

**PSEUDO RESIDUAL - FREE BUBBLE FUNCTIONS
FOR THE STABILIZATION OF CONVECTION -
DIFFUSION - REACTION PROBLEMS**

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ABSTRACT

PSEUDO RESIDUAL - FREE BUBBLE FUNCTIONS FOR THE STABILIZATION OF CONVECTION - DIFFUSION - REACTION PROBLEMS

Convection - diffusion - reaction problems may contain thin regions in which the solution varies abruptly. The plain Galerkin method may not work for such problems on reasonable discretizations, producing non-physical oscillations. The Residual - Free Bubbles (RFB) can assure stabilized methods, but they are usually difficult to compute, unless in special limit cases. Therefore it is important to devise numerical algorithms that provide cheap approximations to the RFB functions, contributing a good stabilizing effect to the numerical method overall. In my thesis we will examine a stabilization technique, based on the RFB method and particularly designed to treat the most interesting case of small diffusion in one and two space dimensions for both steady and unsteady convection - diffusion - reaction problems. We replace the RFB functions by their cheap, but efficient approximations which retain the same qualitative behavior. We compare the method with other stabilized methods.

ÖZET

KONVEKSİYON - DİFÜZYON - REAKSİYON PROBLEMLERİNİN STABİLİZASYONU İÇİN HEMEN HEMEN KALANSIZ FONKSİYONLAR

Konveksiyon - difüzyon - reaksiyon problemleri çözümün aniden deđiřtiđi dar alanlar içerebilirler. Standard Galerkin metodu makul ayrıştırılmalarda bu tür problemler için fiziksel olmayan salınımlar üreterek çalışmayabilir. Residual - Free Bubbles (RFB) metodu bu durumu çözen stabilize edilmiş bir metottur, ama RFB fonksiyonlarını bazı özel durumlar hariç elde etmek zordur. Bu yüzden RFB fonksiyonlarına ucuz bir şekilde yaklaşımlar sağlayan sayısal algoritmalar önemlidir. Bu tezde RFB metoduna dayanan bir boyutta ve iki boyutta hem durađan hemde durađan olmayan konveksiyon - difüzyon - reaksiyon problemleri için özellikle difüzyon katsayısının küçük olduđu durumlar için çalışan bir stabilizasyon tekniđini inceleyeceđiz. RFB fonksiyonlarını aynı kaliteyi gösteren kolay elde edilir ama etkili yaklaşımları ile yer deđiřtireceđiz. Metodu başka stabilize edilmiş metodlar ile kıyaslayacađız.

TABLE OF CONTENTS

LIST OF FIGURES	viii
LIST OF TABLES	x
CHAPTER 1. INTRODUCTION	1
1.1. Introduction.....	1
1.2. Layout of the Thesis.....	2
CHAPTER 2. PSEUDO RESIDUAL - FREE BUBBLES FOR STEADY CONVECTION - DIFFUSION - REACTION PROBLEMS IN ONE DIMENSION	4
2.1. A Review of RFB Method in One Dimension	4
2.2. Pseudo - RFB in One Dimension.....	6
2.2.1. Diffusion - Dominated Regime	7
2.2.2. Convection - Dominated Regime.....	8
2.2.3. Reaction - Dominated Regime.....	8
2.3. Numerical Experiments	8
2.3.1. Test 1 (Diffusion - Dominated Regime).....	9
2.3.2. Test 2 (Convection - Dominated Regime).....	9
2.3.3. Test 3 (Reaction - Dominated Regime)	10
2.3.4. Test 4 (Internal Layer Problem)	11
CHAPTER 3. PSEUDO RESIDUAL - FREE BUBBLES FOR CONVECTION - DIFFUSION - REACTION PROBLEMS IN TWO DIMENSIONS .	15
3.1. A Review of RFB Method in Two Dimensions	15
3.2. Pseudo RFB in Two Dimensions	16
3.2.1. Diffusion - Dominated Regime	18
3.2.2. Convection - Dominated Regime.....	18
3.2.2.1. One Inflow Edge	19
3.2.2.2. Two Inflow Edges.....	20
3.2.2.3. Numerical Tests.....	21
3.2.3. Reaction - Dominated Regime.....	29

3.2.3.1. Two Inflow Edges	29
3.2.3.2. One Inflow Edge	30
3.2.3.3. Numerical Tests	31
CHAPTER 4. PSEUDO RESIDUAL - FREE BUBBLES FOR UNSTEADY CONVECTION - DIFFUSION - REACTION PROBLEMS	41
4.1. Pseudo Residual - Free Bubbles for Unsteady Convection - Diffusion - Reaction Problems in One Dimension.....	41
4.1.1. Numerical Tests	43
4.1.1.1. Test 1 (Choice of CFL Numbers)	43
4.1.1.2. Test 2 (Convection - Dominated Regime)	44
4.1.1.3. Test 3 (Convection - Dominated Regime with Different Initial Condition)	44
4.1.1.4. Test 4 (Reaction - Dominated Regime)	45
4.2. Pseudo Residual - Free Bubbles for Unsteady Convection - Diffusion - Reaction Problems in Two Dimensions	45
4.2.1. Numerical Tests	47
4.2.1.1. Test 5 (Convection - Dominated Regime)	47
CHAPTER 5. CONCLUSION	54
REFERENCES	55

LIST OF FIGURES

<u>Figure</u>	<u>Page</u>
Figure 2.1. Standard Galerkin finite element method with $\epsilon = 0.001$, $\beta = 1$, $\sigma = 1$ and $h = 0.02$ subject to homogeneous boundary condition.	5
Figure 2.2. Comparison of exact solution (curved line) of the optimal bubble with its piecewise linear approximation for problem parameters $\epsilon = 0.005$, $\beta = 1$, $\sigma = 0.001$ (left) and $\epsilon = 0.0001$, $\beta = 1$, $\sigma = 0.001$ (right).	6
Figure 2.3. Optimal ξ in convection - dominated regime.	9
Figure 2.4. Error rates in L_2 and H_1 norms when the problem (2.1) is in diffusion - dominated regime.	10
Figure 2.5. Approximate solutions when the problem (2.1) is in convection dominated regime.	12
Figure 2.6. Error rates in L_2 and H_1 norms when the problem (2.1) is in convection - dominated regime.	12
Figure 2.7. Numerical approximations when the problem (2.1) is in reaction dominated regime.	13
Figure 2.8. Numerical approximations with an internal layer when the problem (2.1) is in reaction dominated regime.	14
Figure 3.1. Configuration of internal nodes for element has one inflow edge (left) and two inflow edge (right).	19
Figure 3.2. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with one inflow edge, when $\theta = 72^\circ$, $N = 20$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$	20
Figure 3.3. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with two inflow edge, when $\theta = 72^\circ$, $N = 20$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$	22
Figure 3.4. Configuration of test problem 1.	23
Figure 3.5. Elevation plots of approximate solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$	25
Figure 3.6. Elevation plots of exact solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$	25
Figure 3.7. Contour plots of approximate solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$	26
Figure 3.8. Contour plots of exact solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$	26

Figure 3.9. Error rates in L_2 (left) and H_1 (right) norms for the test problem 1 for different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$	27
Figure 3.10. Comparison of two method with respect to L_2 norm (left) and H_1 norm (right) for $\epsilon = 10^{-4}, \sigma = 10^{-3}$ with $N = 10, 20, 40, 80$	27
Figure 3.11. Statement of thermal boundary layer problem.	29
Figure 3.12. Elevation plots (left) of approximate solutions of the test problem 2 and corresponding contour plots (right).	33
Figure 3.13. Elevation plots of approximate solutions of the test problem 3 (top) and corresponding contour plots (below).	34
Figure 3.14. Pseudo - bubble functions b_1, b_2 and b_3 in a typical element with two inflow edge, when $\theta = 72^\circ, N = 10, \epsilon = 10^{-3}$ and $\sigma = 10, 100, 500$	35
Figure 3.15. Pseudo - bubble functions b_1, b_2 and b_3 in a typical element with one inflow edge, when $\theta = 72^\circ, N = 10, \epsilon = 10^{-3}$ and $\sigma = 10, 100, 500$	35
Figure 3.16. Elevation plots (top) of approximate solutions and corresponding contour plots of test problem 4 for $\epsilon = 10^{-4}, \beta = (\cos 72^\circ, \sin 72^\circ)$ and various reaction terms ($\sigma = f = 0.001, 1, 10, 20, 50, 1000$).	36
Figure 3.17. Elevation plots (left) of approximate solutions of the test problem 2 and corresponding contour plots (right).	37
Figure 3.18. Configuration of test problem 6.	38
Figure 3.19. Uniform (top) and nonuniform (below) triangular elements used in discretization of the domain of the test problem 6.	38
Figure 3.20. Elevation plots (top) of approximate solutions of test problem 6 and corresponding contour plots (below) in reaction dominated regime with uniform meshes.	39
Figure 3.21. Elevation plots (top) of approximate solutions of test problem 6 and corresponding contour plots (below) in reaction dominated regime with nonuniform meshes.	40
Figure 4.1. Comparisons of three methods in convection - dominated regime with respect to $L^\infty(0, T; L^1(I))$ norm.	44
Figure 4.2. Error rates in $L^\infty(0, T; L^1(I))$ norm for various CFL numbers.	48
Figure 4.3. Approximate solutions of test problem 2.	49
Figure 4.4. Approximate solutions of test problem 3.	50
Figure 4.5. Approximate solutions of test problem 4.	51
Figure 4.6. Approximate solutions of test problem 5 at different time steps.	52
Figure 4.7. Approximate solutions of test problem 5 at different time steps.	53

LIST OF TABLES

<u>Table</u>		<u>Page</u>
Table 2.1.	Errors in L_2 norm for various values of h when the problem (2.1) is in diffusion - dominated regime.	9
Table 2.2.	Errors in H_1 norm for various values of h when the problem (2.1) is in diffusion - dominated regime.	10
Table 2.3.	Errors in L_2 norm for various values of h when the problem (2.1) is in convection - dominated regime.	13
Table 2.4.	Errors in H_1 norm for various h when the problem (2.1) is in convection - dominated regime.	13
Table 3.1.	Errors of the test problem 1 in L_2 norm for various N with $\sigma = 10^{-3}$ and different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$	28
Table 3.2.	Errors of the test problem 1 in H_1 norm for various N with $\sigma = 10^{-3}$ and different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$	28

CHAPTER 1

INTRODUCTION

1.1. Introduction

Convection - diffusion - reaction (CDR) problem is one of the most frequently used model problem in science and engineering. This model problem describes how the concentration of a number of substances (e.g., pollutants, chemicals, electrons) distributed in a medium changes under the influence of three processes, namely convection, diffusion and reaction. *Convection* refers to the movement of a substance within a medium (e.g., water or air). *Diffusion* refers to the movement of the substance from an area of high concentration to an area of low concentration, resulting in the uniform distribution of the substance. A chemical *reaction* is a process that results in the inter-conversion of chemical substance. Thus simulations of convection - diffusion - reaction equations are required in various applications. Numerical simulations of convection - diffusion - reaction problems have been studied actively during the last thirty five years.

A characteristic feature of solutions of convection - diffusion - reaction problems is the presence of sharp layers. When convection or reaction dominates, there are physical effects in the problem that occur on a scale which is much smaller than the smallest one representable on the computational grid. However such effects have a strong impact on the larger scale. It is known that plain Galerkin method produces undesired oscillations that pollute whole domain in the presence of under-resolved layers.

Petrov-Galerkin method changing the shape of the test functions is one of the earliest attempts to cure this situation. In order to gain the control of derivatives Streamline-Upwind Petrov Galerkin (SUPG) method which is first proposed in (Brooks & Hughes 1982) is a much more general approach where the variational formulation is augmented. The advantages of this method are its great generality to analyze and to derive the error bounds. The main drawback of SUPG method is the presence of a stabilizing parameter that needs to be properly chosen.

Another approach is Residual-Free-Bubble (RFB) method which is based on enriching the finite element space. It is first studied in (Baiocchi et al. 1993) to find a suitable value of stabilizing parameter for SUPG method. The main problem with this method is that it requires the solution of a local PDE. Cheap approximate solutions to this

local problem were designed by several researchers (Baiocchi et al. 1993), (Neslitürk 1999), (Brezzi et al. 1998), (Brezzi et al. 2003), (Şendur & Neslitürk 2011). Link-Cutting Bubble (LCB) strategy aims to stabilize the Galerkin method by using a suitable refinement near the layer region. LCB strategy uses the piecewise linear bubble functions to find the suitable sub-grid nodes. It works as the plain Galerkin method on augmented meshes. It is extended to time-dependent convection - diffusion - reaction problem in one dimension in (Asensio et al. 2007). One of the drawback of this strategy is that in limit regimes sub-grid nodes are very close to the original nodes so undesired oscillations may occur at sub-grid nodes near layers for unsteady problems. Hence, in numerical simulations one has to exclude the sub-grid nodes. Another drawback of LCB strategy is that in two dimensions it is very difficult to implement because of its technique.

Pseudo Residual-Free Bubble (P-RFB) method aims to get sub-grid nodes to approximate bubble functions cheaply using piecewise linear functions (Şendur & Neslitürk 2011). The main advantage of P-RFB method is that it can be implemented in two dimensions (Şendur et al. 2012). Another advantage of this method is that since integrals of P-RFB functions are directly used when constructing the mass matrix, a smaller mass matrix is used with respect to the mass matrix constructed in LCB strategy.

In my thesis we will examine P-RFB method for both steady and unsteady convection - diffusion - reaction problems in one and two space dimensions.

1.2. Layout of the Thesis

Chapter 2 reviews RFB method and P-RFB method in one dimension for steady convection - diffusion - reaction problems. Comparisons are done between P-RFB method, LCB strategy and SUPG method in different regimes. Approximate solutions and error rates in L_2 norm are given.

Chapter 3 deals with steady convection - diffusion - reaction problems in two dimensions and examines P-RFB method in different regimes. A comparison is done between P-RFB and SUPG methods. Approximate solutions in different regimes are given.

Chapter 4 is devoted to extension of P-RFB method to unsteady convection - diffusion - reactions problems. Variational formulations of P-RFB method, LCB strategy and SUPG method are given in one dimension. CFL numbers at which P-RFB method, LCB strategy and SUPG method work best with Crank-Nicolson scheme are determined. Then comparisons between the methods at these CFL numbers are done. Finally, the

thesis extends P-RFB method to unsteady convection - diffusion - reaction problems in two dimensions. Variational formulations of P-RFB and SUPG methods are given. A comparison between these two methods with Bacward-Euler scheme is established.

CHAPTER 2

PSEUDO RESIDUAL - FREE BUBBLES FOR STEADY CONVECTION - DIFFUSION - REACTION PROBLEMS IN ONE DIMENSION

In this section, we will show a stabilization method for one - dimensional steady convection - diffusion - reaction problems, designed to treat the most interesting case of small diffusion, but able to adapt one regime to another continuously which is studied in (Şendur & Neslitürk 2011). This method aims to approximate the RFB functions efficiently but cheaply without compromising the accuracy. The pseudo bubbles are chosen to be piecewise linear on a suitable sub-grid that, the position of whose nodes are determined by minimizing the residual of local differential problems with respect to L_1 norm (Şendur & Neslitürk 2011). Location of sub-grid nodes in (Şendur & Neslitürk 2011) coincides with the location of sub-grid nodes in (Brezzi et al. 2003) when the problem is in reaction - dominated regime.

2.1. A Review of RFB Method in One Dimension

Consider the two point boundary value problem

$$\begin{cases} \mathcal{L}u = -\epsilon u'' + \beta u' + \sigma u = f(x) \text{ on } I, \\ u(0) = u(1) = 0, \end{cases} \quad (2.1)$$

where $I = (0, 1)$. Let $T_h = \{K\}$ be a decomposition of I where $K = (x_{k-1}, x_k)$, $k = 1, \dots, N$. For simplicity we shall assume that the subintervals are uniform so that length of each subinterval is h . We also assume that diffusion coefficient ϵ is positive constant and convection field β and reaction field σ are non-negative constants. It is well known that when diffusion coefficient ϵ is small with respect to β or σ , Galerkin method produces oscillations as depicted in Fig. 2.1. To treat this case several stabilized methods have been introduced such as SUPG (Streamline - Upwind Petrov/Galerkin) method which is first described in (Brooks & Hughes 1982) and the RFB method which is based on augmenting the finite element space of linear basis functions. RFB method can be summarized as

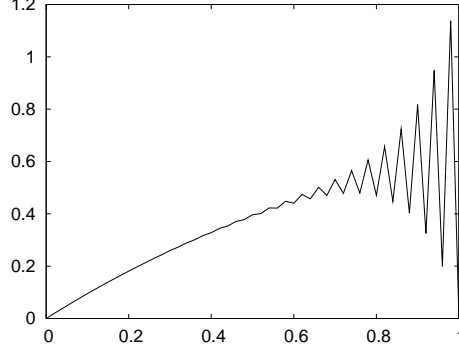


Figure 2.1. Standard Galerkin finite element method with $\epsilon = 0.001$, $\beta = 1$, $\sigma = 1$ and $h = 0.02$ subject to homogeneous boundary condition.

follows. Let start with recalling abstract variational formulation of problem (2.1): Find $u \in H_0^1(I)$ such that

$$a(u, v) = (f, v), \quad \forall v \in H_0^1(I), \quad (2.2)$$

where

$$a(u, v) = \epsilon \int_I u'v' dx + \int_I (\beta u)'v dx + \int_I \sigma uv dx. \quad (2.3)$$

Define V_h subspace of $H_0^1(I)$ as finite - dimensional space. Then Galerkin finite element method reads: Find $u_h \in V_h$ such that

$$a(u_h, v_h) = (f, v_h), \quad \forall v_h \in V_h. \quad (2.4)$$

Now, decompose the space V_h as $V_h = V_L \oplus V_B$, where V_L is the space of continuous piecewise linear polynomials and $V_B = \bigoplus_K B_K$ with $B_K = H_0^1(K)$. From this decomposition every $v_h \in V_h$ can be written in the form $v_h = v_L + v_B$, where $v_L \in V_L$ and $v_B \in V_B$. Bubble component u_B of u_h satisfy the original differential equation in an element K strongly, i.e.

$$\mathcal{L}u_B = -\mathcal{L}u_L + f \quad \text{in} \quad K, \quad (2.5)$$

subject to boundary condition,

$$u_B = 0 \quad \text{on} \quad \partial K. \quad (2.6)$$

Since the support of bubble u_B is contained within the element K we can make a static condensation for the bubble part, getting directly the V_L - projection u_L of the solution u_h (Brezzi & Russo 1993). This can be done as follows. Using $V_h = V_L \oplus V_B$, the finite element approximation reads: Find $u_h = u_L + u_B$ in V_h such that

$$a(u_L, v_L) + a(u_B, v_L) = (f, v_L), \quad \forall v_L \in V_L. \quad (2.7)$$

From equations (2.5) and (2.6), u_B is identified by the linear part u_L and source function

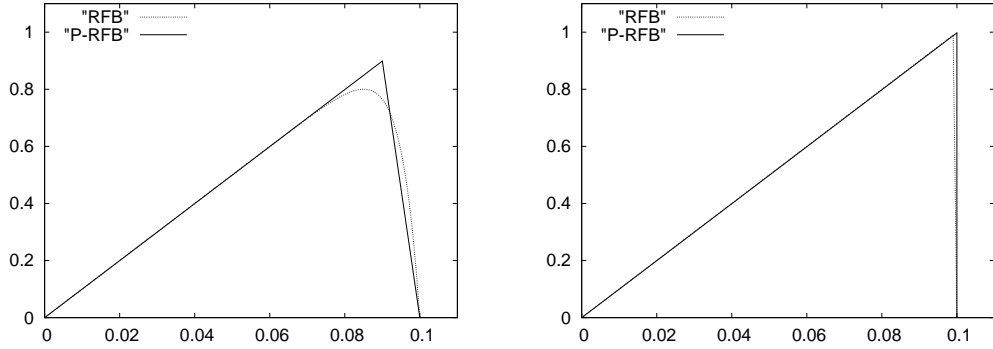


Figure 2.2. Comparison of exact solution (curved line) of the optimal bubble with its piecewise linear approximation for problem parameters $\epsilon = 0.005$, $\beta = 1$, $\sigma = 0.001$ (left) and $\epsilon = 0.0001$, $\beta = 1$, $\sigma = 0.001$ (right).

f , which is as complicated as solving the original differential equation. Therefore, it is important to bring a cheap approximation to the bubble function which gives a similar stabilization effect as shown in Fig. 2.2 .

2.2. Pseudo - RFB in One Dimension

In order to make an efficient linear approximation to the bubbles, locations of sub-grid nodes are crucial. This is accomplished by a minimization process with respect

to L_1 norm in the presence of layers (Şendur & Neslitürk 2011). Let z_1 and z_2 be two sub-grid in a typical element $K = (x_{k-1}, x_k)$ such that $x_{k-1} < z_1 < z_2 < x_k$ on which we approximate the bubble functions. Assume that f is a piecewise linear function with respect to discretization. Then the residual in (2.5) becomes a linear function and it is reasonable to consider bubble functions B_i ($i = 1, 2$) defined by

$$\mathcal{L}B_i = -\mathcal{L}\varphi_i \quad \text{in } K, \quad B_i = 0 \quad \text{on } \partial K, \quad i = 1, 2, \quad (2.8)$$

where φ_1, φ_2 are the restrictions of the piecewise linear basis functions for V_L to K . Further define B_f such that

$$\mathcal{L}B_f = f \quad \text{in } K, \quad B_f = 0 \quad \text{on } \partial K. \quad (2.9)$$

Let $B_i^*(x) = \alpha_i b_i(x)$ be the classical Galerkin approximation of B_i through (2.8), that is

$$a(B_i^*, b_i)_K = (-\mathcal{L}\varphi_i, b_i)_K, \quad i = 1, 2, \quad (2.10)$$

where b_i is a piecewise linear function with

$$b_i(x_{k-1}) = b_i(x_k) = 0, \quad b_i(z_i) = 1, \quad i = 1, 2. \quad (2.11)$$

Using numerical integration and properties of bubble functions one can get explicit expressions of α_1 and α_2 as follows:

$$\alpha_1 = \frac{3\beta + (\xi - 2h)\sigma}{2h(\frac{3\epsilon}{\xi(h-\xi)} + \sigma)}, \quad \alpha_2 = -\frac{3\beta + (2h - \eta)\sigma}{2h(\frac{3\epsilon}{\eta(h-\eta)} + \sigma)}, \quad (2.12)$$

where $\xi = z_1 - x_{k-1}$, $\eta = x_k - z_2$, $\delta = z_2 - z_1$. Now it remains to choose z_i . The main idea behind determining the locations of sub-grid nodes is to minimize residual with respect to L_1 norm coming out from equation (2.8). That is, choose z_i such that

$$J_i = \int_K |\mathcal{L}B_i^* + \mathcal{L}\varphi_i| dx, \quad i = 1, 2, \quad (2.13)$$

is minimum (Şendur & Neslitürk 2011).

2.2.1. Diffusion - Dominated Regime

The problem is assumed to be diffusion - dominated when $6\epsilon > \beta h^2/9$ (Şendur & Neslitürk 2011). In this regime, stabilization is not needed and a uniform sub-grid is chosen as $\xi = \eta = \delta = h/3$ (Şendur & Neslitürk 2011).

2.2.2. Convection - Dominated Regime

The problem is convection - dominated if $6\epsilon < \beta h^2/9$ with $3\beta \geq \sigma h$. The following lemma which is given in (Şendur & Neslitürk 2011) suggests an optimal position for z_2 .

Lemma 1 In convection - dominated case, the point $\eta_e = \frac{-3\beta + \sqrt{9\beta^2 + 24\epsilon\sigma}}{2\sigma}$ minimizes the integral (2.13) for $i = 2$.

There are several possibilities for ξ in convection - dominated regime. To determine the optimal ξ , we look at the errors in L_2 norm for various values of ξ . We set the diffusion coefficient $\epsilon = 10^{-5}$, the convective field to $\beta = 1$ and reaction term to $\sigma = 1$ with external source $f = 1$. From Fig. 2.3 we can see that optimal ξ is $h - \eta$ and error in L_2 norm is of order 2. Thus in convection - dominated regime we take $\eta = \eta_e$ and $\xi = h - \eta$.

2.2.3. Reaction - Dominated Regime

In reaction - dominated regime position of z_2 is as in convection - dominated regime. Note that the problem is in reaction - dominated regime if $6\epsilon \leq \beta h^2/9$ with $3\beta < \sigma h$. After the minimization of the integral J_1 , ξ , η and δ are suggested as follows in (Şendur & Neslitürk 2011):

$$\xi_e = \frac{3\beta + \sqrt{9\beta^2 + 24\epsilon\sigma}}{2\sigma}, \quad \eta = \eta_e, \quad \xi = \min\{h - \eta, \xi_e\}, \quad \delta = (h - \eta - \xi). \quad (2.14)$$

2.3. Numerical Experiments

In this section, we report some numerical experiments to illustrate the performance of P-RFB (Şendur & Neslitürk 2011), Link - Cutting Bubble Strategy (Brezzi et al. 2003)

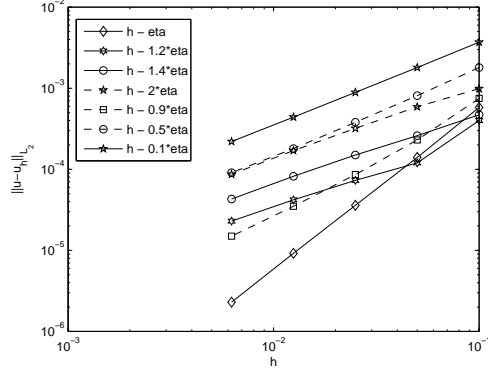


Figure 2.3. Optimal ξ in convection - dominated regime.

and SUPG method. Stabilization parameter $\tau = 1/(2\sigma + \frac{2\beta}{h} + \frac{12\epsilon}{h^2})$ for SUPG method is taken from (Asensio et al. 2007). In this chapter all tests are done in the unit interval (0.1) and uniform meshes are used.

2.3.1. Test 1 (Diffusion - Dominated Regime)

We start with the advection - diffusion - reaction problem (2.1) subject to homogeneous Dirichlet boundary condition when the problem is diffusion dominated. The diffusion coefficient is set to $\epsilon = 1$. The convective field is set to $\beta = 1$ and the reaction term to $\sigma = 1$ with external force $f = 1$. Table 2.1. and Table 2.2. show the values of errors in L_2 and H_1 norms for $h = 0.05, 0.025, 0.0125, 0.00625$, respectively. Fig 2.4.

Table 2.1. Errors in L_2 norm for various values of h when the problem (2.1) is in diffusion - dominated regime.

	h=0.05	h=0.025	h=0.0125	h=0.00625
P-RFB	0.00018	0.000046	0.000011	0.0000029
LCB	0.00019	0.000047	0.000011	0.0000030
SUPG	0.00018	0.000045	0.000011	0.0000028

shows the error rates in L_2 and H_1 norms. In diffusion dominated regime all the three

Table 2.2. Errors in H_1 norm for various values of h when the problem (2.1) is in diffusion - dominated regime.

	h=0.05	h=0.025	h=0.0125	h=0.00625
P-RFB	0.012	0.0061	0.0030	0.0015
LCB	0.012	0.0061	0.0030	0.0015
SUPG	0.012	0.0061	0.0030	0.0015

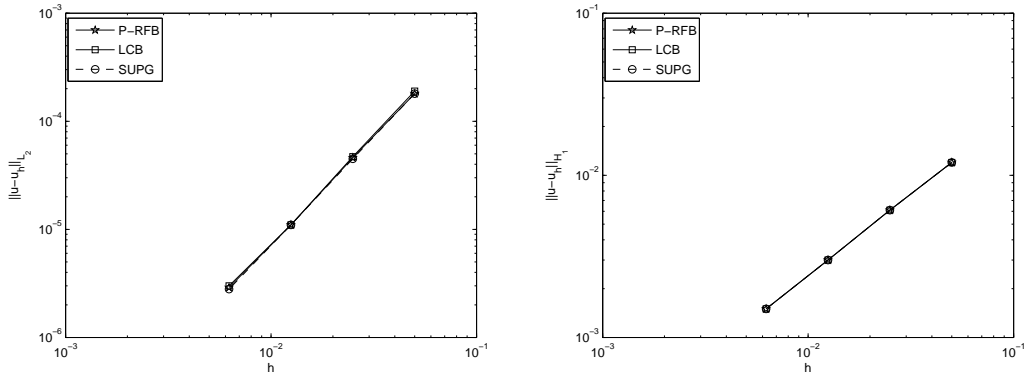


Figure 2.4. Error rates in L_2 and H_1 norms when the problem (2.1) is in diffusion - dominated regime.

methods turn into Standard Galerkin finite element method and they give approximately the same results.

2.3.2. Test 2 (Convection - Dominated Regime)

Our second numerical experiment is a test problem taken from (Brezzi et al. 2003) which is an advection - diffusion - reaction problem (2.1) subject to homogeneous Dirichlet boundary condition when the convection term is dominated. 11 nodes are used for numerical approximations. The diffusion coefficient is set to $\epsilon = 0.00001$, convection term to $\beta = 1$ and reaction term is set to $\sigma = 1$. We assume external force $f = 1$. Fig 2.5 shows the numerical approximations. Errors in L_2 and H_1 norms are reported in Table 2.3. and Table 2.4. respectively. Fig. 2.6 shows the error rates for

$h = 0.05, 0.025, 0.0125, 0.00625$. In convection - dominated regime error in L_2 norm is of order 2 and in H_1 norm is of order 1 for the three methods. SUPG method produces an oscillation near boundary layer.

2.3.3. Test 3 (Reaction - Dominated Regime)

We now consider the advection - diffusion - reaction problem (2.1) subject to homogenous Dirichlet boundary condition when reaction term is dominated. The diffusion coefficient is set to $\epsilon = 0.00001$, convective field to $\beta = 1$ and reaction term is set to $\sigma = 100$. We assume $f = 100$. For numerical approximations (Fig. 2.7) 21 nodes are used. All the methods works fine in reaction dominated regime but SUPG method produces oscillations again near boundary layers.

2.3.4. Test 4 (Internal Layer Problem)

Our last experiment is as in previous one advection - diffusion - reaction problem (2.1) subject to Dirichlet boundary condition when reaction term is dominated but an internal layer exists. The diffusion coefficient is set to $\epsilon = 0.00001$, convection term to $\beta = 1$ and reaction term is set to $\sigma = 50$. External force f is piecewise defined such that $f = -50$ for $x \leq 0.5$ and $f = 50$ for $x > 0.5$. 41 nodes are used for numerical approximations. From Fig 2.8 we can say that Pseudo - RFB is able to capture the internal layer more accurately than the other ones. SUPG method produces oscillations near both internal layer and boundary layer.

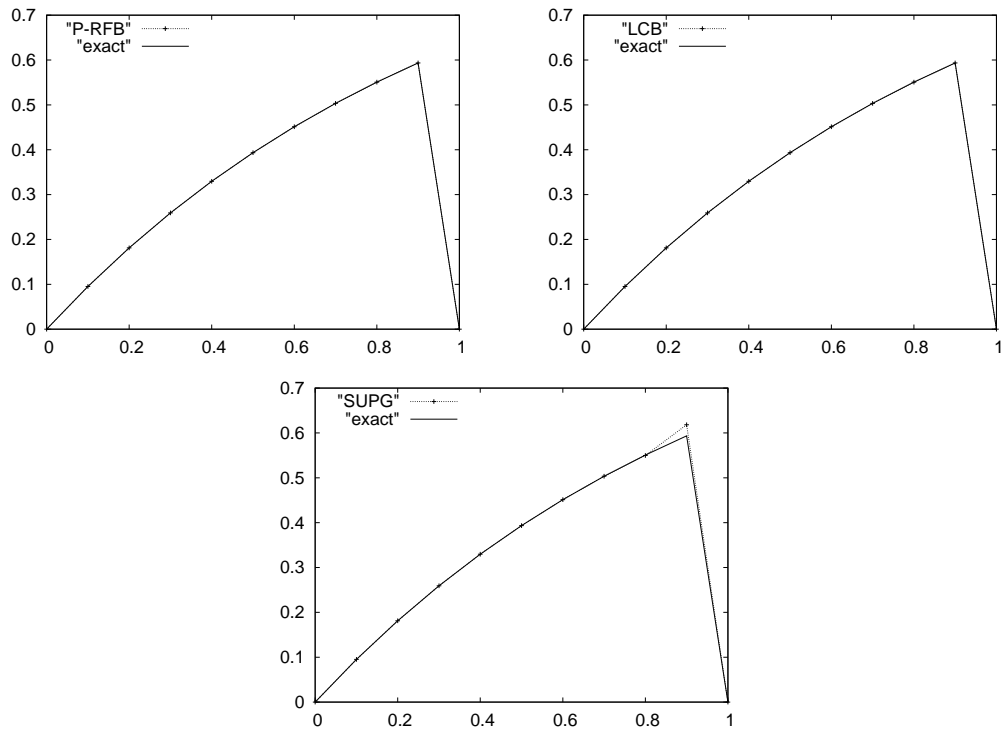


Figure 2.5. Approximate solutions when the problem (2.1) is in convection dominated regime.

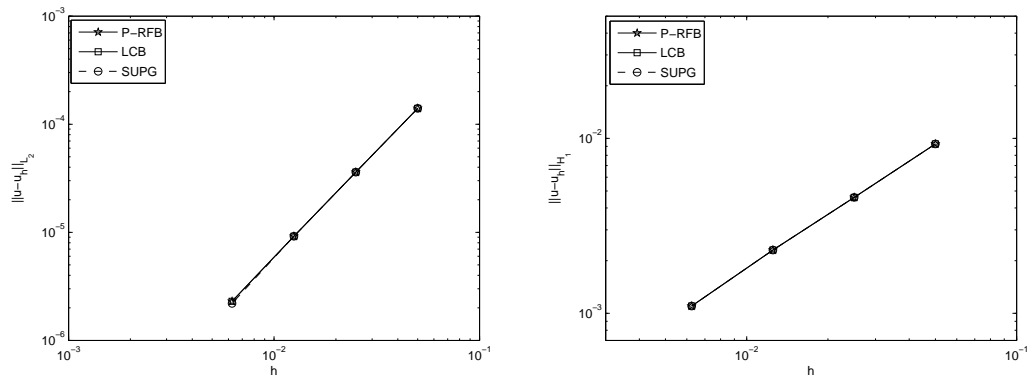


Figure 2.6. Error rates in L_2 and H_1 norms when the problem (2.1) is in convection - dominated regime.

Table 2.3. Errors in L_2 norm for various values of h when the problem (2.1) is in convection - dominated regime.

	h=0.05	h=0.025	h=0.0125	h=0.00625
P-RFB	0.00014	0.000036	0.0000092	0.0000023
LCB	0.00014	0.000036	0.0000092	0.0000023
SUPG	0.00014	0.000036	0.0000091	0.0000022

Table 2.4. Errors in H_1 norm for various h when the problem (2.1) is in convection - dominated regime.

	h=0.05	h=0.025	h=0.0125	h=0.00625
P-RFB	0.0093	0.0046	0.0023	0.0011
LCB	0.0093	0.0046	0.0023	0.0011
SUPG	0.0093	0.0046	0.0023	0.0011

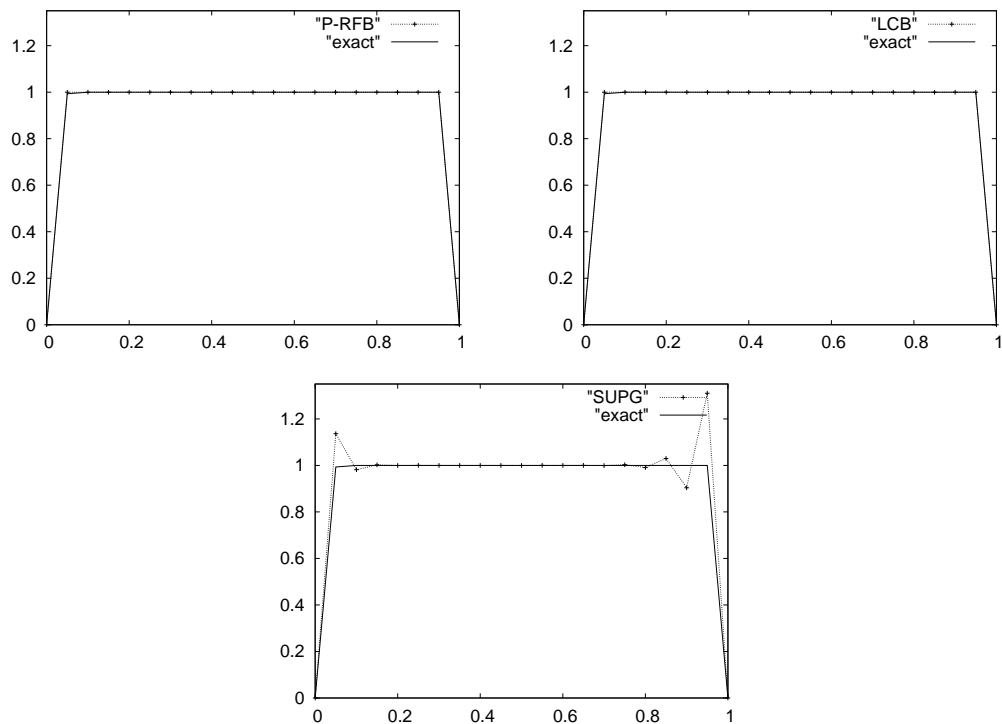


Figure 2.7. Numerical approximations when the problem (2.1) is in reaction dominated regime.

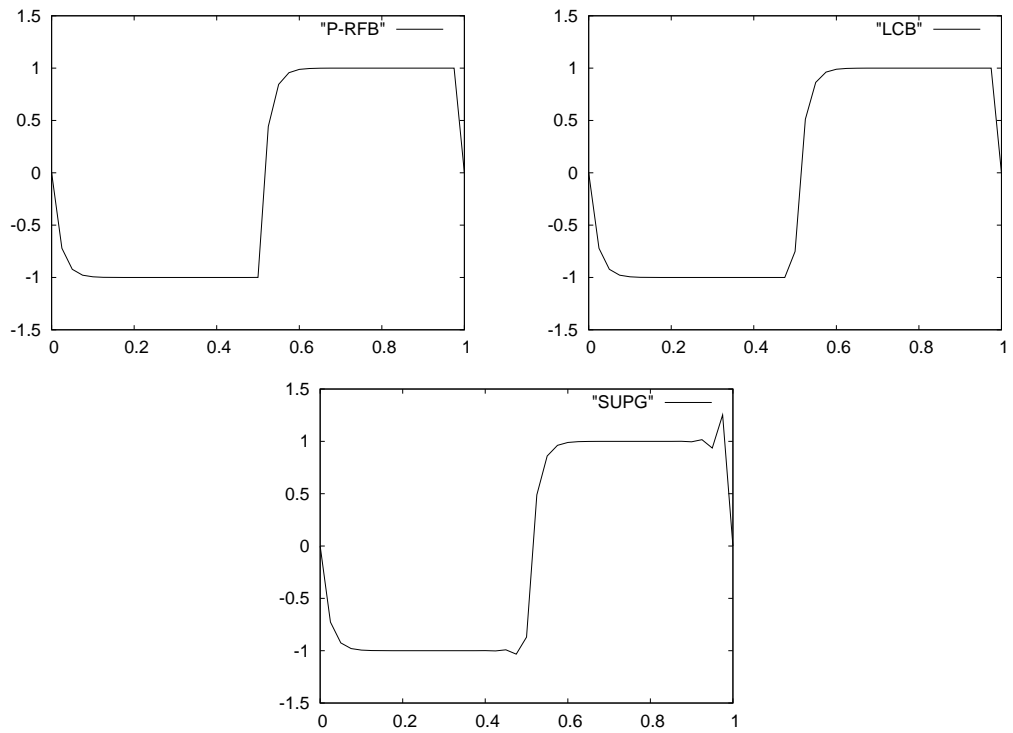


Figure 2.8. Numerical approximations with an internal layer when the problem (2.1) is in reaction dominated regime.

CHAPTER 3

PSEUDO RESIDUAL - FREE BUBBLES FOR CONVECTION - DIFFUSION - REACTION PROBLEMS IN TWO DIMENSIONS

This section is devoted to the application of the Pseudo Residual - free Bubble functions for the stabilization of two - dimensional steady convection - diffusion - reaction problems. In one dimension two sub-grid nodes are sufficient. But in two dimensions three sub-grid nodes are necessary in each triangular element to approximate the bubble functions. Presence of three sub-grid nodes in an element makes LCB strategy very difficult to apply in two dimensions. However, since only integrals of Pseudo Residual - free bubble functions are directly used in calculations without modifying the given mesh, it is easier to implement P-RFB method in two dimensions when the positions of sub-grid nodes are in hand. Positions of these three sub-grid nodes are determined by minimizing the residual of local differential problems with respect to L_1 norm as in one dimension (Şendur et al. 2012).

3.1. A Review of RFB Method in Two Dimensions

Consider the elliptic convection - diffusion - reaction problem on polygonal domain Ω in $2D$

$$\begin{cases} \mathcal{L}u = -\epsilon\Delta u + \beta.\nabla u + \sigma u = f \text{ on } \Omega, \\ u = 0 \text{ on } \partial\Omega, \end{cases} \quad (3.1)$$

where the diffusion coefficient ϵ is positive constant, convection term β and reaction term σ are non-negative constants. Let T_h be a decomposition of the domain Ω in to triangles K , and let $h_k = \text{diam}(K)$ with $h = \max_{K \in T_h} h_k$. We assume that T_h is admissible (non - overlapping triangles, their union reproduces the domain) and shape regular (the triangles verify a minimum angle condition). We start by considering the abstract variational

formulation of the problem (3.1): Find $u \in H_0^1(\Omega)$ such that

$$a(u, v) = (f, v) \quad \forall v \in H_0^1(\Omega) \quad (3.2)$$

where $a(u, v) = \epsilon \int_{\Omega} \nabla u \cdot \nabla v + \int_{\Omega} (\beta \cdot \nabla u) v + \int_{\Omega} \sigma u v$ and $(f, v) = \int_{\Omega} f v$. Define V_h as a finite dimensional subspace of $H_0^1(\Omega)$. Then standard Galerkin finite element method reads: Find $u_h \in V_h$ such that

$$a(u_h, v_h) = (f, v_h) \quad \forall v_h \in V_h. \quad (3.3)$$

We now decompose the space V_h such that $V_h = V_L \oplus V_B$, where V_L is the space of continuous piecewise linear polynomials and $V_B = \bigoplus_K B_K$ with $B_K = H_0^1(K)$. Then $v_h = v_L + v_B$ can be uniquely written where $v_L \in V_L$ and $v_B \in V_B$. From the decomposition of V_h into V_L and V_B , we require the bubble component u_B of u_h to satisfy the original differential equation in K strongly i.e.,

$$\mathcal{L}u_B = -\mathcal{L}u_L + f \quad \text{in } K \quad (3.4)$$

subject to boundary conditions,

$$u_B = 0 \quad \text{on } \partial K. \quad (3.5)$$

By the static condensation procedure, (Brezzi & Russo 1993) the method reads: Find $u_h = u_L + u_B$ in V_h such that

$$a(u_L, v_L) + a(u_B, v_L) = (f, v_L) \quad \forall v_L \in V_L. \quad (3.6)$$

The bubble component should be computed to solve (3.6). From equations (3.4) and (3.5) bubble function u_b is identified by the linear part u_L and the source function f which is as complicated as solving the original differential equation. So it is important to get a cheap approximation for the RFB functions which gives a similar stabilization effect (Şendur et al. 2012).

3.2. Pseudo RFB in Two Dimensions

In order to make an efficient linear approximation to the bubble functions, locations of sub-grid nodes are crucial. Let P_i ($i = 1, 2, 3$) be these sub-grid nodes. Location of those sub-grid nodes are determined by a minimization process with respect to L_1 norm in the presence of layers (Şendur et al. 2012). Assume that f is a piecewise linear function with respect to discretization. Then the residual in (3.4) becomes a linear function and it is reasonable to consider bubble functions B_i ($i = 1, 2$) defined by

$$\mathcal{L}B_i = -\mathcal{L}\varphi_i \quad \text{in } K, \quad B_i = 0 \quad \text{on } \partial K, \quad i = 1, 2, 3 \quad (3.7)$$

where φ_1, φ_2 and φ_3 are the restrictions of the piecewise linear basis functions for V_L to K . Further define B_f such that

$$\mathcal{L}B_f = f \quad \text{in } K, \quad B_f = 0 \quad \text{on } \partial K. \quad (3.8)$$

Since

$$u_L|_K = \sum_{i=1}^3 c_i \varphi_i \quad (3.9)$$

we can write

$$u_B|_K = \sum_{i=1}^3 c_i B_i + B_f \quad (3.10)$$

with the same coefficient c_i . From here

$$\mathcal{L}u_B = -\mathcal{L}u_L + f \quad \text{in } K. \quad (3.11)$$

That is, equation (3.4) is automatically satisfied (Şendur et al. 2012). Let $B_i^*(x) = \alpha_i b_i(x)$ be the classical Galerkin approximation of B_i through (3.7) that is,

$$a(B_i^*, b_i)_K = (-\mathcal{L}\varphi_i, b_i)_K, \quad i = 1, 2 \quad (3.12)$$

where b_i is a piecewise linear function such that

$$b_i(V_j) = 0 \quad \text{and} \quad b_i(P_i) = 1 \quad \forall i, j = 1, 2, 3 \quad (3.13)$$

where V_i are the vertices of K . From equation (3.12) one can easily get

$$\alpha_i = \frac{-(\mathcal{L}\varphi_i, b_i)}{a(b_i, b_i)} = \frac{-(\mathcal{L}\varphi_i, b_i)}{\epsilon \|\nabla b_i\|_K^2 + \sigma \|b_i\|_K^2} \quad i = 1, 2, 3 \quad (3.14)$$

where in equation (3.14) the following fact is used (Şendur et al. 2012);

$$\int_K (\beta \cdot \nabla b_i) b_i = \int_K \nabla \cdot (\beta b_i) b_i - \int_K (\nabla \cdot \beta) b_i b_i = \int_{\partial K} (\beta b_i b_i) \cdot da - \int_K 0 * b_i b_i = 0 + 0 = 0. \quad (3.15)$$

To determine the location of internal points, L_1 minimization process is applied to the following integral coming out from the bubble equation (3.7) (Şendur et al. 2012)

$$J_i = \int_K |\mathcal{L}B_i^* + \mathcal{L}\varphi_i|, \quad i = 1, 2, 3. \quad (3.16)$$

Before giving the explicit expression of internal nodes for different regimes, we will give additional notation about element geometry. Edges of K are denoted by e_i opposite to V_i , length of e_i by $|e_i|$, the midpoint of edge e_i by M_i , the outward unit normal to e_i by n^i , $\nu_i = |e_i|n^i$ and $\beta_{\nu_i} = (\beta, \nu_i)$. If $\beta_{\nu_1} < 0$, $\beta_{\nu_2} > 0$ and $\beta_{\nu_3} > 0$ then the element has only one inflow edge and if $\beta_{\nu_1} > 0$, $\beta_{\nu_2} < 0$ and $\beta_{\nu_3} < 0$ then the element has two inflow edges as depicted in Fig 3.1.

3.2.1. Diffusion - Dominated Regime

Location of P_i along the median from V_i is defined as

$$P_i = (1 - t_i)M_i + t_i V_i, \quad 0 < t_i < 1, \quad i = 1, 2, 3. \quad (3.17)$$

t_1, t_2 , and t_3 are defined for both one inflow and two inflow edge as $t_1 = t_2 = t_3 = 1/3$ (Şendur et al. 2012). That is when the problem is in diffusion dominated regime the sub-grid nodes are at the barycentre of triangular element.

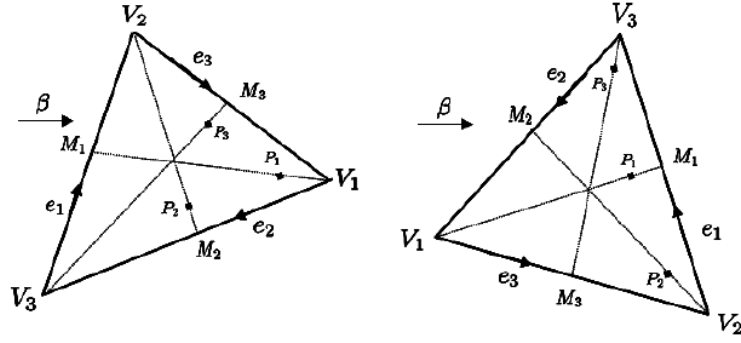


Figure 3.1. Configuration of internal nodes for element has one inflow edge (left) and two inflow edge (right).

3.2.2. Convection - Dominated Regime

We consider the both one inflow edge element and two inflow edges element and we start with one inflow edge.

3.2.2.1. One Inflow Edge

Location of P_i along the median from V_i is defined as

$$P_i = (1 - t_i)M_i + t_iV_i, \quad 0 < t_i < 1, \quad i = 1, 2, 3. \quad (3.18)$$

The problem is in convection - dominated regime if $\epsilon \leq \epsilon_1^*$ with $2\sigma|K| < \min\{\beta_{v_2}, \beta_{v_3}\}$ where

$$\epsilon_1^* = \frac{2|K|(-3\beta_{v_1} + \sigma|K|)}{9(|e_1|^2 + |e_2|^2 + |e_3|^2)}. \quad (3.19)$$

The following lemma which is given in (Şendur et al. 2012) suggests an optimal position for P_1 along the median from V_1 .

Lemma 1 If the inflow boundary make up of one edge, then the point $t_1^* = 1 - \frac{-\rho_1 + \sqrt{\rho_1^2 + \lambda_1}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 1$ in convection - dominated flows where $\rho_1 =$

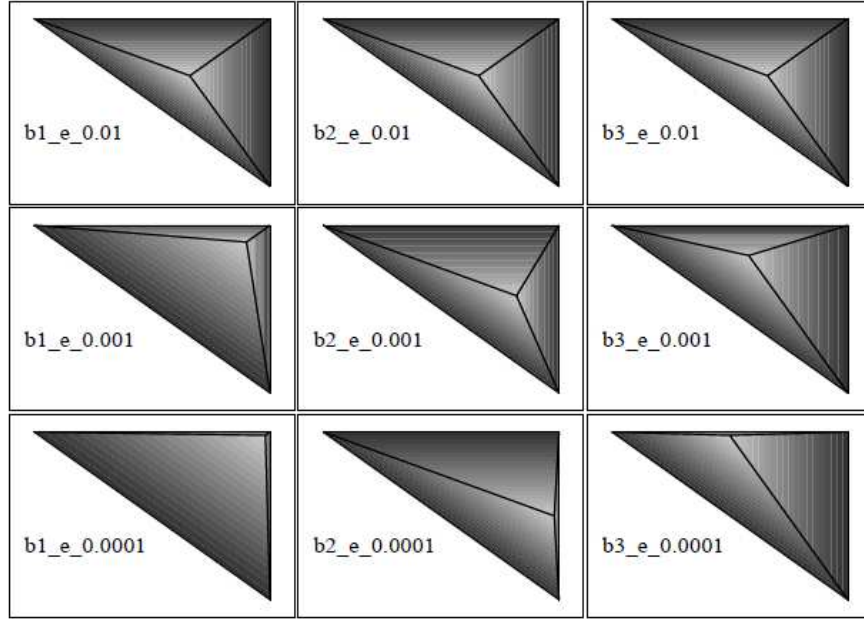


Figure 3.2. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with one inflow edge, when $\theta = 72^\circ, N = 20, \epsilon = 10^{-2}, 10^{-3}, 10^{-4}$.

$$-2\beta_{\nu_1}|K| + 3\epsilon|e_2 - e_3|^2 \text{ and } \lambda_1 = 24\epsilon\sigma|K|^2(|e_2|^2 + |e_3|^2).$$

The choice of other two points P_2 and P_3 should be consistent with the physics of the problem. Thus in convection dominated regime we take

$$\begin{cases} t_1 = t_1^* & \text{if } \epsilon < \epsilon_1^*, \\ t_1 = 1/3 & \text{otherwise,} \\ t_2 = t_3 = \min\{1/3, 1 - t_1^*\}. \end{cases} \quad (3.20)$$

In Fig 3.2 the behaviours of approximate bubble functions in a typical element K with one inflow edge, for $\beta = (\cos 72^\circ, \sin 72^\circ)$, $\sigma = 0.001$ and various ϵ are displayed. The first column of the figure represents the bubble function b_1 for decreasing values of diffusion ($\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$). The corresponding numerical results for b_2 and b_3 are shown in columns 2 and 3 respectively.

3.2.2.2. Two Inflow Edges

Now let the inflow boundary make up of two edges and let e_2 and e_3 be the inflow ones. The problem is convection dominated if $\epsilon \leq \min\{\epsilon_1^*, \epsilon_2^*\}$ where

$$\epsilon_i^* = \frac{2|K|(-3\beta_{\nu_i} + \sigma|K|)}{9(|e_1|^2 + |e_2|^2 + |e_3|^2)} \quad i = 1, 2. \quad (3.21)$$

The following lemmas suggest optimal positions for P_2 and P_3 . Proof of the lemmas are given in (Şendur et al. 2012).

Lemma 2 If the inflow boundary make up of two edges, then the point $t_2^* = 1 - \frac{-\rho_2 + \sqrt{\rho_2^2 + \lambda_2}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 2$ in convection - dominated flows where $\rho_2 = -2\beta_{\nu_2}|K| + 3\epsilon|e_1 - e_3|^2$ and $\lambda_2 = 24\epsilon\sigma|K|^2(|e_1|^2 + |e_3|^2)$.

Lemma 3 If the inflow boundary make up of two edges, then the point $t_3^* = 1 - \frac{-\rho_3 + \sqrt{\rho_3^2 + \lambda_3}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 3$ in convection - dominated flows where $\rho_3 = -2\beta_{\nu_3}|K| + 3\epsilon|e_1 - e_2|^2$ and $\lambda_3 = 24\epsilon\sigma|K|^2(|e_1|^2 + |e_2|^2)$.

For convection dominated regime, the choice of other point P_1 should be consistent with the physics of the problem. Thus we take

$$t_2 = t_2^*, \quad t_3 = t_3^*, \quad t_1 = \min\{1/3, 1 - t_2^*, 1 - t_3^*\}. \quad (3.22)$$

In Fig 3.3 the behaviours of pseudo - bubble functions in a typical element K with two inflow edge, for $\beta = (\cos 72^\circ, \sin 72^\circ)$, $\sigma = 0.001$ and various ϵ are displayed. The first column of the figure represents the bubble function b_1 for decreasing values of diffusion ($\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$). The corresponding numerical results for b_2 and b_3 are shown in columns 2 and 3 respectively.

3.2.2.3. Numerical Tests

In this section, we present some numerical experiments to assess the accuracy and performance of P-RFB method. We shall report errors in L_2 and H_1 norms and a comparison is done between SUPG and P-RFB methods in terms of L_2 and H_1 norms. In our calculations we take different partitions of domain Ω . N represents the number of element in each x and y direction for uniformly partitioned domains.

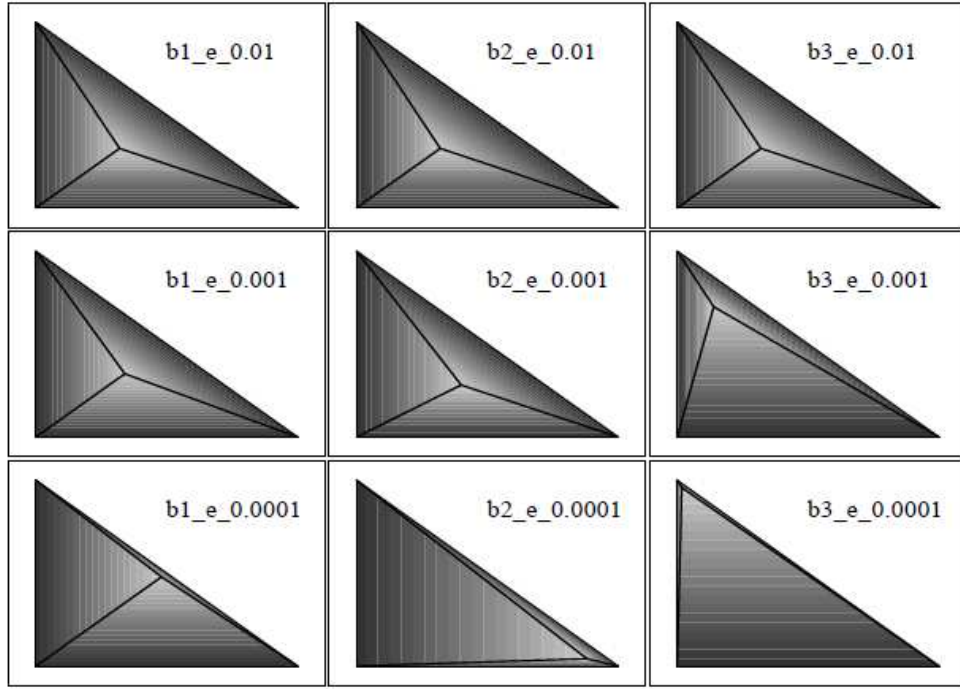


Figure 3.3. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with two inflow edge, when $\theta = 72^\circ, N = 20, \epsilon = 10^{-2}, 10^{-3}, 10^{-4}$.

Test 1 (Convection - dominated regime)

We start with considering the advection - diffusion - reaction equation (3.1) on a unit square that can be solved analytically. We consider following problem

$$-\epsilon \Delta u + (1, 0) \cdot \nabla u + \sigma u = 0, \quad (3.23)$$

subject to boundary conditions (see Fig 3.4)

$$u = \begin{cases} 0, & \text{if } y = 0, 0 \leq x \leq 1, \\ 0, & \text{if } x = 1, 0 \leq y \leq 1, \\ 0, & \text{if } y = 1, 0 \leq x \leq 1, \\ \sin(\pi y), & \text{if } x = 0, 0 \leq y \leq 1. \end{cases} \quad (3.24)$$

Analytical solution of test problem 1:

Let $u(x, y) = h(x)g(y)$ be our solution. Substituting $u(x, y)$ into the equation (3.23)

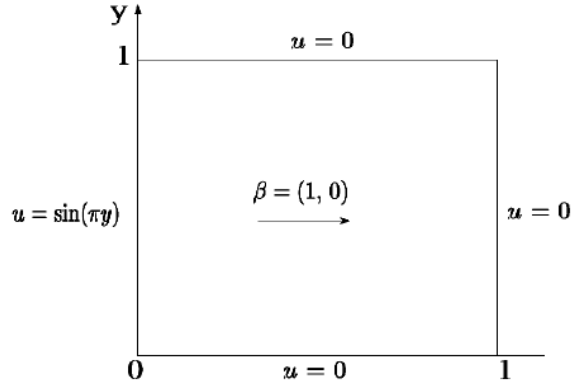


Figure 3.4. Configuration of test problem 1.

we get

$$-\epsilon h''g - \epsilon g'' + h'g + \sigma hg = 0. \quad (3.25)$$

Separating the variables in equation (3.25)

$$-\epsilon \frac{h''}{h} + \frac{h'}{h} + \sigma = \epsilon \frac{g''}{g} = -\lambda \quad (3.26)$$

where λ is a constant. From equation (3.26) and the given boundary conditions

$$\epsilon g'' + \lambda g = 0, \quad g(0) = 0, \quad g(1) = 0 \quad (3.27)$$

$$\epsilon h'' - h' - h(\lambda + \sigma), \quad h(1) = 0. \quad (3.28)$$

Equation (3.27) is a two point boundary value problem and its solution is of the form

$$g(y) = c_1 \sin\left(\sqrt{\frac{\lambda_n}{\epsilon}} y\right) \quad (3.29)$$

where $\lambda_n = \epsilon n^2 \pi^2$, $n = 1, 2, 3, \dots$ and c_1 is a constant. Solution of equation (3.28) is of

the form

$$h(x) = e^{\frac{x}{2\epsilon}} \left(c_2 \sinh \left(\frac{\sqrt{1 + 4\epsilon(\sigma + \epsilon n^2 \pi^2)}}{2\epsilon} (x - 1) \right) \right) \quad (3.30)$$

where c_2 is a constant. From superposition principle

$$u(x, y) = \sum_{n=1}^{\infty} A_n e^{\frac{x}{2\epsilon}} \sinh \left(\frac{\sqrt{1 + 4\epsilon(\sigma + \epsilon n^2 \pi^2)}}{2\epsilon} (x - 1) \right) \sin(n\pi y). \quad (3.31)$$

Using orthogonality of sin function and last boundary condition

$$A_1 = \frac{1}{\sinh \left(-\frac{\sqrt{1+4\epsilon(\sigma+\epsilon\pi^2)}}{2\epsilon} \right)}, \quad A_n = 0 \quad \text{for } n = 2, 3, \dots \quad (3.32)$$

Hence our solution is

$$u(x, y) = e^{\frac{x}{2\epsilon}} \frac{1}{\sinh \left(-\frac{\sqrt{1+4\epsilon(\sigma+\epsilon\pi^2)}}{2\epsilon} \right)} \sinh \left(\frac{\sqrt{1 + 4\epsilon(\sigma + \epsilon \pi^2)}}{2\epsilon} (x - 1) \right) \sin(\pi y). \quad (3.33)$$

Elevation plots of approximate and exact solutions for $\sigma = 10^{-3}$ and for different diffusions ($\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$) with $N = 10, 20, 40$ are represented respectively in Fig 3.5 and Fig 3.6. The columns represent the solutions with a certain ϵ and increasing N . Corresponding contour plots are represented in Fig 3.7 and Fig 3.8 respectively. In Table 3.1 and Table 3.2 errors in L_2 and H_1 norms are reported respectively. In Fig 3.9 error rates are represented in L_2 and H_1 norms respectively. It can be seen from numerical calculations that the error in L_2 norm is of order 2 and in H_1 norm is of order 1 which are the expected orders. The method works fine in limit regimes. In Fig 3.10 a comparison between SUPG and P-RFB method is represented with respect to L_2 and H_1 norm. Stabilization parameter for SUPG method $\tau = 1 / (\frac{4\epsilon}{h_k^2} + \frac{2|\beta|}{h_k} + \sigma)$ where h_k is an appropriate measure for the size of the mesh cell, is taken from (Codina 1998). SUPG and P-RFB methods approximately have the same quality in convection dominated regime.

Test 2 (Thermal boundary layer problem)

Now we consider a problem taken from (Neslitürk 1999). Let us consider a

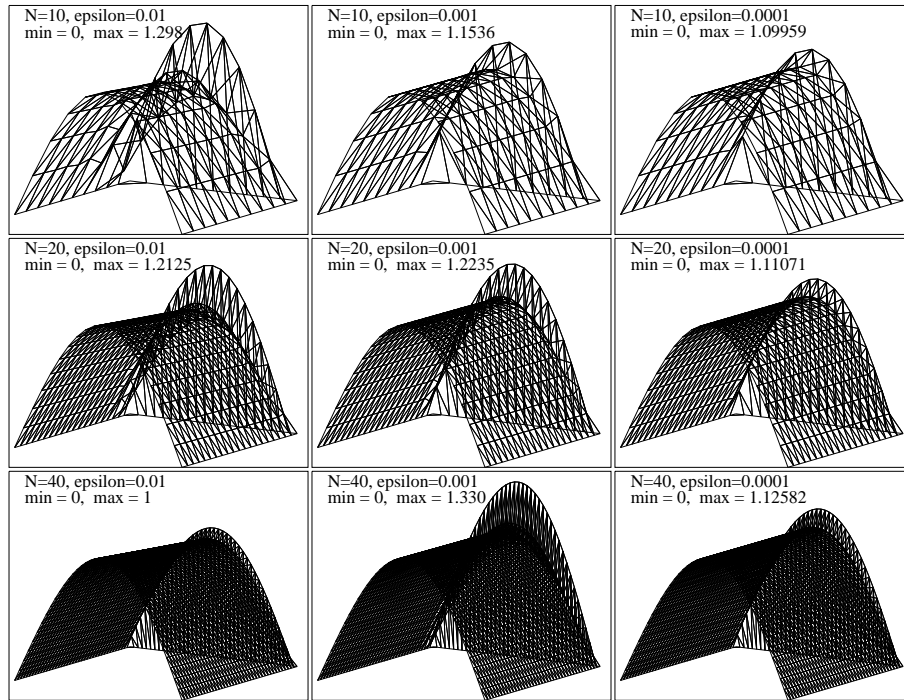


Figure 3.5. Elevation plots of approximate solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$.

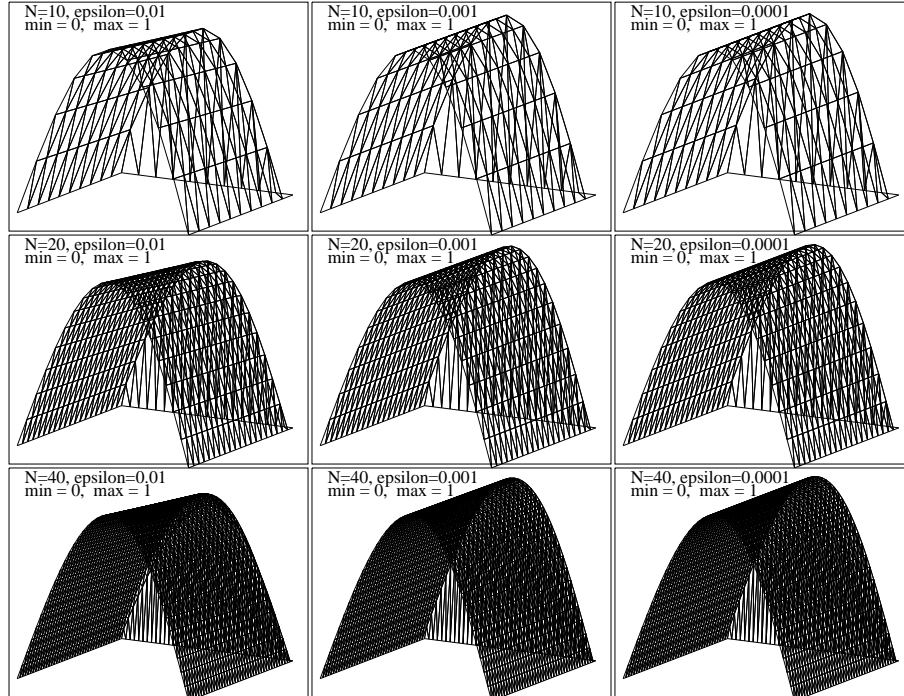


Figure 3.6. Elevation plots of exact solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$.

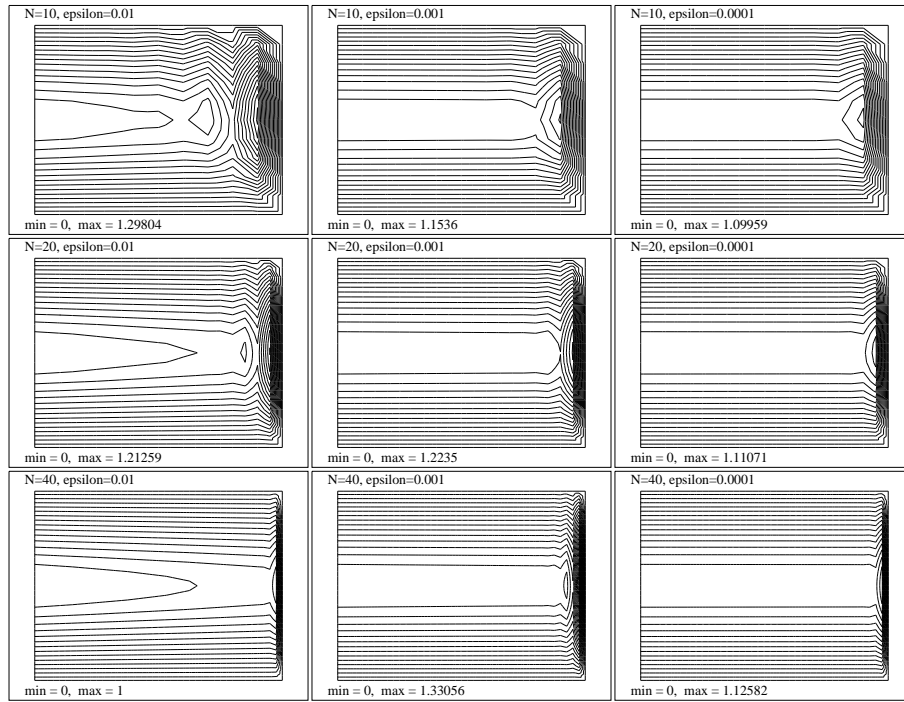


Figure 3.7. Contour plots of approximate solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$.

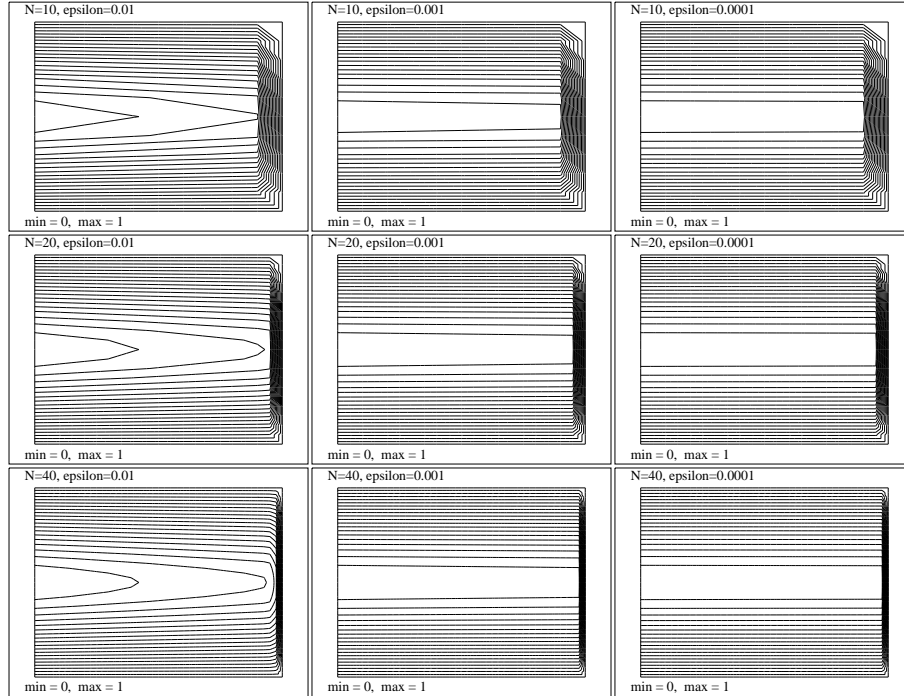


Figure 3.8. Contour plots of exact solutions of the test problem 1 for $\sigma = 10^{-3}$, $\epsilon = 10^{-2}, 10^{-3}, 10^{-4}$ with $N = 10, 20, 40$.

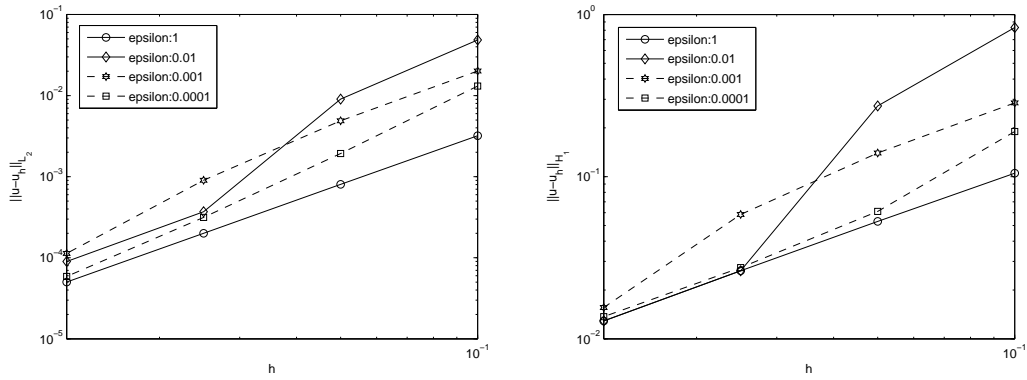


Figure 3.9. Error rates in L_2 (left) and H_1 (right) norms for the test problem 1 for different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$.

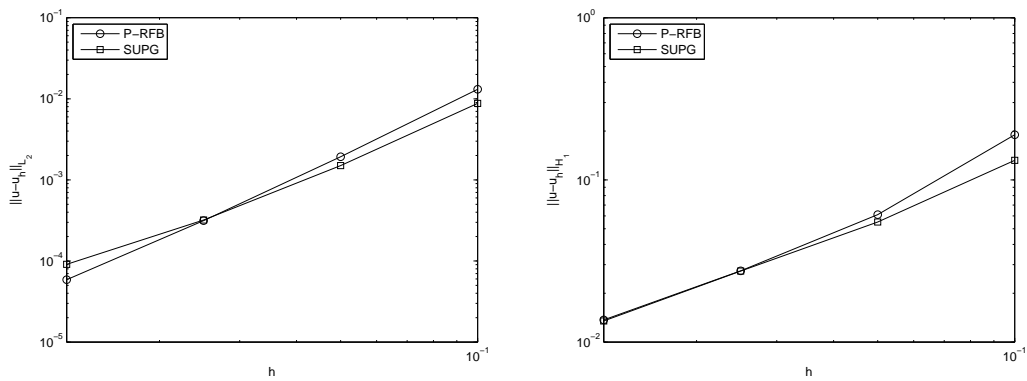


Figure 3.10. Comparison of two method with respect to L_2 norm (left) and H_1 norm (right) for $\epsilon = 10^{-4}, \sigma = 10^{-3}$ with $N = 10, 20, 40, 80$.

Table 3.1. Errors of the test problem 1 in L_2 norm for various N with $\sigma = 10^{-3}$ and different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$

	N=10	N=20	N=40	N=80
$\epsilon=1$	0.003202	0.000804	0.000200	0.0000501
$\epsilon=0.01$	0.0486	0.00905	0.000369	0.0000899
$\epsilon=0.001$	0.0201	0.00489	0.000903	0.000113
$\epsilon=0.0001$	0.0131	0.00193	0.000314	0.0000587

Table 3.2. Errors of the test problem 1 in H_1 norm for various N with $\sigma = 10^{-3}$ and different diffusions $\epsilon = 1, 10^{-2}, 10^{-3}, 10^{-4}$.

	N=10	N=20	N=40	N=80
$\epsilon=1$	0.105	0.0530	0.0263	0.01288
$\epsilon=0.01$	0.832	0.273	0.0263	0.0129
$\epsilon=0.001$	0.285	0.140	0.0585	0.0156
$\epsilon=0.0001$	0.19	0.0611	0.0275	0.0137

rectangular domain of sides 1.0 and 0.5, subject to following boundary conditions

$$u = \begin{cases} 1, & \text{if } x = 0, 0 \leq y \leq 0.5, \\ 1, & \text{if } y = 0.5, 0 \leq x \leq 1, \\ 0, & \text{if } y = 0, 0 \leq x \leq 1, \\ 2y, & \text{if } x = 1, 0 \leq y \leq 0.5. \end{cases} \quad (3.34)$$

The flow is taken as $\beta = (2y, 0)$ (see Fig 3.11). In each element we consider the variable component of flow as constant i.e. we take the average value of $2y$ at nodes in each element. This problem may be viewed as the simulation of the development of a thermal boundary layer on a fully developed flow between two parallel plates, where the top plate is moving with velocity equal to one and the bottom plate is fixed. In our test we take the diffusion $\epsilon = 10^{-5}$ and the reaction term $\sigma = 10^{-3}$. In Fig 3.12 the elevation plots of approximate solutions and corresponding contour plots are presented for $N = 10, 20, 40$.

Test 3 (Propagation of discontinuity on boundary through the wind)

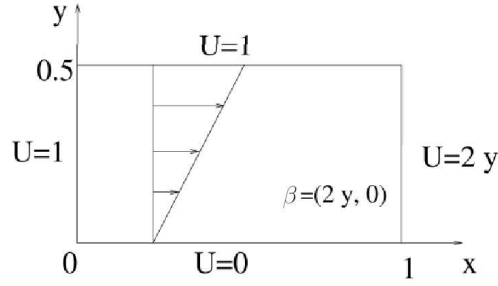


Figure 3.11. Statement of thermal boundary layer problem.

Our last problem for convection - dominated regime is about propagation of discontinuity on boundary. We use a uniform triangulations on unit square. We take diffusions $\epsilon = 10^{-2}, 10^{-3}$, convective field $\beta = (\cos 72^\circ, \sin 72^\circ)$ and reaction term $\sigma = 10^{-3}$ with $N = 20, 40, 80$. In Fig 3.13 elevation plots of approximate solutions and their corresponding contour plots are presented. The first column of the figure represents the approximate solutions and their corresponding contour plots for decreasing diffusions ($\epsilon = 10^{-2}, 10^{-3}$).

3.2.3. Reaction - Dominated Regime

Again we consider both one inflow edge element and two inflow edges element. We start with considering the two inflow edges element.

3.2.3.1. Two Inflow Edges

The problem is reaction - dominated if $\epsilon \leq \min\{\epsilon_2^*, \epsilon_3^*\}$ with $\sigma|K| > 3\beta_{\nu_1}$ (Şendur et al. 2012). Position of P_2 and P_3 are as in convection - dominated regime. It remains to define location of P_1 . Location of P_i along the median from V_i is defined as

$$P_i = (1 - t_i)M_i + t_iV_i, \quad 0 < t_i < 1, \quad i = 1, 2, 3. \quad (3.35)$$

The following lemma suggests optimal position for P_1 . Proof of the lemma is given in (Şendur et al. 2012).

Lemma 4 If the inflow boundary make up of two edges, then the point $t_1^{**} = 1 -$

$\frac{\rho_1 + \sqrt{\rho_1^2 + \lambda_1}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 1$ in reaction - dominated flows where $\rho_1 = 2\beta_{\nu_1}|K| - 3\epsilon|e_2 - e_3|^2$ and $\lambda_1 = 24\epsilon\sigma|K|^2(|e_2|^2 + |e_3|^2)$.

Thus we take t_1, t_2 and t_3 as follows (Şendur et al. 2012) :

$$\begin{cases} t_2 = t_2^*, \\ t_3 = t_3^*, \\ t_1 = \max\{\min\{1/3, 1 - t_2, 1 - t_3\}, t_1^{**}\}. \end{cases} \quad (3.36)$$

In Fig 3.14 the behaviours of pseudo - bubble functions in a typical element K with two inflow edges, for $\beta = (\cos 72^\circ, \sin 72^\circ)$, $\epsilon = 10^{-3}$ and various σ are displayed. The first column of the figure represents the bubble function b_1 for increasing values of reaction ($\sigma = 10, 100, 500$). The corresponding numerical results for b_2 and b_3 are shown in column 2 and 3 respectively.

3.2.3.2. One Inflow Edge

In this case, the problem is reaction - dominated if (Şendur et al. 2012)

$$\epsilon \leq \epsilon_1^* \quad \text{with} \quad \sigma|K| > 3\max\{\beta_{\nu_2}, \beta_{\nu_3}\}. \quad (3.37)$$

Position of P_1 is as in convection - dominated regime. It remains to define locations of P_2 and P_3 . The following lemmas suggests optimal positions for P_2 and P_3 . Proofs of the lemmas are given in (Şendur et al. 2012).

Lemma 5 If the inflow boundary make up of one edge, then the point $t_2^{**} = 1 - \frac{\rho_2 + \sqrt{\rho_2^2 + \lambda_2}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 2$ in reaction-dominated flows where $\rho_2 = 2\beta_{\nu_2}|K| - 3\epsilon|e_1 - e_3|^2$ and $\lambda_2 = 24\epsilon\sigma|K|^2(|e_1|^2 + |e_3|^2)$.

Lemma 6 If the inflow boundary make up of one edge, then the point $t_3^{**} = 1 - \frac{\rho_3 + \sqrt{\rho_3^2 + \lambda_3}}{2\sigma|K|^2}$ minimizes the integral (3.16) for $i = 3$ in reaction - dominated flows where $\rho_3 = 2\beta_{\nu_3}|K| - 3\epsilon|e_1 - e_2|^2$ and $\lambda_3 = 24\epsilon\sigma|K|^2(|e_1|^2 + |e_2|^2)$.

Thus we take t_1, t_2 and t_3 as follows (Şendur et al. 2012) :

$$\begin{cases} t_1 = t_1^*, \\ t_2 = \max\{1 - t_1, t_2^{**}\}, \\ t_3 = \max\{1 - t_1, t_3^{**}\}. \end{cases} \quad (3.38)$$

In Fig 3.15 the behaviours of pseudo - bubble functions in a typical element K with one inflow edge, for $\theta = 72^\circ$, $\epsilon = 10^{-3}$ and various σ are displayed. The first column of the figure represents the bubble function b_1 for increasing values of reaction ($\sigma = 10, 100, 500$). The corresponding numerical results for b_2 and b_3 are shown in column 2 and 3 respectively.

3.2.3.3. Numerical Tests

Now we presents three numerical experiments to asses the quality of P-RFB method in reaction dominated regime. Our first and second test show continuous transition of sub-grid nodes from one regime to another. Third test is done when the problem is reaction dominated without external source.

Test 4 (Continuous transition from one regime to another)

This test problem is convection - diffusion - reaction problem (3.1) taken from (Asensio et al. 2004). We take $\epsilon = 10^{-4}$, $\beta = (\cos 72^\circ, \sin 72^\circ)$ with various reaction terms ($\sigma = f = 0.001, 1, 10, 20, 50, 1000$) with $N = 20$. Elevation plots of approximate solutions and their corresponding contour plots are presented in Fig 3.16. From Fig 3.16 we can say that P-RFB method has continuous transition between convection - dominated regime and reaction - dominated regime.

Test 5 (Continuous transition from one regime to another)

Now, we consider convection - diffusion - reaction problem (3.1) with $\epsilon = 10^{-3}$, $f = 1$ and $\beta = (\cos 72^\circ, \sin 72^\circ)$ with homogenous Dirichlet boundary conditions. In Fig 3.17 elevation plots of approximate solutions for the given data are presented with increasing reaction from left to right and from top to bottom. From Fig 3.17 we can say that P-RFB method satisfies continuous transition between convection - dominated regime and reaction dominated regime for this problem.

Test 6 (Reaction - dominated regime)

Our last test problem is taken from (Franca & Valentin 2000). Problem configurations are displayed in Fig 3.18. In this problem we test our method with uniform

and nonuniform meshes (see Fig 3.19). Our discretizations consist of 200 and 400 elements. We take $\epsilon = 10^{-4}$, $\beta = (0.15, 0.1)$ and $f = 0$ for various values of reaction ($\sigma = 10, 10^2, 10^3$). In Fig 3.20 and Fig 3.21 elevation plots of approximate solutions and corresponding contour plots for uniform and nonuniform discretizations are presented respectively. As we see from Fig 3.20 and Fig. 3.21 when the problem is in reaction dominated regime, P-RFB method works perfect.

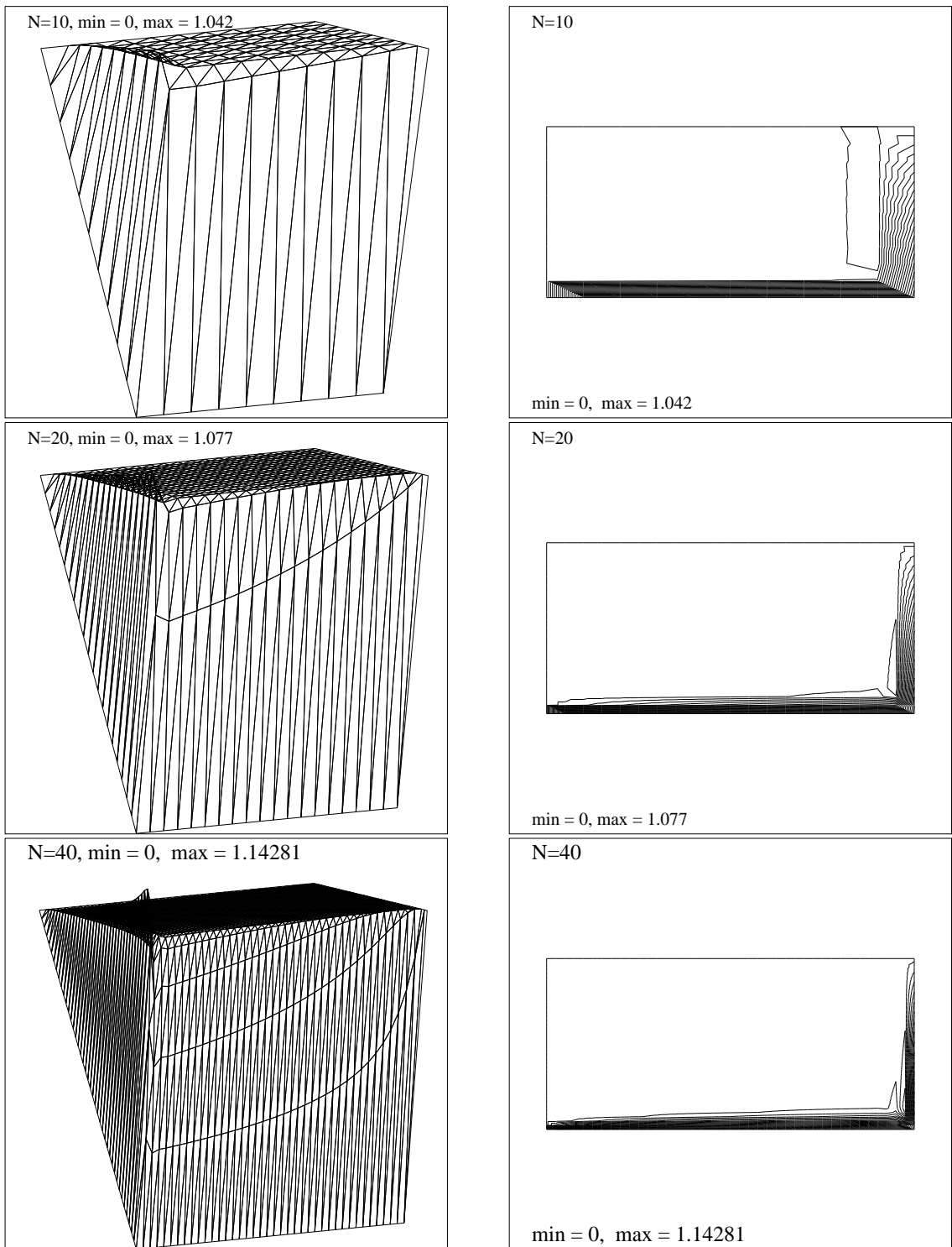


Figure 3.12. Elevation plots (left) of approximate solutions of the test problem 2 and corresponding contour plots (right).

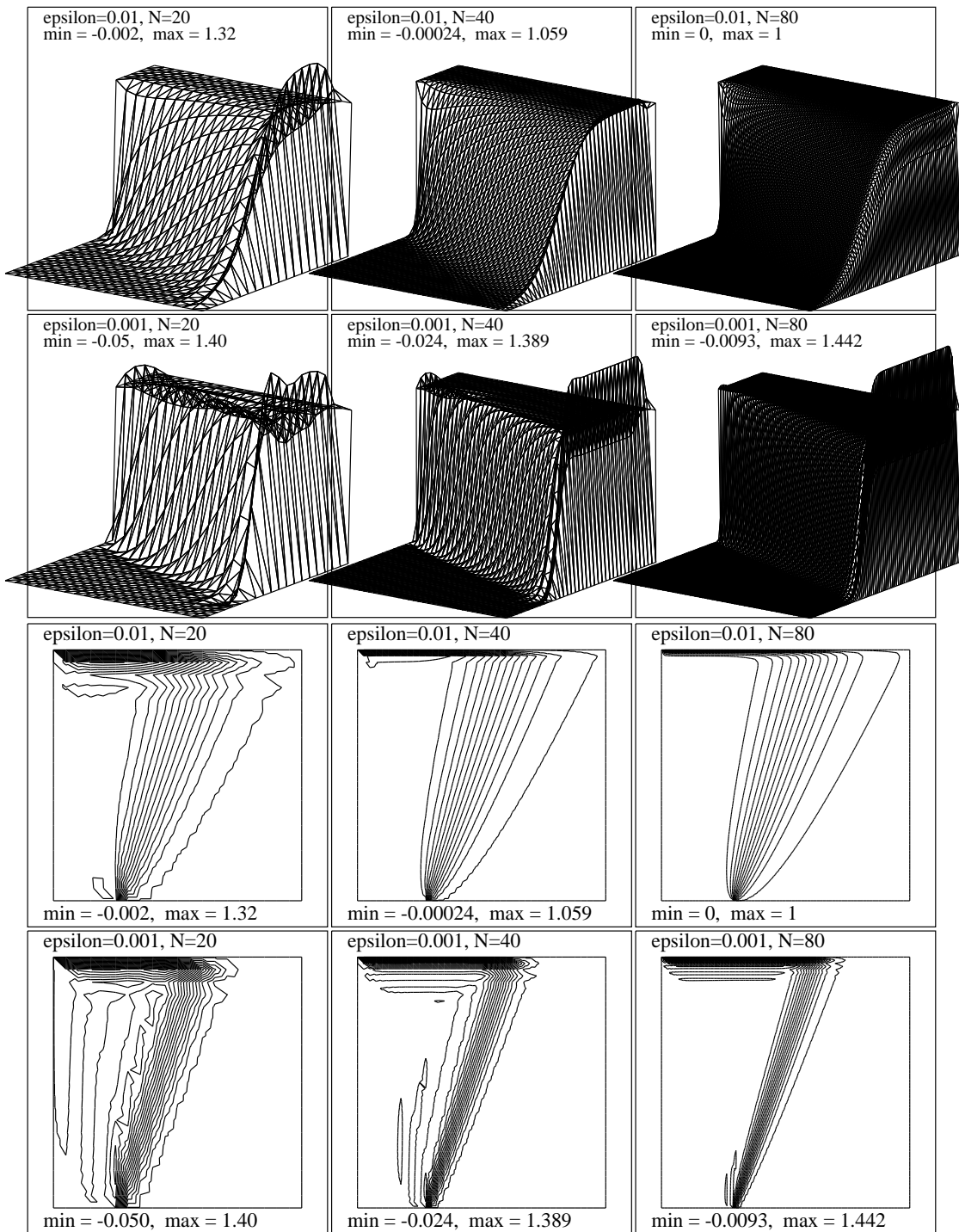


Figure 3.13. Elevation plots of approximate solutions of the test problem 3 (top) and corresponding contour plots (below).

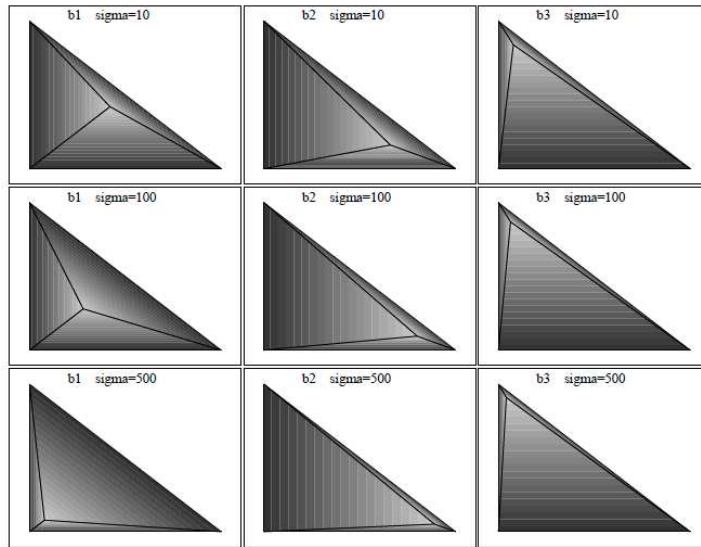


Figure 3.14. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with two inflow edge, when $\theta = 72^\circ, N = 10, \epsilon = 10^{-3}$ and $\sigma = 10, 100, 500$.

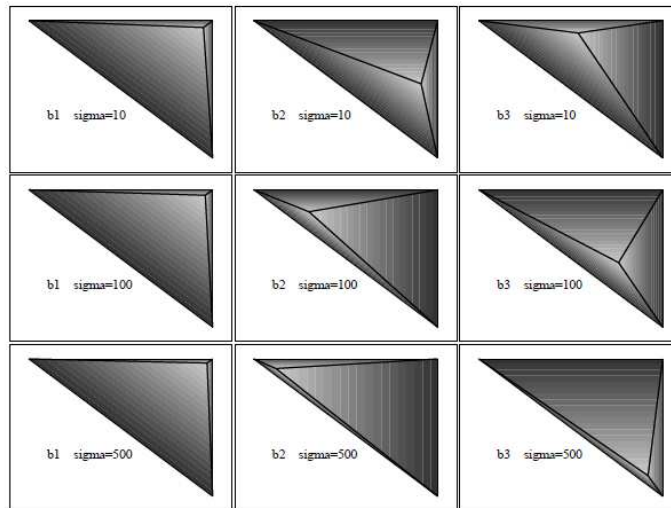


Figure 3.15. Pseudo - bubble functions b_1 , b_2 and b_3 in a typical element with one inflow edge, when $\theta = 72^\circ, N = 10, \epsilon = 10^{-3}$ and $\sigma = 10, 100, 500$.

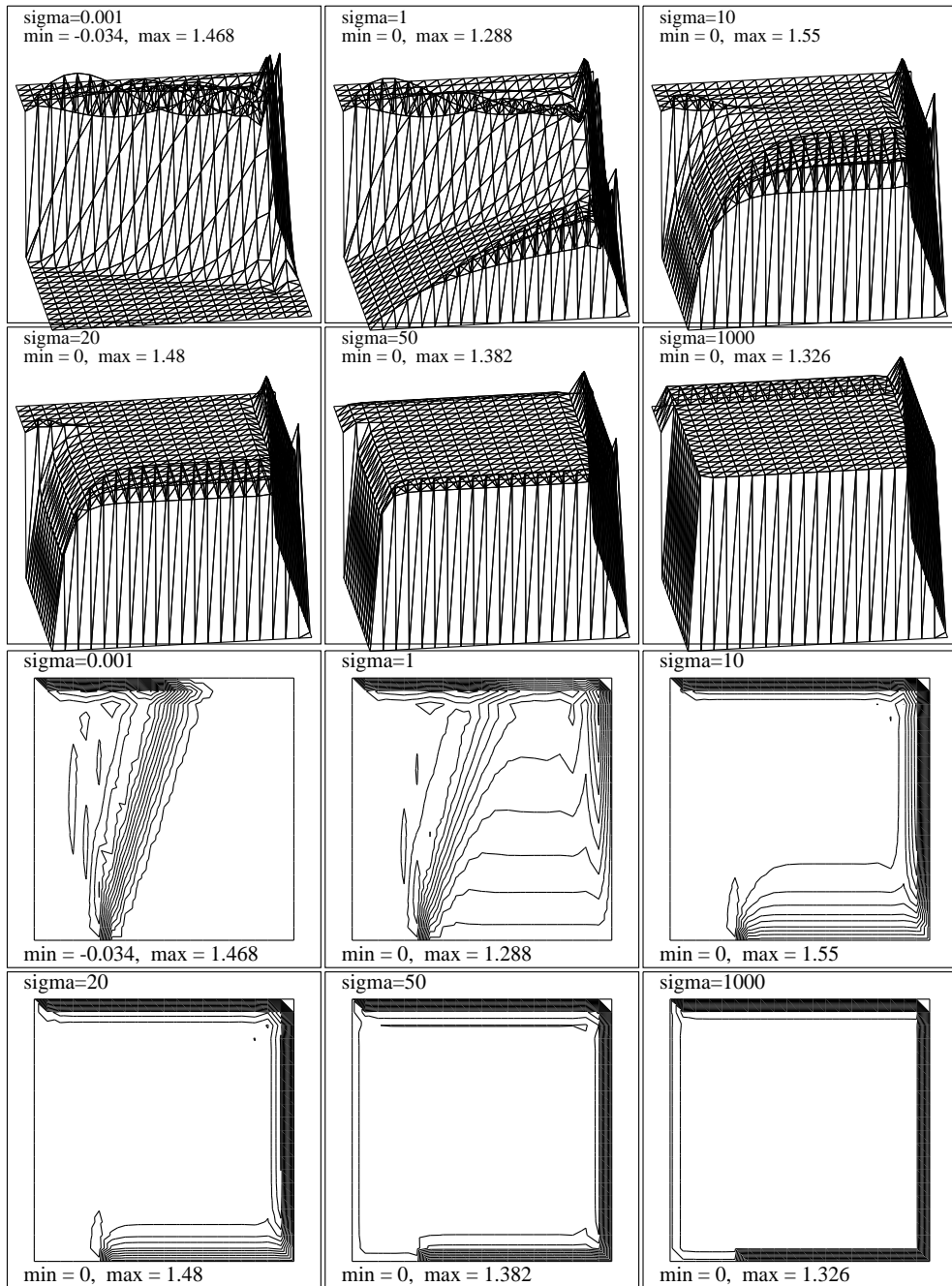


Figure 3.16. Elevation plots (top) of approximate solutions and corresponding contour plots of test problem 4 for $\epsilon = 10^{-4}$ $\beta = (\cos 72^\circ, \sin 72^\circ)$ and various reaction terms ($\sigma = f = 0.001, 1, 10, 20, 50, 1000$).

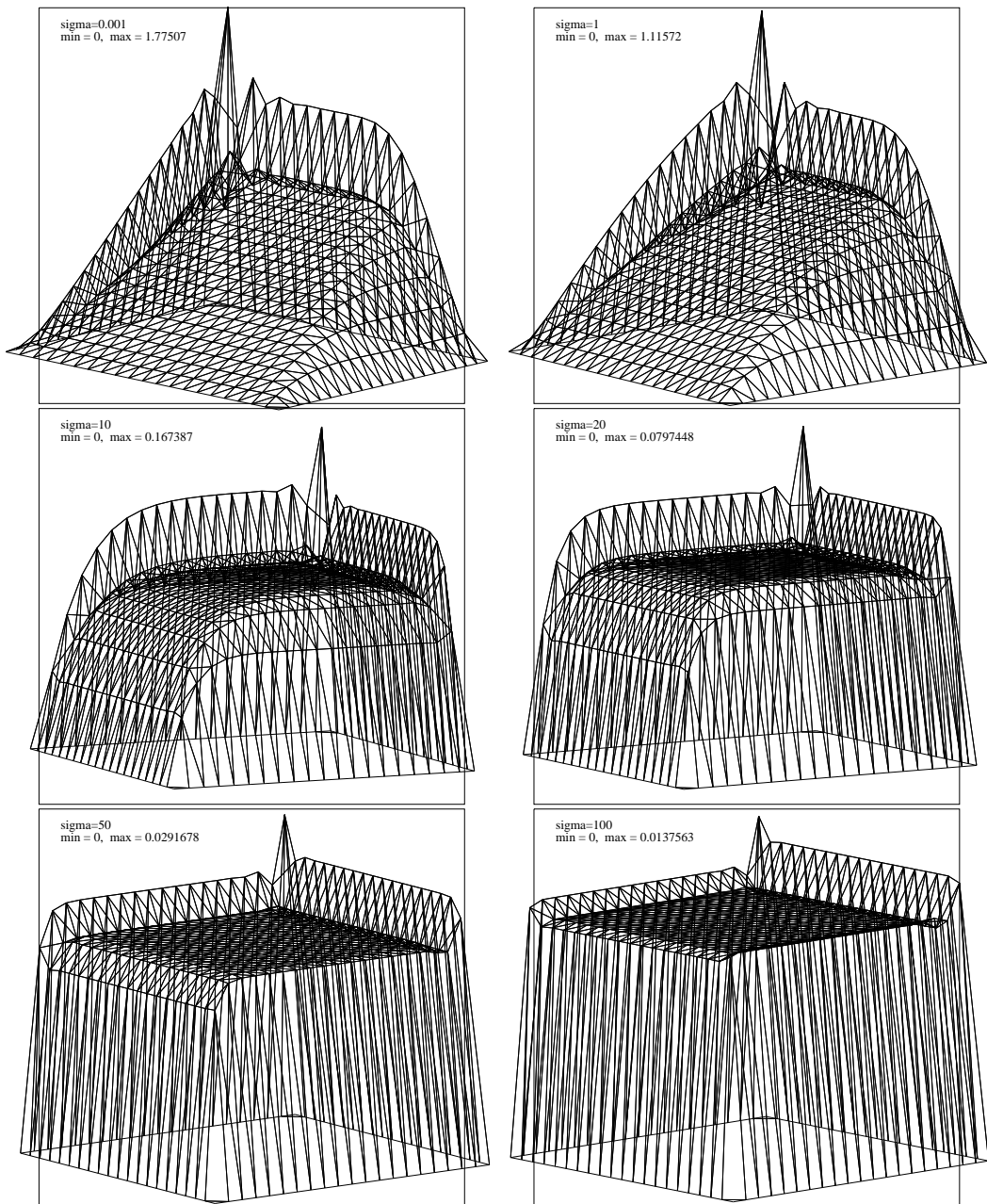


Figure 3.17. Elevation plots (left) of approximate solutions of the test problem 2 and corresponding contour plots (right).

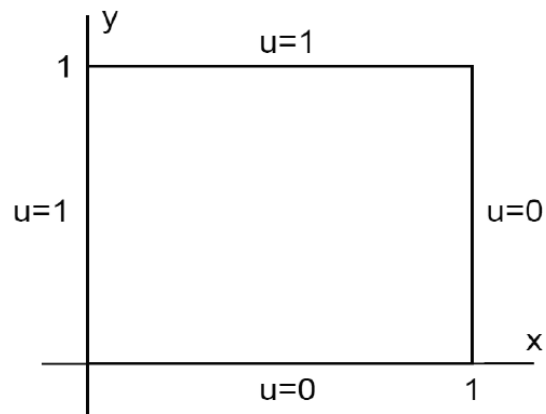


Figure 3.18. Configuration of test problem 6.

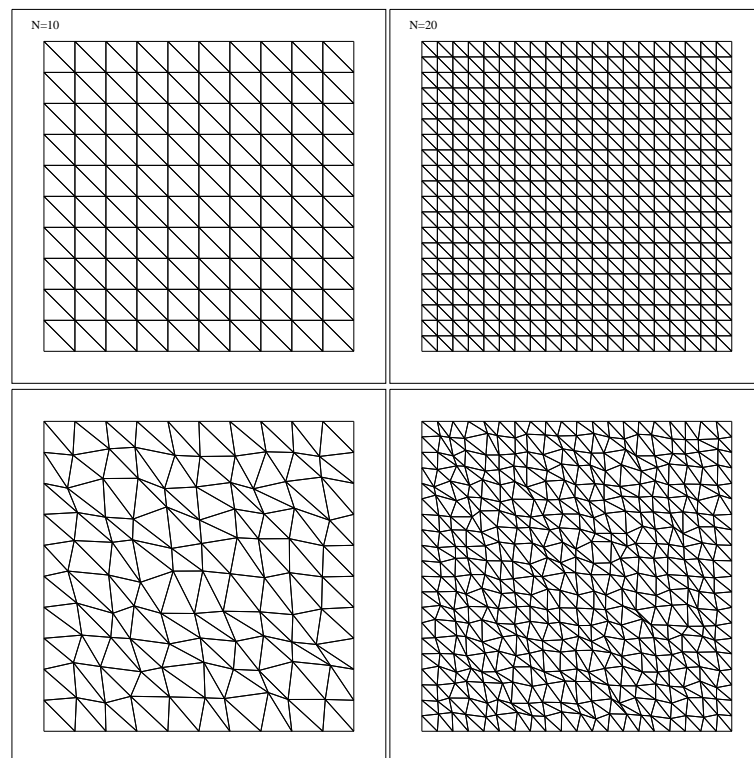


Figure 3.19. Uniform (top) and nonuniform (below) triangular elements used in discretization of the domain of the test problem 6.

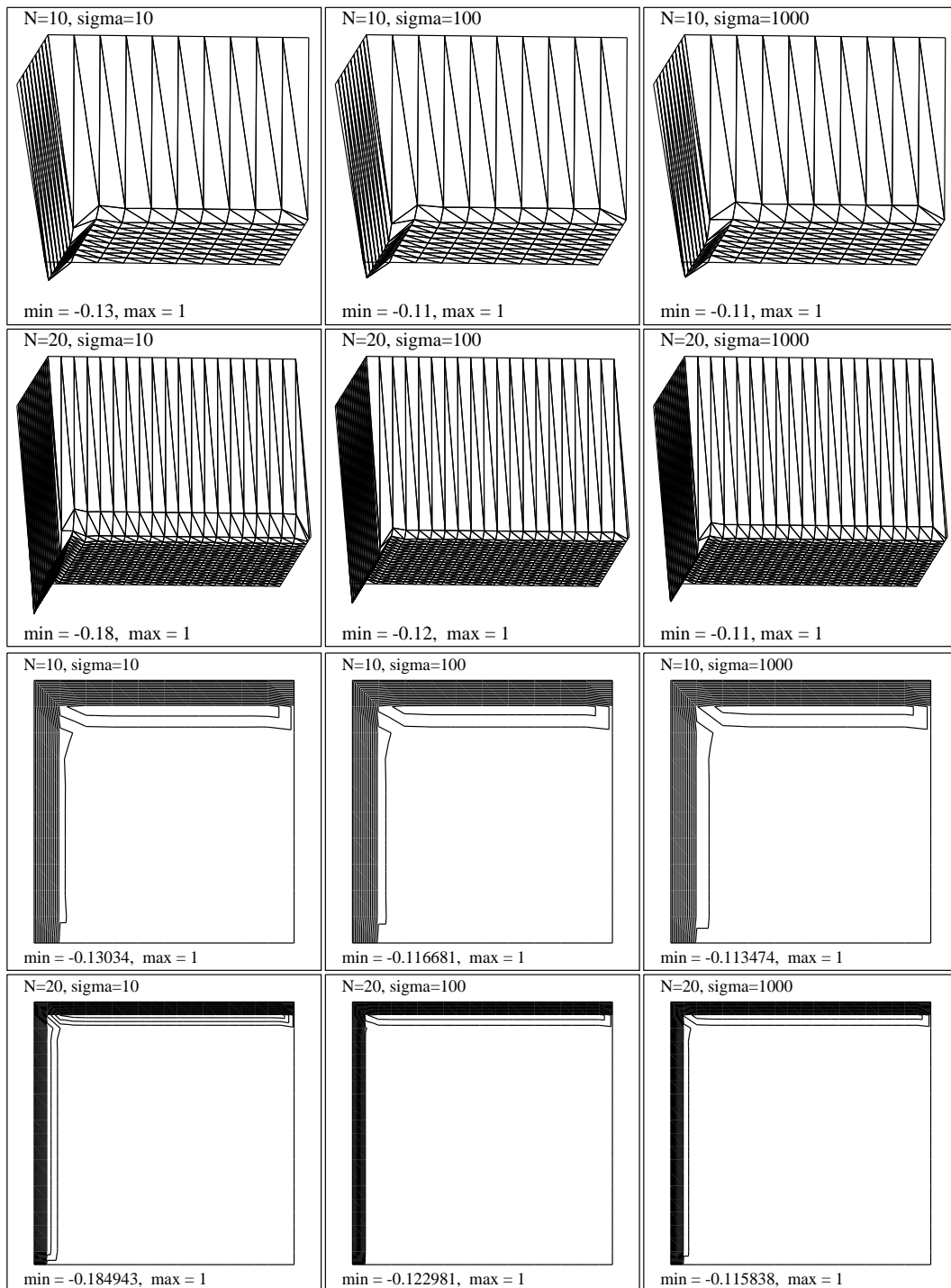


Figure 3.20. Elevation plots (top) of approximate solutions of test problem 6 and corresponding contour plots (below) in reaction dominated regime with uniform meshes.

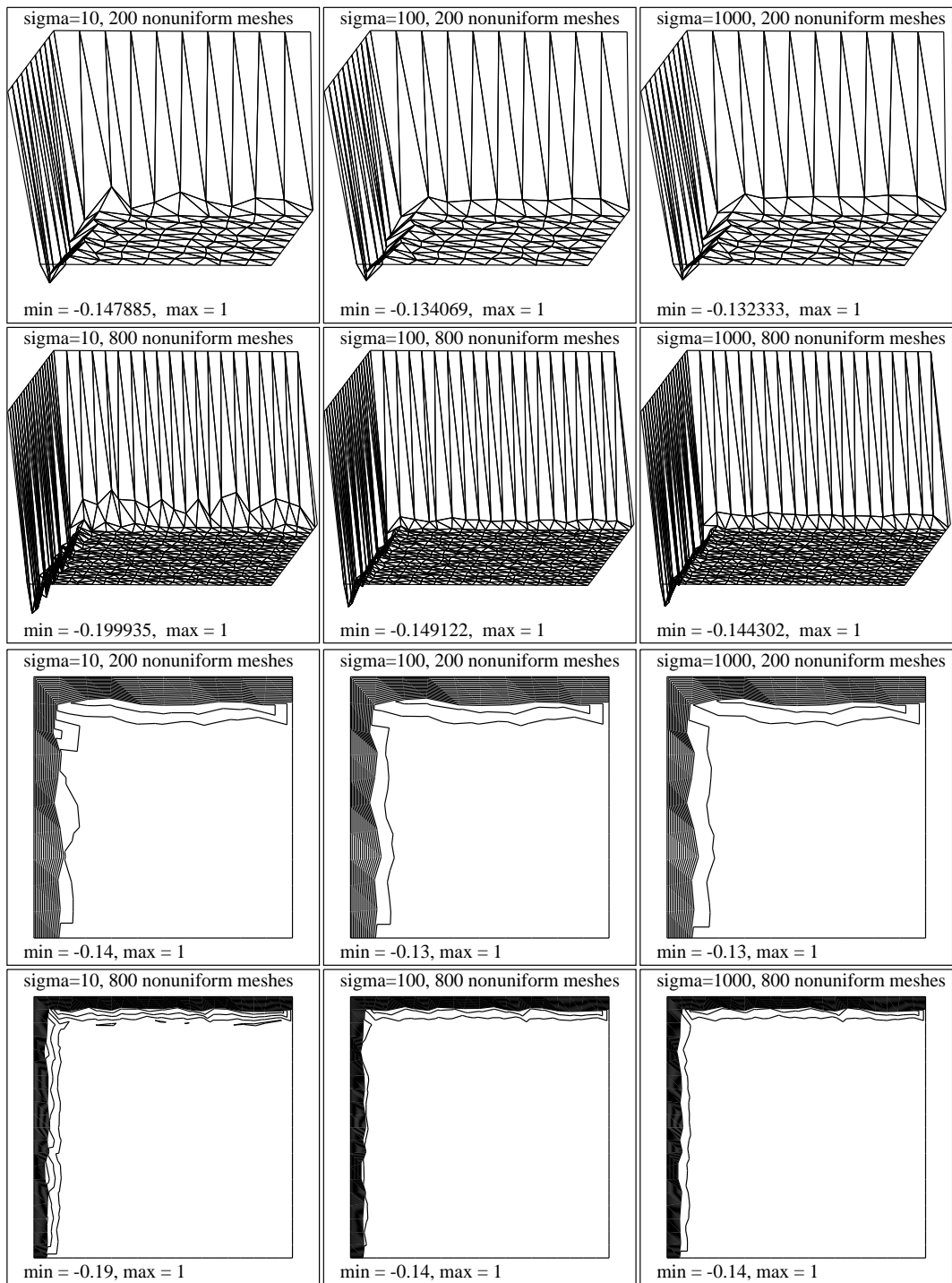


Figure 3.21. Elevation plots (top) of approximate solutions of test problem 6 and corresponding contour plots (below) in reaction dominated regime with nonuniform meshes.

CHAPTER 4

PSEUDO RESIDUAL - FREE BUBBLES FOR UNSTEADY CONVECTION - DIFFUSION - REACTION PROBLEMS

4.1. Pseudo Residual - Free Bubbles for Unsteady Convection - Diffusion - Reaction Problems in One Dimension

In this section we focus on unsteady convection - diffusion - reaction problem for the case of small diffusion. The standard Galerkin method produces undesired oscillations with well - known time discretizations. To cure this situation we apply Pseudo - RFB method to unsteady convection - diffusion - reaction problem (4.1) and we compare results with SUPG and LCB for different initial conditions and problem parameters. For the unsteady problem we have two types of partial differentiation of different nature. On the one hand we discretize first in space then we use a time integrator which is referred as *FEs_FDt*. On the other hand we first discretize time derivative then discretize in space resulting family of steady differential equations which is referred as *FDt_FEs*. The first is generally known as **method of lines** and second is known as **horizontal method of lines**. In both cases we use Crank - Nicolson scheme which is second order accurate and unconditionally stable. For space discretization we use stabilized finite element methods Pseudo - RFB (Şendur & Neslitürk 2011), Link - Cutting Bubble (LCB) (Brezzi et al. 2003) and Stream Line Upwind Petrov Galerkin (SUPG) method. We consider the following problem;

$$\begin{cases} u_t - \epsilon u_{xx} + \beta u_x + \sigma u = f(x) & \text{in } I \times (0, T), \\ u = 0 & \text{on } \partial I \times (0, T), \\ u = u^0 & \text{on } I \times \{0\}, \end{cases} \quad (4.1)$$

where I is the interval $(0, L)$ and the coefficients $\epsilon > 0$ and $\sigma \geq 0$ and β are assumed to be piecewise constants for the sake of simplicity. Let $[0, T]$ be the time interval. Consider uniform partition $\{0 = t_0 < t_1 \dots < t_N = T\}$ of this time interval with time - step size

$\Delta t = T/N$. Then time discretization of (4.1) by Crank - Nicolson scheme gives

$$\begin{aligned} \frac{1}{\Delta t}u^{n+1} + \frac{1}{2}\mathcal{L}u^{n+1} &= \frac{1}{2}(f^{n+1} + f^n) + \frac{1}{\Delta t}u^n - \frac{1}{2}\mathcal{L}u^n, \\ n = 0, 1, \dots, N-1 \quad u^0 &= u(0), \end{aligned} \quad (4.2)$$

where $\mathcal{L} = -\epsilon\partial_{xx} + \beta\partial_x + \sigma I$ and I denotes the identity operator. After time discretization standard Galerkin reads: For $n = 0, 1, \dots, N-1$, find $u_h^{n+1} \in V_h$ such that $\forall v_h \in V_h$

$$\frac{1}{\Delta t}(u_h^{n+1}, v_h) + \frac{1}{2}a(u_h^{n+1}, v_h) = \frac{1}{2}(f^{n+1} + f^n, v_h) + \frac{1}{\Delta t}(u_h^n, v_h) - \frac{1}{2}a(u_h^n, v_h), \quad (4.3)$$

where $a(u_h^{n+1}, v_h) = \epsilon((u_h^{n+1})', v_h') + \beta((u_h^{n+1})', v_h) + \sigma(u_h^{n+1}, v_h)$. Discretizing first in space then in time, one get the same equation (4.3) for standard Galerkin method. LCB strategy reads the same equation with standard Galerkin method on augmented meshes (Asensio et al. 2007). But when calculating the sub-grid nodes in *F Dt_FEs* modified problem parameters are used. SUPG methods reads: For $n = 0, 1, \dots, N-1$, find $u_h^{n+1} \in V_h$ such that $\forall v_h \in V_h$

$$\begin{aligned} \frac{1}{\Delta t}(u_h^{n+1}, v_h) + \tau(u_h^{n+1}, \beta v_h') + \frac{1}{2}a(u_h^{n+1}, v_h) + \tau\frac{1}{2}a(u_h^{n+1}, \beta v_h') &= \\ \frac{1}{2}(f^{n+1} + f^n, v_h) + \tau\frac{1}{2}(f^{n+1} + f^n, \beta v_h') + \frac{1}{\Delta t}(u_h^n, v_h) + & \\ \tau\frac{1}{\Delta t}(u_h^n, \beta v_h') - \frac{1}{2}a(u_h^n, v_h) - \tau\frac{1}{2}a(u_h^n, \beta v_h'). & \end{aligned} \quad (4.4)$$

Stabilization parameter is taken from (Asensio et al. 2007) and for *F Dt_FEs* it is defined as

$$\tau = \left(\frac{2}{\Delta t} + \sigma + \frac{|\beta|}{h_k} + \frac{6\epsilon}{h_k^2} \right)^{-1}, \quad (4.5)$$

and for *F Es_F Dt* it is defined as

$$\tau = \left(2\sigma + \frac{2|\beta|}{h_k} + \frac{12\epsilon}{h_k^2} \right)^{-1}. \quad (4.6)$$

In extended space $V_h = V_L \oplus V_B$, P-RFB method reads: For $n = 0, 1, \dots, N-1$, find $u_h^{n+1} \in V_h$ such that $\forall v_h \in V_h$

$$\frac{1}{2}\epsilon \left((u_h^{n+1})', v_h' \right) + \frac{1}{2}\beta \left((u_h^{n+1})', v_h \right) + \left(\frac{\sigma}{2} + \frac{1}{\Delta t} \right) (u_h^{n+1}, v_h) = \frac{1}{\Delta t}(u_h^n, v_h) - \frac{1}{2}a(u_h^n, v_h) \quad (4.7)$$

where $u_h^n = c_1^n \psi_1 + c_2^n \psi_2 + c_1^n \alpha_1 b_1 + c_2^n \alpha_2 b_2 + \lambda_1 \alpha_1 b_1 + \lambda_2 \alpha_2 b_2$. Here c_1^n and c_2^n are solutions at time step n at one element nodes. ψ_1 and ψ_2 are linear basis functions and $\lambda_1 = \lambda_2 = -f/\sigma$. Since $\epsilon/2$, $\beta/2$ and $\sigma/2 + 1/\Delta t$ play the role of diffusion, advection and reaction coefficients, when calculating sub-grid nodes in *FDt_FEs* we use these modified parameters. For *FEs_FDt* original problem parameters are used to calculate the sub-grid nodes.

4.1.1. Numerical Tests

In this section we report some numerical experiments to illustrate the performance of the P-RFB method, SUPG method and LCB strategy. We compare the three methods with $L^\infty(0, T; L^1(I))$ norm and give numerical simulations for different problem parameters and different initial conditions. We take a uniform partition of unit interval into subintervals of length $h = 1/M$ where M is an integer.

4.1.1.1. Test 1 (Choice of CFL Numbers)

Our first test is unsteady convection - diffusion - reaction problem (4.1) subject to homogenous Dirichlet boundary condition. We choose a smooth initial condition which is defined in equation 4.7. We set diffusion coefficient to $\epsilon = 10^{-4}$, advection coefficient to $\beta = 1$ and reaction term to $\sigma = 10^{-3}$ with $f = 0$. We set final time to $T = 0.2$. We use 20, 40, 80, 160, 320 uniform meshes to calculate the error in $L^\infty(0, T; L^1(I))$ norm when $CFL = 1, 0.05, 0.025, 0.01$ where $CFL = \frac{\Delta t |\beta|}{h}$. We compare the three methods with respect to $L^\infty(0, T; L^1(I))$ norm at which CFL they work best in convection - dominated regime. In this respect we take 20, 40 and 80 meshes to do comparisons of methods in this regime. From Fig. 4.2 we say that Pseudo - RFB method works best when $CFL = 1$ for both *FDt_FEs* and *FEs_FDt*, LCB strategy method works best when $CFL = 0.025$ which is consistent with proposed in (Asensio et al. 2007) for both *FDt_FEs* and *FEs_FDt*. SUPG method works best when $CFL = 0.025$ for *FDt_FEs* and works best when $CFL = 0.5$ for *FEs_FDt*. From Fig. 4.1 it is easy to see that in limit regime P-RFB is the best. It is consistent because in limit regime Pseudo - RFB functions approximate RFB functions better in limiting case.

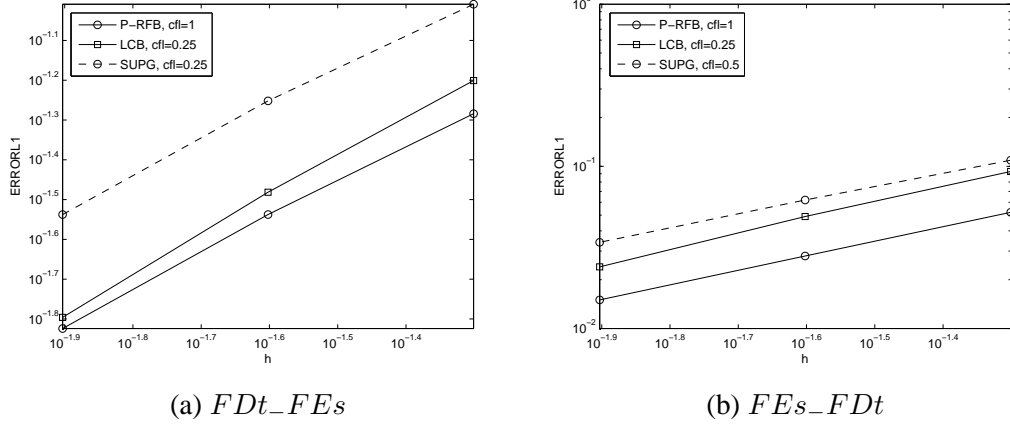


Figure 4.1. Comparisons of three methods in convection - dominated regime with respect to $L^\infty(0, T; L^1(I))$ norm.

$$u(0, x) = \begin{cases} \sin(2\pi x) & \text{if } x \leq 0.5, \\ 0 & \text{if } x > 0.5. \end{cases} \quad (4.8)$$

4.1.1.2. Test 2 (Convection - Dominated Regime)

In this test problem we have considered the equation of first test problem one but with $\epsilon = 10^{-6}$ and with initial data

$$u(0, x) = \begin{cases} 1 & \text{if } |x - 0.3| \leq 0.1, \\ 0 & \text{otherwise.} \end{cases} \quad (4.9)$$

We take 80 uniform meshes. In Fig. 4.3 approximate solutions for three methods are presented at which CFL they work best for both FDt_FEs and FEs_FDt . We see from Fig. 4.3 that results of P-RFB method are perfect for both FDt_FEs and FEs_FDt .

4.1.1.3. Test 3 (Convection - Dominated Regime with Different Initial Condition)

This test is devoted to a different initial condition:

$$u(0, x) = \begin{cases} e^{100x} \sin(10\pi x) & \text{if } 0 \leq x \leq 0.1, \\ 0 & \text{otherwise.} \end{cases} \quad (4.10)$$

We set diffusion coefficient to $\epsilon = 10^{-6}$, convective field to $\beta = 1$ and reaction term to $\sigma = 10^{-6}$ with $f = 0$. We take $M = 80$ and set the final time $T = 0.4$. In Fig. 4.4 approximate solutions for three methods are presented at which CFL number they work best. As in the previous results of test problem results of Pseudo - RFB method are perfect for this delicate initial condition.

4.1.1.4. Test 4 (Reaction - Dominated Regime)

In this test we consider the reaction dominated case with zero initial condition. We set diffusion coefficient to $\epsilon = 10^{-6}$, convective field to $\beta = 1$ and reaction term and external source to $\sigma = f = 100$. We take $M = 40$ and set the final time $T = 1.0$. In Fig. 4.5 approximate solutions for three methods are presented at which CFL number they work best. Pseudo - RFB and LCB give good results. However SUPG methods produces undesired oscillations near boundary layer.

4.2. Pseudo Residual - Free Bubbles for Unsteady Convection - Diffusion - Reaction Problems in Two Dimensions

This section is devoted to time - dependent convection - diffusion - reaction problems in two dimensions. As in one dimensional case standard Galerkin produces undesired oscillations for unsteady convection - diffusion - reaction problems in 2D. We apply P-RFB method and SUPG method to cure this situation. We discretize first in space then we use Backward-Euler for time integration which is strongly stable. Consider the

parabolic convection - diffusion - reaction problem

$$\begin{cases} \frac{\partial u}{\partial t} - \epsilon \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) + \beta \cdot \left(\frac{\partial u}{\partial x}, \frac{\partial u}{\partial y} \right) + \sigma u = f(t, x, y) \text{ on } \Omega \times (0, T), \\ u = 0 \text{ on } \partial\Omega \times (0, T), \quad u(0, x, y) = u^0 \text{ on } \Omega \times \{0\}, \end{cases} \quad (4.11)$$

where the diffusion coefficient ϵ is positive constant, convection term β and reaction term σ are non-negative constants. Let T_h be a decomposition of the domain Ω in to triangles K and let $h_k = \text{diam}(K)$ with $h = \max_{K \in T_h} h_k$. We assume that T_h is admissible (non-overlapping triangles, their union reproduces the domain) and shape regular (the triangles verify a minimum angle condition). Let $[0, T]$ be the time interval. Consider uniform partition $\{0 = t_0 < t_1 \dots < t_N = T\}$ of this time interval with time-step size $\Delta t = T/N$. Then standard Galerkin reads with time discretization of (4.11) by Backward - Euler scheme: For $n = 0, 1, \dots, N - 1$, find $u_h^{n+1} \in V_h$ such that

$$\left(\frac{u_h^{n+1} - u_h^n}{\Delta t}, v_h \right) + a(u_h^{n+1}, v_h) = (f(\cdot, t^{n+1}), v_h) \quad \forall v_h \in V_h \quad (4.12)$$

where u_h^n represents the approximation of $u(\cdot, t^n)$ and

$$a(u_h^n, v_h) = \epsilon \int_{\Omega} \left(\frac{\partial u_h^n}{\partial x}, \frac{\partial u_h^n}{\partial y} \right) \cdot \left(\frac{\partial v_h}{\partial x}, \frac{\partial v_h}{\partial y} \right) + \int_{\Omega} \beta \cdot \left(\frac{\partial u_h^n}{\partial x}, \frac{\partial u_h^n}{\partial y} \right) v_h + \int_{\Omega} \sigma u_h^n v_h. \quad (4.13)$$

Pseudo - RFB method reads in extended space $V_h = V_L \oplus V_B$: For $n = 0, 1, \dots, N - 1$, find $u_h^{n+1} \in V_h$ such that $\forall v_h \in V_h$

$$\left(\frac{u_h^{n+1} - u_h^n}{\Delta t}, v_h \right) + a(u_h^{n+1}, v_h) = (f(\cdot, t^{n+1}), v_h) \quad (4.14)$$

where $u_h^n = c_1^n \psi_1 + c_2^n \psi_2 + c_3^n \psi_3 + c_1^n \alpha_1 b_1 + c_2^n \alpha_2 b_2 + c_3^n \alpha_3 b_3 + \lambda_1 \alpha_1 b_1 + \lambda_2 \alpha_2 b_2 + \lambda_3 \alpha_3 b_3$. Here c_1^n , c_2^n and c_3^n are solutions at time step n at one element nodes. ψ_1 , ψ_2 and ψ_3 are linear basis functions. $\lambda_1 = \lambda_2 = \lambda_3 = -f/\sigma$ for external source f is constant.

SUPG methods reads: For $n = 0, 1, \dots, N - 1$, find $u_h^{n+1} \in V_h$ such that $\forall v_h \in V_h$

$$\begin{aligned} & \frac{1}{\Delta t}(u_h^{n+1}, v_h) + \tau(u_h^{n+1}, \beta \cdot \nabla v_h) + a(u_h^{n+1}, v_h) + \tau a(u_h^{n+1}, \beta \nabla v_h) = \\ & \frac{1}{2}(f^{n+1} + f^n, v_h) + \tau \frac{1}{2}(f^{n+1} + f^n, \beta \cdot \nabla v_h) + \frac{1}{\Delta t}(u_h^n, v_h) + \\ & \tau \frac{1}{\Delta t}(u_h^n, \beta \cdot \nabla v_h). \end{aligned} \quad (4.15)$$

Stabilization parameter is taken from (Asensio et al. 2007) and it is defined as

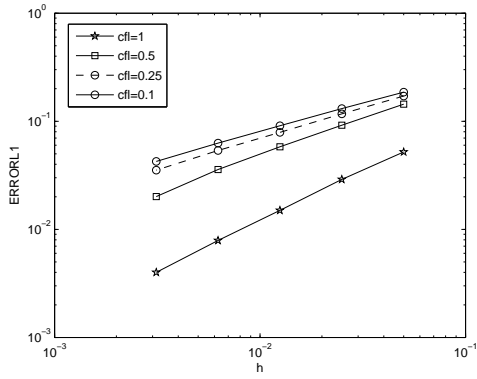
$$\tau = \left(2\sigma + \frac{2|\beta|}{h_k} + \frac{12\epsilon}{h_k^2} \right)^{-1}. \quad (4.16)$$

4.2.1. Numerical Tests

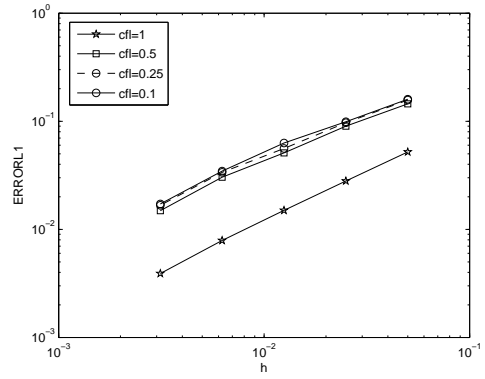
In this section we report a test problem to compare Pseudo - RFB and SUPG method. LCB strategy has not being extended to two dimensions so far. We do our test with discretizing first in space then in time with Backward - Euler scheme. We use 12800 uniform triangular elements on unit square.

4.2.1.1. Test 5 (Convection - Dominated Regime)

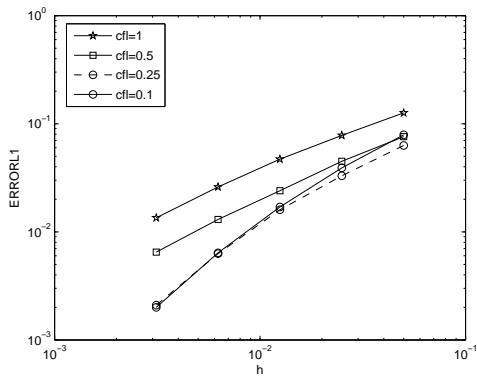
We set diffusion coefficient to $\epsilon = 10^{-5}$, advection coefficient to $\beta = (\cos(\pi/4), \sin(\pi/4))$ and reaction term to $\sigma = 10^{-3}$ with $f = 0$. We set final time to $T = 0.5$. We do 50 time steps. In Fig.4.6 and Fig.4.7 approximate solutions are presented at different time steps.



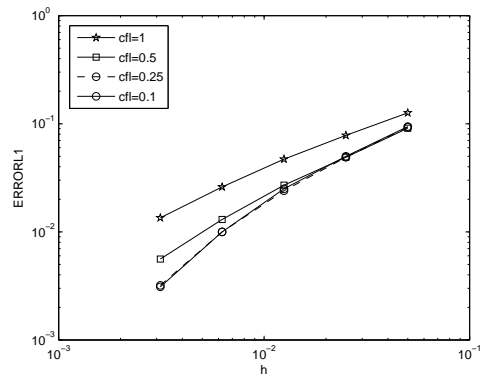
(a) P-RFB (FDt_FEs)



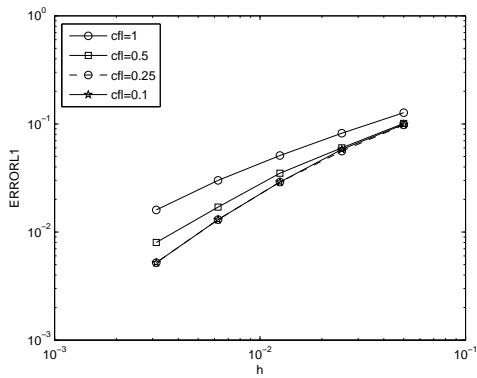
(b) P-RFB (FEs_FDt)



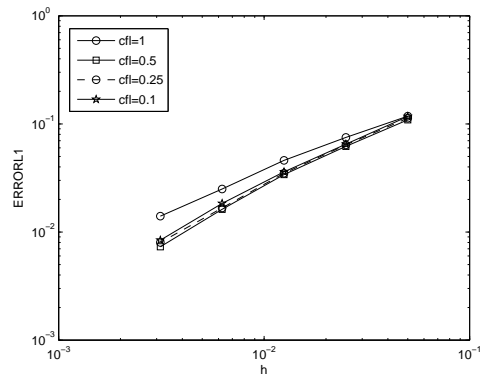
(c) LCB (FDt_FEs)



(d) LCB (FEs_FDt)

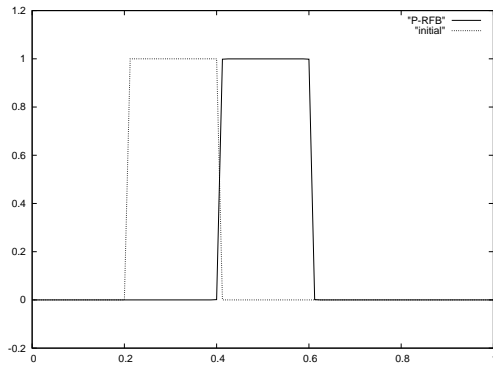


(e) SUPG (FDt_FEs)

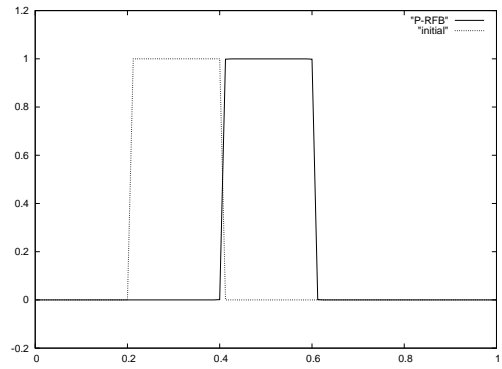


(f) SUPG (FEs_FDt)

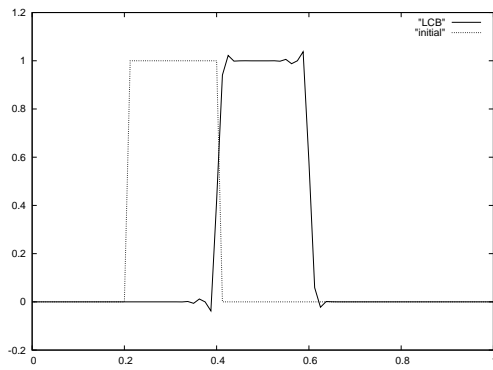
Figure 4.2. Error rates in $L^\infty(0, T; L^1(I))$ norm for various CFL numbers.



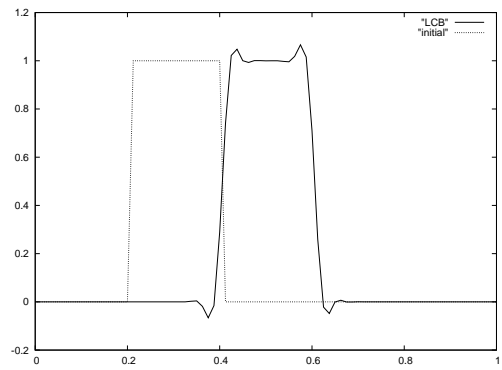
(a) P-RFB for $CFL = 1$ (FDt_FEs)



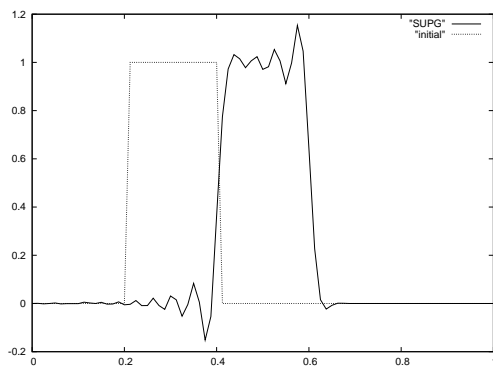
(b) P-RFB for $CFL = 1$ (FEs_FDt)



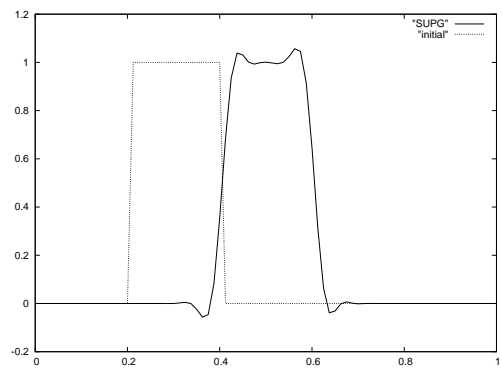
(c) LCB for $CFL = 0.25$ (FDt_FEs)



(d) LCB for $CFL = 0.25$ (FEs_FDt)

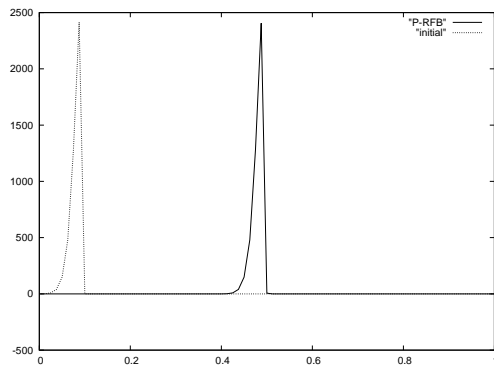


(e) SUPG for $CFL = 0.25$ (FDt_FEs)

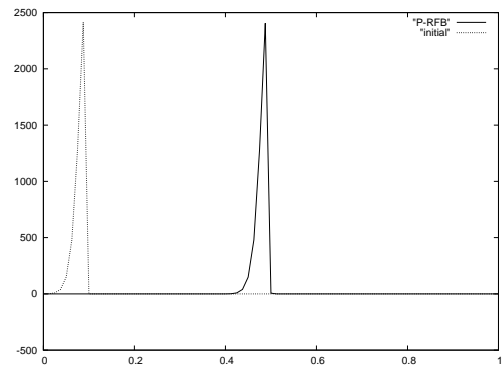


(f) SUPG for $CFL = 0.5$ (FEs_FDt)

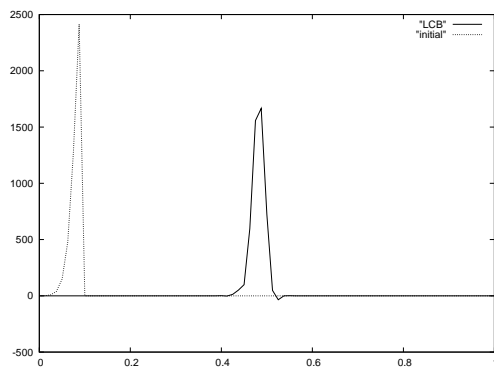
Figure 4.3. Approximate solutions of test problem 2.



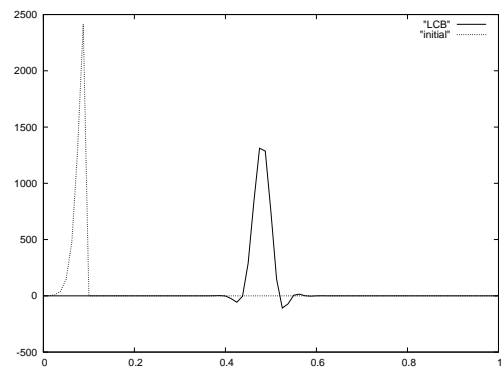
(a) P-RFB for $CFL = 1$ (FDt_FEs)



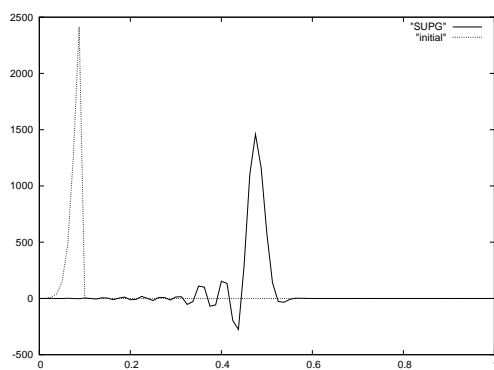
(b) P-RFB for $CFL = 1$ (FEs_FDt)



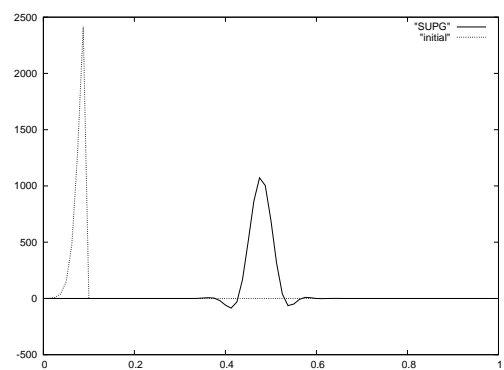
(c) LCB for $CFL = 0.25$ (FDt_FEs)



(d) LCB for $CFL = 0.25$ (FEs_FDt)

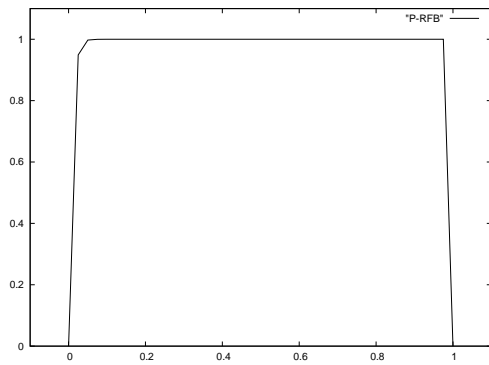


(e) SUPG for $CFL = 0.25$ (FDt_FEs)

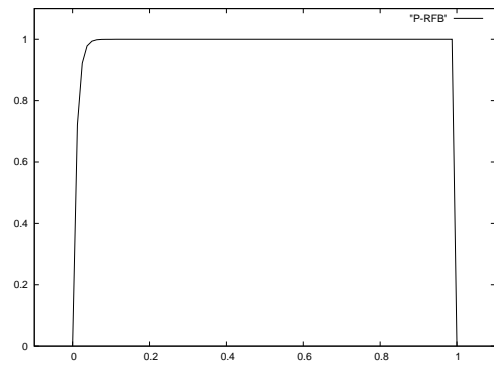


(f) SUPG for $CFL = 0.5$ (FEs_FDt)

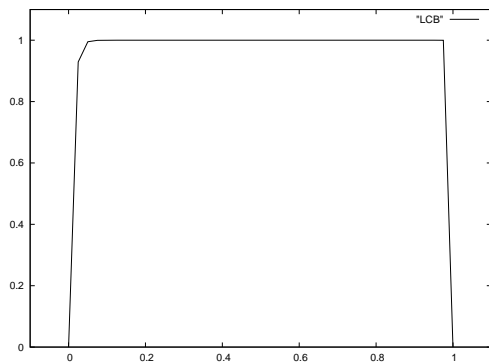
Figure 4.4. Approximate solutions of test problem 3.



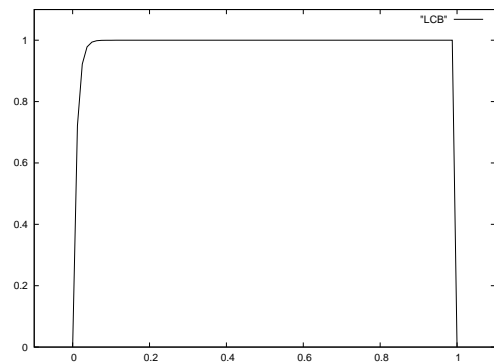
(a) P-RFB for $CFL = 1$ (FDt_FEs)



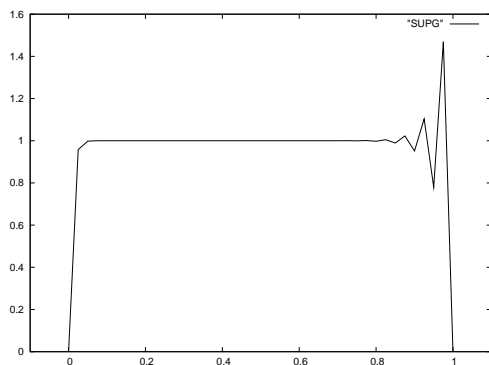
(b) P-RFB for $CFL = 1$ (FEs_FDt)



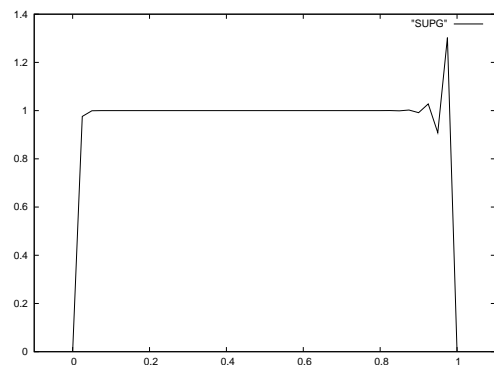
(c) LCB for $CFL = 0.25$ (FDt_FEs)



(d) LCB for $CFL = 0.25$ (FEs_FDt)

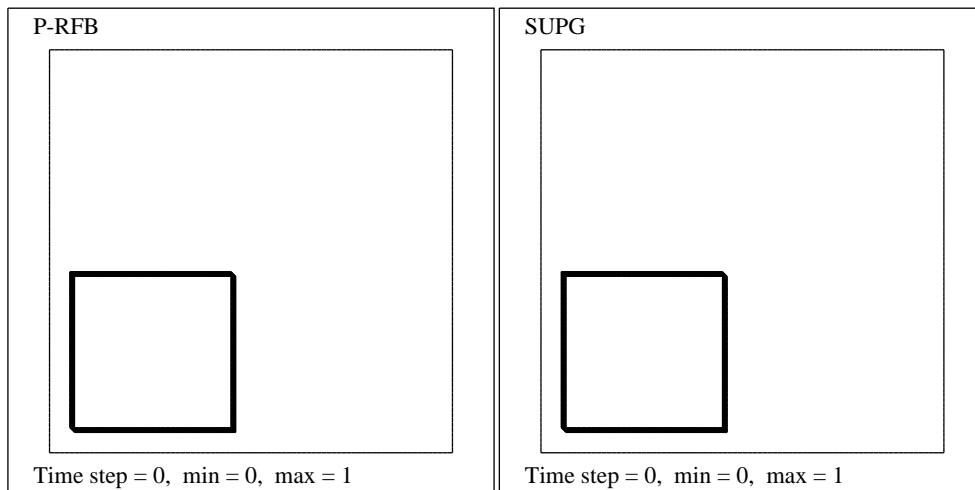


(e) SUPG for $CFL = 0.25$ (FDt_FEs)

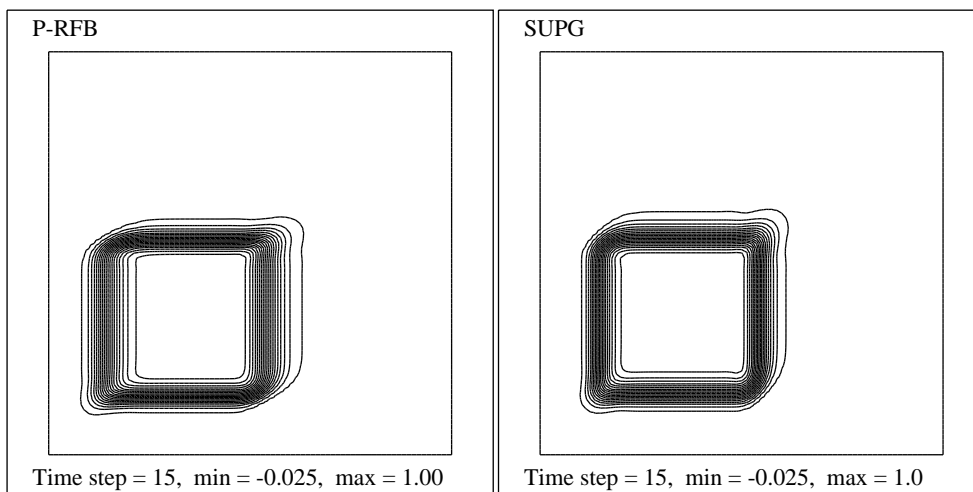


(f) SUPG for $CFL = 0.5$ (FEs_FDt)

Figure 4.5. Approximate solutions of test problem 4.

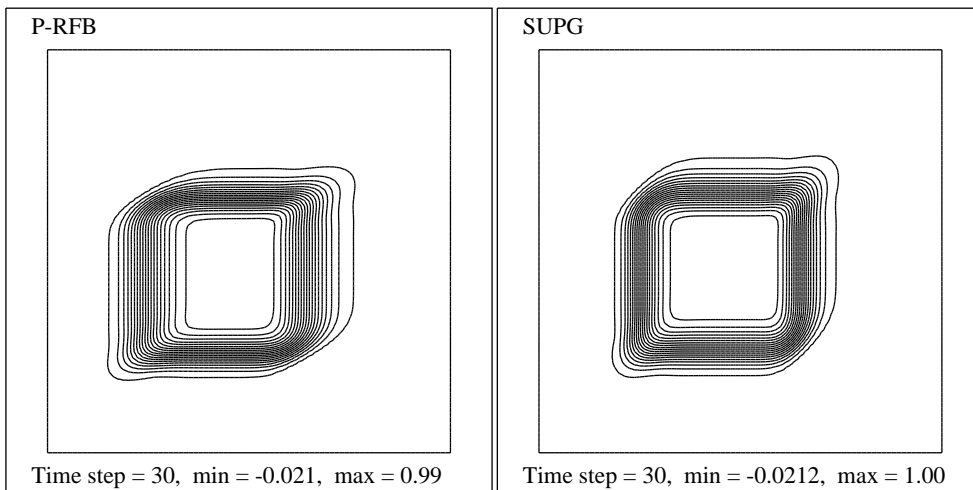


T=0

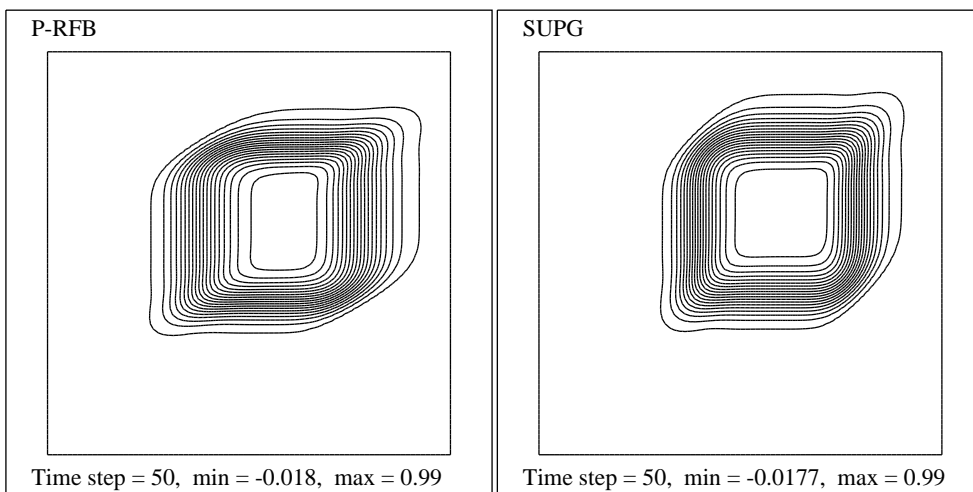


T=0.15

Figure 4.6. Approximate solutions of test problem 5 at different time steps.



T=0.3



T=0.5

Figure 4.7. Approximate solutions of test problem 5 at different time steps.

CHAPTER 5

CONCLUSION

Here we studied Pseudo Residual-Free Bubbles method for both steady and unsteady convection-diffusion-reaction equations in one and two dimensions. In detail we primarily applied the method to steady problem . We approximated the RFB functions with piecewise linear functions using two sub-grid nodes in one dimension. We compared P-RFB method with LCB strategy and SUPG method.

For the case of two dimensions, three sub-grid nodes are used to approximate the bubbles with piecewise linear functions. Numerical experiments have been given to assess the performance of the method. We looked at the error rates in L_2 and H_1 norms.

For unsteady problems in one dimension, two kinds of discretizations have been considered. The first one is discretization first in time then discretization in space which is known as horizontal method of lines. The second one is discretization first in space then in time which is known as method of lines. For the horizontal method of lines modified sub-grid nodes are used. We have tested the method with Crank-Nicolson scheme and compared with other stabilized methods.

Finally, we adapted P-RFB method to unsteady convection-diffusion-reaction problems in two dimensions with Backward-Euler scheme. We applied just method of lines and compared P-RFB with SUPG method at different time steps.

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