh nodes } X_i \in \bar\Omega, \quad (32)$$

where $m = 0$ for the Bakhvalov mesh (a) and $m = 2$ for the Shishkin mesh (b).

Table 1. Maximum nodal errors $|U-u|$ in the numerical method [7] (upper part) and additional errors $|\tilde{U}-U|$ induced by using an ordered set of boundary points instead of an explicit parametrization of the domain (lower part)

	Bakhvalov mesh			Shishkin mesh		
N	$\varepsilon=10^{-2}$	$\varepsilon=10^{-4}$	$\varepsilon=10^{-8}$	$\varepsilon=10^{-2}$	$\varepsilon=10^{-4}$	$\varepsilon=10^{-8}$
32	3.745e-3	3.842e-3	3.843e-3	3.915e-2	3.947e-2	3.948e-2
64	9.296e-4	9.534e-4	9.536e-4	1.318e-2	1.325e-2	1.325e-2
128	2.333e-4	2.388e-4	2.388e-4	4.004e-3	4.400e-3	4.401e-3
256	5.854e-5	5.967e-5	5.968e-5	1.008e-3	1.430e-3	1.430e-3
32	4.764e-3	7.745e-6	1.586e-9	3.157e-3	6.711e-6	6.641e-10
64	1.248e-3	2.060e-6	4.206e-10	1.105e-3	1.786e-6	1.765e-10
128	3.436e-4	5.177e-7	1.061e-10	3.514e-4	4.482e-7	4.423e-11
256	8.607e-5	1.480e-7	3.035e-11	8.812e-5	1.475e-7	1.460e-11

Proof. We invoke the theory of Z-fields, imitating the proofs of [7, Lemma 3.19, Theorem 3.20]. Set $\bar{p} := C_3 h^2 |\ln h|^m$, where $C_3 > 0$ is a sufficiently large constant. Now combining Lemma 2.3 with (25a), (30a) and (31), we conclude that the functions equal to $\beta(x_{ij};\pm p)$ at $\tilde{x}_{ij}$ and $\beta(X_i;\pm p)$ at $X_i \in \Omega^h_\sigma$ are discrete sub- and supers-solutions, where '$-$' is used for the sub-solution and '$+$' is used for the super-solution. Since our discrete operator $\tilde{F}^h$ is a Z-field—see [9], [7, §3.2]—by [7, Lemma 3.6], there exists a discrete solution $\tilde{U}$ between our sub- and super-solutions. Using (8) and Lemma 4.2, observe that $|x_{ij}-\tilde{x}_{ij}| = O(r_{ij}h^2)$ combined with $|\nabla\beta_{ij}| \le C[1+\varepsilon^{-1}e^{-\gamma_0 r_{ij}/\varepsilon}]$ implies $\beta(x_{ij}) = \beta(\tilde{x}_{ij}) + O(h^2)$. Hence our discrete solution $\tilde{U}(X_i)$ is between $\beta(X_i;-p) - O(h^2)$ and $\beta(X_i;p) + O(h^2)$ for *all* mesh nodes $X_i \in \bar{\Omega}$, which combined with (7) and (A3), yields the desired error estimate. □

5 Numerical Results

Our model problem is (1) in the domain Ω—see Figure 2 and [7, §7]—in which

$$b(x,u) = \big(u-\bar{u}_0(x)\big)u\big(u+\bar{u}_0(x)\big), \qquad \bar{u}_0(x) = x_1^2 + x_1 + 1. \tag{33}$$

Here $\pm\bar{u}_0(x)$ are two stable solutions and 0 is an unstable solution of the corresponding reduced problem. The boundary condition $g(x) = (x_1 - x_1^2)/3$ satisfies (A2) for both $\pm\bar{u}_0$; see Figure 1. We present numerical results for the solution u near $\bar{u}_0$; see Figure 1 (left); the results for the solution near $-\bar{u}_0$ are similar.

Table 1 gives numerical results for the Bakhvalov and Shishkin meshes with the parameter $\gamma_0 := 3\sqrt{2}/5$. The upper part of the table shows maximum nodal errors $\max_i |U_i - u(X_i)|$—which are computed as described in [8, §4]—for the numerical method [7], which requires an explicit parametrization of the domain. The lower part of the table shows the additional errors $\max_i |\tilde{U}_i - U_i|$ induced by switching to the method of §4, which instead uses an ordered set of boundary points. The errors in the lower part of the table are comparable with the errors in the upper part and decay very fast as ε tends to 0.

In summary, the numerical results support our error estimates of Theorems 3.1 and 4.5. Thus, we observe that even if no explicit parametrization of the domain is available, the modification of the numerical method [7], which we presented in this paper, produces reliable computed solutions.

References

1. N. S. Bakhvalov: On the optimization of methods for solving boundary value problems with boundary layers. *Zh. Vychisl. Mat. Mat. Fis.* **9** (1969) 841–859 (in Russian).
2. I. A. Blatov: Galerkin finite element method for elliptic quasilinear singularly perturbed boundary problems. I. *Differ. Uravn.* **28** (1992) 1168–1177 (in Russian). Translation in *Differ. Equ.* **28** (1992) 931–940.
3. C. Clavero, J. L. Gracia, E. O'Riordan: A parameter robust numerical method for a two dimensional reaction-diffusion problem. *Math. Comp.* **74** (2005) 1743–1758.
4. C. M. D'Annunzio: *Numerical analysis of a singular perturbation problem with multiple solutions*, Ph.D. Dissertation. University of Maryland at College Park, 1986 (unpublished).
5. P. C. Fife: Semilinear elliptic boundary value problems with small parameters. *Arch. Rational Mech. Anal.* **52** (1973) 205–232.
6. P. Grindrod: *Patterns and Waves: the theory and applications of reaction-diffusion equations.* Clarendon Press, Oxford, 1991.
7. N. Kopteva: Maximum norm error analysis of a 2d singularly perturbed semilinear reaction-diffusion problem. *Math. Comp.* to appear.
8. N. Kopteva, M. Stynes: Numerical analysis of a singularly perturbed nonlinear reaction-diffusion problem with multiple solutions. *Appl. Numer. Math.* **51** (2004) 273-288.
9. J. Lorenz: *Nonlinear singular perturbation problems and the Enquist-Osher scheme.* Report 8115, Mathematical Institute, Catholic Univerity of Nijmegen, 1981 (unpublished).
10. J. M. Melenk: *hp–finite element methods for singular perturbations.* Springer, 2002.
11. J. D. Murray: *Mathematical Biology.* Springer-Verlag, Berlin, 1993.
12. N. N. Nefedov: The method of differential inequalities for some classes of nonlinear singularly perturbed problems with internal layers. *Differ. Uravn.* **31** (1995) 1142–1149 (in Russian). Translation in *Differ. Equ.* **31** (1995) 1077–1085.
13. A. A. Samarski: *Theory of Difference Schemes.* Nauka, Moscow, 1989 (in Russian).
14. A. H. Schatz, L. B. Wahlbin: On the finite element method for singularly perturbed reaction-diffusion problems in two and one dimensions. *Math. Comp.* **40** (1983) 47–89.
15. G. I. Shishkin: *Grid approximation of singularly perturbed elliptic and parabolic equations.* Ur. O. Ran, Ekaterinburg, 1992 (in Russian).
16. G. Sun, M. Stynes: A uniformly convergent method for a singularly perturbed semilinear reaction-diffusion problem with multiple solutions. *Math. Comp.* **65** (1996) 1085–1109.
17. A. B. Vasil'eva, V. F. Butuzov, L. V. Kalachev: *The boundary function method for singular perturbation problems.* SIAM Studies in Applied Mathematics, 14. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 1995.