

INTERIOR LAYERS IN A REACTION–DIFFUSION EQUATION WITH A DISCONTINUOUS DIFFUSION COEFFICIENT

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This paper is dedicated to G. I. Shishkin on the occasion of his 70th birthday

Abstract. In this paper a problem arising in the modelling of semiconductor devices motivates the study of singularly perturbed differential equations of reaction–diffusion type with discontinuous data. The solutions of such problems typically contain interior layers where the gradient of the solution changes rapidly. Parameter–uniform methods based on piecewise–uniform Shishkin meshes are constructed and analysed for such problems. Numerical results are presented to support the theoretical results and to illustrate the benefits of using a piecewise–uniform Shishkin mesh over the use of uniform meshes in the simulation of a simple semiconductor device.

Key Words. Diffusion Reaction Equations, Singularly Perturbed Differential Equations, Finite Difference Methods on Fitted Meshes.

1. Introduction

The solutions of singularly perturbed differential equations with smooth data exhibit steep gradients in narrow layer regions adjacent to part or all of the boundary of the domain. When the data for the problem is not smooth, additional interior layers can appear in the solutions of these singularly perturbed problems. There are two broad classes of interest within singularly perturbed problems: problems of reaction–diffusion type and problems of convection–diffusion type. In this paper, we examine numerical methods for singularly perturbed ordinary differential equations of reaction–diffusion type with non-smooth data. Our interest is in the design and analysis of parameter–uniform numerical methods, for which the error constants in the associated asymptotic error bounds are independent of any singular perturbation parameters.

Farrell et al. [7] constructed and analysed a parameter–uniform method for a reaction–diffusion problem of the form: find $u \in C^1(0, 1)$ such that

$$(1.1) \quad -(\varepsilon u)' + r(x)u = f(x), \quad x \in (0, 1) \setminus \{d\}, \quad u(0), \quad u(1) \text{ given}, \quad r(x) \geq 0,$$

where r, f were allowed to be discontinuous at a point $d \in (0, 1)$ and ε was a positive small parameter. The method consisted of a standard difference operator combined with an appropriate piecewise–uniform Shishkin [6] mesh and it was shown in [7] to be essentially a first order parameter–uniform method. By using a different discretization at the interface, Roos and Zarin [11] analysed a second order method for the case when the source term f is discontinuous and $\varepsilon \leq CN^{-1}$. A first order

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numerical method was analysed in [8] for a nonlinear version of (1.1), where $r(x)u$ is replaced by $r(u)u$ and the source term f is allowed to be possibly discontinuous at some point d . Two dimensional versions of problem (1.1) with point sources were considered in [3, 2] where the parameter uniform convergence of numerical methods incorporating Shishkin meshes was examined.

In this paper, we return to the one dimensional problem (1.1) with possible point sources included, but we add some new features into the problem class. Firstly, we allow the diffusion coefficient ε to be variable, $\varepsilon = \varepsilon(x)$, and to be possibly discontinuous. Such discontinuous diffusion coefficients can arise, for example, in the modelling of phase transitions. Moreover, this means that the resulting problem is a two parameter singularly perturbed problem. In the context of parameter–uniform methods, this forces one to ensure that the convergence of the numerical approximations is independent of both singular perturbation parameters. In addition, we also consider the effect of interfacing a reaction–diffusion equation with an equation with no reactive term ($r \equiv 0$) on one side of the interface $x = d$. The examination of this second class of problems was motivated by a modelling problem from the area of semiconductor devices. The resulting interior layer in the solution can be weaker than in the case of (1.1), but we see below that it is still desirable to use an appropriate fitted mesh in order to achieve parameter–uniform convergence. In §2,3,4, a priori bounds on the continuous solutions are established, which are used in §5 to construct an appropriate fitted mesh. Combining this fitted mesh with a finite difference operator in conservative form, it is shown in §6 that the resulting numerical method is essentially a globally second order parameter–uniform numerical method [6] for both of the problem classes being considered. Parameter–uniform convergence estimates for the appropriately scaled fluxes are also given. Numerical results in §7 are presented to support the theoretical results.

In §8, we consider a class of linear singularly perturbed ordinary differential equations of reaction–diffusion type with non–smooth data, associated with a nonlinear singularly perturbed ordinary differential equation arising in the modelling of a Metal Oxide Semiconductor (MOS) capacitor. To determine the capacitance of this nonlinear device over a practical range of applied voltages, it is necessary to approximate the scaled derivative of the solution of the associated linear singularly perturbed problems over a wide range of the singular perturbation parameter. Parameter–uniform methods are designed for this purpose. At the end of the paper, we observe an improvement in the accuracy of the capacitance when a suitably fitted mesh is employed within the numerical algorithm.

In passing we note that the piecewise–uniform mesh used in this paper is only one of a family of possible layer–adapted meshes [10] which could be used for this singularly perturbed problem. In particular, it is well established that Bakhvalov [1] meshes outperform piecewise–uniform meshes by typically obtaining parameter–uniform convergence orders of $O(N^{-p})$ as opposed to $O((N^{-1} \ln N)^p)$ for the piecewise–uniform meshes. Likewise, in the case of ordinary differential equations, many possible analytical approaches exist [10] to establish these theoretical results. In this paper, we choose the classical analytical approach of stability and consistency, suitably modified for singularly perturbed problems, to establish our theoretical results. The main reason for this choice and, also, for our choice of a piecewise–uniform mesh, is that this same approach has been extended to a wide class of singularly perturbed partial differential equations [13].

Throughout this paper C (sometimes subscripted) is a generic constant that is independent of the singular perturbation parameters $\varepsilon_1, \varepsilon_2$ and the discretization parameter N .

2. Two classes of reaction–diffusion problems

Consider the singularly perturbed reaction–diffusion equation (1.1) with discontinuous data on the unit interval $\Omega = (0, 1)$. Let $\Omega_1 = (0, d)$ and $\Omega_2 = (d, 1)$. Denote the jump at the point d in any function by $[\omega](d) = \omega(d+) - \omega(d-)$. Our first problem class is given by:

find $u_\varepsilon \in C^0(\bar{\Omega}) \cap C^2(\Omega_1 \cup \Omega_2)$ such that

$$\begin{aligned} (2.1a) \quad & -(\varepsilon(x)u'_\varepsilon)' + r(x)u_\varepsilon = f, \quad x \in \Omega_1 \cup \Omega_2, \\ (2.1b) \quad & u_\varepsilon(0) = B_0, \quad u_\varepsilon(1) = B_1, \\ (2.1c) \quad & [-\varepsilon u'_\varepsilon](d) = Q'_1, \\ (2.1d) \quad & [f](d) = Q_2, \quad [r](d) = Q_3, \end{aligned}$$

$$(2.1e) \quad \varepsilon(x) = \begin{cases} \varepsilon_1 p(x), & x \in \Omega_1 \\ \varepsilon_2 p(x), & x \in \Omega_2 \end{cases}, \quad p(x) \geq \underline{p} > 0, \quad x \in \Omega_1 \cup \Omega_2,$$

where $\varepsilon_1 > 0, \varepsilon_2 > 0$ are singular perturbation parameters,

$$(2.1f) \quad |Q'_1| \leq C(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2}),$$

$$(2.1g) \quad r(x) \geq r_0 > 0, \quad \frac{r(x)}{p(x)} > \beta > 0, \quad x \in \Omega_1 \cup \Omega_2,$$

and $\varepsilon_1, \varepsilon_2$ are sufficiently small so that

$$(2.1h) \quad \sqrt{\varepsilon_i \beta} |p'(x)| \leq r(x) - \beta p(x), \quad \forall x \in \Omega_1 \cup \Omega_2, \quad i = 1, 2.$$

In particular, equations (2.1d) and (2.1e) above indicate that all the coefficients in (2.1a) may exhibit a jump at $x = d$, while equation (2.1c) allows for a jump in the flux $(-\varepsilon u'_\varepsilon)$ at $x = d$. The constraint (2.1h) on the magnitude of $|p'|$ is required in Corollary 2.1 to establish the parameter–uniform stability of the solution. Note that if $p(x)$ is piecewise constant, then this stability constraint is automatically satisfied.

We will also examine a second problem class given by: find $u_\varepsilon \in C^0(\bar{\Omega}) \cap C^2(\Omega_1 \cup \Omega_2)$ such that (2.1a-e) are satisfied and

$$(2.2a) \quad |Q'_1| \leq C_1 \sqrt{\varepsilon_1} + C_2 \varepsilon_2,$$

$$(2.2b) \quad r(x) \geq r_0 > 0, \quad \frac{r(x)}{p(x)} > \beta > 0, \quad x \in \Omega_1, \quad r(x) \equiv 0, \quad x \in \Omega_2,$$

$$(2.2c) \quad f(x) = \begin{cases} f_1(x), & x \in \Omega_1 \\ \varepsilon_2 f_2(x), & x \in \Omega_2 \end{cases},$$

and ε_1 is sufficiently small so that

$$(2.2d) \quad \sqrt{\varepsilon_1 \beta} |p'(x)| \leq r(x) - \beta p(x), \quad \forall x \in \Omega_1.$$

In this second problem class, the inhomogeneous term $f(x)$ is suitably scaled so that the solutions u_ε are uniformly bounded. For both problem classes, we assume throughout the paper that $r, p, f \in C^4(\Omega \setminus \{d\})$. Let L_ε denote the linear operator given by

$$L_\varepsilon \omega := \begin{cases} -(\varepsilon(x)\omega')' + r(x)\omega, & x \neq d \\ [-\varepsilon\omega'](d), & x = d \\ \omega(x), & x = \{0, 1\}. \end{cases}$$

Then L_ε satisfies the following minimum principle on $\bar{\Omega}$.

Lemma 2.1. *Suppose that a function $\omega \in C^0(\bar{\Omega}) \cap C^2(\Omega_1 \cup \Omega_2)$ satisfies $L_\varepsilon \omega(x) \geq 0$, $\forall x \in \bar{\Omega}$. Then $\omega(x) \geq 0$, $\forall x \in \bar{\Omega}$.*

Proof. We consider the problems (2.1) and (2.2) separately. In the case of problem (2.1), when $r(x) > 0$, $x \in \Omega_1 \cup \Omega_2$ we argue as follows. Let x_* be any point at which ω attains its minimum value in $\bar{\Omega}$ and assume that $\omega(x_*) < 0$. With the above assumption on the boundary values, either $x_* \in \Omega_1 \cup \Omega_2$ or $x_* = d$. If $x_* \in \Omega_1 \cup \Omega_2$ then $\omega'(x_*) = 0$, $\omega''(x_*) \geq 0$ and so $L_\varepsilon \omega(x_*) = -(\varepsilon \omega')'(x_*) + r(x_*)\omega(x_*) < 0$, which is false. If $x_* = d$, then $\omega'(d^-) \leq 0$ and $\omega'(d^+) \geq 0$. We are led to a contradiction if either of these inequalities are strict. Hence $\omega \in C^1(\Omega)$ and $\omega'(d) = 0$. Recalling that $\omega(d) < 0$ it follows that there exists a neighbourhood $N_h = (d - h, d)$ such that $\omega(x) < 0$ for all $x \in N_h$. Now choose a point $x_1 \in N_h$ such that $\omega(x_1) > \omega(d)$. It follows from the Mean Value Theorem that, for some $x_2 \in N_h$,

$$(\varepsilon \omega')(x_2) = \varepsilon(x_2) \frac{\omega(d) - \omega(x_1)}{d - x_1} < 0.$$

Note that when $\omega'(d) = 0$ then $\varepsilon \omega' \in C^0(\bar{N}_h) \cap C^1(N_h)$. So there exists some $x_3 \in N_h$,

$$(\varepsilon \omega')'(x_3) = \frac{\varepsilon \omega'(d) - \varepsilon \omega'(x_2)}{d - x_2} = \frac{-\varepsilon \omega'(x_2)}{d - x_2} > 0.$$

Note also that $\omega(x_3) < 0$, since $x_3 \in N_h$. Thus

$$L_\varepsilon \omega(x_3) = -(\varepsilon \omega')'(x_3) + r(x_3)\omega(x_3) < 0,$$

which is the required contradiction.

In the case of problem (2.2) (when $r(x) \equiv 0$, $x \in \Omega_2$), note that if the minimum point $x_* \in \Omega_2$ then to avoid a contradiction we must have $\omega(x) \equiv \omega(x_*)$, $\forall x \in \bar{\Omega}_2$. Complete the proof using the arguments above. \square

Corollary 2.1. *If u_ε is a solution of problem (2.1) and $\varepsilon_1, \varepsilon_2$ are sufficiently small so that (2.1h) is satisfied, then*

$$\|u_\varepsilon\|_{\bar{\Omega}} \leq \max\{|u_\varepsilon(0)|, |u_\varepsilon(1)|, \frac{1}{r_0} \|f\|_{\Omega_1 \cup \Omega_2}\} + C \frac{|Q'_1|}{\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2}}.$$

Proof. Consider the barrier function

$$G(x) = \begin{cases} e^{-\sqrt{\frac{\beta}{\varepsilon_1}}(d-x)}, & x \leq d \\ e^{-\sqrt{\frac{\beta}{\varepsilon_2}}(x-d)}, & x > d \end{cases},$$

which has the property that for sufficiently small $\varepsilon_1, \varepsilon_2$ (such that $\sqrt{\varepsilon_i \beta} |p'| \leq r - p\beta$, $i = 1, 2$),

$$L_\varepsilon G = \begin{cases} ((r - p\beta) - \sqrt{\varepsilon_1 \beta} p') G \\ (\sqrt{\varepsilon_1} p(d^-) + \sqrt{\varepsilon_2} p(d^+)) \sqrt{\beta} \\ ((r - p\beta) + \sqrt{\varepsilon_2 \beta} p') G \end{cases} \geq \begin{cases} 0, & x < d \\ p(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2}) \sqrt{\beta}, & x = d \\ 0, & x > d \end{cases}.$$

Then, use the barrier functions

$$\Psi_\pm(x) = \max\{|u_\varepsilon(0)|, |u_\varepsilon(1)|, \frac{1}{r_0} \|f\|_{\Omega_1 \cup \Omega_2}\} + \left(\frac{|Q'_1|}{p(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2}) \sqrt{\beta}}\right) G \pm u_\varepsilon(x)$$

to complete the proof. \square

Corollary 2.2. *If u_ε is a solution of problem (2.2), ε_1 is sufficiently small so that (2.1h) is satisfied and $|Q'_1| \leq C_1 \sqrt{\varepsilon_1} + C_2 \varepsilon_2$, then*

$$\|u_\varepsilon\|_{\bar{\Omega}} \leq \max\{|u_\varepsilon(0)|, |u_\varepsilon(1)|, C \|f_1\|_{\Omega_1}, C \|f_2\|_{\Omega_2}\} + C(C_1 + C_2).$$

Proof. Consider the barrier functions

$$G(x) = \begin{cases} \frac{1}{\sqrt{\varepsilon_1}} e^{-\sqrt{\frac{\beta}{\varepsilon_1}}(d-x)}, & x < d \\ \frac{1}{\sqrt{\varepsilon_1}}, & x > d \end{cases}, \quad P(x) = \begin{cases} \int_d^1 \frac{t}{p(t)} dt, & x \leq d \\ \int_x^1 \frac{t}{p(t)} dt, & x > d \end{cases},$$

which have the properties that

$$L_\varepsilon G = \begin{cases} ((r - p\beta) - \sqrt{\varepsilon_1\beta}p')G, & x < d \\ p(d^-)\sqrt{\beta}, & x = d \\ 0, & x > d \end{cases}, \quad L_\varepsilon P = \begin{cases} rP(d), & x < d \\ \varepsilon_2 d, & x = d \\ \varepsilon_2, & x > d \end{cases}.$$

Then, for sufficiently small ε_1 , use the barrier functions

$$\Psi_\pm(x) = \max\{|u_\varepsilon(0)|, |u_\varepsilon(1)|, \frac{1}{r_0}\|f_1\|_{\Omega_1}, KP(x)\} + \left(\frac{C_1\sqrt{\varepsilon_1}}{p(d^-)\sqrt{\beta}}\right)G \pm u_\varepsilon(x),$$

where $K := \max\{\|f_2\|_{\Omega_2}, \frac{C_2}{d}\}$, to complete the proof. □

Theorem 2.1. *Each of the problems (2.1) and (2.2) has a unique solution.*

Proof. We modify the corresponding argument from [7]. The proof is by construction. Let y_1, y_2 be particular solutions of the differential equations

$$-(\varepsilon y_1')' + r(x)y_1 = f, \quad x \in \Omega_1 \quad \text{and} \quad -(\varepsilon y_2')' + r(x)y_2 = f, \quad x \in \Omega_2.$$

Define $\phi_1(x), \phi_2(x) \in C^2(\Omega) \cap C^0(\bar{\Omega})$ as the solutions of the boundary value problems

$$\begin{aligned} -(\varepsilon^* \phi_1')' + r^*(x)\phi_1 &= 0, \quad x \in \Omega, \quad \phi_1(0) = 1, \quad \phi_1(1) = 0; \\ -(\varepsilon_* \phi_2')' + r_*(x)\phi_2 &= 0, \quad x \in \Omega, \quad \phi_2(0) = 0, \quad \phi_2(1) = 1, \end{aligned}$$

where $\varepsilon^*, \varepsilon_*, r^*, r_* \in C^1(\Omega)$ are appropriate extensions of the functions so that e.g.

$$\begin{aligned} r^*(x) &= r(x), \quad x \in \Omega_1, \quad r^*(x) \geq 0.5\beta > 0, \quad x \in \bar{\Omega}, \\ \varepsilon_*(x) &= \varepsilon(x), \quad x \in \Omega_2, \quad C\varepsilon_2 \geq \varepsilon_*(x) \geq 0.5\varepsilon_2 > 0, \quad x \in \bar{\Omega}. \end{aligned}$$

In the case of (2.2), where $r(x) \equiv 0, x \in \Omega_2$, then take $r_*(x) \equiv 0, x \in \bar{\Omega}$. Note that ϕ_1 and ϕ_2 cannot have an internal maximum or minimum. Hence

$$0 < \phi_1, \phi_2 < 1, \quad \phi_1' < 0, \phi_2' > 0, \quad x \in (0, 1).$$

Then we construct the solution as follows:

$$y(x) = \begin{cases} y_1(x) + (u_\varepsilon(0) - y_1(0))\phi_1(x) + A\phi_2(x), & x \in \Omega_1, \\ y_2(x) + B\phi_1(x) + (u_\varepsilon(1) - y_2(1))\phi_2(x), & x \in \Omega_2, \end{cases}$$

where A, B are constants chosen so that $y \in C^0(\Omega)$ and $[\varepsilon y'](d) = -Q_1'$. The constants A, B exist as

$$\left| \begin{array}{cc} \phi_2(d) & -\phi_1(d) \\ \varepsilon(d^-)\phi_2'(d) & -\varepsilon(d^+)\phi_1'(d) \end{array} \right| > 0.$$

Uniqueness follows from the previous corollaries. □

3. A priori bounds on the derivatives of the solution of problem (2.1)

To establish the parameter-robust properties of the numerical methods involved in this paper, the following decomposition of u_ε into regular v_ε and singular w_ε components will be useful. The regular component v_ε is defined as the solution of

$$L_\varepsilon v_\varepsilon = f, \quad x \in \Omega_1 \cup \Omega_2, \quad r(x)v_\varepsilon(x) = f(x), \quad x \in \{0, d^-, d^+, 1\};$$

and the singular component w_ε is given by

$$\begin{aligned} L_\varepsilon w_\varepsilon &= 0, \quad x \in \Omega_1 \cup \Omega_2, \\ [w_\varepsilon(d)] &= -[v_\varepsilon(d)], \quad [\varepsilon w'_\varepsilon(d)] = -[\varepsilon v'_\varepsilon(d)] - Q'_1, \\ w_\varepsilon(0) &= u_\varepsilon(0) - v_\varepsilon(0), \quad w_\varepsilon(1) = u_\varepsilon(1) - v_\varepsilon(1). \end{aligned}$$

Note that, in general, $v_\varepsilon, w_\varepsilon \notin C^0(\bar{\Omega})$. In fact, $v_\varepsilon, w_\varepsilon$ are multi-valued at $x = d$. As before, the singular component w_ε is well defined and is given by

$$(3.1) \quad w_\varepsilon(x) = \begin{cases} w_\varepsilon(0)\psi_1(x) + A_1\psi_2(x), & x \in \Omega_1 \\ A_2\psi_3(x) + w_\varepsilon(1)\psi_4(x), & x \in \Omega_2 \end{cases},$$

where $\psi_i(x), i = 1, 2, 3, 4$ are the solutions of the boundary value problems

$$\begin{aligned} (3.2a) \quad & -(\varepsilon\psi'_1)' + r(x)\psi_1 = 0, \quad x \in \Omega_1, \quad \psi_1(0) = 1, \quad \psi_1(d) = 0; \\ (3.2b) \quad & -(\varepsilon\psi'_2)' + r(x)\psi_2 = 0, \quad x \in \Omega_1, \quad \psi_2(0) = 0, \quad \psi_2(d) = 1; \\ (3.2c) \quad & -(\varepsilon\psi'_3)' + r(x)\psi_3 = 0, \quad x \in \Omega_2, \quad \psi_3(d) = 1, \quad \psi_3(1) = 0; \\ (3.2d) \quad & -(\varepsilon\psi'_4)' + r(x)\psi_4 = 0, \quad x \in \Omega_2, \quad \psi_4(d) = 0, \quad \psi_4(1) = 1. \end{aligned}$$

The constants $A_1 = A_2 + [v_\varepsilon(d)]$ are chosen so that the jump conditions at $x = d$ are satisfied. One can show that

$$\begin{aligned} A_2 &= \frac{[v_\varepsilon(d)](\varepsilon\psi'_2)(d^-) + w_\varepsilon(0)(\varepsilon\psi'_1)(d^-) - w_\varepsilon(1)(\varepsilon\psi'_4)(d^+) - [\varepsilon v'_\varepsilon(d)] - Q'_1}{(\varepsilon\psi'_3)(d^+) - (\varepsilon\psi'_2)(d^-)} \\ A_1 &= \frac{[v_\varepsilon(d)](\varepsilon\psi'_3)(d^+) + w_\varepsilon(0)(\varepsilon\psi'_1)(d^-) - w_\varepsilon(1)(\varepsilon\psi'_4)(d^+) - [\varepsilon v'_\varepsilon(d)] - Q'_1}{(\varepsilon\psi'_3)(d^+) - (\varepsilon\psi'_2)(d^-)}. \end{aligned}$$

Define the barrier function

$$B_{\varepsilon_1}(x) = e^{-x\sqrt{\beta/\varepsilon_1}}.$$

Observe that $\sqrt{\varepsilon_1}B'_{\varepsilon_1} = \sqrt{\beta}B_{\varepsilon_1}$, $\varepsilon_1 B''_{\varepsilon_1} = \beta B_{\varepsilon_1}$ and $B_{\varepsilon_1}(0) = 1$. Hence, (for ε_1 sufficiently small) we have

$$-(\varepsilon_1 p B'_{\varepsilon_1})' + r B_{\varepsilon_1} = (r - \beta p - \sqrt{\beta \varepsilon_1} p') B_{\varepsilon_1} \geq 0.$$

Lemma 3.1. *Assume the $\varepsilon_1, \varepsilon_2$ are sufficiently small so that (2.1h) is satisfied and that $|Q'_1| \leq C(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2})$. For each integer k , satisfying $0 \leq k \leq 4$, the regular and singular components v_ε and w_ε of the problem (2.1) satisfy the bounds.*

$$\begin{aligned} |v_\varepsilon^{(k)}(x)| &\leq \begin{cases} C + C\varepsilon_1^{1-\frac{k}{2}} (|w_\varepsilon(0)|B_{\varepsilon_1}(x) + B_{\varepsilon_1}(d-x)), & x \in \Omega_1 \\ C + C\varepsilon_2^{1-\frac{k}{2}} (|w_\varepsilon(1)|B_{\varepsilon_2}(1-x) + B_{\varepsilon_2}(x-d)), & x \in \Omega_2 \end{cases}, \\ |w_\varepsilon^{(k)}(x)| &\leq \begin{cases} C\varepsilon_1^{-\frac{k}{2}} (|w_\varepsilon(0)|B_{\varepsilon_1}(x) + B_{\varepsilon_1}(d-x)), & x \in \Omega_1 \\ C\varepsilon_2^{-\frac{k}{2}} (|w_\varepsilon(1)|B_{\varepsilon_2}(1-x) + B_{\varepsilon_2}(x-d)), & x \in \Omega_2 \end{cases}, \end{aligned}$$

where C is a constant independent of $\varepsilon_1, \varepsilon_2$.

Proof. Note that $u_\varepsilon = v_\varepsilon + w_\varepsilon$ and

$$|v_\varepsilon(d^-)| + |v_\varepsilon(d^+)| + \|v_\varepsilon\|_{\Omega_1 \cup \Omega_2} \leq C, \quad \|u_\varepsilon\|_{\Omega} \leq C + C \frac{|Q'_1|}{(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2})}.$$

Hence if $|Q'_1| \leq C(\sqrt{\varepsilon_1} + \sqrt{\varepsilon_2})$ then $|w_\varepsilon(d^-)| + |w_\varepsilon(d^+)| \leq C$. Bounding the derivatives separately on the intervals Ω_1 and Ω_2 (for example, see [6]), we get that for $0 \leq k \leq 4$,

$$(3.3) \quad |u_\varepsilon^{(k)}(x)| \leq C + C \begin{cases} \varepsilon_1^{-\frac{k}{2}} (|w_\varepsilon(0)|B_{\varepsilon_1}(x) + B_{\varepsilon_1}(d-x)), & x \in \Omega_1 \\ \varepsilon_2^{-\frac{k}{2}} (|w_\varepsilon(1)|B_{\varepsilon_2}(1-x) + B_{\varepsilon_2}(x-d)), & x \in \Omega_2 \end{cases}.$$

On the domain Ω_1 , the regular component is of the form

$$v_\varepsilon(x) = \frac{f(x)}{r(x)} + \varepsilon_1 z_{\varepsilon_1}(x),$$

where the remainder term z_{ε_1} satisfies the boundary value problem

$$L_\varepsilon z_{\varepsilon_1} = (p(\frac{f}{r}))', \quad z_{\varepsilon_1}(0) = z_{\varepsilon_1}(d) = 0.$$

Apply the bounds (3.3) to the remainder to derive the bounds on $|v_\varepsilon^{(k)}(x)|$.

Consider the boundary layer function $\psi_1(x)$ defined in (3.2a). From the maximum principle, we can deduce that for ε_1 sufficiently small, $0 \leq \psi_1(x) \leq B_{\varepsilon_1}(x)$ and $\varepsilon_1 |(p\psi'_1)'(x)| \leq CB_{\varepsilon_1}(x)$. Note that $\psi'_1(x) < 0$ and by the Mean Value Theorem, using the argument from [1], we have that $|\psi'_1(x)| \leq C\varepsilon_1^{-1/2}B_{\varepsilon_1}(x)$. Differentiate the differential equation (3.2a) to obtain bounds on the third and fourth derivatives of $\psi_1(x)$. Appropriate bounds on the other layer functions $\psi_i(x), i = 2, 3, 4$ can be deduced in an analogous fashion and then we can deduce that the constants in (3.1) satisfy $|A_2| \leq C$ and $|A_1| \leq C$. The bounds on w_ε and its derivatives follow. \square

4. A priori bounds on the derivatives of the solution of problem (2.2)

In the case of problem (2.2), the regular component is continuous and satisfies

$$L_\varepsilon v_\varepsilon = f, \quad x \in \Omega_1 \cup \Omega_2, \\ r(0)v_\varepsilon(0) = f(0), \quad r(d^-)v_\varepsilon(d) = f(d^-), \quad v_\varepsilon(1) = u_\varepsilon(1).$$

The singular component w_ε is hence also continuous and is given by

$$L_\varepsilon w_\varepsilon = 0, \quad x \in \Omega_1 \cup \Omega_2, \\ [\varepsilon w'_\varepsilon(d)] = -[\varepsilon v'_\varepsilon(d)] - Q'_1, \quad w_\varepsilon(0) = u_\varepsilon(0) - v_\varepsilon(0), \quad w_\varepsilon(1) = 0.$$

The singular component w_ε is explicitly given by

$$w_\varepsilon(x) = \begin{cases} w_\varepsilon(0)\psi_1(x) + A\psi_2(x), & x \in \Omega_1 \\ A\psi_5(x), & x \in \Omega_2 \end{cases}, \\ \text{where } -(\varepsilon\psi'_5)' = 0, \quad x \in \Omega_2, \quad \psi_5(d) = 1, \quad \psi_5(1) = 0, \\ \text{and } A = \frac{w_\varepsilon(0)(\varepsilon\psi'_1)(d^-) - [\varepsilon v'_\varepsilon(d)] - Q'_1}{(\varepsilon\psi'_5)(d^+) - (\varepsilon\psi'_2)(d^-)} = \mathcal{O}\left(\frac{\sqrt{\varepsilon_1} + \varepsilon_2 + |Q'_1|}{\varepsilon_2 + \sqrt{\varepsilon_1}}\right).$$

Lemma 4.1. *Assume that ε_1 is sufficiently small so that (2.2d) is satisfied and that $|Q'_1| \leq C(\sqrt{\varepsilon_1} + \varepsilon_2)$. For each integer k , satisfying $0 \leq k \leq 4$, the regular and singular components v_ε and w_ε of the problem (2.2) satisfy the bounds.*

$$|v_\varepsilon^{(k)}(x)| \leq \begin{cases} C + C\varepsilon_1^{1-\frac{k}{2}} (|w_\varepsilon(0)|B_{\varepsilon_1}(x) + B_{\varepsilon_1}(d-x)), & x \in \Omega_1 \\ C, & x \in \Omega_2 \end{cases},$$

$$|w_\varepsilon^{(k)}(x)| \leq \begin{cases} C\varepsilon_1^{-\frac{k}{2}} (|w_\varepsilon(0)|B_{\varepsilon_1}(x) + B_{\varepsilon_1}(d-x)), & x \in \Omega_1 \\ C, & x \in \Omega_2 \end{cases},$$

where C is a constant independent of $\varepsilon_1, \varepsilon_2$.

5. Discrete Problem

On $\Omega_1 \cup \Omega_2$ a piecewise-uniform mesh of N mesh intervals is constructed as follows. The interval $\bar{\Omega}_1$ is subdivided into the three subintervals

$$[0, \sigma_1], \quad [\sigma_1, d - \sigma_1] \quad \text{and} \quad [d - \sigma_1, d]$$

for some σ_1 that satisfies $0 < \sigma_1 \leq \frac{d}{4}$. On $[0, \sigma_1]$ and $[d - \sigma_1, d]$ a uniform mesh with $\frac{N}{8}$ mesh-intervals is placed, while on $[\sigma_1, d - \sigma_1]$ has a uniform mesh with $\frac{N}{4}$ mesh-intervals. The subintervals $[d, d + \sigma_2], [d + \sigma_2, 1 - \sigma_2], [1 - \sigma_2, 1]$ are treated analogously for some σ_2 satisfying $0 < \sigma_2 \leq \frac{1-d}{4}$. The interior points of the mesh are denoted by

$$(5.1) \quad \Omega_\varepsilon^N = \{x_i : 1 \leq i \leq \frac{N}{2} - 1\} \cup \{x_i : \frac{N}{2} + 1 \leq i \leq N - 1\}.$$

Let $h_i = x_i - x_{i-1}$ be the mesh step and $\bar{h}_i = (h_{i+1} + h_i)/2$. Clearly $x_{\frac{N}{2}} = d$ and $\bar{\Omega}_\varepsilon^N = \{x_i\}_0^N$. In the case of problem (2.1) we take

$$(5.2) \quad \sigma_1 = \min \left\{ \frac{d}{4}, 2\sqrt{\frac{\varepsilon_1}{\beta}} \ln N \right\}, \quad \sigma_2 = \min \left\{ \frac{1-d}{4}, 2\sqrt{\frac{\varepsilon_2}{\beta}} \ln N \right\}.$$

In the case of problem (2.2)

$$(5.3) \quad \sigma_1 = \min \left\{ \frac{d}{4}, 2\sqrt{\frac{\varepsilon_1}{\beta}} \ln N \right\}, \quad \sigma_2 = \frac{1-d}{4}.$$

Let h^+ (h^-) be the fine mesh interval sizes on the right (left) side of $x = d$ and $h = \max\{h^-, h^+\}$. Thus $h^- = 8\sigma_1 N^{-1}$, $h^+ = 8\sigma_2 N^{-1}$. Define the discrete finite difference operator L_ε^N as follows. For any mesh function Z , define

$$L_\varepsilon^N Z := \begin{cases} -\varepsilon_i \delta^2 Z(x_i) + r(x_i)Z(x_i), & x_i \neq d, \\ -\varepsilon_i \delta^2 Z(d) + \bar{r}(d)Z(d), & x_i = d, \\ Z(x_i), & x_i = \{0, 1\}, \end{cases}$$

where $\varepsilon_i \delta^2 Z(x_i) := (\bar{\varepsilon}(x_i)D^+ Z(x_i) - \bar{\varepsilon}(x_{i-1})D^- Z(x_i)) \frac{1}{\bar{h}_i}$

$$\bar{\varepsilon}(x_i) := \frac{\varepsilon(x_{i+1}^-) + \varepsilon(x_i^+)}{2}; \quad \bar{r}(d) := \frac{h^- r(d - h^-) + h^+ r(d + h^+)}{h^- + h^+};$$

$$D^+ v(x_i) := \frac{v(x_{i+1}) - v(x_i)}{x_{i+1} - x_i}, \quad D^- v(x_i) := D^+ v(x_{i-1}).$$

Since the system matrix L_ε^N is an M-matrix, the finite difference operator L_ε^N has properties analogous to those of the differential operator L_ε .

Lemma 5.1. *Suppose that a mesh function W satisfies $L_\varepsilon^N W(x_i) \geq 0$ for all $x_i \in \bar{\Omega}_\varepsilon^N$, then $W(x_i) \geq 0$ for all $x_i \in \bar{\Omega}_\varepsilon^N$.*

The discrete problem is: find U_ε such that

$$(5.4a) \quad -\varepsilon_i \delta^2 U_\varepsilon(x_i) + r(x_i) U_\varepsilon(x_i) = f(x_i), \quad x_i \in \Omega_\varepsilon^N,$$

$$(5.4b) \quad -\varepsilon_i \delta^2 U_\varepsilon(d) + \bar{r}(d) U_\varepsilon(d) = \bar{f}(d) + \frac{Q'}{h}, \quad x_i = d,$$

$$(5.4c) \quad U_\varepsilon(0) = u_\varepsilon(0), \quad U_\varepsilon(1) = u_\varepsilon(1),$$

$$(5.4d) \quad \text{where } \bar{f}(d) := \frac{h^- f(d-h^-) + h^+ f(d+h^+)}{h^- + h^+}.$$

6. Error analysis

We begin by examining the truncation error for $x_i \neq d$, where

$$\begin{aligned} & (\varepsilon_i \delta^2) u_\varepsilon(x_i) - (\varepsilon u'_\varepsilon)'(x_i) = \varepsilon(x_i) (\delta^2 u_\varepsilon(x_i) - u''_\varepsilon(x_i)) \\ & + \frac{\varepsilon'(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_{i-1}}^{x_{i+1}} \int_{s=x_i}^t u''_\varepsilon(s) ds dt \right) + \frac{D^+ u_\varepsilon(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_i}^{x_{i+1}} \int_{s=x_i}^t \varepsilon''(s) ds dt \right) \\ & - \frac{D^- u_\varepsilon(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_{i-1}}^{x_i} \int_{s=t}^{x_i} \varepsilon''(s) ds dt \right) \\ & = \varepsilon(x_i) (\delta^2 u_\varepsilon(x_i) - u''_\varepsilon(x_i)) + \frac{\varepsilon'(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_{i-1}}^{x_{i+1}} \int_{s=x_i}^t \int_{p=x_i}^s u'''_\varepsilon(p) dp ds dt \right) \\ & + \frac{D^+ u_\varepsilon(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_i}^{x_{i+1}} \int_{s=x_i}^t \int_{p=x_i}^s \varepsilon'''(p) dp ds dt \right) \\ & - \frac{D^- u_\varepsilon(x_i)}{h_i + h_{i+1}} \left(\int_{t=x_{i-1}}^{x_i} \int_{s=t}^{x_i} \int_{p=x_i}^s \varepsilon'''(p) dp ds dt \right) \\ & + \frac{\varepsilon''(x_i)}{4} (h_i^2 \delta^2 u_\varepsilon(x_i) + \frac{h_{i+1}^2 - h_i^2}{h_i} D^+ u_\varepsilon(x_i)). \end{aligned}$$

In the case of problem (2.1), by classical estimates and Lemma 3.1, we have that for all $i \neq N/2$,

$$|\varepsilon(x_i) (\frac{d^2}{dx^2} - \delta^2) v_\varepsilon(x_i)| \leq \begin{cases} C\varepsilon(x_i)(x_{i+1} - x_{i-1})|v_\varepsilon|_3 & \leq C\sqrt{\varepsilon(x_i)}N^{-1} \\ C\varepsilon(x_i)h^2|v_\varepsilon|_4 \leq CN^{-2}, & x_{i+1} - x_i = x_i - x_{i-1} = h, \end{cases}$$

where $|v|_k := \max \left| \frac{d^k v}{dx^k} \right|$, $\forall k \in \mathbb{N}$, and we also have

$$|\varepsilon(x_i) (\frac{d^2}{dx^2} - \delta^2) w_\varepsilon(x_i)| \leq \begin{cases} C\varepsilon(x_i)(x_{i+1} - x_{i-1})|w_\varepsilon|_3 & (a) \\ C\varepsilon(x_i)h^2|w_\varepsilon|_4, \quad x_{i+1} - x_i = x_i - x_{i-1} = h & (b) \\ C\varepsilon(x_i) \max_{x \in [x_{i-1}, x_{i+1}]} |w''_\varepsilon(x)|. & (c) \end{cases}$$

Using (c) in the outer-layer regions $[\sigma_1, d - \sigma_1] \cup [d + \sigma_2, 1 - \sigma_2]$ gives

$$|\varepsilon(x_i) (\frac{d^2}{dx^2} - \delta^2) w_\varepsilon(x_i)| \leq CN^{-2}.$$

Using (b) within the layer regions $(0, \sigma_1) \cup (d - \sigma_1, d) \cup (d, d + \sigma_2) \cup (1 - \sigma_2, 1)$,

$$|\varepsilon(x_i) (\frac{d^2}{dx^2} - \delta^2) w_\varepsilon(x_i)| \leq C\sigma_j^2 \varepsilon_j^{-1} N^{-2} \leq C(N^{-1} \ln N)^2.$$

Hence

$$|\varepsilon(x_i) (\frac{d^2}{dx^2} - \delta^2) w_\varepsilon(x_i)| \leq C(N^{-1} \ln N)^2, \quad x_i \neq d.$$

Using the decomposition $u_\varepsilon = v_\varepsilon + w_\varepsilon$ and the bounds on the derivatives of these components, we conclude that for $x_i \neq d$

$$|L_\varepsilon^N(U_\varepsilon - u_\varepsilon)(x_i)| \leq \begin{cases} C\sqrt{\varepsilon(x_i)}N^{-1} + C(N^{-1} \ln N)^2 \\ C(N^{-1} \ln N)^2 & \text{if } x_{i+1} - x_i = x_i - x_{i-1}. \end{cases}$$

At the point $x_i = d$,

$$\begin{aligned} & \bar{h}(-\varepsilon_i\delta^2 + \bar{r}(d))(U_\varepsilon - u_\varepsilon)(d) \\ &= \frac{1}{h^+} \int_{t=d}^{d+h^+} \int_{s=d}^t (\varepsilon u'_\varepsilon)'(s) ds dt \\ & - \frac{1}{h^-} \int_{t=d-h^-}^d \int_{s=d}^t (\varepsilon u'_\varepsilon)'(s) ds dt + \bar{h}(\bar{f}(d) - \bar{r}(d)u_\varepsilon(d)) \\ & + \frac{1}{h^+} \int_{t=d}^{d+h^+} (\bar{\varepsilon}(d) - \varepsilon(t))u'_\varepsilon(t) dt + \frac{1}{h^-} \int_{t=d-h^-}^d (\varepsilon(t) - \bar{\varepsilon}(d-h^-))u'_\varepsilon(t) dt \\ &= -\frac{1}{h^+} \int_{t=d}^{d+h^+} \int_{s=d}^t (f - ru_\varepsilon)(s) ds dt \\ & + \frac{1}{h^-} \int_{t=d-h^-}^d \int_{s=d}^t (f - ru_\varepsilon)(s) ds dt + \bar{h}(\bar{f}(d) - \bar{r}(d)u_\varepsilon(d)) + \mathcal{O}(\bar{h}^2) \\ &= \frac{1}{h^+} \int_{t=d}^{d+h^+} \int_{s=d}^t \int_{p=s}^{d+h^+} + \frac{1}{h^-} \int_{t=d-h^-}^d \int_{s=d}^t \int_{p=d-h^-}^s (f - ru_\varepsilon)'(p) dp ds dt \\ & + \frac{h^+r(d+h^+)}{2} \int_{t=d}^{d+h^+} u'_\varepsilon(t) dt + \frac{h^-r(d-h^-)}{2} \int_{t=d-h^-}^d u'_\varepsilon(t) dt + \mathcal{O}(\bar{h}^2). \end{aligned}$$

Hence,

$$|(-\varepsilon_i\delta^2 + \bar{r}(d))(U_\varepsilon - u_\varepsilon)(d)| \leq CN^{-1} \ln N.$$

Theorem 6.1. *In the case of both problems (2.1) and (2.2) we have that*

$$\max_{x_i \in \Omega_\varepsilon^N} |U_\varepsilon(x_i) - u_\varepsilon(x_i)| \leq C(N^{-1} \ln N)^2,$$

where C is a constant independent of $\varepsilon_1, \varepsilon_2$ and N .

Proof. We outline the proof for problem (2.1). Minor modifications to this proof will yield the proof for (2.2). Note that for problem (2.2) the mesh is uniform on Ω_2 . Consider first the case where $\sigma_1 < 1/4$ and $\sigma_2 < 1/4$. Define the mesh functions ω_1, ω_2 to be

$$\omega_1(x_j) = \prod_{i=1}^j (1 + \frac{\sqrt{\beta}h_i}{\sqrt{2\varepsilon_1}}); \quad \omega_2(x_j) = \prod_{i=j}^N (1 + \frac{\sqrt{\beta}h_i}{\sqrt{2\varepsilon_2}})^{-1}.$$

Note the following properties of these mesh functions

$$\begin{aligned} D^- \omega_1(x_i) &= \frac{\sqrt{\beta}}{\sqrt{2\varepsilon_1}(1 + \sqrt{\beta}h_i/\sqrt{2\varepsilon_1})} \omega_1(x_i) \quad ; \quad D^+ \omega_1(x_i) = \frac{\sqrt{\beta}}{\sqrt{2\varepsilon_1}} \omega_1(x_i); \\ D^+ \omega_2(x_i) &= -\frac{\sqrt{\beta}}{\sqrt{2\varepsilon_2}(1 + \sqrt{\beta}h_i/\sqrt{2\varepsilon_2})} \omega_2(x_i) \quad ; \quad D^- \omega_2(x_i) = -\frac{\sqrt{\beta}}{\sqrt{2\varepsilon_2}} \omega_2(x_i). \end{aligned}$$

This implies that for $0 < x_i < d$

$$-\varepsilon_1 p(x_i) \delta^2 \omega_1(x_i) + r(x_i) \omega_1(x_i) \geq (r(x_i) - \beta p(x_i)) \omega_1(x_i) > 0$$

and, hence, for ε_1 sufficiently small and $x_i < d$

$$-\varepsilon_i \delta^2 \omega_1(x_i) + r(x_i) \omega_1(x_i) \geq (r(x_i) - \beta p(x_i)) \omega_1(x_i) + \mathcal{O}(\sqrt{\varepsilon_1} \|p'\|) \omega_1(x_i) \geq 0.$$

Define the three barrier functions $\zeta_1(x_i)$, $\zeta_2(x_i)$, $\zeta_3(x_i)$ as follows

$$\zeta_1(x_i) = \begin{cases} \frac{x_i}{\sigma_1}, & 0 \leq x_i \leq \sigma_1 \\ 1, & \sigma_1 \leq x_i \leq 1 - \sigma_2 \\ \frac{1-x_i}{1-\sigma_2}, & 1 - \sigma_2 \leq x_i \leq 1, \end{cases} ; \zeta_2(x_i) = \begin{cases} \frac{\omega_1(x_i)}{\omega_1(d-\sigma_1)}, & 0 \leq x_i \leq d - \sigma_1 \\ 1, & d - \sigma_1 \leq x_i \leq d + \sigma_2 \\ \frac{\omega_2(x_i)}{\omega_2(d+\sigma_2)}, & d + \sigma_2 \leq x_i \leq 1 \end{cases} ;$$

$$\zeta_3(x_i) = \begin{cases} \frac{\omega_1(x_i)}{\omega_1(d)}, & 0 \leq x_i \leq d \\ \frac{\omega_2(x_i)}{\omega_2(d)}, & d \leq x_i \leq 1 \end{cases} .$$

Use the mesh function

$$\Xi(x_i) = C(N^{-1} \ln N)^2 \left(1 + \sum_{j=1}^3 \zeta_j(x_i)\right) \pm U_\varepsilon - u_\varepsilon$$

to conclude that $\|u_\varepsilon - U_\varepsilon\| \leq C(N^{-1} \ln N)^2$. In the case when $\sigma_1 = 1/4$ (or $\sigma_2 = 1/4$) use $\omega_1(x_i) = x_i$ (or $\omega_2(x_i) = 1 - x_i$). \square

Theorem 6.2. [5] *In the case of problem (2.1),*

$$|D^+(U_\varepsilon - u_\varepsilon)(x_i)| \leq \begin{cases} CN^{-1} \ln N / \sqrt{\varepsilon_1}, & x_i \in [0, \sigma_1] \cup [d - \sigma_1, d], \text{ if } \sigma_1 < 0.25, \\ CN^{-1} \ln N / \sqrt{\varepsilon_2}, & x_i \in [1 - \sigma_2, 1] \cup [d, d + \sigma_2], \text{ if } \sigma_2 < 0.25, \\ CN^{-1} (\ln N)^2, & \text{otherwise.} \end{cases}$$

In the case of problem (2.2),

$$|D^+(U_\varepsilon - u_\varepsilon)(x_i)| \leq \begin{cases} CN^{-1} \ln N / \sqrt{\varepsilon_1}, & x_i \in [0, \sigma_1] \cup [d - \sigma_1, d], \text{ if } \sigma_1 < 0.25, \\ CN^{-1} (\ln N)^2, & \text{otherwise.} \end{cases}$$

We have the parameter-uniform global error bound

Corollary 6.1. [6, pp. 55-56] *In the case of problems (2.1) and (2.2)*

$$\|u_\varepsilon - \bar{U}_\varepsilon\| \leq C(N^{-1} \ln N)^2,$$

where \bar{U}_ε is the piecewise linear interpolant of U_ε .

Let us finally examine the error in the scaled derivatives. Define the boundary layer widths to be:

$$\tau_1 = \sqrt{\frac{\varepsilon_1}{\beta}} \ln \frac{1}{\varepsilon_1}, \quad \tau_2 = \sqrt{\frac{\varepsilon_2}{\beta}} \ln \frac{1}{\varepsilon_2}.$$

Theorem 6.3. [5] *In the case of problem (2.1),*

$$|(D^+U_\varepsilon - u'_\varepsilon)(x_i)| \leq \begin{cases} CN^{-1} (\ln N)^2 / \sqrt{\varepsilon_1} & x_i \in [0, \tau_1] \cup [d - \tau_1, d] \\ CN^{-1} (\ln N)^2 / \sqrt{\varepsilon_2} & x_i \in [1 - \tau_2, 1] \cup [d, d + \tau_2] \\ CN^{-1} (\ln N)^2 & \text{otherwise.} \end{cases}$$

In the case of problem (2.2),

$$|(D^+U_\varepsilon - u'_\varepsilon)(x_i)| \leq \begin{cases} CN^{-1} (\ln N)^2 / \sqrt{\varepsilon_1} & x_i \in [0, \tau_1] \cup [d - \tau_1, d] \\ CN^{-1} (\ln N)^2 & \text{otherwise.} \end{cases}$$

7. Numerical results

In this section both the global and the nodal errors and their corresponding orders of convergence are estimated using the double mesh principle [6]. Define the parameter uniform double mesh nodal differences D^N to be

$$D^N := \max_{(\varepsilon_1, \varepsilon_2) \in R_\varepsilon} D_\varepsilon^N \quad \text{and} \quad D_\varepsilon^N := \max_{x_i \in \bar{\Omega}_\varepsilon^N} |U_\varepsilon^N(x_i) - \bar{U}_\varepsilon^{2N}(x_i)|,$$

where \bar{U}_ε^{2N} is the piecewise linear interpolant of the mesh function U_ε^{2N} onto $[0, 1]$. Here R_ε is the range of the singular perturbation parameters over which the numerical performance of the schemes will be tested. In this paper, we have taken R_ε to be

$$R_\varepsilon := \{(\varepsilon_1, \varepsilon_2) | \varepsilon_1 = 2^0, 2^{-2}, \dots, 2^{-40}, \varepsilon_2 = 2^0, 2^{-2}, \dots, 2^{-40}\}.$$

Define the double mesh global differences \bar{D}^N to be

$$\bar{D}^N := \max_{(\varepsilon_1, \varepsilon_2) \in R_\varepsilon} \bar{D}_\varepsilon^N \quad \text{and} \quad \bar{D}_\varepsilon^N := \max_{x_i \in \bar{\Omega}_\varepsilon^N \cup \bar{\Omega}_\varepsilon^{2N}} |\bar{U}_\varepsilon^N(x_i) - \bar{U}_\varepsilon^{2N}(x_i)|.$$

From these quantities the parameter-robust orders of nodal p^N and global convergence \bar{p}^N are computed from

$$p^N := \log_2\left(\frac{D^N}{D^{2N}}\right), \quad \bar{p}^N := \log_2\left(\frac{\bar{D}^N}{\bar{D}^{2N}}\right).$$

When an exact solution is available we compute the parameter-uniform nodal error E^N and the corresponding convergence rate p_E^N defined as

$$E^N := \max_{(\varepsilon_1, \varepsilon_2) \in R_\varepsilon} E_\varepsilon^N, \quad E_\varepsilon^N := \max_{x_i \in \bar{\Omega}_\varepsilon^N} |U_\varepsilon^N(x_i) - u_\varepsilon(x_i)|, \quad p_E^N := \log_2\left(\frac{E^N}{E^{2N}}\right).$$

We also examine the relative error Q^N in the fluxes at the interface $x = d$ and their corresponding convergence rates q^N defined by

$$Q_\varepsilon^N := \begin{cases} \frac{|D^- U_\varepsilon^N(d) - D^- U_\varepsilon^{2N}(d)|}{|D^- U_\varepsilon^N(d)|}, & \text{if } \varepsilon_1 \leq \varepsilon_2 \\ \frac{|D^+ U_\varepsilon^N(d) - D^+ U_\varepsilon^{2N}(d)|}{|D^+ U_\varepsilon^N(d) - [\varepsilon u'_\varepsilon]_d|}, & \text{if } \varepsilon_1 > \varepsilon_2 \end{cases}, \quad Q^N := \max_{(\varepsilon_1, \varepsilon_2) \in R_\varepsilon} Q_\varepsilon^N, \quad q^N := \log_2\left(\frac{Q^N}{Q^{2N}}\right).$$

The different definitions given above for Q_ε^N only differ by a factor of CN^{-1} . This choice of approximation to the relative error in the flux at d was required to reduce the probability of round-off errors accumulating for extreme values of the ratio of ε_1 to ε_2 .

Again, when an exact solution is available, we use the exact value of the flux to compute the relative error and its convergence rate from

$$Q_{E,\varepsilon}^N := \begin{cases} \frac{|D^- U_\varepsilon^N(d) - u'_\varepsilon(d^-)|}{|u'_\varepsilon(d^-)|}, & \text{if } \varepsilon_1 \leq \varepsilon_2 \\ \frac{|D^+ U_\varepsilon^N(d) - u'_\varepsilon(d^+)|}{|u'_\varepsilon(d^+) - [\varepsilon u'_\varepsilon]_d|}, & \text{if } \varepsilon_1 > \varepsilon_2 \end{cases}, \quad Q_E^N := \max_{(\varepsilon_1, \varepsilon_2) \in R_\varepsilon} Q_{E,\varepsilon}^N, \quad q_E^N := \log_2\left(\frac{Q_E^N}{Q_E^{2N}}\right).$$

7.1. Example 1. Consider the following problem, from the class (2.2), whose exact solution $u_{\varepsilon x}$ is easily determined. Find $u_\varepsilon \in C^1[0, 1]$ such that

$$(7.1a) \quad -(\varepsilon u'_\varepsilon)' + r u_\varepsilon = f, \quad x \neq 0.5, \quad u_\varepsilon(0) = 1, \quad u_\varepsilon(1) = 0,$$

$$(7.1b) \quad \begin{cases} \varepsilon_1, & 0 \leq x \leq 0.5 \\ \varepsilon_2, & 0.5 < x \leq 1 \end{cases}; \quad r = \begin{cases} 1, & 0 \leq x < 0.5 \\ 0, & 0.5 < x \leq 1 \end{cases}; \quad f = \begin{cases} 1, & 0 \leq x \leq 0.5 \\ \varepsilon_2, & 0.5 < x \leq 1. \end{cases}$$

	N=64	N=128	N=256	N=512	N=1024	N=2048
E^N	0.001276	0.0004609	0.000157	5.131e-05	1.624e-05	5.011e-06
p_E^N	1.421	1.469	1.553	1.614	1.66	1.696
Q_E^N	0.1077	0.06485	0.03788	0.02166	0.01218	0.006769
q_E^N	0.6651	0.7316	0.7756	0.8067	0.8298	0.8479

TABLE 1. Performance of the fitted mesh scheme (5.4), (5.1), (5.3) applied to (7.1).

	N=64	N=128	N=256	N=512	N=1024	N=2048
E^N	0.835	0.822	0.797	0.7513	0.7263	0.6806
p_E^N	0.01149	0.02273	0.04448	0.08529	0.04874	0.09385
Q_E^N	1	1	1	1	1	0.9999
q_E^N	1.29e-07	5.16e-07	2.064e-06	8.255e-06	3.302e-05	0.0001321

TABLE 2. Performance of the scheme (5.4) on a uniform mesh applied to (7.1).

The results in Tab. 1 indicate that the rate of nodal convergence is tending towards the rate $(N^{-1} \ln N)^2$ predicted by Theorem 6.1 and that the rate of convergence of the flux is in agreement with the rates predicted by Theorem 6.3. These rates of convergence should be compared to the lack of convergence on a uniform mesh given in Tab. 2.

	N=64	N=128	N=256	N=512	N=1024	N=2048
D^N	0.02217	0.008099	0.002748	0.000964	0.0003221	0.000105
p^N	1.074	1.453	1.559	1.511	1.581	1.617
\bar{D}^N	0.02217	0.008099	0.002748	0.000964	0.0003221	0.000105
\bar{p}^N	1.074	1.453	1.559	1.511	1.581	1.617
Q^N	0.2729	0.2574	0.1975	0.1433	0.09493	0.05852
q^N	1.132	0.08439	0.3821	0.4629	0.5942	0.6978

TABLE 3. Performance of the fitted mesh scheme (5.4), (5.1), (5.2) applied to problem (7.2).

7.2. Example 2. Consider the particular problem: find $u_\varepsilon \in C^0[0, 1]$ such that

$$(7.2a) \quad -(\varepsilon u'_\varepsilon)' + r u_\varepsilon = f,$$

$$(7.2b) \quad u_\varepsilon(0) = f(0)/r(0), \quad u_\varepsilon(1) = f(1)/r(1),$$

$$(7.2c) \quad \varepsilon(x) = \begin{cases} \varepsilon_1(1+x), & 0 \leq x \leq 0.5 \\ \varepsilon_2(2-x)^2, & 0.5 < x \leq 1 \end{cases}; \quad r = \begin{cases} 1-x, & 0 \leq x < 0.5 \\ 1+x, & 0.5 < x \leq 1 \end{cases};$$

$$(7.2d) \quad f = x^2, \quad x \neq 0.5, \quad [\varepsilon u'_\varepsilon]_d = \sqrt{\varepsilon_1}.$$

The example (7.2) in this section comes from the problem class (2.1). In this example, the diffusion coefficient is variable and there is a point source in the data. The results presented in Tables 3 and 4 again display the advantages of using a fitted mesh over a uniform mesh.

	N=64	N=128	N=256	N=512	N=1024	N=2048
D^N	0.1131	0.1121	0.1116	0.1114	0.1113	0.1112
p^N	0.0234	0.01239	0.006376	0.003237	0.001641	0.0008698
\bar{D}^N	0.1904	0.1906	0.1907	0.1907	0.1907	0.1907
\bar{p}^N	-0.002289	-0.001224	-0.0006321	-0.000304	-7.8e-05	0.0002638
Q^N	10.51	6.641	5.59	5.177	4.991	4.902
q^N	3.128	0.6621	0.2484	0.1109	0.0527	0.02585

TABLE 4. Performance of the scheme (5.4) on a uniform mesh applied to problem (7.2).



FIGURE 1. One dimensional Metal-Oxide-Semiconductor (MOS) Structure

8. A Modelling Problem

Consider the one dimensional Metal-Oxide-Semiconductor (MOS) structure depicted in Fig. 1, consisting of a slab of uniformly p-doped silicon of thickness t_{Si} and a layer of silicon-dioxide of thickness t_{ox} . One ohmic contact is placed at the oxide end of the device (Gate) and one at the semiconductor end (Bulk). Let N_A be the density of p-type dopant ions in the semiconductor and N_{ox} be the density of ionized impurities in the oxide. This structure is used as a nonlinear capacitor in integrated circuits, therefore the interest in numerical simulations is focused on accurately predicting the capacitance per unit area $C(V_A) := \frac{\partial Q}{\partial V_A}$ where Q indicates the total net charge per unit area in the semiconductor and V_A is the voltage applied at the Gate. We will show below that this problem gives rise to a diffusion-reaction problem with coefficients that are discontinuous and whose magnitude spans several orders of magnitude as V_A varies within the range of practically admissible values. This clearly demands for the use of a parameter-uniform numerical method, whose pointwise accuracy is independent of the magnitude of the equation coefficients.

If we choose the X axis to be normal to the Si/SiO₂ interface and its origin to be in correspondence with the bulk contact, the electric potential $V(X)$ in the device can be computed as a solution of the following nonlinear problem [9, 12]

$$(8.1a) \quad \frac{d}{dX} \left(\frac{\kappa}{q} \frac{dV(X)}{dX} \right) - \rho(X, V(X)) = 0, \quad 0 \leq X \leq L = t_{Si} + t_{ox},$$

$$(8.1b) \quad V(0) = V_0, \quad V(L) = V_L,$$

$$(8.1c) \quad \kappa(X) = \kappa_0 \kappa_{Si} \chi_{[0, t_{Si}]} + \kappa_0 \kappa_{ox} \chi_{(t_{Si}, L]},$$

where κ_0 is the electrical permittivity of free space and κ_{Si}, κ_{ox} denote the relative permittivity of silicon and of silicon-dioxide respectively and $\chi_{[0, t_{Si}]}$ denotes the indicator function of the interval $[0, t_{Si}]$. Assuming a uniform temperature and

that Maxwell–Boltzmann statistics apply, the net charge density $\rho(X, V(X))$ is given by

$$(8.1d) \quad \rho(X, V(X)) = n_i \left[-\exp\left(\frac{V}{V_{th}}\right) + \exp\left(-\frac{V}{V_{th}}\right) \right] \chi_{[0, t_{Si}]} + D(X),$$

where the intrinsic carrier density n_i and the thermal voltage V_{th} are constants depending only on the temperature and $D(X)$ denotes the volume density of fixed charged impurities. As we have assumed uniform p -type doping,

$$(8.1e) \quad D(X) = D_{Si} \chi_{[0, t_{Si}]} + D_{ox} \chi_{(t_{Si}, L]},$$

where $D_{Si} = -N_A < 0$ and $D_{ox} \ll D_{Si}$. The boundary values of V in (8.1) are

Quantity	Symbol	Value / Range
constants		
Electric permittivity of free space	κ_0	$8.810 \times 10^{-12} \text{ F/m}$
Unitary electric charge	q	$1.6022 \times 10^{-19} \text{ A s}$
Relative permittivity of Silicon	κ_{Si}	11.7
Relative permittivity of Silicon Dioxide	κ_{ox}	3.9
Thermal voltage at room temperature	V_{th}	$26 \times 10^{-3} \text{ V}$
Oxide voltage	V_{ox}	0.6 V
Silicon Intrinsic carrier density in at 300K	n_i	10^{-10} m^{-3}
device parameters		
Density of acceptor impurities	N_A	$10^{10} - 10^{25} \text{ m}^{-3}$
Net density of trapped charges in oxide gate	N_{ox}	$10^6 - 10^{13} \text{ m}^{-3}$
Oxide gate thickness	t_{ox}	$10^{-9} - 10^{-7} \text{ m}$
Bulk thickness	t_{Si}	$10^{-7} - 10^{-6} \text{ m}$
Applied voltage at the gate	V_A	0 – 10 V

TABLE 5. Typical values of relevant physical quantities appearing in (8.1)

set as follow

- the value of V at the Bulk contact is set by enforcing charge neutrality

$$\rho(0, V(0)) = 0 \Rightarrow V(0) \simeq V_{th} \ln\left(\frac{|D_{Si}|}{n_i}\right) =: V_0,$$

- the value at the gate contact equals the applied voltage V_A displaced by the contact built-in potential

$$V(L) = V_A + V_{ox} =: V_L.$$

Remark 8.1. Applying Gauß's theorem to (8.1), we get that the charge is given by

$$Q = \int_0^{t_{Si}} q\rho \, dX = - \left. \frac{d(\kappa V)}{dX} \right|_0^{t_{Si}}.$$

That is, the charge Q equals the flux of the electric displacement vector through the boundary of the semiconductor.

It is convenient for the subsequent discussion to rescale our unknown V with respect to its values at the boundary and to rescale the domain to be $(0, 1)$. Hence, we define the nondimensional quantity w , the scaled spatial coordinate x and the scaled junction location d by

$$w := \frac{V - V_0}{V_L - V_0}, \quad x := \frac{X}{L} \quad \text{and} \quad d := \frac{t_{Si}}{L}.$$

Furthermore, we define the following nondimensional coefficients:

$$\begin{cases} \varepsilon := \frac{\kappa (V_L - V_0)}{q L^2 |D_{Si}|}, & \alpha := \frac{V_L - V_0}{V_{th}}, \quad f := \frac{D}{|D_{Si}|}, \\ \theta := \frac{n_i}{|D_{Si}|} \exp\left(\frac{V_0}{V_{th}}\right), & \gamma := \frac{n_i}{|D_{Si}|} \exp\left(-\frac{V_0}{V_{th}}\right). \end{cases}$$

Note that ε will have different values on either side of the junction. We arrive at the following scaled nonlinear problem

$$(8.2) \quad \begin{cases} -(\varepsilon w')' + [\theta e^\alpha w - \gamma e^{-\alpha w}] \chi_{[0,d]} = f, & x \in (0, 1), \\ w(0) = 0, & w(1) = 1. \end{cases}$$

For any given value \bar{V} of the applied voltage V_A , an approximation to the capacitance can be computed as follows. Let \bar{w} be the solution of (8.2) for $V_A = \bar{V}$. By perturbing the boundary value at $x = 1$ by a small amount $\delta w \ll 1$ we get the following perturbed problem

$$\begin{cases} -(\varepsilon(\bar{w} + y))' + [\theta e^\alpha (\bar{w} + y) - \gamma e^{-\alpha (\bar{w} + y)}] \chi_{[0,d]} = f, & x \in (0, 1), \\ (\bar{w} + y)(0) = 0, & (\bar{w} + y)(1) = 1 + \delta w. \end{cases}$$

By linearizing the zero order term and recalling that \bar{w} is a solution of (8.2), we get

$$\begin{cases} -(\varepsilon y')' + [\theta \alpha e^\alpha \bar{w} + \gamma \alpha e^{-\alpha \bar{w}}] y \chi_{[0,d]} = 0, & x \in (0, 1), \\ y(0) = 0, & y(1) = \delta w. \end{cases}$$

This is linear and so we can set $\delta w = 1$ without loss of generality, and arrive at the following class of linear problems. Find u such that

$$(8.3) \quad \begin{cases} -(\bar{\varepsilon} u')' + \bar{r}(x)u = 0, & x \in (0, 1), \\ u(0) = 0, & u(1) = 1, \end{cases}$$

$$(8.4) \quad r(x) = \alpha(\theta e^\alpha \bar{w} + \gamma e^{-\alpha \bar{w}})\chi_{[0,d]}, \quad \bar{r}(x) = \frac{r(x)}{\|r\|}, \quad \bar{\varepsilon} = \frac{\varepsilon}{\|\varepsilon\|}$$

and the scaled capacitance is given by

$$(8.5) \quad c = (\varepsilon u)'|_0^d.$$

Note that the coefficient \bar{r} in (8.3) vanishes in $(d, 1]$ and is a function of \bar{w} , which is the unknown solution of the nonlinear problem (8.2). In this paper we focused on linear problems only. The theory developed in the earlier sections is not immediately applicable to the nonlinear problem (8.2). To produce a fair comparison between the performance of a uniform mesh method and a fitted mesh method applied to the linear problem (8.3) we use the same value for the coefficient \bar{r} in both cases, which is computed from solving (8.2). To reduce to a minimum the impact of inaccuracies in the computation of \bar{r} we use a much finer mesh for the solution of (8.2) than for (8.3). Although the detailed description of the solution strategy for the nonlinear problem is beyond the scope of the present paper, we wish to note that the Newton iteration algorithm used to solve (8.2) consists in the solution of a sequence of problems each of a form analogous to (8.3). This justifies the use of a suitably fitted piecewise uniform mesh for the solution of (8.2) as well. The computed values for the

coefficient $r(x)$ in (8.3) as a function of V_A are displayed in Fig. 2b. In this figure, we observe that away from the interior layer, the coefficient $r(x)$ can become arbitrary small and, moreover, this coefficient contains its own layers. Hence, the theory we have developed in the earlier sections of this paper is not directly applicable with this effect. However, in [4] it is shown, in the case of a reaction–diffusion problem where the coefficient of the reactive term contains its own layer and tends to zero within the layer, that the parameter-uniform convergence of second order is retained using the same piecewise–uniform mesh as is described here. Hence, below we examine the numerical output from using a fitted mesh of the form (5.1), (5.3) with the transition parameter β taken to be $1/2$. This choice can be justified by considering that, as is apparent from the definitions in (8.4), $0 < \bar{r}(x) < 1, x \in (0, d)$ and that numerical computations for physically acceptable values of the parameters produce values of \bar{r} such that $\bar{r} \geq 1/2$ within the layer region.

8.1. Simulation of a 1-D MOS Capacitor. In Figs. 2, 3 we consider the simulation of an MOS capacitor with the following specific data

$$(8.6) \quad t_{Si} = 10^{-5} \text{ m}, t_{ox} = 10^{-7} \text{ m}, N_A = 10^{22} \text{ m}^{-3}, D_{ox} = 0 \text{ m}^{-3}.$$

It is worth noting that the scaled diffusion coefficient ε/ρ , as shown in Fig. 2a, spans several orders of magnitude for $0 \leq \|V_A\| \leq 4V$. In Fig. 3 the values of the capacitance $C^N \equiv -\varepsilon D^- U^{200}(d) + \varepsilon D^+ U^{200}(0)$ computed using a uniform mesh and a fitted mesh are compared. Fig. 3a shows that both methods qualitatively predict the expected behaviour of C , with a minimum corresponding to the threshold voltage and an asymptotic value for large voltages of $\frac{K_0 K_{ox}}{t_{ox}}$ corresponding to that of a metal plate capacitor. Fig. 3b shows that in the range of values for the applied voltage V_A where the nonlinear behaviour of the device is stronger, the capacitance computed on the fitted mesh is approximately five times more accurate than the capacitance computed on a uniform mesh.

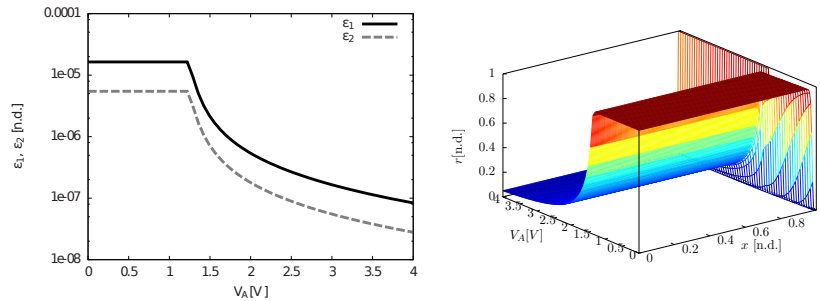


FIGURE 2. The scaled diffusion coefficient $\bar{\varepsilon}$ and the scaled reaction coefficient \bar{r} as a function of the applied voltage V_A and of position x .

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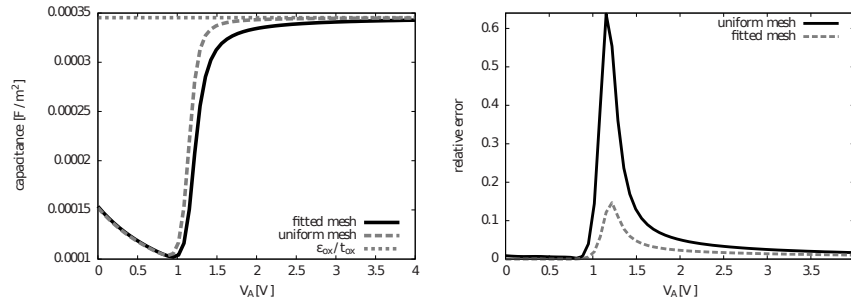


FIGURE 3. (a) The capacitance C (given by the scaled capacitance c defined in (8.5) multiplied by $\frac{q|D_{Si}|L}{V_L - V_0}$) as a function of the applied voltage V_A and (b) its relative error, both computed using a uniform mesh and a fitted mesh with $N = 200$.

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