Impact of Mixed Boundary Conditions on Non-Premixed Combustion Model with a Low Diffusion Rate and Discontinuous Data: Higher Order Numerical Analysis

Karlstad Applied Analysis Seminar

Dr. Pratibhamoy Das
Department of Mathematics,
Indian Institute of Technology Patna, India.

@ Karlstad University, Sweden

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Introduction– Boundary Layer Originated Problems

Example:

$$\begin{cases} -\varepsilon u''(x) + u(x) = 0, \quad 0 < \varepsilon \ll 1, \quad x \in (0,1), \\ u(0) = 0, \quad u(1) = 1. \end{cases} \tag{1.1}$$

Exact Solution: $u(x) = \dfrac{\exp(x/\sqrt{\varepsilon}) - \exp(-x/\sqrt{\varepsilon})}{\exp(1/\sqrt{\varepsilon}) - \exp(-1/\sqrt{\varepsilon})}.$

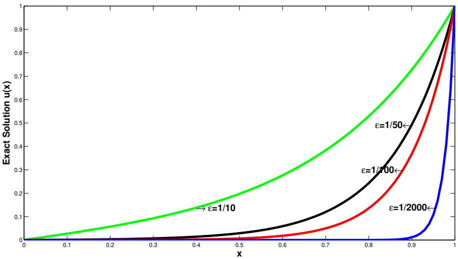


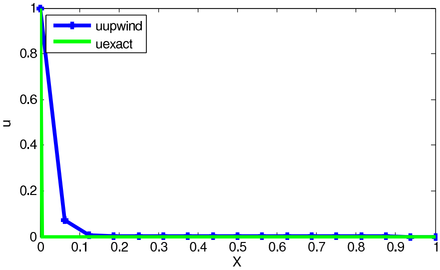
Figure: Comparison of the solution plots for various values of ε with number of mesh intervals $N = 100$

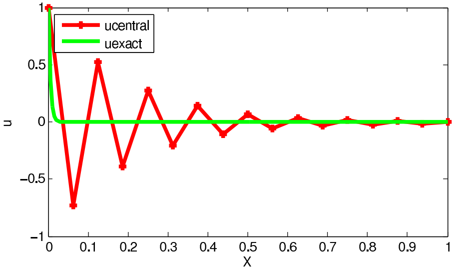
Numerical Difficulties

Consider the following problem

$$\begin{cases} \varepsilon u_\varepsilon'' + 2u_\varepsilon' = 0, & x \in (0,1), \\ u_\varepsilon(0) = 1, \quad u_\varepsilon(1) = 0. \end{cases}$$

Approximate solutions corresponding to the Upwind and Central Difference Schemes with 16 number of uniform partitions and $\varepsilon = .01$;





- Multiscale behavior of solutions leads to a big challenge for developing proper numerical schemes.
- On equidistant meshes, classical numerical methods converge if $\varepsilon \geq N^{-1}$. [RST08]
- Adaptive mesh may lead to optimal (or nearly optimal) convergence. [RST08]
- Computational cost increases for coupled system in 1D/2D.

- **ε-uniformly convergent scheme:** A numerical method is ε-uniformly convergent, if

$$\sup_{0<\varepsilon\leq 1} \|u(x_i) - U_i^N\|_{\Omega^N} \leq C\ N^{-p}, \quad p > 0, \quad N \geq N_0,$$

where u is exact solution, U^N is numerical solution, C is independent of mesh points x_i, mesh size and the parameter ε in the discretized domain Ω^N.

- **Aim**-To obtain higher order accurate ε-uniformly convergent approximation for problems having discontinuous data, and the effect of mixed conditions on the layer phenomena.

Mesh Adaptivity: Piecewise Uniform Mesh

- **Uniform mesh:** $\Omega^N \equiv \{0 = x_0 < x_1 < \cdots < x_{N-1} < x_N = 1\}$ where $x_i = i/N$.
- **Piecewise Uniform Mesh:** [RST08] For problems having discontinuous data, define discrete domain $\bar{\Omega}^N$ as a piece-wise uniform layer adaptive mesh having N mesh intervals.
- Domain $\bar{\Omega}^- = [0, d] = [0, \tau_1] \cup (\tau_1, d - \tau_1] \cup (d - \tau_1, d]$, where

$$\tau_1 = \min\left\{\frac{d}{4}, k^* \ln N\right\},$$

  and $d = x_{N/2}$ and $k^* = 2\sqrt{\varepsilon}/\sqrt{\alpha}$.
- Similarly, the domain $\bar{\Omega}^+ = [d, 1]$ is subdivided into the three sub-intervals.
- Each sub-intervals $(\tau_1, d - \tau_1]$ and $(d + \tau_2, 1 - \tau_2]$, a uniform mesh with $\frac{N}{4}$.
- $(0, \tau_1]$, $(d - \tau_1, d]$, $(d, d + \tau_2]$ and $(1 - \tau_2, 1]$, a uniform mesh with $\frac{N}{8}$ mesh points are placed.
- Hence, the discrete domain
  $\Omega^N = \Omega_1^N \cup \Omega_2^N$, where $\Omega_1^N = \{x_j\}_{j=1}^{\frac{N}{2}-1}$, $\Omega_2^N = \{x_j\}_{j=\frac{N}{2}+1}^{N-1}$ and $x_{\frac{N}{2}} = d$.

Non-premixed Combustion: Overview

- **Non-premixed combustion:** Fuel and oxidizer are not mixed before entering the combustion zone.
- Reaction occurs at the **interface** where the two meet.
- Flame structure determined by **diffusion rate** of reactants.
- Hottest region: near the **stoichiometric mixture**.

Modeling requires:

- Species and energy conservation equations,
- Turbulence and chemical kinetics models,
- Diffusion and mixing processes.

Non-premixed Combustion Model

Mathematical model of nonlinear form:

$$\varepsilon u'' + f(x,u) = g(x), \quad x \in (-1,1), \tag{1.2}$$

$$u(-1) = u(1) = 1. \tag{1.3}$$

- ε –small parameter, ratio of diffusive to reactive effects.
- $x = 0$: position of the flame (fuel-oxidizer interface).

Burke–Schumann Approximation

For $f(x,u) = u^2 - x^2$, $g(x) = 0$:

$$u_1(x) = x, \quad u_2(x) = -x$$

- $u - x$: fuel mass fraction.
- $u + x$: oxidizer mass fraction.
- Stable path: $u(x) = |x|$ **–Burke–Schumann approximation.**

$$u_\varepsilon(x) = |x| + O\left(\frac{\varepsilon^{1/3}}{\sigma}\left(1 + \frac{\sigma|x|}{\varepsilon^{1/3}}\right)^{-2}\right)$$

Flame thickness: $O(\varepsilon^{1/3})$

Aim of the Work

Objective

Investigate the impact of **mixed boundary conditions** on:

- Asymptotic behavior of nonlinear solutions,
- Efficiency of identifying the flame region,
- Reduction in flame width.

Catalytic Reaction Model

Nonlinear mixed boundary value problem:

$$\varepsilon u'' = u - u^3, \quad x \in (0,1), \tag{1.4}$$

$$u(0) - u'(0) = A, \quad u(1) + u'(1) = B. \tag{1.5}$$

Physical context:

- Isothermal reaction within a catalyst pellet.
- Balance between diffusion and reaction rates.

Catalytic Reaction Setup

Simplified governing equation:

$$u'' = \Psi^2 F(u), \quad x \in (0,1)$$

- u: normalized reactant concentration,
- Ψ: Thiele modulus (reaction vs diffusion),
- $F(u) = u^n$: nonlinear reaction rate.

Boundary conditions:

$$u'(0) = 0, \quad u(1) + \Sigma u'(1) = 1$$

Σ^{-1}: Sherwood number (mass transfer capability).

Boundary Layer Phenomenon

For $\varepsilon = \Psi^{-2} \ll 1$:

$$\varepsilon u'' = u^n, \quad u'(0) = 0, \quad u(1) + \Sigma u'(1) = 1$$

- When $\Sigma = 0$: strong boundary layer near $x = 1$.
- Reactant concentration decreases:
  - exponentially for $n = 1$,
  - algebraically for $n \geq 2$.

$$\lim_{\varepsilon \to 0^+} u_\varepsilon(x) = 0, \quad x \in [0, 1 - \delta]$$

Effect of Mass Transfer Resistance

For $\Sigma > 0$:

- Resistance to mass transfer from bulk to pellet.
- Solution behaves as:

$$u_\varepsilon(1) = \begin{cases} O(\varepsilon), & n = 1, \\ O(\varepsilon^{1/(n+1)}), & n > 2. \end{cases}$$

- No boundary layer as $\varepsilon \to 0^+$.

Broader Applications

Nonlinear singularly perturbed problems appear in:

- Michaelis–Menten enzyme kinetics,
- Schrödinger equations,
- Turing's model for pattern formation,
- Reaction–diffusion systems with Robin boundary conditions.

Need: Robust numerical algorithms that:

- Handle low regularity of solutions,
- Are stable on uniform meshes,
- Improve convergence for nonlinear boundary layers.

Non-linear Reaction-Diffusion Problem

We start with the following class of mixed boundary value problems having discontinuous source term:

$$Tu := -\varepsilon u''(x) + f(x, u(x)) = g(x) \text{ on } \Omega^- \cup \Omega^+, \tag{1.6}$$

$$\beta_0 u(0) := \mu_1 u(0) - \mu_2 u'(0) = \phi, \quad \beta_1 u(1) := \mu_3 u(1) + \mu_4 u'(1) = \psi. \tag{1.7}$$

- Here $\Omega^- = (0, d)$, $\Omega^+ = (d, 1)$ and $\Omega = \Omega^- \cup \Omega^+$, $\bar{\Omega}^- = [0, d], \bar{\Omega}^+ = [d, 1]$.
- We take $g(d-) \neq g(d+)$ for $d \in \mathcal{D} = (0, 1)$, and $\mu_1^2 + \mu_2^2 \neq 0$, $\mu_3^2 + \mu_4^2 \neq 0$, $\mu_2, \mu_4 \geq 0$.
- The jump of ζ at d is denoted by $[\zeta](d) = \zeta(d+) - \zeta(d-)$.
- **Assumption:** For all $x \in \bar{\Omega}$, we consider

$$\alpha^* \geq \frac{\partial f(x, u(x))}{\partial u} \geq \alpha > 0, \text{ for some constants } \alpha, \alpha^* \in \mathbb{R}. \tag{1.8}$$

Analytical Properties

- It is to be noted that $u(x) \notin C^2(\mathcal{D})$. Also $u(d+) = u(d-)$.
- Due the appearance of the discontinuity on g, the solution $u(x)$ exhibits an additional interior layer of width $O(\sqrt{\varepsilon})$ at $x = d$ [MMS21],
- Note that the sharpness of boundary layers at $x = 0, 1$ [MQ15], depend on the type of Robin boundary conditions.

Theorem

The given problem has a solution $u \in C^0(\bar{\Omega}) \cap C^1(\mathcal{D}) \cap C^2(\Omega^- \cup \Omega^+)$.

The uniqueness of the solution under the assumptions in (1.8) is similar to the linear version of the current problem. It also satisfies the maximum principle [FMOS98].

Decomposition of the Solution and Derivative Bounds

Decompose $u(x)$ into a smooth component $s(x)$ and a singular component $t(x)$ so that: $u(x) = s(x) + t(x)$,

Theorem

For every $x \in \Omega$, we have the following bounds for $s^{(k)}(x)$ and $\tilde{t}^{(k)}(x)$

$$
\begin{aligned}
&\left|s^{(k)}(x)\right| \leq C, \quad k = 0,1,2,3, && \left|s^{(4)}(x)\right| \leq C\,\varepsilon^{-1/2}, \\
&\left|\tilde{t}^{(k)}(x)\right| \leq C\mathcal{B}_1(x), \quad k = 0,1, && \left|\tilde{t}^{(k)}(x)\right| \leq C\varepsilon^{-\frac{(k-1)}{2}}\mathcal{B}_1(x), \quad k = 2,3,4, \\
&\left|\hat{t}^{(k)}(x)\right| \leq C\mathcal{B}_2(x), \quad k = 0,1, && \left|\hat{t}^{(k)}(x)\right| \leq C\varepsilon^{-\frac{(k-1)}{2}}\mathcal{B}_2(x), \quad k = 2,3,4,
\end{aligned}
$$

where C is independent of ε.

$$\mathcal{B}_1(x) = e^{-x\sqrt{\alpha/\varepsilon}} + e^{-(d-x)\sqrt{\alpha/\varepsilon}}, \quad \text{on } \bar{\Omega}^-, \; \mathcal{B}_2(x) = e^{-(x-d)\sqrt{\alpha/\varepsilon}} + e^{-(1-x)\sqrt{\alpha/\varepsilon}} \quad \text{on } \bar{\Omega}^+.$$

Discrete Problem

The discrete formulation corresponding to (1.6)-(1.7) is provided by:

$$
\begin{aligned}
T^N U_i &\equiv -\varepsilon\delta^2 U_i + f\left(x_i, U_i\right) = g_i \text{ on } \Omega^N, && (1.9)\\
T^N_{d_*} U_{\frac{N}{2}} &\equiv D^+_* U_{\frac{N}{2}} - D^-_* U_{\frac{N}{2}} = 0, && (1.10)\\
\beta^N_0 U_0 &\equiv \mu_1 U_0 - \mu_2 D^- U_0 = \phi,\ \beta^N_1 U_N := \mu_3 U_N + \mu_4 D^- U_N = \psi. && (1.11)
\end{aligned}
$$

At the point of discontinuity $x_{N/2} = d$, we can define two types of discrete schemes:

$$T^N_d U_{\frac{N}{2}} \equiv D^+ U_{\frac{N}{2}} - D^- U_{\frac{N}{2}} = 0, \tag{1.12}$$

or

$$T^N_{d_*} U_{\frac{N}{2}} \equiv \frac{-U_{\frac{N}{2}+2} + 4U_{\frac{N}{2}+1} - 3U_{\frac{N}{2}}}{2h_{\frac{N}{2}+1}} - \frac{U_{\frac{N}{2}-2} - 4U_{\frac{N}{2}-1} + 3U_{\frac{N}{2}}}{2h_{\frac{N}{2}}} = 0, \tag{1.13}$$

where $h_{\frac{N}{2}+1}$ and $h_{\frac{N}{2}}$ are the right and left step sizes around the point $x_{N/2}$ respectively.

Hybrid Scheme

Remark

If we replace (1.10) by $T_d^N U_{\frac{N}{2}} \equiv D^+ U_{\frac{N}{2}} - D^- U_{\frac{N}{2}} = 0$, *the matrix associated with the boundary condition forms an M-matrix and uniformly first-order accurate.*

Now put the values $U_{N/2+2}$ and $U_{N/2-2}$ from (1.9) in (1.13), to get

$$T_D^N U_{N/2} \equiv \frac{1}{2h}\left[-\left(2-\frac{a_{\frac{N}{2}-1} h^2}{\varepsilon}\right) U_{\frac{N}{2}-1} + 4U_{\frac{N}{2}} - \left(2-\frac{a_{\frac{N}{2}+1} h^2}{\varepsilon}\right) U_{\frac{N}{2}+1}\right] = \frac{h}{2\varepsilon}\left(g_{\frac{N}{2}+1} + g_{\frac{N}{2}-1}\right),$$

Lemma

Assume that $\frac{N^2}{\ln^2 N} \geq \frac{2\alpha^*}{\alpha}$, *where* $\alpha^* = \max_{x\in\bar{\Omega}} a(x)$ *and* $\alpha = \min_{x\in\bar{\Omega}} a(x)$. *Then the matrix associated with (1.13) forms an M-matrix.*

So, from the above lemma, we conclude that the operator T_M^N satisfies the discrete maximum principle, which directly leads to the following stability result.

Convergence on Interior points

Theorem

For any mesh functions V and W with
$\beta_0^N V_0 = \beta_0^N W_0$, $\beta_1^N V_N = \beta_1^N W_N$, $(D_*^+ - D_*^-) V_{\frac{N}{2}} = (D_*^+ - D_*^-) W_{\frac{N}{2}}$, *we have*

$$|V_i - W_i| \leq C \left| T^N (V_i - W_i) \right|, \text{ for } i \neq \frac{N}{2}.$$

Theorem

Let u be the solution of (1.6) -(1.7) and U be the solution of (1.9) - (1.11). Then for $x_i \in \Omega^N$, we have $|(U - u)(x_i)| \leq C(N^{-1} \ln N)^2$.

Remark

The order of convergence for the present Robin-type semi-linear reaction-diffusion problem is almost second order at all the interior points except the region of discontinuity.

Convergence on Boundary points

Theorem

Let u be the solution of (1.6) -(1.7) and U be the solution of (1.9) - (1.11). Then for $x_i \in \Omega^N$, we have

$$|\beta_0^N (U - u)(0)| \leq C\sqrt{\varepsilon} N^{-1} \ln N,$$

$$|\beta_1^N (U - u)(1)| \leq C\sqrt{\varepsilon} N^{-1} \ln N.$$

Remark

The point-wise rate of convergences for the present Robin type semi-linear reaction-diffusion problem at boundary points is almost second order, for sufficiently small values of ε, say $\sqrt{\varepsilon} \leq CN^{-1}$.

Main Theorem

Theorem

Let u be the solution of (1.6) - (1.7) and U be the solution of (1.9) - (1.11)using the scheme (1.13). Then, $\left|(U-u)\left(x_{N/2}\right)\right| \leq C(N^{-1}\ln N)^2$.

Remark

The above three point scheme (used at the point of discontinuity) can be also used at the mixed boundary condition to obtain a higher order numerical approximation. Note that the condition $\sqrt{\varepsilon} \leq CN^{-1}$ will not be required, which is mentioned in Remark 3, in this case. Similar things happen with scaled boundary conditions too.

Theorem

Let u be the solution of (1.6) -(1.7) and U be the solution of (1.9) - (1.11). Then, for $x_i \in \bar{\Omega}^N$,

$$|(U-u)(x_i)| \leq C\left(N^{-1}\ln N\right)^2.$$

Numerical Example

Example 1

Let us consider the following nonlinear reaction-dominated problem with discontinuous source term:

$$-\varepsilon u'' + (1-u^2)u = \begin{cases} 0.1 - x(x-0.5), & \text{for} \quad 0 < x < .5, \\ -0.2 - (x-1)(x-0.5), & \text{for} \quad .5 < x < 1, \end{cases} \tag{1.14}$$

with any one of the following boundary conditions:

(a) $u(0) = 0, u(1) = 0,$

(b) $\beta_0 u(0) := 2u(0) - u'(0) = 1, \quad \beta_1 u(1) := 8u(1) + u'(1) = 8,$

(c) $\beta_0 u(0) := 2u(0) - \sqrt{\varepsilon}u'(0) = 1, \quad \beta_1 u(1) := 8u(1) + \sqrt{\varepsilon}u'(1) = 8.$

Error Formula

- Errors and orders are evaluated as

$$E_{\varepsilon}^{N} = \max_{0 \le i \le N} \left| (U_{\varepsilon}^{N} - U_{\varepsilon}^{2N})(x_i) \right|, \quad r^{N} = \log_2(E_{\varepsilon}^{N} / E_{\varepsilon}^{2N}).$$

- $S_1 = \{1, 10^{-1}, \cdots, 10^{-8}\}$, $S_2 = \{\varepsilon \in S_1 \big|, \varepsilon \le N^{-1}\}$. For Newton iteration, we took tolerance 10^{-6}.

Table: Almost second-order accuracy with uniform errors at the whole domain, for Example 1.14(a) using the scheme (1.13).

N	32	64	128	256	512	1024	2048	4096	8192
$\varepsilon \in S_1$	4.7277e-3 1.0372	2.3038e-3 1.4703	8.3144e-4 1.5515	2.8366e-4 1.6469	9.0582e-5 1.6917	2.8041e-5 1.7230	8.4942e-6 1.7485	2.5280e-6 1.7689	7.4177e-7

Error and Order Tables

Table: Almost second-order accuracy with uniform errors at the interior points (except the point of discontinuity) for Example 1.14 (b), using the scheme (1.12). (See Remark 2)

N	32	64	128	256	512	1024	2048	4096	8192
$\varepsilon \in S_2$	3.4569e-2 1.1699	1.5364e-2 1.4743	5.5297e-3 1.9295	1.4516e-3 1.9245	3.8241e-4 1.9094	1.0180e-4 1.8994	2.7286e-5 1.8958	7.3326e-6 1.8965	1.9695e-6

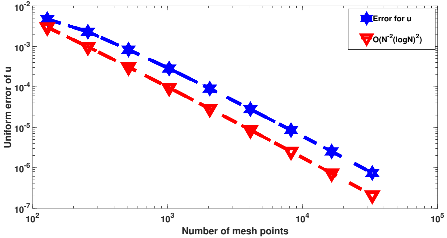
Table: Almost second-order accuracy with uniform errors on the whole domain, for Example 1.14 (b), (See Remark 3) using the scheme (1.13).

N	32	64	128	256	512	1024	2048	4096	8192
$\varepsilon \in S_2$	3.4569e-2 1.1699	1.5364e-2 1.4743	5.5297e-3 1.9295	1.4516e-3 1.9245	3.8241e-4 1.9094	1.0180e-4 1.8994	2.7286e-5 1.8958	7.3326e-6 1.8965	1.9695e-6

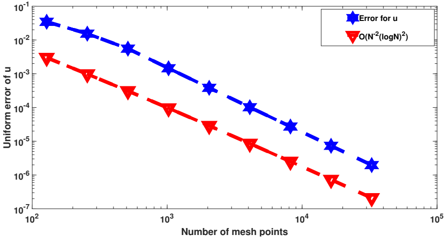
Error and Order Tables

Table: Uniform errors and corresponding rates of convergences throughout the discrete domain for Example 1.14 (c) using the scheme (1.13).

N	32	64	128	256	512	1024	2048	4096	8192
$\varepsilon \in S_1$	3.4569e-2	1.5364e-2	7.3353e-3	3.2617e-3	1.5174e-3	7.5133e-4	3.6501e-4	1.7982e-4	8.9241e-5
	1.1699	1.0666	1.1693	1.1040	1.0141	1.0415	1.0213	1.0108	



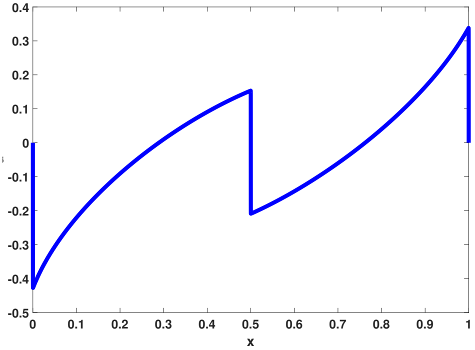
(a) Example 1.14 (a)



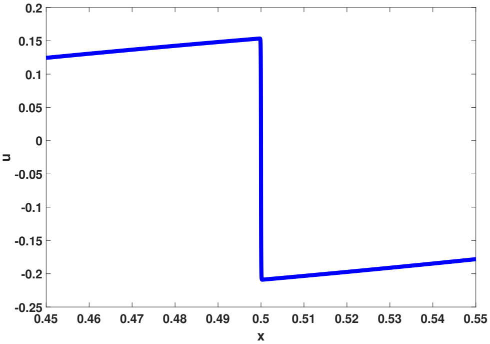
(b) Example 1.14 (b)

Figure: Loglog plot for Example 1.14 through scheme (1.13), where $\varepsilon \in S_2$.

Solution Plot



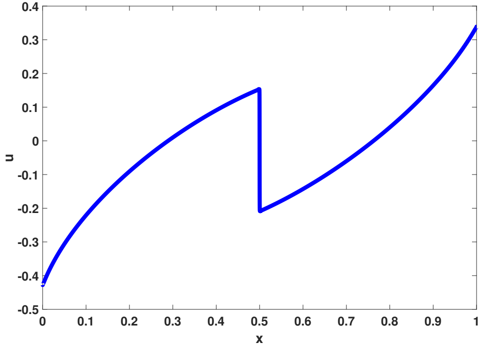
(a) Boundary and Interior Layers



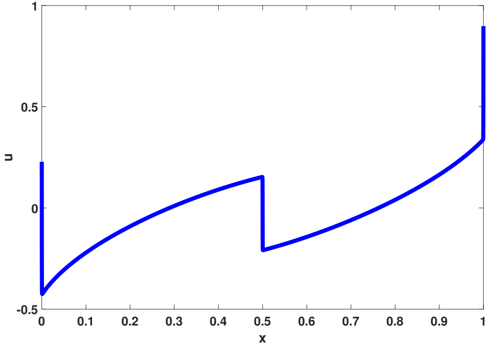
(b) Magnified version near the point of discontinuity

Figure: Example 1.14(a) with $\varepsilon = 10^{-8}, N = 128$ through scheme 1.13.

Solution plot



(a) Example 1.14 (b)



(b) Example 1.14 (c)

Figure: Boundary and interior layers appearances with respect to different boundary conditions of Example 1.14 with $\varepsilon = 10^{-8}, N = 128$ through scheme 1.13.

Collaborations & Communications

This work is a collaborative work with Dr. Shridhar Kumar (IISER Thiruvananthapuram), and Dr. R. Ishwariya (Amrita Vishwavidyapeetham).

Shridhar Kumar, Ishwariya R and Pratibhamoy Das. Impact of Mixed Boundary Conditions and Non-smooth Data on Layer Originated Non-premixed Combustion Problems: Higher Order Convergence Analysis. *Studies in Applied Mathematics*, 2024, https://doi.org/10.1111/sapm.12763

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Thank You