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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 occassion 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

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

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].