Chapter 1

Introduction

It is widely known that various forms of ordinary differential equations or systems can be employed to describe a wide range of phenomena in biology, chemistry, engineering, and physics. Often, these mathematical problems are extremely difficult (or even impossible) to solve exactly, necessitating the use of numerical solutions. There are numerous numerical techniques available in the literature for this purpose. Nevertheless, some problems pose particularly daunting challenges that defy conventional analytical and numerical techniques. Among these enigmatic equations lie the "singularly perturbed problems" (SPPs), a class of differential equations with remarkable attributes and profound applications.

1.1 A brief background

The concept of singular perturbations has been in existence for slightly over a century, although the specific term "singular perturbation" was coined in the 1940s by Friedrichs and Wasow [3]. Typically, these problems can be described using differential equations (ordinary/partial) featuring at least one small parameter, popularly known as the "perturbation parameter(s)". When these parameters are not zero but are very small, the solution exhibits thin transition layers, often adjacent to the boundaries of the domain of interest, where it varies rapidly. These regions are usually referred to as *boundary layers* in fluid mechanics, *edge layers* in solid mechanics, *skin layers* in electrical applications, *shock layers* in fluid and solid mechanics, *transition points* in quantum mechanics and *Stokes lines and surfaces* in mathematics.

In fluid and gas dynamics, the existence of boundary layers was unknown to the world prior to the early twentieth century. It was Prandtl who revolutionized the theoretical understanding of many flow phenomena when he presented his seminal paper [4] in the Third International Congress of Mathematicians held at Heidelberg in 1904. Here, the small parameter is the inverse Reynolds number and the equations are based on the classical Navier-Stokes equation of fluid mechanics. This analysis, coupled with small-Reynolds-number-approximations that were developed at about the same time (1910), prepared the ground for a century of singular perturbation in fluid mechanics. Several early mathematical papers concerning singularly perturbed problems appeared in the 1930s, but they had limited long-term impact. The initial noteworthy advancement in the exploration of singularly perturbed problems can be seen in the doctoral thesis [5] of Wasow in 1941. Nonetheless, it was the pioneering research conducted by Friedrichs and Wasow [3, 6] that propelled the theory of singular perturbations to unprecedented levels of significance and recognition. Over the past few decades, this branch of mathematics has grown to extraordinary proportions. Despite the fact that numerous effective approaches have been developed, considerable progress is still being made, and essential research is underway. For the further reading on the historical development of singularly perturbed problems, we refer [7–9] to the readers.

1.2 Singularly perturbed problems

In 2009, Linß [10] provided the formal definition of singularly perturbed problems which is norm dependent. In the context of singularly perturbed problems, it turns out that maximum norm is most appropriate norm for the error measurement. The discussion in [11, 12] is quite helpful in this regard.

Definition 1.1. Let $\mathcal{S}$ be a function space with some norm $\|\cdot\|_{\mathcal{S}}$, $\mathcal{D} \subset \mathbb{R}^n$ be a parameter domain, and $u_\varepsilon \in \mathcal{S}$ be the solution of continuous problem $(\mathcal{P}_\varepsilon)$ for all $\varepsilon \in \mathcal{D}$. The continuous function $u_\varepsilon : \mathcal{D} \to \mathcal{S}$, $\varepsilon \mapsto u_\varepsilon$ is said to be *regular* for $\varepsilon \to \varepsilon_\star \in \partial\mathcal{D}$ if there exist a function $u_\star$ such that

$$\lim_{\varepsilon \to \varepsilon_\star} \|u_\varepsilon - u_\star\|_{\mathcal{S}} = 0,$$

otherwise u_ε is said to be *singular* for $\varepsilon \to \varepsilon_\star$, and the problem $(\mathcal{P}_\varepsilon)$ is said to be **singularly perturbed problem**.

Several examples of singularly perturbed problems can be found in the book of Miller et al. [13]. One key characteristic of these problems is their tendency to exhibit layer phenomena within the domain of interest. Consequently, the solution or its derivatives undergo rapid fluctuations within specific areas of the domain, while maintaining a smooth behavior outside of these zones. These areas exhibiting rapid changes are termed ‘layer regions,’ whereas the regions where solutions exhibit smooth behavior are designated as ‘regular regions.’ When these layer regions are situated near the boundaries of the domain, they are termed ‘boundary layer regions.’ Conversely, if the layer regions manifest within the interior of the domain, they are known as ‘interior layer regions.’

Many applied mathematicians have taken a keen interest in this mathematical area and have made significant contributions to the numerical treatment of SPPs. This interest stems from the fact that SPPs are not only limited to fluid dynamics but extend their relevance to a wide range of fields, including elasticity, quantum mechanics, electrical networks, chemical reactor theory, gas porous electrodes theory, aerodynamics, plasma dynamics, oceanography, diffraction theory, reaction-diffusion processes, and various other domains.

1.3 Numerical treatment of SPPs

Numerical analysis and asymptotic analysis are two principal approaches for addressing SPPs. These approaches have historically developed independently due to their distinct objectives and nature of the problems they tackle. There are quite a few books [7, 14–26] in this field that either deal with the asymptotic analysis or with numerical analysis of SPPs. Numerical analysis aims to provide precise quantitative solutions to specific problems, while asymptotic analysis seeks to offer insights into the qualitative characteristics of a family of problems. Numerical methods are designed to handle a wide range of problem types and prioritize user-friendliness. In contrast, asymptotic methods treats comparatively restricted classes of problems and demands a deeper understanding of the anticipated solution behavior beforehand. Given this disparity, it is advisable to consider numerical analysis over straightforward asymptotic analysis when dealing with SPPs.

Standard or classical numerical method includes Finite Difference Method (FDM), Finite Element Method (FEM), and Finite Volume Method (FVM). It is well established that that when any discretization method is applied to a parameter-dependent problem, its performance is influenced by that parameter. Consequently, unless an exceedingly high number of mesh points are utilized, standard numerical methods struggle to provide reasonably accurate approximations of the exact solution for all perturbation parameter values. This issue leads to unbounded truncation errors. Further, when the parameter equals zero, order of the differential equation decreases, resulting in a reduced number of initial or boundary conditions [13]. These limitations served as the driving force for researchers to seek robust numerical approaches that consistently perform effectively regardless of the perturbation parameter's magnitude. In literature, these techniques are commonly referred to as **parameter-uniform, parameter-robust, or uniformly convergent methods**. This method ensures that both the convergence rate and the error constant remain unaffected by changes in the perturbation parameter. Throughout this thesis, our primary objective is to design and employ such parameter-uniform numerical methods to obtain approximate solutions for various classes of SPPs.

In order to construct uniformly convergent methods, there are primarily two common approaches for the numerical treatment of SPPs. Here, we briefly describe the both approaches.

- **Fitted Operator Methods (FOMs):** The method was initially introduced by Allen and Southwell [27] in 1955 as a solution to the problem of a viscous fluid flow past a cylinder. In this approach, the conventional finite difference operator, which corresponds to the continuous problem, is substituted with a modified finite difference operator on a uniform mesh. This modified operator incorporates either a fitting factor, often of exponential nature, or a denominator function. This modification enhance the stability and ensure that the truncation error remains bounded with respect to the perturbation parameter. Nonetheless, extending this techniques to nonlinear and higher-dimensional problems poses significant challenges. Further information regarding fitted operator methods can be found in [13, 26–31].

- **Fitted Mesh Methods (FMMs):** This method consists of a simple discretization scheme applied to the specially chosen nonuniform meshes which adapt to the singularly perturbed nature of the problem. One notable benefit of FMMs compared to FOMs is their ability to handle nonlinear and higher-dimensional problems, even those with complex domain structures, with greater ease [13]. Numerous works involving FMMs have been reported in the literature for various classes of SPPs [10, 13, 32, 33].

These specially chosen nonuniform meshes are referred to as layer-adapted or fitted meshes. Such meshes can be further classified into two categories.
(i) A priori meshes: If sufficient a priori information regarding the location and width of the layer is available, then one can construct a priori layer-adapted meshes. The concept of such meshes was initially explored approximately sixty years ago by Bakhvalov [34] within the context of a reaction-diffusion problem. Thereafter, researchers like Gartland [35], Liseikin [36, 37], Vulanovic [38], and others developed such meshes for convection-diffusion problems. Note that constructing these meshes is very complex, and extending them to higher dimensions presents considerable difficulty. Further research in this direction gained momentum with the introduction of piecewise-uniform grids by Shishkin [39]. Due to their straightforward structure, these meshes have garnered significant attention and are commonly referred to as Shishkin meshes. For more comprehensive information on these grids, we refer to the book [11] and the references therein.

(ii) A posteriori meshes: In real-world situations, it is frequently the scenario when there is a lack of prior information regarding the exact solution of the problem, for instance, phenomena such as the interaction of waves on the ocean's surface, the multi-phase flow through porous materials, and the formation of patterns in Hele-Shaw shells. This results in the development of layer-adapted meshes, which differ from a priori meshes in the sense that they don't necessarily require any prior knowledge about the solution and its derivatives. A posteriori meshes are highly nonuniform grids developed using a posteriori error estimates. In this approach, an algorithm begins with an initial unsophisticated mesh and subsequently identifies layers, generates a mesh tailored to these layers solely based on intermediate computed solutions and mesh information. In general, a posteriori error estimates can underlie any suitable moving mesh algorithms, however, in this thesis we have used the algorithm originally proposed by De Boor [40] which is based on the equidistribution principle [41].

An arbitrary mesh $\{t_i\}_{i=0}^{N}$ satisfies the equidistribution principle if there exists a positive monitor function $M_E(u(t),t)$ such that

$$\int_{t_{j-1}}^{t_j} M_E(u(z),z)dz = \int_{t_j}^{t_{j+1}} M_E(u(z),z)dz,\ j = 1,2,\ldots,N-1,$$

where N is the number of mesh-intervals. Equivalently,

$$\int_{t_{j-1}}^{t_j} M_E(u(z),z)dz = \frac{1}{N}\int_{0}^{T} M_E(u(z),z)dz, \quad j = 1,2,\ldots,N.$$

A key to the success to this approach of mesh adaptation is in the selection of a proper monitor function. Several factors influence the effectiveness of this choice, including the nature of the problem at hand, the specific numerical discretization method employed, and norm of the error used. According to Ren and Russell [42], three types of monitor functions are suggested: those based on arc length, a combination of curvature and gradient, and those derived from truncation errors or solution residuals. Many researchers have explored arc length monitor functions, however, it has been pointed out in [43] that the arc length-based monitor function is unsuitable for reaction-diffusion type problems. Beckett and Meckenzie proposed a curvature-based monitor function in [44, 45], which proves effective for a broader range of singularly perturbed problems.

An alternative approach for selecting a suitable monitor function involves relying on the a posteriori error analysis of SPPs. This involves using the derived a posteriori error bound as the monitor function, which ensures the convergence of the method. Unlike the a priori error analysis, one doesn't require a priori information regarding the continuous solution and its behavior, for deriving the a posteriori error estimates. Pioneering work in this regard has been conducted by Kopteva and her collaborators in their papers [43, 46, 47] and related references. Inspired by this, we have conducted a thorough a posteriori error analysis for various categories of SPPs within this thesis.

1.4 Literature review

In this section, we provide an overview of the research documented in the literature concerning the numerical treatment of different classes of SPPs, which will be discussed in the subsequent chapters of this thesis.

1.4.1 Singularly perturbed nonlinear problems with integral boundary conditions

Integral equations are a very important class of mathematical problems that appear in modeling of various physical phenomena in several branches of applied sciences and engineering, such as fluid dynamics, elasticity, mathematical finance, population dynamics, mathematical image processing, electromagnetic inverse problems [48], options pricing under jump diffusion [49], and transient radiative transfer [50, 51].

Some studies of problems in ordinary and partial differential equations with integral boundary conditions are done in [52–60], however the problems in all these papers are of regular type (i.e. they are not singularly perturbed). There is enormous literature available on studies of singularly perturbed differential equations with non-integral initial/boundary conditions (see [2, 61–68] and the references therein). However, studies of first-order nonlinear singularly perturbed differential equations with integral initial/boundary conditions are limited. In [69], the nonlinear equation is discretized using the backward Euler scheme and the boundary condition by a composite right-rectangle rule. The piecewise-uniform Shishkin mesh is used to resolve the layers. The method is proved to be uniformly convergent of $\mathcal{O}(N^{-1} \ln N)$. Recently, in [70], problem is discretized using the same scheme as in [69], but the mesh is generated using the equidistribution of the arc-length monitor function. The method is proved to be uniformly convergent of $\mathcal{O}(N^{-1})$. Therefore, the construction of high-order numerical schemes for these problems is indeed necessary.

1.4.2 Singularly perturbed nonlinear parameterized problems with integral boundary condition

Parameterized boundary value problems often arise in thermodynamics and physics, helping us to understand the various phenomena, such as exothermic and isothermal chemical reactions, the steady-state temperature distributions, and the oscillation of a mass attached by two springs [71–74]. When a small parameter is multiplied with the highest order derivative of parameterized problems, it is known as singularly perturbed parameterized problems. In the last two decades, substantial work has been reported in research literature on numerical methods for nonlinear singularly perturbed parameterized problems with Dirichlet boundary conditions (see [66, 67, 75–78] and the references therein). However, a very few works have been reported on nonlinear singularly perturbed parameterized problems with integral boundary conditions. In [79], almost first-order parameter-uniform convergence of a finite difference scheme on Shishkin mesh is established. In [80], the same scheme is analyzed on Bakhvalov mesh and proved to be first-order parameter-uniformly convergent. Recently, the posteriori error estimate approach is used in [70] for a class of non parameterized problems with integral boundary conditions. Clearly, a posteriori error analysis for parameterized nonlinear SPPs with integral boundary condition is lacking in the literature.

1.4.3 Singularly perturbed Volterra delay integro-differential equations

Volterra integro-differential equations (VIDEs) frequently arise in various fields, such as chemistry, biology, insurance mathematics, viscoelasticity, and demography [81]. These equations involve an unknown function under the integral sign with a variable upper limit of the integration [82]. When a small perturbation parameter ε is multiplied with the highest order differential term of such VIDEs, these equations are termed singularly perturbed Volterra integro-differential equations (SPVIDEs). Many physical phenomena, such as diffusion-dissipation processes, epidemic dynamics, synchronous control systems, and filament stretching problems [83–86], are governed by SPVIDEs. One can see [87] for a survey of early findings in the theoretical and numerical analysis of SPVIDEs. In the last two decades, a substantial amount of work has been reported in the literature for singularly perturbed Volterra integro-differential equations without delay (see [66, 88–94] and the references therein), as well as for singularly perturbed delay differential equations (see [95–102] and the references therein). However, very little progress has been observed in the numerical analysis of singularly perturbed delay Volterra integro-differential equations. In particular, some development can be found in [103], where an almost first-order convergent finite difference scheme on Shishkin type mesh is proposed. Note that the work of [103] is restricted to Shishkin meshes only. It is evident that a priori and a posteriori error analysis for SPVIDEs with a delay argument is lacking in the literature.

1.4.4 Coupled systems of nonlinear singularly perturbed problems

The systems of multiscale problems involving small perturbation parameters are a frequently arising class in physical sciences and engineering [104–106]. A first-order convergent numerical method on Shishkin mesh is given in [107]. In [108], the authors first derived a priori bounds and then proposed an almost second order convergent numerical method using a hybrid finite difference scheme on Shishkin mesh under the restriction $\varepsilon_1, \varepsilon_2 \leq CN^{-1}$. In [2], the authors presented a general error analysis framework for the first and second order convergent schemes on both Shishkin and Bakhvalov meshes. Recently, in [109], the problem is discretized by a second order weighted monotone hybrid finite difference scheme on equidistributed meshes. The meshes are constructed via equidistribution of a monitor function based on the discrete analogue of the a priori error estimates involving the derivatives of the exact solution. Apparently, a posteriori error analysis for the concerned problem has not been attempted yet.

1.4.5 Coupled systems of singularly perturbed Volterra integro-differential equations

Studies of systems of Volterra integro-differential equations have sparked a lot of interest in the applied sciences. The general concepts and the essential characteristics of such problems can be used in a variety of practical situations, for instance, in actuarial sciences [110], population growth models [111], epidemic studies [112], and ecology [113]. The numerical treatment of systems of SPVIDEs is even more difficult due to the presence of overlapping layers. We refer to [66, 88, 88, 91, 103, 114–120] and the sources therein for a basic understanding of the numerical treatment of SPVIDEs. Bijura [121] considered a system of SPVIDEs and presented an algorithm for the construction of asymptotic solutions. Recently, a system of SPVIDEs is considered in [1] and the first-order convergence rate is reported in the maximum norm. They carried out a posteriori error analysis for the finite difference scheme, but unfortunately, it suffers from mathematical drawbacks. Further, the scheme in [1] posed some additional restrictions on the data. This motivated us to derive a new scheme and conduct its a posteriori error analysis for a system of SPVIDEs.

1.5 Objective of the thesis

The review of existing literature highlights a noticeable gap in the context of a posteriori error analysis for singularly perturbed problems other than linear and scalar types. Given that many real-world phenomena are described by nonlinear models, whether scalar or system-based, it becomes particularly intriguing to derive a posteriori error estimates for such problems. Although numerous research papers have conducted a priori error analyses for linear and nonlinear problems, they often require separate analysis to establish the convergence of discrete schemes on various layer-adapted meshes. Consequently, there is a pressing need for a theoretically simpler approach in this direction. These gaps in literature have spurred our motivation to contribute to this area.

To fulfill this purpose, we have systematically considered the following important classes of singularly perturbed problems throughout the thesis.

(i) First-order nonlinear singularly perturbed problems with integral boundary condition.

(ii) First-order nonlinear singularly perturbed parameterized problems with integral boundary condition.

(iii) First-order linear singularly perturbed delay Volterra integro-differential equations.

(iv) Coupled systems of first-order nonlinear singularly perturbed problems.

(v) Coupled systems of first-order linear singularly perturbed Volterra integro-differential equations.

Overall, the main objective of this thesis is to develop and analyze parameter-uniform convergent schemes on layer-adapted meshes for various classes of singularly perturbed problems. A significant emphasis has been placed on establishing a general error analysis framework that allows to deduce uniform convergence on various layer-adapted meshes conveniently within a single framework. Recognizing the ubiquitous need for error estimates that do not rely on prior knowledge of the exact solution and its derivatives, providing a posteriori error estimates is another vital contribution of this work.

1.6 Outline of the thesis

We continue with a few words about the structure of the thesis. The thesis is structured into six chapters, each containing distinct components of the research work. Now, let us briefly describe the material included in the thesis.

Chapter 1 provides an in-depth review of the historical progress made in the field of singularly perturbed problems and their numerical treatment. It also includes a concise literature survey related to the problems addressed in the thesis, along with a presentation of the thesis objectives.

Chapter 2 focuses on the construction of high-order uniformly convergent numerical methods for the class of nonlinear singularly perturbed problems with integral boundary condition. The discretization of the problem consists of a hybrid scheme defined on an arbitrary nonuniform mesh. A unified error analysis framework is introduced, and uniform convergence on various layer-adapted meshes is proved. Further, we propose adaptive generation of meshes based on a suitable monitor function and the mesh equidistribution principle. Numerical results align well with the proposed theory.

In Chapter 3, we examine a first-order nonlinear singularly perturbed parameterized problem with integral boundary condition. To discretize this problem, we employ the implicit Euler scheme for the nonlinear problem, whereas a composite right rectangle rule is applied to the integral boundary condition. A priori as well as a posteriori error analysis is developed for the proposed scheme. Optimal first-order uniform convergence is shown on both a priori and a posteriori meshes. Numerical results are consistent with our theoretical findings.

In Chapter 4, we address the first-order linear singularly perturbed delay Volterra integro-differential equation that exhibits multiple-layer phenomena. The discretization consists of an implicit difference scheme for the derivative term and a composite numerical integration rule for the integral term. A priori and a posteriori error analysis for the proposed discrete scheme is carried out. A comparison of uniformly accurate results is shown on these meshes. Further, numerical experiments are conducted, which support the theory.

Chapter 5 focuses on the development of a high-order convergent adaptive numerical method for a system of first-order singularly perturbed nonlinear differential equations with distinct perturbation parameters. The problem is discretized by a hybrid finite difference scheme, for which a posteriori error estimate in the maximum norm is derived. The layer-adapted meshes are generated using the equidistribution of the monitor function, chosen based on the derived a posteriori error estimate. Numerical results are presented that validate the theory and show the effectiveness of the present numerical method.

Finally, in Chapter 6, we examine a system of Volterra integro-differential equations with initial conditions. The derivative term in these equations is multiplied with distinct small positive parameters giving rise to overlapping layers. We propose a numerical scheme that avoids the extra condition on the problem's data required by the scheme of Liang et al. [1]. We derive a priori and a posteriori error bounds for the proposed scheme and further rectify the shortcomings of a posteriori error estimation in Liang et al. [1]. Numerical results are presented in the form of graphs and tables that validate the proposed theory.

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