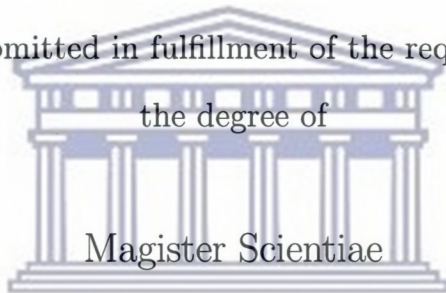# NUMERICAL TREATMENT OF NON-LINEAR

SINGULAR PERTURBATION PROBLEMS

by

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A thesis submitted in fulfillment of the requirements for

the degree of

Magister Scientiae

in the

Department of Mathematics and Applied Mathematics

University of the Western Cape
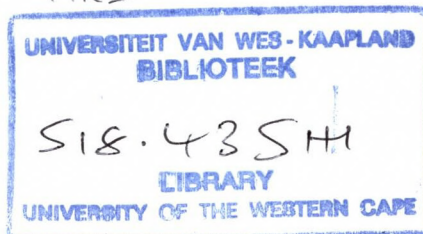
Supervisor: Dr. Kailash C. Patidar

November 2007

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Abstract

NUMERICAL TREATMENT OF NON-LINEAR SINGULAR PERTUR-BATION PROBLEMS

A. Shikongo

This thesis deals with the design and implementation of some novel numerical methods for nonlinear singular perturbations problems (NSPPs). We provide a survey of asymptotic and numerical methods for some NSPPs in past decade. By considering two test problems, rigorous asymptotic analysis is carried out. Based on this analysis, suitable numerical methods are designed, analyzed and implemented in order to have some relevant results of physical importance. Since the asymptotic analysis provides only qualitative information, the focus is more on the numerical analysis of the problem which provides the quantitative information.

Keywords: Non-linear Singular Perturbation Problems, Asymptotic Analysis, Numerical Analysis, Fitted Mesh Finite Difference Methods, Fitted Operator Finite Difference Methods, Stability, Error Estimates, Convergence, Enzyme Kinetics.

November 2007

i

Declaration

I declare that *Numerical Treatment of non-linear Singular Perturbation Problems* is my own work, that it has not been submitted before for any degree or examination in any other university, and that all the sources I have used or quoted have been indicated and acknowledged as complete references.

Albert Shikongo   November 2007

Signed:..

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Albert Shikongo

iii

Contents

iv

v

UNIVERSITY *of the*

WESTERN CAPE

vi

List of Figures

UNIVERSITY *of the*

WESTERN CAPE

vii

List of Tables

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Publications: A part of this thesis has been submitted in form of the following research reports whose modified versions are being submitted as research paper(s) to some international journals for publication:

1. **K.C. Patidar and A. Shikongo**, Some non-linear singular perturbation models and techniques for their solution, Report Nr. UWC-MRR 2006/06, University of the Western Cape, December 2006.

2. **K.C. Patidar and A. Shikongo**, A novel numerical method for solving a non-linear singular perturbation problem arising in enzyme kinetics, Report Nr. UWC-MRR 2007/04, University of the Western Cape, November 2007.

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ix

Chapter 1

Introduction

Nonlinear Singular Perturbation Problems (SPPs) governing mathematical models appear in many interesting applications in engineering fields. H. L. Dryden describes it in his National Advisory Committee for Aeronautics, Washington 25, D.C. that the concept of the boundary layer is diffused into mechanical engineering, hydraulics and chemical engineering. Similarly, studies of heat transfer, diffusion, and evaporation in moving fluids were greatly aided by the knowledge of the boundary layer flow.

The above information indicates that there has been some successful interaction between scientists and engineers which has resulted in an almost exponential growth of research on boundary layer flow in recent years. To this end, it will be paramount to highlight an account of some recent developments (both theoretical and applied) on non-linear singular perturbation models. We include some of the works that use the singular perturbation techniques to solve some other problems in recent years. Such inclusions are limited due to the non-availability of literature and therefore, we apologize if there are any omissions.

1.1 Nonlinear Singular Perturbation Problems

Consider the following ordinary differential equation (ODE)

$$a_n(x)\frac{d^n y}{dx^n} + a_{n-1}(x)\frac{d^{n-1}y}{dx^{n-1}} + \cdots + a_1(x)\frac{dy}{dx} + a_0(x)y = g(x), \;\; n \in Z^+.$$

An ODE which cannot be expressed in the form of the above ODE is called a non-linear ODE.

If $0 < \varepsilon << 1$ (known as the singular perturbation parameter) is multiplied to the highest derivative term of a non-linear ODE, then such a problem is known as a non-linear SPP provided that the following condition holds

$$\lim_{\varepsilon \to 0} y(x, \varepsilon) \neq y_{reduced}(x)$$

(where $y(x, \varepsilon)$ and $y_{reduced}(x)$ denote the solutions to a non-linear SPP when $0 < \varepsilon << 1$ and $\varepsilon = 0$ respectively), in the sense that its solution has an asymptotic expansion (c.f. Appendix A) that is not uniformly valid in the domain of interest. The part of the domain where the two solutions do not agree constitutes the layer region. When a layer is located near the boundary, the SPP is referred as a boundary layer problem, whereas if the layer is located inside the domain of interest, the SPP is known as an interior layer problem. These layers become very sharp as $\varepsilon \to 0$. See Figure 1.1 for the case of boundary layers.

1.2 Problems Associated With the Non-linear Singular Perturbation Problems

There are two major problems inherent in a non-linear SPP. The first is the layer issue whereas the second one is the type of non-linearity which could be

2
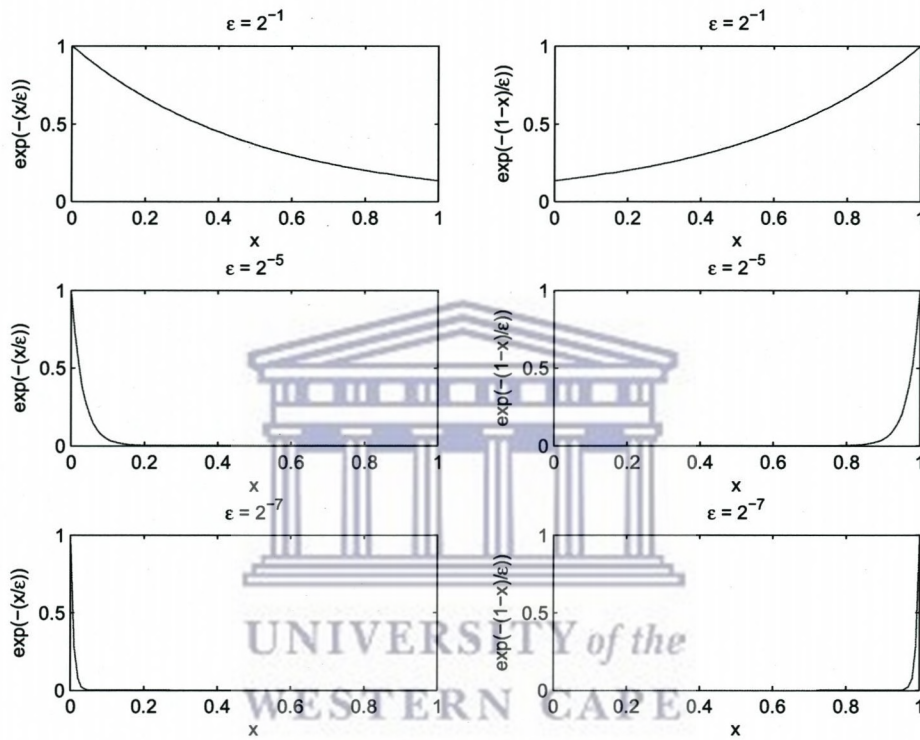
Figure 1.1: Profiles of the left and right boundary layer functions: $\exp(-x/\varepsilon)$ and $\exp(-(1-x)/\varepsilon)$, for different values of ε. Total grid points taken in each case are 100.

3

- smooth analytical functions such as powers, sinusoids and exponentials.

- bilinear terms consisting of state variables multiplied by independent variables

- a set of linear relations valid in different regions.

Depending on each case, the solution profile change significantly and therefore additional care is required in designing appropriate numerical methods.

1.3 Some Basic Methods for Solving Non-linear Singular Perturbation Problems

Methods that are devised for solving non-linear SPPs (NSSPs) can broadly be classified into *Asymptotic methods* which are *Qualitative methods* and the *Numerical methods* which are *Quantitative methods*. (The words *Qualitative* and *Quantitative* are self-explanatory.) We discuss both of these approaches.

1.3.1 Asymptotic Methods

There are several asymptotic methods available in the literature to approximate the solution of non-linear SPPs. However the most widely used ones are the following two:

- **The Method of Multiple Scales.** When applied to a SPP, this method yields a single solution valid in the entire domain of interest. Instead of being saddled with the deficiencies of stability theory in dynamic stability analysis one may use the Method of Multiple Scale to analyze a model equation for linear or non-linear dynamic stability.

4

- **The Method of Matched Asymptotic Expansions.** Matched asymptotic expansions yield two solutions, known as inner and outer solutions. The method is much useful when one wishes to investigate these two solutions in their own right. The inner solution can be matched with the outer solution using the Van Dyke matching principle and composite expansions can then be obtained which are valid in the entire domain. It has been discovered that they are quite successful in the calculation of both the free stream and boundary layer solutions for viscous flow past a body at high Reynolds number or Stokes' and Oseen's problems for flow at low Reynolds number.

  Further discussion about above two approaches is postponed until Chapter 2 where we use the method of multiple scales to obtain the width of the boundary layer whereas the methods of matched asymptotic expansion is used to obtain the composite expansion.

In Chapter 2 we have applied asymptotic analysis to a model problem to obtain qualitative information about the solution of a non-linear SPP.

1.3.2 Numerical Methods

Because of the complex nature of the associated terms in the NSPPs, closed form solutions are not easily obtainable and one has to go for some approximation methods. Though the asymptotic methods do provide such approximate solutions but no quantitative information can be obtained with these approaches and therefore one need to use one of the following popular numerical methods.

- Finite Difference Methods

- Finite Element Methods

5

- Spline Approximation Methods.

Further details about some of these numerical approaches will be provided in forth-coming chapters.

1.4 Some Models Describing Non-linear Singularly Perturbed Problems

We list some models in which non-linear singular perturbations problems feature.

1. **Non-premixed combustion** [118].

$$\varepsilon y'' = y^2 - t^2 \equiv h(t, y), \quad -1 < t < 1,$$

and

$$y(-1, \varepsilon) = y(1, \varepsilon) = 1.$$
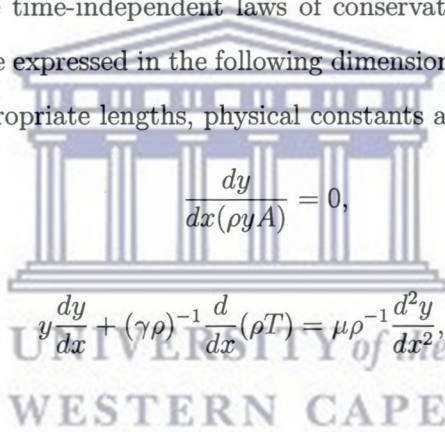
Here ε (assumed to be very small) is a ratio of diffusive effects to the speed of reaction, and t is a distance coordinate, chosen so that $t = 0$ is the location of the flame, where the fuel and the oxidizer meet each other and react. The functions $y - t$ and $y + t$ represent the mass fractions of fuel and oxidizer, respectively.

2. **A catalytic reaction theory** [3]. This physical problem involves an isothermal reaction $A \to B$ which is catalyzed in a pallet of length two. The equation that describes the mass balance between diffusion and reaction inside of the pellet is

$$y'' = \Phi^2 R(y), \ 0 < t < 1,$$

6

where y is the normalized concentration of the reactant A, t is the (dimensionless) distance from the center of the pellet ($t = 0$) to the mouth ($t = 1$), Φ is the Thiele modulus which measures the effect of diffusion as opposed to reaction, and $R(y)$ is the reaction rate term. In particular, Φ^2 is proportional to $\frac{k}{D}$, where D is the diffusion coefficient and k the reaction rate constant.

3. **Steady state flow** [28]. The steady-state flow pattern arising from the injection of a gas at supersonic velocity into a duct of uniform or diverging cross-sectional area when a back pressure is applied. Complications such as the effect of viscous stresses on the duct walls is neglected, and the gas is assumed to be perfect and polytrophic. The time-independent laws of conservation of mass, momentum and energy can be expressed in the following dimensionless form by referring all quantities to appropriate lengths, physical constants and upstream conditions:

$$\frac{dy}{dx(\rho y A)} = 0,$$

$$y\frac{dy}{dx} + (\gamma\rho)^{-1}\frac{d}{dx}(\rho T) = \mu\rho^{-1}\frac{d^2 y}{dx^2},$$

and

$$y\frac{dT}{dx} + (\gamma - 1)T\left[\frac{dy}{dx} + y\frac{d}{dx}(\ln A)\right] - \gamma(\gamma - 1)\frac{\mu}{\rho}\left(\frac{dy}{dx}\right)^2 = \frac{\mu\gamma}{\rho p_r}\frac{d^2 T}{dx^2}.$$

Here x is the dimensionless distance measured from the entrance of the duct, y is the dimensionless velocity of the gas relative to the velocity of sound, ρ is the density, γ is the adiabatic index with a value between 1 and $\frac{5}{3}$, T is the dimensionless cross-sectional area of the duct relative to the area of the duct entrance.

7

4. **Catalytic reaction** [92]. A fixed-bed reactor packed with catalyst in the presence of axial diffusion. The boundary-value problem for the dimensionless concentration γ is then

$$\varepsilon y'' = y' + g(y), \ 0 < x < 1$$

with

$$y(0, \varepsilon) - p_1 y'(0, \varepsilon) = A, \ \ y(1, \varepsilon) = p_2 y'(1, \varepsilon) = B,$$

where x is the dimensionless axial coordinate, ε is the reciprocal of the Peclet number (the diffusional analogy of the Reynolds number), and g is the reaction rate term, of the form $g(y) = y^n$ for an n-th order reaction. The positive terms $p_1 = p_1(\varepsilon)$ and $p_2 = p_2(\varepsilon)$ are mass transport coefficients. If the axial diffusion is weak then ε is small, and the Robin problem is singularly perturbed.

5. **Chemical reaction** [115]. The model

$$\varepsilon y'' = \varepsilon \Theta (1 + \Theta \gamma)^{-1} y'^2 + y^r (1 + \Theta y), \ \ 0 < t < 1,$$

with

$$-y(0, \varepsilon) = 0, \ \ y(1, \varepsilon) + \sum y'(1, \varepsilon) = 1,$$

describes a chemical reaction accompanied by a change in volume [115]. (Note that $\sum$ is the reciprocal of the Sherwood number and not the usual summation notation). More precisely, y represents the dimensionless concentration of a gas A undergoing an isothermal reaction on a flat plate catalytic surface, namely $A \to Bn$. The variable t is the normalized distance from a plane of symmetry to the edge of the reaction. As before, the parameter ε is the reciprocal of the square of the Thiele modulus, and the parameter $\theta \approx n - 1$ is the volume change modulus. For simplicity, the reaction is assumed to be of integral order $l \geq 1$.

8

Some other interesting models can be found in [26].

It should be noted that the methods presented in forthcoming chapters can be experimented for above models after some suitable modifications.

1.5 Literature

For the sake of simplicity, we broadly classify the literature (in the past few years) as the articles based on asymptotic methods and those based on numerical methods. The works are presented chronologically.

1.5.1 Research Works Consisting of Asymptotic Approaches

In this sub-section we list the works which contain one or more than one type of asymptotic approaches.

Using perturbation analysis, Fitt et al. [41] discussed the propagation of a one-dimensional, fluid-filled crack in a hot dry rock geothermal energy reservoir. The model contains a dimensionless parameter that measures the relative importance of the stresses due to local deformation of asperities and the long-range deformation of the crack surface. They found that for some combinations of laws a strained-coordinate analysis is required, whilst for others a matched asymptotic approach is needed.

Happawana et al. [51] established a closed form asymptotically valid solution for the non-similar normal modes for the strongly non-linear discrete system. The equation governing the existence of the non-linear normal mode for the system is singular at the boundaries and depends on a small mistuning parameter. The singularity in the sequence of linear problems obtained for an asymptotic approximation of the solution satisfies conditions for linear differential equations with regular points. Thus,

9

the series equations methodology for linear differential equations with regular singular points to solve the non-linear problem is implemented.

Bouyekhf [21] dealt with the singular perturbations theory for discrete-time non-linear systems. In the first part of the paper a foundation of the method is presented and the proof of the approximations is established. The second part is concerned with an asymptotic expansion for the solution in terms of an outer expansion and a boundary layer correction. The perturbation method is justified by showing that it is equivalent to finding the Taylor expansions of the slow and fast solutions in the decomposition of the solution of the whole system.

Fu and Chen [42], studied the two-point boundary-value optimal problem of a class of non-linear singularly perturbed systems, and gave asymptotic analysis of this class of non-linear systems under composite control, which is the sum of a reduced optimal control, a left boundary layer stabilizing control and a right boundary layer stabilizing control. They showed that the application of composite control results in a final state that is close to the desired state, and in a value of the cost that is close to the optimal cost of the reduced problem. The mid-course guidance system of air-to-ground missiles was used as a numerical example. The results of simulations are in good agreement with those for optimal control.

Shi [98] studied the singular perturbations for the higher-order non-linear vector differential equation. They discussed the construction of the formal asymptotic solution for the problem, based on the O'Malley construction and obtained a uniformly valid approximation.

Weili [117] studied radially symmetric solutions for Poisson equation as the background and discussed the existence, uniqueness and asymptotic estimates of solutions of the singularly perturbed Robin problem for the general non-linear second-order

10

ordinary differential equation with a small positive parameter.

Yan [120] considered singularly perturbed non-linear differential algebraic equations (DAE's), which are decomposed into two auxiliary problems, called the outer and inner problems, respectively. The structure of solutions of the singularity perturbed DAE's is determined by the outer and inner solutions, both of which are proved to exist. Asymptotic expansions for outer and inner solutions are obtained and proved to be uniformly convergent.

Kang [62] used the modified method of multiple scales, to investigate the non-linear bending of a truncated shallow spherical shell of variable thickness without an indeformable rigid body at the center under linear distributed loads along the interior edge. When the geometrical parameter k is larger, the uniformly valid asymptotic solutions of this problem are obtained and the remainder terms are estimated.

Zhou et al. [123], discussed the singular perturbation of non-linear differential equation system with non-linear boundary conditions. Under suitable assumptions, with the asymptotic method of Lyusternik-Vishik and fixed point theory, the existence of the solution of the perturbation problem was proved and its valid asymptotic expansion of higher order was derived.

Belolipetskij [11] studied the problem of cooling a thin-wall sphere filled by a gas for the case of the external heat conducting medium. The mathematical model of this process is the non-linear initial problem for the singular perturbed semilinear equation of thermal conductivity. The analytical dependence of the cooling time on problem parameters is obtained by asymptotic methods.

Evkin and Kalamkarov [39], applied the singular perturbation method in combination with the variational method to the general Reissner's equations describing axially symmetric large deflections of thin composite shells of revolution with varying

11

material and geometrical parameters in meridian direction. The obtained asymptotic non-linear boundary-value problem is significantly simpler in comparison with the original one. The asymptotic model has the following advantages: Number of the geometrical and stiffness parameters of shell is effectively reduced, and singularities are eliminated without loss of the accuracy of the solution. The simple asymptotic formulae have been derived in case of completed shells.

Garbey [45] presented several applications of (local) Fourier basis combined with corrector techniques via the superposition principle to compute solutions of boundary-value problems. Their methodology is inspired by the well-known corrector technique used in asymptotic singular perturbation theory, see, for example, [36]. They built solvers for time dependent boundary-value problems and singular perturbation problems using Fourier expansions combined to additional convenient set of time independent basis functions to enforce the boundary conditions. The algorithms are very well suited for parallel computing because they rely mainly on FFTs and basis functions given analytically or computed (in parallel) once and for all.

Van Horssen [108] presented a perturbation method based on integrating vectors and multiple scales for singularly perturbed systems of ordinary differential equations. It was shown how asymptotic approximations for first integrals for such systems can be constructed on long time-scales. To show how this perturbation method actually works, the method was applied to a linear spring-mass system, to a first order linear ordinary differential equation, and to a non-linear spring-mass system.

Wang and Jin [113], studied a third order singularly perturbed boundary-value problem by means of differential inequality theories. Based on the given results of second order non-linear boundary-value problem, the upper and lower solutions method of third order non-linear boundary-value problems was established by making use of

12

Volterra type integral operator. Specific upper and lower solutions were constructed, and existence and asymptotic estimates of solutions under suitable conditions were obtained. The result shows that it seems to be new to apply these techniques to solving these kinds of third order singularly perturbed boundary-value problem. An example was given to demonstrate the applications.

Djennoune and Bettayeb [32] investigated a balancing method for a class of non-linear singularly perturbed systems. The main result presented there shows that the well-known 'two-stages' strategy used with singular perturbations in control theory can be extended to compute a balancing form of non-linear singularly perturbed systems.

Gaitsgory and Nguyen [43], developed an averaging technique for non-linear multi-scale singularly perturbed control systems. Issues concerning the existence and structure of limit occupational measures sets generated by such systems are discussed. General results are illustrated with special cases.

1.5.2 Research Works Consisting of Numerical Approaches

In this sub-section we list the works which contain one or more than one type of numerical approaches.

In [40], Ezzine and Ben-Daya explored the continuous realizations of iterative processes emanating from interior point optimization algorithms, and their connection with non-linear singularly-perturbed ordinary differential equations. This mathematical connection provides a theoretical framework for the analysis of the dynamical properties long known and exploited in interior point-based optimization techniques. In addition, this connection is used to show that the logarithmic barrier function is indeed, in some sense, optimum.

13

Taiwo [102] presented a parameter expansion method for two-point non-linear singularly perturbed boundary-value problem for second order ordinary differential equation. Newton's linearization scheme is used to linearize the non-linear problems. In Okoro et al. (Ref.[1] in the above paper) linear problems were treated. The numerical results obtained for some examples show that the parameter expansion becomes more accurate as the value of epsilon approaches zero when compared with the standard collocation method, at no extra computational effort. For favourable problems to exponential fitting reported in Ref.[2] in [102], the proposed method in this paper is less accurate. It is however more general in application than the exponential fitting.

Pan et al. [86] investigated the stabilization problem of two classes of non-linear singularly perturbed systems via dynamic output feedback. Firstly, they consider the non-linear singularly perturbed systems in which the non-linearities are continuously differentiable. Secondly, they examined the non-linear singularly perturbed systems in which the non-linearities are not necessarily continuously differentiable but satisfy the global Lipschitz condition. Combining the dynamic output feedback controller that stabilizes the reduced-order model of the linear part of the non-linear singularly perturbed system with the quasi-stability result of Persidskii, they proposed a two-step compensating scheme to stabilize the original non-linear singularly perturbed system under consideration for a sufficiently small ε.

Bouyekhf and Moudni [21] introduced a model of singular perturbation for discrete-time non-linear systems. This paper is aimed at validating the proposed model. In fact, a discrete version of the well-known Tikhonov's theorem on singular perturbation of continuous-time systems is established. The second aim is to study stability problems of such systems. Sufficient conditions for both asymptotic and exponential

14

stability are obtained. As a result, significant order reduction of stability problems is achieved. This is achieved by allowing a small parameter whose upper bound is estimated. Finally a simple example is given to illustrate the applications of the results.

Huang [56] dealt with the boundary-value problem for second order singularly perturbed non-linear system by the technique and method of diagonalization. The existence of the solution and its asymptotic properties were discussed for some special cases.

Bagagiolo and Bardi [8] studied the singular perturbation of optimal control problems for non-linear systems with constraints on the fast state variables and a cost functional either of Bolza type or involving the exit time of the system from a given domain. Under a controllability assumption on the fast variables, they show that these variables become controls in the limit problem. Their method consists of passing to the limit in the associated Hamilton-Jacobi-Bellman (HJB) equations by means of some tools in the theory of viscosity solutions.

Bouyekhf and Moudni [22] treated a class of discrete-time non-linear systems which have two-time-scales. Using the singular perturbation theory in a systematic way, they presented a mode-decoupling approach which yields two separate subsystems containing the slow and fast parts. Furthermore, they presented a two-time-scale analysis and design procedure for stabilization and regulation.

Budd et al. [20] studied the effect of using grid adaptation on the numerical solution of model convection-diffusion equations with a conservation form. The grid adaptation technique studied is based on moving a fixed number of mesh points to equidistribute a generalization of the arc-length of the solution. In particular, a parameter-dependent monitor function is introduced which incorporates fixed meshes,

15

approximate arc-length equidistribution, and equidistribution of the absolute value of the solution, in a single framework. Thus the resulting numerical method is a coupled non-linear system of equations for the mesh spacings and the nodal values.

Djennoune et al. [31] investigated digital implementation of continuous-time composite control feedback for a class of non-linear singularly perturbed systems. Although starting with a stabilizing control feedback, the sampling process may destroy the stability properties of the resulting closed-loop system. In this paper, multi-rate measurements (slow variables are measured at a rate slower than that of fast variables) are considered. Sufficient conditions on the slow and fast sampling periods, which preserve exponential stability properties, are established.

Kanzawa and Oishi [63] defined a new concept of an imperfect singular solution as an approximate solution which becomes a singular solution by adding a suitable small perturbation to the original equations. A numerical method is presented for proving the existence of imperfect singular solutions of non-linear equations with guaranteed accuracy. A few numerical examples are also presented for illustration.

Liu and Pan [73], extended Ortiz and Samara's operational approach to the Tau Method to the numerical solution of systems of linear and non-linear ordinary differential equations (ODEs), together with initial or boundary conditions. They lead to accurate results through the use of simple algorithms. A Tau software called TAUSYS3 for mixed-order systems of ODEs was written based on this approach. In this paper they gave a brief description of the Tau Method, the structure of the Tau program, and the testing of the TAUSYS3. They considered several examples and report results of high accuracy. These include linear and non-linear, stiff and singular perturbation problems for ordinary and systems of ordinary differential equations in which the solution may not be unique.

16

Bensassi et al. [12] investigated the problem of constructing the discretized and decomposed system for a singularly perturbed non-linear continuous-time system. Thus, they use two schemes namely decomposition-discretization and discretization-decomposition. By using two discretization methods inspired from Euler's methodology they illustrate the decomposition of system by means of two periods (fast and slow), and a method for the choice of these periods is given. The comparison of the obtained subsystems from each scheme leads them to propose two different designs of multi-rate digital controls.

Grammel and Shi [48], investigated the problem of asymptotics of Lyapunov exponents for a class of singularly perturbed non-linear systems. They defined the maximal and minimal Lyapunov exponents for the underlying systems and show, via an averaging technique, that under certain conditions, the extremal Lyapunov exponents of the original system converge to the extremal Lyapunov exponents of the averaged slow subsystem when the singular perturbation parameter tends to zero. For low-dimensional systems, the existence of Lipschitz, continuous composite state feedbacks, which asymptotically provide the minimal Lyapunov exponents, can be shown. An example is given to illustrate the potential of the proposed technique and show that the designed controller is robust for sufficiently small perturbations.

Tuan and Hosoe [106], proposed a direct approach to the Lur'e problem for singularly perturbed systems (SPS). In contrast to previous results, the feedback connection between the linear and non-linear parts of SPS is allowed to depend essentially on both the slow and the fast variables. The Lur'e problem for multi-parameter SPS (MSPS) is studied by the same framework.

Bouyekhf et al. [16] studied a class of discrete-time non-linear systems which depend on a small parameter. Using the singular perturbation theory in a systematic

17

way, they gave a trajectory approximation result based on the decomposition of the model into reduced and boundary layer models. This decomposition is used to analyze optimal control via maximum principle of such systems. As a result, significant order reduction of optimal control problems is achieved.

Suzuki [101] studied singular perturbation problem for non-linear difference equations with a small parameter. He considered analytic solutions for the systems and apply the theorem of boundary layer corrections for singular perturbation problem for differential equations to the difference systems.

Van Horssen [108] developed a perturbation method based on integrating vectors for initial value problems for regularly and singularly perturbed, weakly non-linear ordinary differential equations. In this paper they gave an overview of earlier results and discussed the possibilities to apply this perturbation method to other problems.

Wang and Hu [112], presented a new approach, based on the center manifold theorem, to reducing the dimension of non-linear time-delay systems composed of both stiff and soft substructures. To complete the reduction process, the dynamic equation of a delayed system is first formulated as a set of singularly perturbed equations that exhibit dynamic behavior evolving in two different time scales.

Assawinchaichote and Nguang [6], considered the problem of designing a fuzzy observer-based controller for a class of non-linear singularly perturbed systems described by Takagi-Sugeno-Kang (TSK) fuzzy model. Fast and slow decomposition approach is utilized to derive a fuzzy observer-based controller which stabilizes this class of singularly perturbed non-linear systems.

Cakir and Amiraliyev [25], presented a singularly perturbed boundary-value problem with nonlocal conditions. The appropriate solution exhibits boundary layer behavior for small positive values of the perturbation parameter. An exponentially

18

fitted finite difference scheme on a non-equidistant mesh is constructed for solving this problem. The uniform convergence analysis in small parameter is given.

Kadalbajoo and Patidar [59, 60] used "spline in tension" and "spline in compression" to solve singularly perturbed non-linear two point boundary-value problems.

Kelley [66] discussed the problem of computing approximations of solutions of singularly perturbed two-point boundary-value problems which possesses the square of the first derivative. It was assumed that the quadratic term was a full participant in the differential equation. The analysis showed the use of method of super and subsolutions to verify the approximations which gave unified approach to the analysis of quadratic, quasilinear and semilinear problems.

Boglaev [17] dealt with discrete monotone iterative algorithms for solving a non-linear singularly perturbed parabolic reaction-diffusion problem. Firstly, the monotone method (known as the method of lower and upper solutions) is applied to computing a non-linear difference scheme obtained after discretization of the continuous problem. Secondly, a monotone domain decomposition algorithm based on a modification of the Schwartz alternating method is constructed. This monotone algorithm solves only linear discrete systems at each iterative step of the iterative process. The rate of convergence of the monotone domain decomposition algorithm is estimated. Numerical experiments are presented.

Bykov et al. [24] considered the problem of a pressure-driven flame in an inert porous medium filled with a flammable gaseous mixture. In the frame of reference attached to an advancing combustion wave and after a suitable non-dimensionalization the corresponding mathematical description of the problem includes three highly non-linear ordinary differential equations. The system is rewritten in the form of a singularly perturbed system of ordinary differential equations and is analyzed analytically

19

by the geometrical version of the asymptotic method of integral manifolds. They also provide some numerical results validating the theoretical outcomes.

Jorge and Bujanda [58], presented their new methods to integrate efficiently reaction-diffusion parabolic problems with non-linear reaction terms. In order to obtain uniform and unconditional convergence, such methods combine the advantages of alternating direction methods, the additive Runge-Kutta methods designed by Cooper and Sayfy for non-linear stiff problems as well as the use of Shishkin meshes in the singularly perturbed case. The resulting algorithms are only linearly implicit and they have the same order of computational complexity, per time step, that any explicit method has. They show some numerical experiences which illustrate the good properties of their schemes predicted by the theoretical results.

Kopteva and Stynes [69], considered a non-linear reaction-diffusion two-point boundary-value problem with multiple solutions. Its second-order derivative is multiplied by a small positive parameter epsilon, which induces boundary layers. Using dynamical systems techniques, asymptotic properties of its discrete sub- and super-solutions are derived. These properties are used to investigate the accuracy of solutions of a standard three-point difference scheme on layer-adapted meshes of Bakhvalov and Shishkin types.

Wang [114] presented a boundary-value method for solving a class of non-linear, singularly perturbed two-point boundary-value problems with a boundary layer at the left of the underlying interval. This method is based on ideas of singular perturbation analysis by constructing a modified problem with a boundary layer correction. He dealt with the boundary layer separately, and used a series method. The condition at infinity is applied to the corresponding Padé approximates of the obtained series solution.

20

Boglaev [15] dealt with discrete monotone iterative algorithms for solving a non-linear singularly perturbed convection-diffusion problem. A block monotone domain decomposition algorithm based on a Schwartz alternating method and on block iterative scheme is constructed. This monotone algorithm solves only linear discrete systems at each iterative step of the iterative process and converges monotonically to the exact solution of the non-linear problem. He also estimated the rate of convergence of the block monotone domain decomposition algorithm.

The other interesting articles which the readers may find interesting are [27, 29, 61, 64, 70, 80, 97].

1.6   Scope of this Thesis

It is also evident that the works under asymptotic methods are less compared to those of the numerical methods. This is due to the fact that a lot of difficulties arise in developing asymptotic solutions. No matter how complicated the process becomes, the resulting solution is mostly a qualitative one. It is only semi-quantitative and that is what necessitates the appropriate numerical methods. However, these asymptotic approaches are still of great importance because the little information which one can gather about the qualitative features of the solutions helps a lot in the construction of sophisticated numerical softwares. To this end, we provide details on how to develop asymptotic analysis for particular problems in Chapter 2, and thus in Chapter 4, we design and experiment a novel numerical method whereas some theoretical results are presented in Chapter 3. To extend our ideas and approaches, we solve another problem in Chapter 5 which arise in enzyme kinetics where again the essential qualitative information is obtained via asymptotic analysis and then reliable

21

numerical methods are devised. Finally we conclude the contents and main outcomes in this thesis in Chapter 6 where we also indicate our future research plans.

1.7 Summary

We have explained in this chapter, what is meant by a non-linear singular perturbation problem and presented some models governing non-linear singularly perturbed phenomena from the literature. Then a literature review is provided where we considered the works based on both the asymptotic and the numerical approaches for their solution.

Based on the survey of the research works in recent years, it is clear that non-linear SPPs are part and parcel of most of the real life problems. Such non-linear SPPs are solved as part of many simulations of physical processes. The scope of this thesis is also indicated in this chapter.
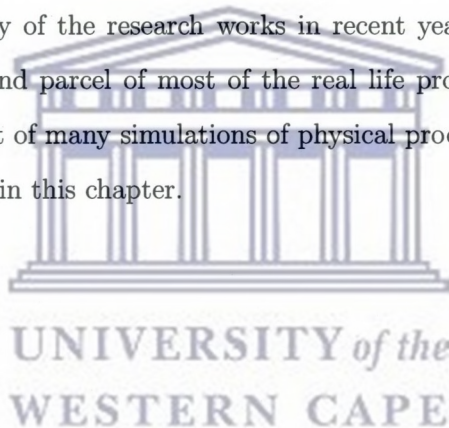
Chapter 2

Asymptotic Analysis for a Model Problem

In this chapter we discuss the importance of the asymptotic analysis by considering a particular non-linear singular perturbation problem. We provide necessary details for this problem. However, an extensive amount of work (involving asymptotic analysis) can be found in [82].

The asymptotic analysis

- provides qualitative information about the solution

- provides way(s) to determine the location of the layer(s)

- helps us to determine the width of the layer(s).

To explain the procedure, we consider the following singularly perturbed non-linear two-point boundary-value problem

$$\varepsilon y'' + yy' - xy = 0, \tag{2.1}$$

$$y(0) = \alpha \text{ and } y(1) = \beta, \tag{2.2}$$

where $0 < \varepsilon << 1$, and α, β are real numbers independent of ε.

Since ε is multiplied to the highest derivative term, boundary layer(s) is (are) expected. However, the location of the layer depends on the sign of the coefficient y of y'. But y is a function of its values α and β at the boundaries, therefore the location of the layer(s) depends(s) on the values of α and β.

2.1 Construction of the Outer Solution

We construct the outer solution y^0 by using asymptotic expansions,

$$y_{as} := y(x, \varepsilon) = \sum_{j=0}^{k} \varepsilon^j y_j(x), \tag{2.3}$$

where $k \in \mathbb{Z}^+$.

Plugging (2.3) into the equation (2.1) and in the boundary conditions (2.2), we obtained the following (when $k = 1$)

$$\varepsilon \frac{d^2}{dx^2} \left(\sum_{j=0}^{1} \varepsilon^j y_j(x) \right) + \sum_{j=0}^{1} \varepsilon^j y_j(x) \frac{d}{dx} \left(\sum_{j=0}^{1} \varepsilon^j y_j(x) \right) - x \sum_{j=0}^{1} \varepsilon^j y_j(x) = 0$$

with

$$\sum_{j=0}^{1} \varepsilon^j y_j(0) = \alpha \text{ and } \sum_{j=0}^{1} \varepsilon^j y_j(1) = \beta. \tag{2.4}$$

Further simplifications yield

$$\varepsilon[\varepsilon^0 y_0''(x) + \varepsilon y_1''(x)] + [\varepsilon^0 y_0(x) + \varepsilon y_1(x)][\varepsilon^0 y_0'(x) + \varepsilon y_1'(x)] - x[\varepsilon^0 y_0(x) + \varepsilon y_1(x)] = 0$$

and

$$\varepsilon^0 y_0(0) + \varepsilon y_1(0) = \alpha \text{ and } \varepsilon^0 y_0(1) + \varepsilon y_1(1) = \beta. \tag{2.5}$$

24

Now we equate the coefficients of like powers of ε.

Coefficients of ε^0:

$$y_0(x)y_0'(x) - xy_0(x) = 0 \qquad (2.6)$$
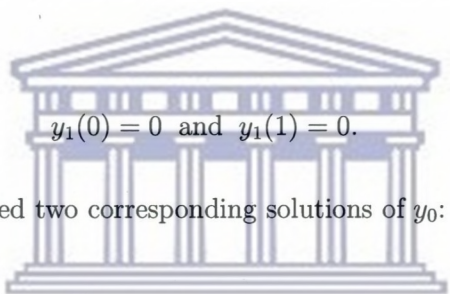
and

$$y_0(0) = \alpha \ \text{ and } \ y_0(1) = \beta. \qquad (2.7)$$

Coefficients of ε^1:

$$y_0''(x) + y_0'(x)y_1(x) + y_0(x)y_1'(x) - xy_1(x) = 0 \qquad (2.8)$$

and

$$y_1(0) = 0 \ \text{ and } \ y_1(1) = 0. \qquad (2.9)$$

Solving (2.6) we obtained two corresponding solutions of y_0:

$$y_0(x) = 0 \qquad (2.10)$$

and

$$y_0(x) = \frac{x^2}{2} + c_0. \qquad (2.11)$$

We see that (2.10) does not satisfy the general boundary conditions and therefore it must be dropped.

Imposing the associated boundary conditions on the second solution we obtained

$$y_0(x) = \frac{x^2}{2} + \alpha \qquad (2.12)$$

25

and

$$y_0(x) = \frac{x^2}{2} + \beta - \frac{1}{2}.$$ (2.13)

Coefficients of ε^1:

$$y_0''(x) + y_0'(x)y_1(x) + y_0(x)y_1'(x) - xy_1(x) = 0$$ (2.14)

Using (2.12) into (2.14) we find

$$y_1'(x) = -\frac{2}{x^2 + 2x}.$$ (2.15)

Integrating equation (2.15) we obtain

$$y_1(x) = \begin{cases} \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{x + \sqrt{-2\alpha}}{x - \sqrt{-2\alpha}} \right| + c_1 & \text{if } \alpha < 0 \\ -\frac{2}{x} + c_1 & \text{if } \alpha = 0 \\ -\frac{1}{\alpha} \left[\arctan \left(\frac{x}{\sqrt{2\alpha}} \right) + c_1 \right] & \text{if } \alpha > 0 \end{cases}$$ (2.16)

where c_1 is a real constant. Imposing the associated boundary condition on (2.16) we find at $x = 0$

$$c_1 = \begin{cases} 0 & \text{if } \alpha < 0 \\ \text{undefined} & \text{if } \alpha = 0 \\ 0 & \text{if } \alpha > 0 \end{cases}$$ (2.17)

and at $x = 1$

$$c_1 = \begin{cases} \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{1 + \sqrt{-2\alpha}}{1 - \sqrt{-2\alpha}} \right| & \text{if } \alpha < 0 \\ 2 & \text{if } \alpha = 0 \\ -\frac{1}{\alpha} \left[\arctan \left(\frac{1}{\sqrt{2\alpha}} \right) \right] & \text{if } \alpha > 0. \end{cases}$$ (2.18)

26

Hence

$$y_1(x) = \begin{cases} \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{x+\sqrt{-2\alpha}}{x-\sqrt{-2\alpha}} \right| & \text{if } \alpha < 0 \\ -\frac{1}{\alpha} \arctan \left(\frac{x}{\sqrt{2\alpha}} \right) & \text{if } \alpha > 0 \end{cases} \tag{2.19}$$

and

$$y_1(x) = \begin{cases} \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{x+\sqrt{-2\alpha}}{x-\sqrt{-2\alpha}} \right| - \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{1+\sqrt{-2\alpha}}{1-\sqrt{-2\alpha}} \right| & \text{if } \alpha < 0 \\ 2 & \text{if } \alpha = 0 \\ -\frac{1}{\alpha} \left[\arctan \left(\frac{x}{\sqrt{2\alpha}} \right) \right] + \frac{1}{\alpha} \arctan \left(\frac{1}{\sqrt{2\alpha}} \right) & \text{if } \alpha > 0. \end{cases} \tag{2.20}$$

Equation (2.20) does not satisfy the left end boundary condition whereas equation (2.19) does satisfy the left end boundary condition. Therefore equation (2.20) must be discarded.

Hence the corresponding outer solution is given by

$$y^0(x) = \frac{x^2}{2} + \alpha + \varepsilon \begin{cases} \frac{1}{\sqrt{-2\alpha}} \ln \left| \frac{x+\sqrt{-2\alpha}}{x-\sqrt{-2\alpha}} \right| & \text{if } \alpha < 0 \\ -\frac{1}{\alpha} \arctan \left(\frac{x}{\sqrt{2\alpha}} \right) & \text{if } \alpha > 0. \end{cases} \tag{2.21}$$

The outer solution y^0 given by (2.21) may be referred as the left outer solution of problem (2.1).

Similarly using (2.13) into (2.14) we find

$$y_1'(x) = -\frac{2}{x^2 + 2\beta - 1}. \tag{2.22}$$

Following the same technique as in the case of the left outer solution we find that the outer solution in this case is given by

$$y^0(x) = \frac{x^2}{2} + \beta - \frac{1}{2} + \varepsilon \begin{cases} \frac{1}{\sqrt{-(2\beta-1)}} \ln \left| \frac{x+\sqrt{-(2\beta-1)}}{x-\sqrt{-(2\beta-1)}} \right| & \text{if } (2\beta - 1) < 0 \\ -\frac{2}{(2\beta-1)} \arctan \left(\frac{x}{\sqrt{(2\beta-1)}} \right) & \text{if } (2\beta - 1) > 0 \end{cases} \tag{2.23}$$

27

which may be referred as the right outer solution of problem (2.1).

2.2 Prediction of the Boundary Layer

The fact that (2.21) does satisfy the left end boundary condition and does not satisfy the right end boundary condition we denote it by y^l. Similarly we denote the solution in (2.23) by y^r.

If $\alpha = \beta - \frac{1}{2}$, we obtained $\varepsilon = 0$, which violates the condition imposed on ε. Therefore when $\alpha = \beta - \frac{1}{2}$ the corresponding solution must be discarded. When $\alpha \neq \beta - \frac{1}{2}$, y^r is not valid near $x = 0$ and y^l is not valid near $x = 1$, therefore y^r predicts the existence of a boundary layer near the left end boundary condition, whereas y^l predicts the existence of a boundary layer near the right end boundary condition.

2.3 Width of the Layer

To obtain the width of a boundary layer, we investigate the behaviour of the solution y in the boundary layer region and look for the matchable inner solution with the respective constructed outer solution, therefore we introduce the stretching transformations

$$\xi = \frac{x - x_b}{\varepsilon^\nu} \text{ and } y^i = \frac{y(x, \varepsilon)}{\varepsilon^\lambda}$$

where $\nu > 0$, x_b denotes the transition point, (which is not known a priori) and λ is a real number. Substituting the stretching transformations into the main differential

28

equation problem we find

$$\varepsilon^{1-2\nu+\lambda}\frac{d^2y^i}{d\xi^2} + \varepsilon^{2\lambda-\nu}\frac{dy^i}{d\xi} - \varepsilon^{\nu+\lambda}y^i = 0.$$

If $\lambda = 0$ and using the technique of finding the matchable inner solution y^i with either outer solution, we find that $\nu = 1$ is the distinguished limit corresponding to the limiting part

$$\frac{d^2y^i}{d\xi^2} + y^i\frac{dy^i}{d\xi} = 0.$$

Similarly, when $\lambda \neq 0$, and using the same technique we find the corresponding dominant part

$$\frac{d^2y^i}{d\xi^2} + y^i\frac{dy^i}{d\xi} - y^i = 0$$

has the distinguished limit $\nu = \frac{1}{3}$. In view of the technique of matching principles, the distinguished limit thus obtained predict the width of the layer(s)

$$\delta = \begin{cases} O(\varepsilon^1) & \text{if } \lambda = 0 \\ O(\varepsilon^{\frac{1}{3}}) & \text{if } \lambda \neq 0. \end{cases}$$

Moreover if $\lambda \neq 0$, the limiting part is the same as (2.1). Therefore no simplification is achieved by carrying out the expansion. Hence the width of the layer corresponding to $\lambda \neq 0$ must be discarded. Therefore if the layer is near $x = 0$ or near $x = 1$, the width of the such a layer is $\delta = O(\varepsilon)$.

2.4 Summary

In this chapter, we have done necessary asymptotic analysis for a model problem and predicted the location and width of the layer. This information will be useful in constructing an appropriate mesh which is carried out in the next chapter. It should

29

be noted that the aim of this chapter is to provide necessary information about the qualitative behaviour of the solution. Not only that we are not interested in the asymptotic solution of the problem under consideration, it is indeed difficult to find that. This is due to the fact that one again requires to solve non-linear equations while considering coefficients of various powers of ε.

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Chapter 3

Results on the Existence and Uniqueness of the Solution

In this chapter we provide some results first for a quasilinear SPP and then for a general non-linear SPP. Part of the work contained in this chapter is borrowed from [35] where the detailed proofs of some of these results can be found.

3.1 Some Theoretical Results

Consider the homogeneous problem

$$\varepsilon y'' + yy' - y = 0, \ \ 0 < x < 1,$$

$$(3.1)$$

$$y(0) = A(\varepsilon), \ \ y(1) = B(\varepsilon).$$

Lemma 3.1. *Let $y(x, \varepsilon)$ be a solution of (3.1). Then*

$$\min(A(\varepsilon), B(\varepsilon) - 1) \leq y(x, \varepsilon) - x \leq \max(A(\varepsilon), B(\varepsilon) - 1). \qquad (3.2)$$

31

Moreover, if

$$A(\varepsilon) \geq B(\varepsilon) - 1,\tag{3.3}$$
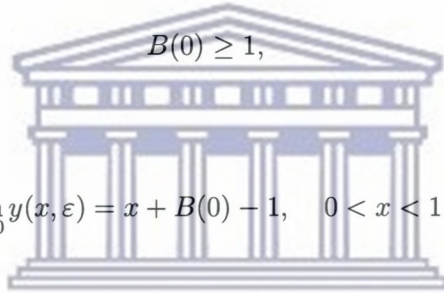
then $y(x, \varepsilon)$ is the unique solution of (3.1).

Proof. See [35].

Theorem 3.2. *Suppose $y(x, \varepsilon)$ is a solution of (3.1) and*

$$A(\varepsilon) \leq 0, \qquad B(0) > 0.\tag{3.4}$$

If

$$B(0) \geq 1,\tag{3.5}$$

then

$$\lim_{\varepsilon \to 0} y(x, \varepsilon) = x + B(0) - 1, \quad 0 < x < 1.\tag{3.6}$$

If

$$0 < B(0) < 1,\tag{3.7}$$

then

$$\lim_{\varepsilon \to 0} y(x, \varepsilon) = \begin{cases} 0, & 0 < x \leq 1 - B(0), \\ x + B(0) - 1, & 1 - B(0) \leq x \leq 1. \end{cases}\tag{3.8}$$

Proof. See [35].

Corollary 3.1. *Suppose*

$$A(0) < 0, \quad B(\varepsilon) \leq 0.$$

32

If

$$A(0) \leq -1, \tag{3.9}$$

then

$$\lim_{\varepsilon \to 0^+} y(x, \varepsilon) = A(0) + x. \tag{3.10}$$

If

$$-1 < A(0) < 0, \tag{3.11}$$

then

$$\lim_{\varepsilon \to 0^+} y(x, \varepsilon) = \begin{cases} A(0) + x, & 0 \leq x \leq -A(0), \\ 0, & -A(0) \leq x < 1. \end{cases} \tag{3.12}$$

Proof. See [35].

Lemma 3.3. *Let $y(x, \varepsilon)$ be a solution of (3.1). Suppose*

$$A(\varepsilon) < 0 < B(\varepsilon). \tag{3.13}$$

Then there is a unique point $C = C(\varepsilon)$ such that

$$y(C, \varepsilon) = 0. \tag{3.14}$$

Moreover, if

$$B(\varepsilon) - A(\varepsilon) < 1, \tag{3.15}$$

then

$$0 < y'(x, \varepsilon) \leq 1, \quad 0 \leq x \leq 1. \tag{3.16}$$

33

If

$$B(\varepsilon) - A(\varepsilon) > 1, \tag{3.17}$$

then

$$y'(x, \varepsilon) \geq 1, \quad 0 \leq x \leq 1. \tag{3.18}$$

Proof. See [35].

Remark 3.4. *If* $B(\varepsilon) - A(\varepsilon) = 1$, *then*

$$y(x, \varepsilon) = A(\varepsilon) + x$$

is the unique solution of (3.1).

Theorem 3.5. *Suppose there is an* $\varepsilon_0 > 0$ *such that (3.13) and (3.15) hold for* $0 < \varepsilon \leq \varepsilon_0$. *Let* $y(x, \varepsilon)$ *be a solution of (3.1). Then*

$$\lim_{\varepsilon_n \to 0+} y(x, \varepsilon_n) = \begin{cases} A(0) + x, & 0 \leq x \leq |A(0)|, \\ 0, & |A(0)| \leq x \leq 1 - B(0), \\ B(0) - 1 + x, & 1 - B(0) \leq x \leq 1. \end{cases} \tag{3.19}$$

Proof. See [35].

The quasilinear equations considered above are linear in y'. In [50] Haber and Levinson (see [84] also) considered the general non-linear equation

$$\varepsilon y'' = f(x, y, y', \varepsilon), \quad 0 < x < 1,$$

$$\tag{3.20}$$

$$y(0) = A, \quad y(1) = B,$$

34

where the "reduced" problem

$$f(x, Y(x), Y'(x), 0) = 0, \quad 0 < x < 1,$$

(3.21)

$$y(0) = A, \quad y(1) = B$$

has an "angular solution"

$$Y(x) = \begin{cases} Y'_L(x), & 0 \le x \le x_0, \\ Y'_R(x), & x_0 \le x \le 1, \end{cases}$$

with

$$Y_L(x_0) = Y_R(x_0), \quad Y'_L(x_0) \ne Y'_R(x_0).$$

Theorem 3.6. [50] *Suppose*

$$\mu_1 = Y'_L(x_0) < Y'_R(x_0) = \mu_2$$

$$f_{y'}(x, Y_L(x), Y'_L(x), 0) \ge k_1 > 0, \quad 0 \le x \le x_0,$$

$$f_{y'}(x, Y_R(x), Y'_R(x), 0) \le -k_2 < 0, \quad x_0 \le x \le 1,$$

and

$$f(x_0, Y_L(x_0), \omega, 0) > 0, \quad \mu_1 < \omega < \mu_2.$$

Then, for ε sufficiently small, there exists a solution $y(x, \varepsilon)$ of the boundary-value problem (3.20) such that

$$\lim_{\varepsilon \to 0} y(x, \varepsilon) = Y(x)$$

35

uniformly on $[0, 1]$ *and*

$$\lim_{\varepsilon_n \to 0+} y'(x, \varepsilon_n) = \begin{cases} Y_L'(x), & 0 \le x < x_0, \\ Y_R'(x), & x_0 < x \le 1 \end{cases}$$

uniformly on $[0, x_0 - \delta]$ *and on* $[x + \delta, 1]$ *for any* $\delta > 0$. *Furthermore, for* ε *small enough,*

$$\mu_1 < y'(x_0, \varepsilon) < \mu_2. \tag{3.22}$$

The solution is unique in the sense that there is no other solution of (3.20) which lies in a sufficiently small neighbourhood of $Y(x)$ *throughout* $[0, 1]$ *for small* $\varepsilon > 0$.

Proof. See [35].

Furthermore, we have the following result.

Lemma 3.7. *Suppose there is an* $\varepsilon_0 > 0$ *such that there exists a solution* $y(x, \varepsilon)$ *of (3.20) for every* ε *with* $0 < \varepsilon \le \varepsilon_0$. *Suppose* $[a, b] \subset [0, 1]$ *is an interval on which*

$$|y(x, \varepsilon)| + |y'(x, \varepsilon)| \le M \tag{3.23}$$

and

$$|f_y'(x, y(x, \varepsilon), y'(x, \varepsilon), \varepsilon)| \le k > 0 \tag{3.24}$$

for two positive constants M *and* k. *Then there is a function* $Y(x) \in C^1(a, b)$ *which satisfies*

$$f(x, Y(x), Y'(x), 0) = 0, \tag{3.25}$$

36

and there is a sequence $\varepsilon_n \to 0+$ such that

$$\lim_{\varepsilon_n \to 0+} y(x, \varepsilon_n) \;=\; Y(x) \quad uniformly \;\; on \quad [a, b],$$

(3.26)

$$\lim_{\varepsilon_n \to 0+} y'(x, \varepsilon_n) \;=\; Y'(x) \quad uniformly \;\; on \quad [a + \delta, b - \delta].$$

Proof. See [35].

3.2   Summary

We have provided some necessary existence and uniqueness results in this chapter.

37

Chapter 4

Fitted Mesh Finite Difference

Method for the Model Problem

In this chapter, we design and implement a fitted mesh finite difference method (FMFDM) for problem (2.1)-(2.2). The reasons for using FMFDM as compared to other approaches is obvious as the

- Finite element users have to use layer adapted meshes (which is not at all trivial)

- Spline approximation users have to use variety of splines (e.g., L, B, cubic splines)

- Collocation users have to choose appropriate basis functions and the proper collocation points (at which the linear combination of the basis function is supposed to satisfy the differential equation) and selection of such collocation points is not trivial

- Multiple shooting users have to solve a large sequence of IVPs involving parameters $t = t_k$ which have to be obtained via methods like Secant, Newton-Raphson,

38

etc., and unless a proper initial approximation is taken, these methods tend to fail

- Continuation Method users

    (i) are puzzled as how to proceed if you don't know the starting solution?

    (ii) have to solve larger system of resulting difference equations (e.g., through RK-4 which will be $4N \times 4N$ system, etc).

Note that to solve the problem $\mathbf{F}(\mathbf{x}) = \mathbf{0}$, the *continuation method* is to consider a $\lambda \in [0, 1]$ and then form

$$\mathbf{g}(\lambda, \mathbf{x}) = \lambda \mathbf{F}(\mathbf{x}) + (1 - \lambda)\left[\mathbf{F}(\mathbf{x}) - \mathbf{F}(\mathbf{x}(0))\right].$$

Now start with a known solution $\mathbf{x}(0)$ of $\mathbf{g}(0, \mathbf{x})$ and proceed (continue) to determine the solution $\mathbf{x}(1)$ of $\mathbf{g}(1, \mathbf{x})$.

It should be noted that we have recently obtained some preliminary results via one or more of the above approaches. However, since they are beyond the scope of this thesis, we are not including them here.

Now before we proceed further, let us fix some notations. We denote by $\mathbf{w}$ the numerical solution obtained via FMFDM. In some cases, the underlying interval is denoted by $[a, b]$ where a and b are arbitrary real constants and N and m are positive integers wheres h_i denotes the mesh size in the subinterval (x_{i-1}, x_i).

The FMFDM is designed on the following mesh (referred to as Shishkin mesh in the literature):

We note that the asymptotic analysis presented in Chapter 2 implies that the layer is located near the left and/or the right end of the interval depending on the

39

relation between α and β in (2.2). We consider here the case when it appears on the left end. The other case can be dealt similarly.

Let the interval $[0, 1]$ be divided into two sub-intervals:

$$[0, 1] := [0, \tau] \cup [\tau, 1].$$

The piecewise uniform mesh (of Shishkin type) in these sub-intervals is designed as follows:

Assuming that $N = 2^m$ with $m \geq 3$, the intervals $(0, \tau)$ and $(\tau, 1)$ are each divided into $N/2$ equal mesh elements.

We define the parameter τ by

$$\tau = \min\{1/2, C \ln N\}. \tag{4.1}$$

Let $x_{j_0} = \tau$ and

$$[0, 1] := 0 = x_0 < x_1 < \ldots < x_{j_0} < \ldots < x_N = 1,$$

with $x_j = h_j - h_{j-1}$, where the mesh spacing is given by

$$h_j = \begin{cases} 2\tau N^{-1}, & j = 1, \ldots, j_0, \\ 2(1 - \tau)N^{-1}, & j = j_0 + 1, \ldots N. \end{cases} \tag{4.2}$$

If $\tau = 1/2$, i.e., $1/2 < 8C \ln N$ then N^{-1} is very small relative to C which is very unlikely in practice and in such a case the method can be analyzed using the standard techniques. We therefore assume that

$$\tau = 8C \ln N. \tag{4.3}$$

Remark 4.1. Some studies have been carried out around the selection of C in the above but no clear guidelines have been obtained so far. Mostly they are all based

40

on trial and error. To avoid such ambiguities, one possible way is to use other type of meshes, for example **Bakhvalov-mesh** [9] or the most recent one **Patidar-mesh** [90], both of which are graded meshes and avoid unnecessary additional grid points as obtained in the Shishkin mesh. However, experimentation with these meshes is currently under progress.

4.1 Fitted Mesh Finite Difference Method

Re-writing (2.1) in the form

$$y''(x_i) = f(x_i, y(x_i), y'(x_i))$$

and then replacing the $y''(x_i)$ and $y'(x_i)$ terms with the central difference approximation, we obtain for each $i = 1, 2, \ldots, N-1$,

$$(D^+D^-)y(x_i) = f\left(x_i, y(x_i), (D^o)y(x_i) - \frac{h_i^2}{6}y'''(\eta_i)\right) + h_i^2\frac{y^{(iv)}}{12}(\xi_i), \qquad (4.4)$$

for some ξ_i and η_i in the interval (x_{i-1}, x_{i+1}) and

$$D^+(y_i) = \frac{y_{i+1} - y_i}{h_{i+1}},$$
$$D^-(y_i) = \frac{y_i - y_{i-1}}{h_i}$$

and

$$D^o(y_i) = \frac{y_{i+1} - y_{i-1}}{h_{i+1} + h_i}.$$

The FMFDM for (2.1)-(2.2) on the above mesh is obtained by deleting the error terms and employing the boundary conditions. Hence, it is give by

$$-(D^+D^-)w_i + f(x_i, w_i, (D^o)w_i) = 0, \; i = 1(1)N-1 \qquad (4.5)$$

41

and

$$w_0 = \alpha, \quad w_N = \beta. \tag{4.6}$$

The $(N-1) \times (N-1)$ non-linear system obtained from this method can be solved by the Newton's method for non-linear systems. We briefly explain this procedure below.

We note that the system (4.5)-(4.6) is of the form

$$\mathbf{F}(\mathbf{w}) = \mathbf{0}, \tag{4.7}$$

where $\mathbf{w} = [w_1, w_2, \cdots, w_{N-1}]^T$.

The Jacobian of $\mathbf{F}(w_1, \ldots, w_{N-1})$ is a tridiagonal matrix $\mathbf{J}$ whose sub-diagonal, diagonal and super-diagonal entries are given by

$$\mathbf{J}_{i,j} = -\frac{h_{i+1}}{h_i} - \frac{h_{i+1}h_i}{h_{i+1}+h_i} f_{y'}\left(x_i, w_i, \frac{w_{i+1}-w_{i-1}}{h_{i+1}+h_i}\right); \; i = j-1 \text{ and } j = 2, \ldots, N-1,$$

$$\mathbf{J}_{i,j} = 1 + \frac{h_{i+1}}{h_i} + h_{i+1}h_i f_y\left(x_i, w_i, \frac{w_{i+1}-w_{i-1}}{h_{i+1}+h_i}\right); \; i = j \text{ and } j = 1, \ldots, N-1,$$

and

$$\mathbf{J}_{i,j} = -1 + \frac{h_{i+1}h_i}{h_{i+1}+h_i} f_{y'}\left(x_i, w_i, \frac{w_{i+1}-w_{i-1}}{h_{i+1}+h_i}\right); \; i = j+1 \text{ and } j = 1, \ldots, N-2.$$

Starting with a suitable initial estimate $\mathbf{w}^{[0]}$, we define

$$\mathbf{w}^{[k+1]} = \mathbf{w}^{[k]} + \Delta\mathbf{w}^{[k]}, \; k = 0, 1, 2, \ldots \tag{4.8}$$

where $\Delta\mathbf{w}^{[k]}$ is the solution of

$$\mathbf{J}\left(\mathbf{w}^{[k]}\right)\Delta\mathbf{w}^{[k]} = -\mathbf{F}\left(\mathbf{w}^{[k]}\right), \; k = 0, 1, 2, \ldots \tag{4.9}$$

Above method is implemented on MATLAB and results thus obtained are discussed below.

42

4.2 Analysis of the Fitted Mesh Finite Difference Methods

It is obvious from the construction above that the local truncation error satisfies

$$|y_j - w_j| \leq \frac{h_j^2}{12} |w_j^{(iv)}|.$$

Since the solution of the problem (2.1)-(2.2) satisfies

$$|y^q(x)| \leq M(1 + \varepsilon^{-q} e^{-\gamma x/\varepsilon})$$

where $q \geq 0$ and γ and M are positive constants independent of ε and the mesh size, we realize that the method is of almost second order because

$$|w_j^{(iv)}| \leq M(1 + \varepsilon^{-4} e^{-\gamma x_j/\varepsilon}).$$

However, more sophisticated analysis follows the standard line as described in various works, see, e.g., [72, 109, 110] and one could obtain the final estimate or the order of $h^2 \ln^2(N)$.

4.3 Numerical Results

In this section, we provide some results obtained by the FMFDM described above for the following test problem

Lemma 4.1. Consider the problem

$$\varepsilon y''(x) + y(x)y'(x) - y(x) = f(x),$$

$$y(0) = 1, \quad y(1) = \exp(-1/\varepsilon).$$

The function $f(x)$ in the above is chosen in such a way that the problem has the exact solution $y(x) = \exp(-x/\varepsilon)$.

43

Table 4.1 contains the maximum errors for various values of N and ε obtained by using the formula

$$\text{Maximum Error} = \max |\mathbf{y} - \mathbf{w}|.$$

Table 4.1: Maximum errors obtained via FMFDM for Example 4.1

ε	$N = 8$	$N = 16$	$N = 32$	$N = 64$	$N = 128$	$N = 256$
10^{-1}	2.45E-02	3.93E-03	1.48E-03	3.73E-04	9.35E-05	2.34E-05
10^{-2}	5.72E-02	1.33E-02	3.05E-03	7.27E-04	2.58E-04	8.80E-05
10^{-3}	6.19E-02	1.54E-02	3.78E-03	9.22E-04	2.58E-04	8.80E-05
10^{-4}	6.24E-02	1.56E-02	3.89E-03	9.70E-04	2.58E-04	8.80E-05
10^{-6}	6.25E-02	1.56E-02	3.91E-03	9.76E-04	2.58E-04	8.80E-05
10^{-8}	6.25E-02	1.56E-02	3.91E-03	9.77E-04	2.58E-04	8.80E-05
10^{-10}	6.25E-02	1.56E-02	3.91E-03	9.77E-04	2.58E-04	8.80E-05
10^{-12}	6.25E-02	1.56E-02	3.91E-03	9.77E-04	2.58E-04	8.80E-05
10^{-14}	6.25E-02	1.56E-02	3.91E-03	9.77E-04	2.58E-04	8.80E-05
10^{-16}	6.25E-02	1.56E-02	3.91E-03	9.77E-04	2.58E-04	8.80E-05

4.4 Summary

This chapter dealt with design of a FMFDM for the model problem (2.1)-(2.2). The method is implemented using MATLAB and the results are presented in Table 4.1.

One can see from the results presented in Table 4.1 that the FMFDM is ε-robust in the sense that the maximum error does not increase (in fact it remain constant)

when ε decreases. This is the most important aspect one is always looking for from a practical point of view. Moreover, the above numerical results are in confirmation with the expected theoretical order of convergence.

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Chapter 5

Fitted Operator Finite Difference Methods for a Problem Arising in Enzyme Kinetics

Unlike the method in the previous chapter, in this chapter, we develop a fitted operator finite difference method (FOFDM) to solve a problem arising in enzyme kinetics.

The practical motivation to solve this problem comes from the fact that when a substance reacts with another substance to form a new substance (referred as a product) one is eager to know the components of each substance involved in the whole process. The cunning way of separating, identifying and determining the relative amounts of the components in each substance used and even in the product formed is part of the procedures used in analytical chemistry. However, such processes can be performed under static conditions referred in the thermodynamic methods in the literature. On the other hand, the dynamic conditions incorporated inside the kinetics methods. In this Chapter we would like to extend our helping hand to any scientist

46

who might be interested in obtaining the aforementioned relative amounts of each substance involved in an enzyme-catalyzed reactions (see [100] for further details on this topic).

Since enzymes are high-molecular-weight molecules that catalyze reactions in biological systems, such reactions become integral part of kinetics methods. One should expect to have a series of chemical equations describing the individual elementary steps by which products are formed from reactants. The rate at which reactants are consumed or products are formed, led to an empirical *rate law* that relates the reaction rate to the concentrations of reactants, products, and intermediates at any instant. Using this law, one is able to translate each reaction which gives a mathematical model. We study the qualitative features of this model via asymptotic analysis and then use these features to develop some a reliable numerical method.

5.1 Problem Description

Consider a substrate S being converted irreversible by a single enzyme E into a product P. The intermediate substrate-enzyme complex is SE.

Law of mass action: *The rate of a chemical reaction is directly proportional to the molecular concentrations of the reacting substances* and therefore the reaction is

$$S + E \xrightarrow{k_1} SE \xrightarrow{k_2} P + E,$$

$$S + E \xrightleftharpoons{k_{-1}} SE,$$

(5.1)

47
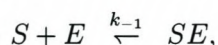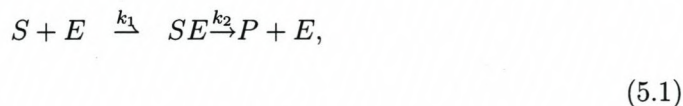
where k_1, k_2 and k_{-1} are proportionality constants.

Introducing s, e, c and p to denote the respective concentrations of S, E, SE and P, we obtain the non-linear autonomous system given

$$\begin{cases} \frac{ds}{dt} = -k_1 se + k_{-1} c \\[2mm] \frac{de}{dt} = -k_1 se + (k_{-1} + k_2)c, \\[2mm] \frac{dc}{dt} = k_1 se - (k_1 + k_2)c \\[2mm] \frac{dp}{dt} = k_2 c, \end{cases} \tag{5.2}$$

with the associated initial conditions $s(0) = s_0 > 0, e(0) = e_0 > 0, c(0) = 0$ and $p(0) = 0$.

In the enzyme-catalyzed reaction (5.1) we expect an enzyme E to be regenerated and a product P to be formed, when the reaction ends. Thus we have to reduce the system (5.2) to the system of the rate of the substrate S and rate of the substrate-enzyme complex SE, in fact the two substances constitute the core of such reactions. To achieve this we add the second and third equation and obtain

$$\frac{d(e+c)}{dt} = 0$$

$$\Rightarrow e(t) = e_0 - c(t), \tag{5.3}$$

and by adding the first, third and fourth equation we obtain

$$\frac{d(s+c+p)}{dt} = 0$$

$$\Rightarrow p(t) = s_0 - s(t) - c(t). \tag{5.4}$$

48

Using equations (5.3) and (5.4) in (5.2) we eliminate the two concentrations e and p from the system (5.2), and eventually obtain

$$\begin{cases} \frac{ds}{dt} = -k_1 e_0 s + (k_1 s + k_{-1})c, & s(0) = s_0, \\ \frac{dc}{dt} = k_1 e_0 s - (k_1 s + k_{-1} + k_2)c, & c(0) = 0. \end{cases} \quad (5.5)$$

It should be noted that this type of elimination often occurs in chemical kinetics, circuit analysis and other fields, due to constraints between variables from physical conservation or mass laws. A biochemist expect that

$$\frac{de}{dt} \approx 0 \Rightarrow \frac{dc}{dt} \approx 0$$

$$\Rightarrow c \approx \frac{k_1 e_0 s}{k_1 s + k_{-1} + k_2} \rightarrow \frac{ds}{dt} = \frac{-k_2 e_0 s}{K + s} \quad \text{where} \quad K \equiv (k_{-1} + k_2)/k_1.$$

The last differential equation can be solved for s.

5.2 Dimensional Analysis

Introducing the dimensionless variables

$$\begin{aligned} \tau &= k_1 e_0 t, \quad \lambda = \frac{k_2}{k_1 s_0}, \quad \kappa = \frac{k_{-1} + k_2}{k_1 s_0}, \\ x(\tau) &= s(t)/s_0, \quad y(\tau) = c(t)/e_0, \quad \varepsilon = e_0/s_0, \end{aligned}$$

into (5.5) and simplifying, we obtain

$$\begin{cases} \frac{dx}{d\tau} = -x + (x + \kappa - \lambda)y, & x(0) = 1, \\ \varepsilon \frac{dy}{d\tau} = x - (x + \kappa)y, & y(0) = 0. \end{cases} \quad (5.6)$$

The value of ε which is e_0/s_0 is typically of the order of $\varepsilon \approx 10^{-6}$. Hence the system is singularly perturbed and information about the location of the layer must be determined.

49

5.3 Prediction of the Boundary Layer

In this section, we discuss how the boundary layer is located using the asymptotic analysis.

Plugging

$$\begin{pmatrix} X(\tau,\varepsilon) \\ Y(\tau,\varepsilon) \end{pmatrix} \sim \sum_{j=0}^{m} \begin{pmatrix} X_j(\tau) \\ Y_j(\tau) \end{pmatrix} \varepsilon^j, \quad m \in \mathbb{Z}^+ \text{ (it is 1 in our case)} \tag{5.7}$$

into (5.6) and simplifying, we obtain

Coefficients of ε^0:

$$\begin{cases} \dot{X}_0 = -\frac{\lambda X_0}{X_0 + \kappa} & \text{with } X_0(0) = 1 \\ Y_0 = \frac{X_0}{X_0 + \kappa} \end{cases} \tag{5.8}$$

Coefficients of ε^1:

$$\begin{cases} \dot{X}_1 = -\frac{\lambda \kappa}{(X_0 + \kappa)^2} X_1 - \frac{X_0 + \kappa - \lambda}{X_0 + \kappa} \dot{Y}_0 & \text{with } X_1(0) = 0 \\ Y_1 = \frac{1}{X_0 + \kappa} \left((1 - Y_0) X_1 - \dot{Y}_0 d\tau \right). \end{cases} \tag{5.9}$$

Note that the problem (5.5) possesses only one initial condition attached to each depended variable and therefore, it is sufficient to use the first order term of (5.7) to predict the location of a boundary layer. Therefore, using terms of $O(\varepsilon^0)$ we notice that

$$Y_0(0) = \frac{1}{1 + \kappa} \neq y(0).$$

Hence we have a layer near $\tau = 0$.

Unlike the FMFDM, the construction of FOFDM does not require knowledge of the width of the layer. However, using the matching principle, it is not hard to find out that the width of the layer is $O(\tau^*)$.

50

Remark 5.1. The reduced system corresponding to (5.6), i.e.,

$$\begin{cases} \frac{dx_0}{d\tau} = -x_0 + (x_0 + \kappa - \lambda)y_0, \quad x_0(0) = 1, \\ 0 = x_0 - (x_0 + \kappa)y_0 \end{cases} \tag{5.10}$$

has the outer solution

$$y_0(\tau) = \frac{x_0(\tau)}{x_0(\tau) + \kappa}. \tag{5.11}$$

Using the outer solution (5.11) into the system (5.10) we obtain the initial-value problem

$$\dot{x}_0 = -\frac{\lambda x_0}{x_0 + \kappa} \quad \text{with } x_0(0) = 1,$$

which is decreasing monotonically to the critical point $x_0 = 0$, and represents the consumption of the substrate S, whereas the outer solution in (5.11) represents the formation of a product P and the regeneration of an enzyme E as the reaction ends.

5.3.1   Stability of Critical Points of the Continuous System

The only critical point of the continuous system (5.6) is $(0,0)$. The eigenvalues of the associated Jacobian matrix at this point are given by

$$\eta_{1,2} := \frac{-\left(1 + \frac{\kappa}{\varepsilon}\right) \pm \sqrt{\left(1 + \frac{\kappa}{\varepsilon}\right)^2 - \frac{4\lambda}{\varepsilon}}}{2}.$$

Now since the determinant of the Jacobian matrix evaluated at the critical point is positive and the real part of both the above eigenvalues is negative, the critical point is stable and attractive, i.e., asymptotically stable ([57]).

5.4 Fitted Operator Finite Difference Method

To approximate the solution of the system (5.6), we consider the following numerical method, referred to as the Fitted Operator Finite Difference Method (FOFDM).

We have used a uniform step-size $\Delta\tau$ to proceed in the infinite interval. Thus $\tau_j = j * \Delta\tau$, $j = 0, 1, \dots$.

Looking at the system (5.6), we find that its solution has a slowly varying component (referred as slow variable) x and a rapidly varying component (referred as fast variable) y. Therefore, the equation corresponding to x can be discretized in an standard way. However, we use a non-standard discretization for the equation containing derivative of y. This non-standard discretization is carried out via one of the Mickens' rules, further details of which can be found in [79, 89].

We consider the constant coefficient homogeneous problem corresponding to the differential equation in y. Corresponding exact scheme is

$$y_j = \exp\left(-\frac{\kappa\tau}{\varepsilon}\right) y_{j-1}.$$

Further simplification to this yields

$$\varepsilon\frac{y_j - y_{j-1}}{\phi} = -\kappa y_j$$

where

$$\phi := \frac{\varepsilon}{\kappa}\left(\exp\left(\frac{\kappa\Delta\tau}{\varepsilon}\right) - 1\right) = \Delta\tau + O\left(\frac{\Delta\tau^2}{\varepsilon}\right).$$

Combining the two facts, we have the following FOFDM for the system problem (5.6):

$$\begin{cases} \frac{x_{j+1} - x_j}{\Delta\tau} = -x_j + (\kappa - \lambda)y_j + x_j y_j \\ \varepsilon\frac{y_j - y_{j-1}}{\phi} = x_j - \kappa y_j - x_j y_j. \end{cases} \tag{5.12}$$

52

Remark 5.2. We have experimented and realized that the other non-standard modelling rules, for instance, "the non-local approximation for the non-linear terms" is not necessary as the stability is obtained just by using the suitable denominator function (in the above case, it is ϕ).

5.5 Analysis of the Fitted Operator Finite Difference Method

In this section, we discuss the stability of the fixed point(s) and the convergence of the FOFDM given by (5.12).

5.5.1 Stability of Fixed Points of the Discrete System

The FOFDM (5.12) can be written as

$$\begin{cases} x_{j+1} = x_j + \Delta\tau\left(-x_j + (\kappa - \lambda)y_j + x_j y_j\right) \equiv F(x_j, y_j) \\ y_j = y_{j-1} + (\phi/\varepsilon)\left(x_j - \kappa y_j - x_j y_j\right) \equiv G(x_j, y_{j-1}) \\ \Rightarrow G(x_j, y_j) = y_j + (\phi/\varepsilon)\left(x_j - \kappa y_{j+1} - x_j y_{j+1}\right). \end{cases} \tag{5.13}$$

The fixed points (x^*, y^*) of the system (5.13) are obtained by setting $F(x^*, y^*)$ and $G(x^*, y^*)$ equal to zero. We check that the only fixed point that satisfies this is $(0, 0)$. Hence the fixed point of (5.13) corresponds to the critical point of the continuous system (5.6). Now evaluating the eigenvalues of the associated Jacobian at this fixed point, we find that the fixed points are asymptotically stable without any step-size restriction. (Note that the same is not true if we use a standard finite difference methods, e.g., forward Euler for the equation in y. In that case, for the fixed point to be asymptotically stable, we would require that $\Delta\tau < 2\varepsilon/(\kappa + \varepsilon)$).

53

5.5.2 Convergence of the Fitted Operator Finite Difference Methods

The local truncation error (LTE) for the method in x satisfies

$$|LTE_x| \leq \frac{\Delta\tau^2}{2}x''(\xi_j), \ \ \xi_j \in (\tau_{j-1}, \tau_j) \tag{5.14}$$

and that for the method in y satisfies (in the more realistic case $\varepsilon < \Delta\tau$)

$$|LTE_y| \leq \frac{\Delta\tau^2}{2}y''(\zeta_j), \ \ \zeta_j \in (\tau_{j-1}, \tau_j). \tag{5.15}$$

Hence, we conclude that the FOFDM is first order accurate.

Remark 5.3. The results presented in Tables 5.1-5.2 are first order accurate which is not possible if we use the FMFDM instead of FOFDM. This is due to the fact that the Shishkin mesh will provide a locking factor $\ln(N)$ in the theoretical order of convergence of the method and therefore the resulting order of convergence would only be $\Delta\tau \ln(N)$ and not $\Delta\tau$ as in the case of FOFDM.

5.6 Numerical Results

In this section, we present some numerical results corresponding to problem (5.6). As noted earlier, the parameter $\varepsilon \approx 10^{-6}$, therefore, we consider a series of ε values and check whether the method is robust with respect to this parameter. (This is important due to the fact that should any non-dimensionalized parameter changes its value, ε will change accordingly (though not significantly)).

Since the exact solution of this problem is not available, we use the well-known double mesh principle [34] to obtain the maximum errors corresponding to each com-

54

ponents x and y, i.e.,

$$\text{Maximum Error in } z = \max_{0 \leq j \leq N} |z_j^N - z_{2j}^{2N}|.$$

where z is the numerical solution vector for x and y.

Tabular results presented for various values of N and ε in Table 5.2 show that the FOFDM is ε-robust. However, since x is a slowly varying component, the results are unaffected by ε. This can be seen from Table 5.1. Finally, the problem being singularly perturbed, there is no need to use the standard methods to solve it and hence we do not add results obtained by them.

5.7 Summary

In this chapter, we considered a problem arising in an enzyme-catalyzed reaction. Using the *law of mass action* we have transformed this reaction into an autonomous system of differential equations. After dimensional analysis, this system is reduced to a singularly perturbed non-linear system of two ODEs. Necessary asymptotic analysis is carried out to predict the location of the layer. This has helped us in deriving the appropriate denominator function from the exact scheme because we have to make a selection from other reductions which are also possible there. Finally, we have designed a FOFDM which we analyzed for stability and convergence. Numerical results are also provided. (Note the the beauty of the FOFDM lies in the fact that we do not need to know the width of the layer as in the case of FMFDM discussed in the previous chapter).

55

Table 5.1: Maximum errors obtained via FOFDM (for x-component)

ε	N=8	N=16	N=32	N=64	N=128
1	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-4}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-12}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-16}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-20}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-24}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-32}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-36}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-40}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04
2^{-48}	1.25E-02	5.98E-03	2.93E-03	1.45E-03	7.22E-04

Table 5.2: Maximum errors obtained via FOFDM (for y-component)

ε	N=8	N=16	N=32	N=64	N=128
1	1.27E-02	6.34E-03	3.18E-03	1.59E-03	7.99E-04
2^{-4}	1.44E-02	1.98E-02	1.52E-02	9.45E-03	5.33E-03
2^{-12}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-16}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-20}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-24}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-32}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-36}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-40}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04
2^{-48}	6.84E-03	3.24E-03	1.58E-03	7.78E-04	3.87E-04

56

Chapter 6

Conclusion and Future Plans

This thesis deals with the analysis and implementation of some reliable numerical methods for non-linear singular perturbation problems (NSPPs).

In the first chapter, we described what is meant by an NSPP. Then we presented some models describing NSPPs and gave a literature review from the past few years. The second chapter deals with the asymptotic analysis for a model problem where we found the necessary qualitative information which is used in designing the numerical method in chapter 4. Some theoretical results about existence and uniqueness of the quasilinear and non-linear SPPs are presented in Chapter 3. A fitted mesh finite difference method is designed, analyzed and implemented in Chapter 4. To gain further insight into the approach, we considered a realistic situation in Chapter 5 where we have solved a problem arising in enzyme kinetics.

Several conclusions are drawn which are mentioned at appropriate places in the individual chapters. Other relevant concerns which form some of our future plans are:

- It is very much surprising that despite the fact that one lacks the analytical

57

theory with regard to finding analytical solution, he/she does not lack the analytical machinery to investigate the qualitative features of the innocent looking mathematical problems. Existence and uniqueness of the solution, existence, location and width of the layers, etc., are just a few examples in support of this statement. To this end we have realized there is a room for improvement and therefore we are currently considering to extend our analysis (i) to find some other qualitative properties, and (ii) for some other research problems such as those for singularly perturbed problems in biology.

- We also intend to do rigorous error analysis of some of the numerical methods (for example, the one in Chapter 2) and simultaneously would like to test the FMFDMs on other meshes such as **Bakhvalov-mesh** [9] and the **Patidar-mesh** [90].

- Another aspect which we are currently dealing with is to improve the order of accuracy. To this end, we have recently obtained some preliminary results using variable mesh shooting type of methods and via some extrapolation techniques. Since they are beyond the scope of this thesis, such works are being dealt elsewhere.

58

Appendix A

Some Useful Results [85]

Definition 1. Let $y(x, \varepsilon)$ denotes the solution of a differential equation involving a small positive parameter ε such that $0 \leq \varepsilon \leq \varepsilon_0$ and let the function $v(x, \varepsilon)$ be defined over the same domain (say $\mathcal{D}$) as the solution $y(x, \varepsilon)$. Then the statement

$$y(x, \varepsilon) = O(v(x, \varepsilon)) \text{ in } \mathcal{D} \text{ as } \varepsilon \to 0 \tag{1}$$

means that for each point $x \in \mathcal{D}$, there exists a positive $k(x)$ and an interval $I := \{0 \leq \varepsilon \leq \varepsilon_0(x)\}$, where ε_0 depends in general on the choice x, such that

$$|y| \leq k|v|$$

for every ε in I. If $\left(\frac{y}{v}\right)$ is defined in $\mathcal{D}$, then (1) implies that $|\frac{y}{v}|$ is bounded above by k. The relation (1) is said to be uniformly valid in $\mathcal{D}$ if k is a constant and ε_0 does not depend on x.

Definition 2. The statement

$$y(x, \varepsilon) = o(v(x, \varepsilon)) \text{ in } \mathcal{D} \text{ as } \varepsilon \to 0$$

means that for each point $x \in \mathcal{D}$ and a given δ, there exists an interval $I := \{0 \leq \varepsilon \leq \varepsilon_0(x, \delta)\}$, which depends in general on the choice of x and δ, such that

$$|y| \leq \delta|v|$$

for all ε in I.

59

Definition 3. Let $\phi_n(\varepsilon)$ with $n = 1, 2, \cdots$ be a sequence of functions of ε such that

$$\phi_{n+1}(\varepsilon) = o(\phi_n(\varepsilon)) \text{ as } \varepsilon \to 0 \text{ for each } n = 1, 2, \cdots.$$

Such a sequence is called an asymptotic sequence. Thus ε^{n-1} with $n = 1, 2, \cdots$ is an asymptotic sequence.

Definition 4. The series

$$\sum_{j=1}^{N} \phi_j(\varepsilon) y_j(x),$$

where the integer N may be finite or infinite, is said to be the asymptotic expansion of y with respect to $\phi_j(\varepsilon)$ as $\varepsilon \to 0$, if for every $M = 1, 2, \cdots, N$

$$y(x, \varepsilon) - \sum_{j=1}^{M} \phi_j(\varepsilon) y_j(x) = o(\phi_M) \text{ as } \varepsilon \to 0$$

which is equivalent to

$$y(x, \varepsilon) - \sum_{j=1}^{M} \phi_j(\varepsilon) y_j(x) = O(\phi_{M+1}) \text{ as } \varepsilon \to 0$$

for each $M = 1, 2, \cdots, N - 1$. The asymptotic expansion is said to hold uniformly in $\mathcal{D}$ if both the order relations hold uniformly there.

60

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