Adaptivity using entropy inequality

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VII Partial differential equations, optimal design and numerics -

Benasque, Spain

1D Elliptic

We consider the following one dimensional steady-state convection diffusion problem as

$$\mathcal{L}u(x) = -\epsilon u''(x) - a(x)u'(x) + b(x)u(x) = f \in (0,1)$$

with B.C. $u(0) = \alpha, u(1) = \beta$, ϵ is a small positive parameter and $x \in [0,1]$. Without loss of generality, we consider $b(x) \geq 0$ and $a(x)$ can change the sign (as in the case of turning point problem) in the given domain $[0,1]$. For $a(x) \geq \gamma > 0$, the above problem has unique solution and exhibit a boundary layer of $O(\epsilon)$ at $x = 0$.

Entropy production

$$2u \times Lu = 2u \times f;$$

Let we define

$$S = u^2 \text{(Entropy)}$$

$$S' = 2uu' \quad ; S'' = 2(uu'' + (u')^2)$$

$$\Rightarrow 2uu'' = S'' - 2(u')^2$$

$$\Rightarrow -\epsilon 2uu'' - 2auu' + 2bu^2 = 2uf$$

$$\Rightarrow -\epsilon(S'' - 2(u')^2) - aS'(x) + 2bS = 2uf$$

$$\Rightarrow P = -\epsilon S'' - aS'(x) - 2uf = -2\epsilon(u')^2 - 2bS \leq 0$$

We label the linear operator on the left hand side (LHS) in the above equation, as the entropy production operator with analogy to similar operators in hyperbolic conservation laws. The continuous operator should obviously be negative for all $x \in [0, 1]$ (as right hand side (RHS) is always negative for all $x \in [0, 1]$).

Example

We consider 1D linear convection-diffusion problem as

$$-\epsilon u'' - 2u' = 0; x \in (0,1), 0 < \epsilon << 1,$$

with boundary conditions

$$u(0) = 1 \text{ and } \quad u(1) = 0;$$

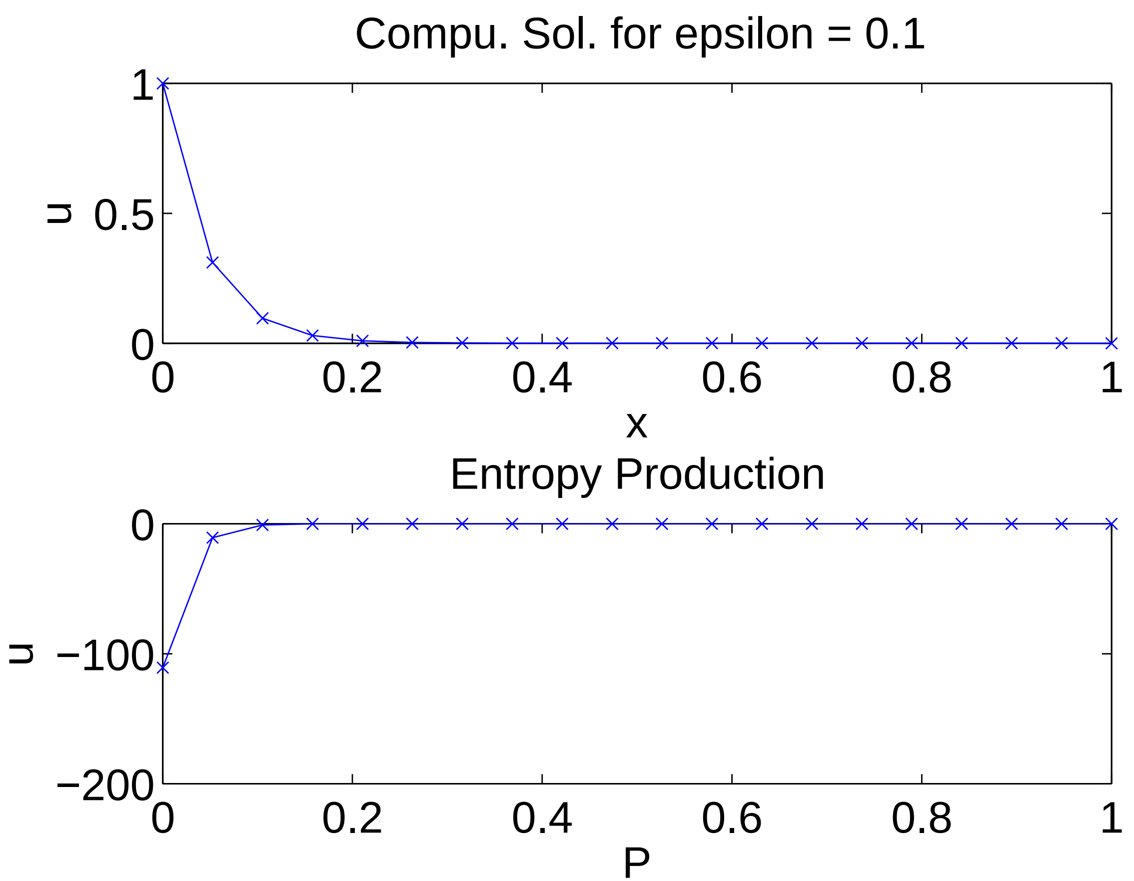
The exact solution is

$$u = \frac{\exp(-2x/\epsilon) - \exp(-2/\epsilon)}{1 - \exp(-2/\epsilon)}.$$

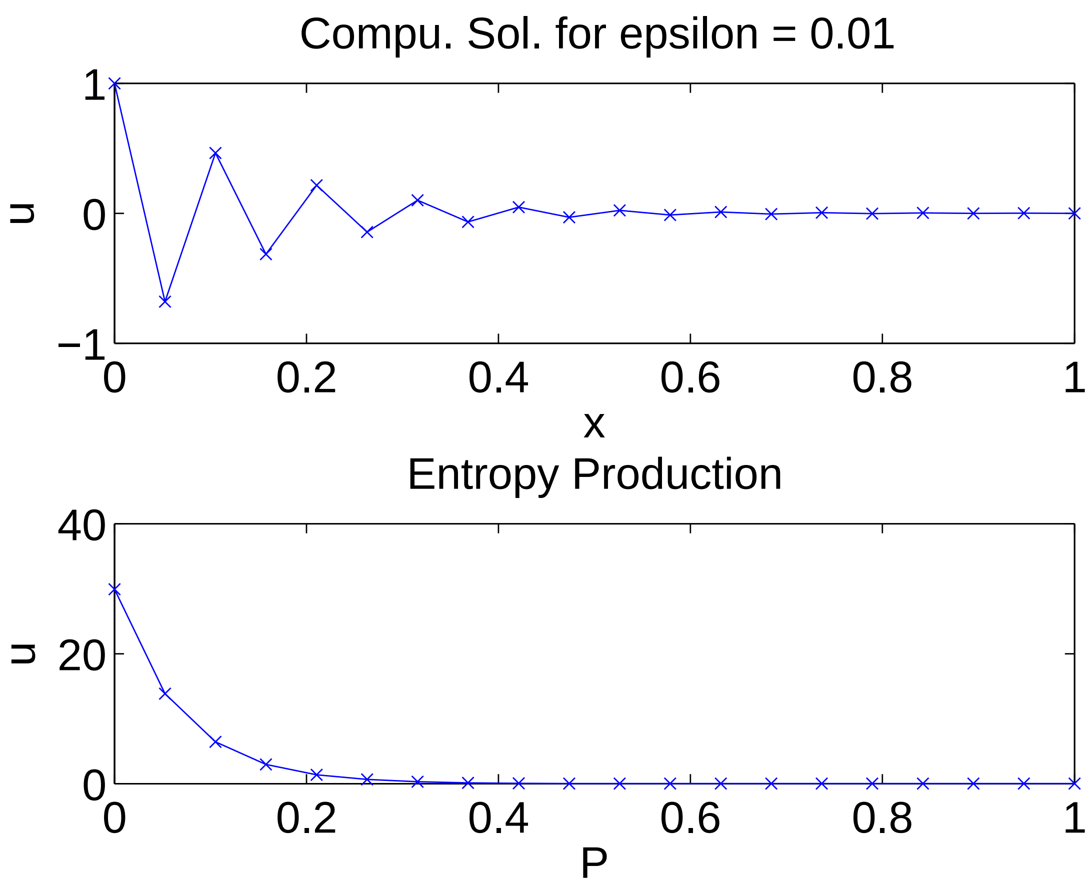
This problem has regular boundary layers of width $O(\epsilon)$ at $x = 0$. When we apply central difference scheme on uniform mesh for this problem, we get

$$(\frac{-\epsilon}{h^2} + \frac{1}{h})u_{i-1} + \frac{2\epsilon}{h^2}u_i + (\frac{-\epsilon}{h^2} - \frac{1}{h})u_{i+1} = 0.$$

Results using Central difference operator

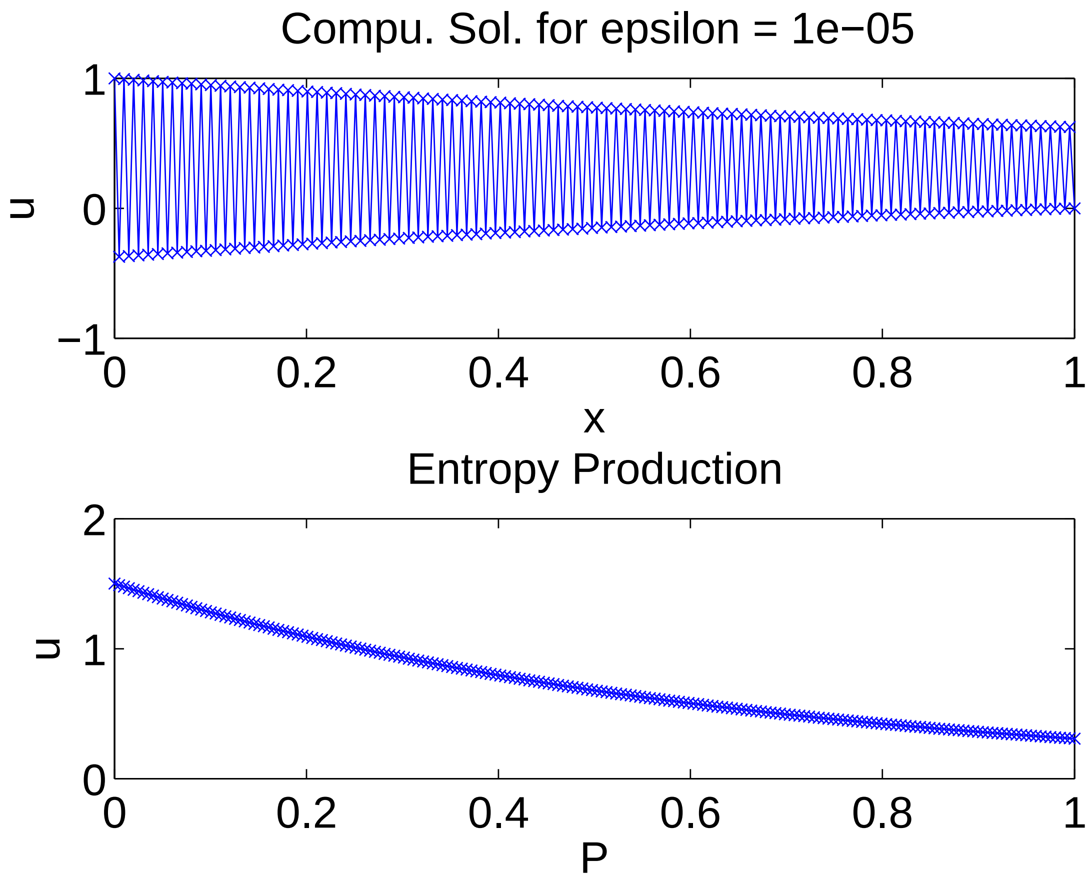


Results



Compu. Sol. for epsilon = 0.01
1
u
0
−1
0
0.2
0.4
0.6
0.8
1
x
Entropy Production
40
u
20
0
0
0.2
0.4
0.6
0.8
1
P

Results


Compu. Sol. for epsilon = 1e−05
u
1
0
−1
0
0.2
0.4
0.6
0.8
1
x
Entropy Production
u
2
1
0
0
0.2
0.4
0.6
0.8
1
P

Results

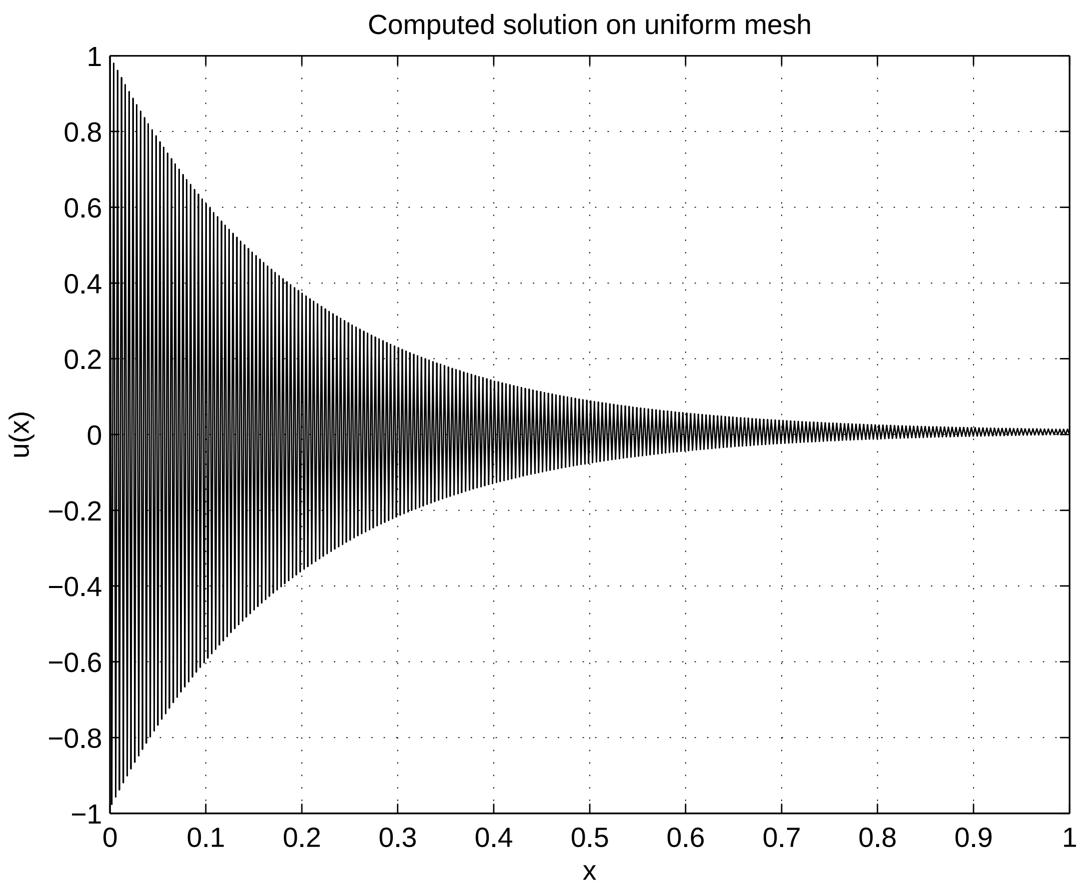


Figure 1: For uniform mesh with $N = 500$ mesh points for $\epsilon = 10^{-5}$

Turning point problem

We consider another 1D linear convection-diffusion problem as

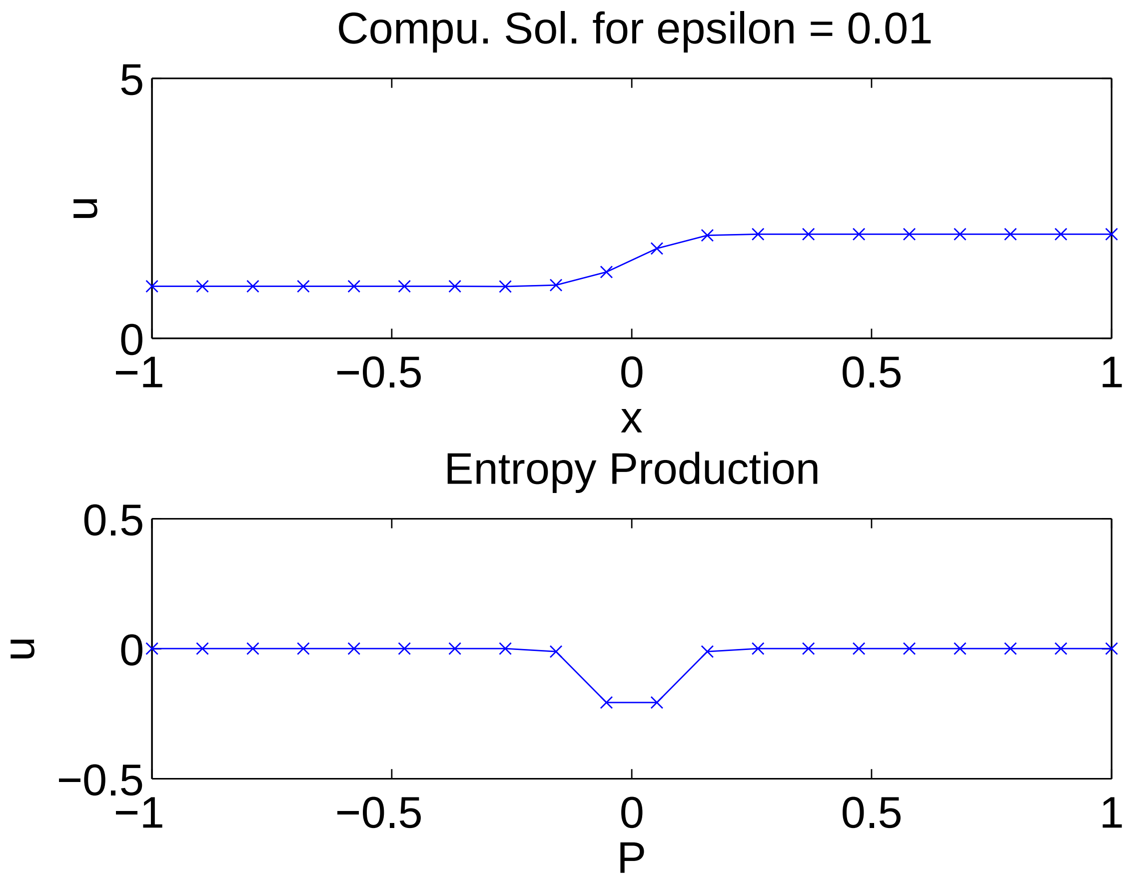
$$-\epsilon u'' - xu' = 0; x \in (-1, 1), 0 < \epsilon << 1,$$

with boundary conditions

$$u(-1) = 1 \text{ and } \quad u(1) = 2;$$

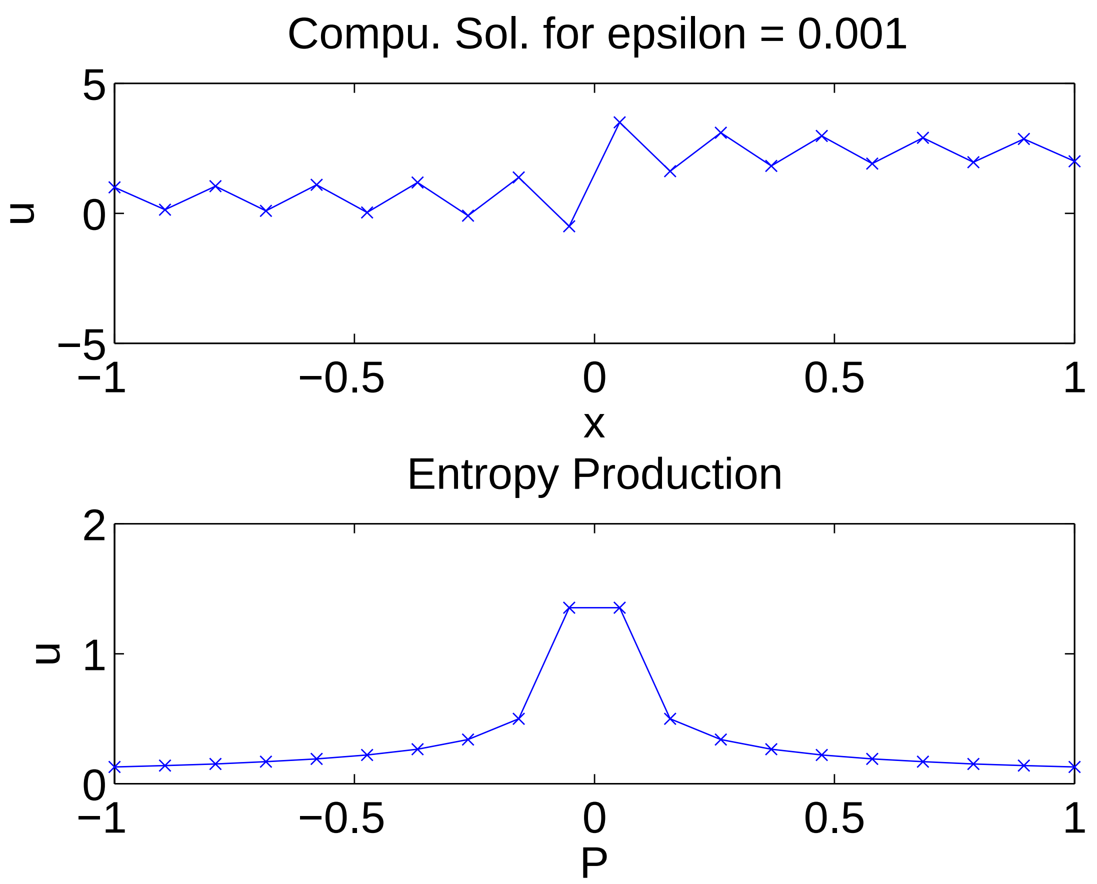
This equation has a interior layer at $x = 0$.

Results



Compu. Sol. for epsilon = 0.01
5
u
0
−1
−0.5
0
0.5
1
x
Entropy Production
0.5
u
0
−0.5
−1
−0.5
0
0.5
1
P

Results



Compu. Sol. for epsilon = 0.001
u
5
0
−5
−1
−0.5
0
0.5
1
x
Entropy Production
u
2
1
0
−1
−0.5
0
0.5
1
P

Main Idea

The central idea is:
(1) Just as the second law of thermodynamics separates unphysical solutions from the physical ones by finding the sign of an entropy variable, it is possible to identify unphysical portions of a numerical solution by finding the sign of an appropriately defined discrete entropy production.
(2) Discretization of entropy inequality is done by exactly repeated the discretization of the original equation operator by operator.

Main Idea

If we calculate the discrete analogue of the left hand side equation in using the same central difference operator by taking $S_i = u_i^2,$ where u_i is the central difference computed solution for equation, we observe that LHS is negative wherever the solution is smooth enough and positive where we have boundary layers (or oscillation in the computed solution of equation. After investigation, we have found that if we write the RHS term $-2bu^2 - 2\epsilon(u')^2$ of equation in difference operator at the i*th* mesh point, we get

$$-2b_i(u_i u_{i-1}) - 2\epsilon(\frac{u_i - u_{i-1}}{x_i - x_{i-1}})(\frac{u_{i+1} - u_i}{x_{i+1} - x_i})$$

Adaptive mesh Generation Algorithm

To generate the adaptive mesh for the convection dominant SPP, we follow the following algorithm:

Step 1: Calculate the entropy with a minimum number of initial uniform mesh points (minimum 3 points in our case).

Step 2: Locate the mesh points where entropy S is positive and then choose the mesh point with the maximum entropy.

Step 3: Add one mesh point on the left and the right side of the location found in step 2.

Step 4: go to Step 1 till all the entropy becomes non positive over the complete mesh.

The resulting mesh is our adapted mesh which is represented by N_a.

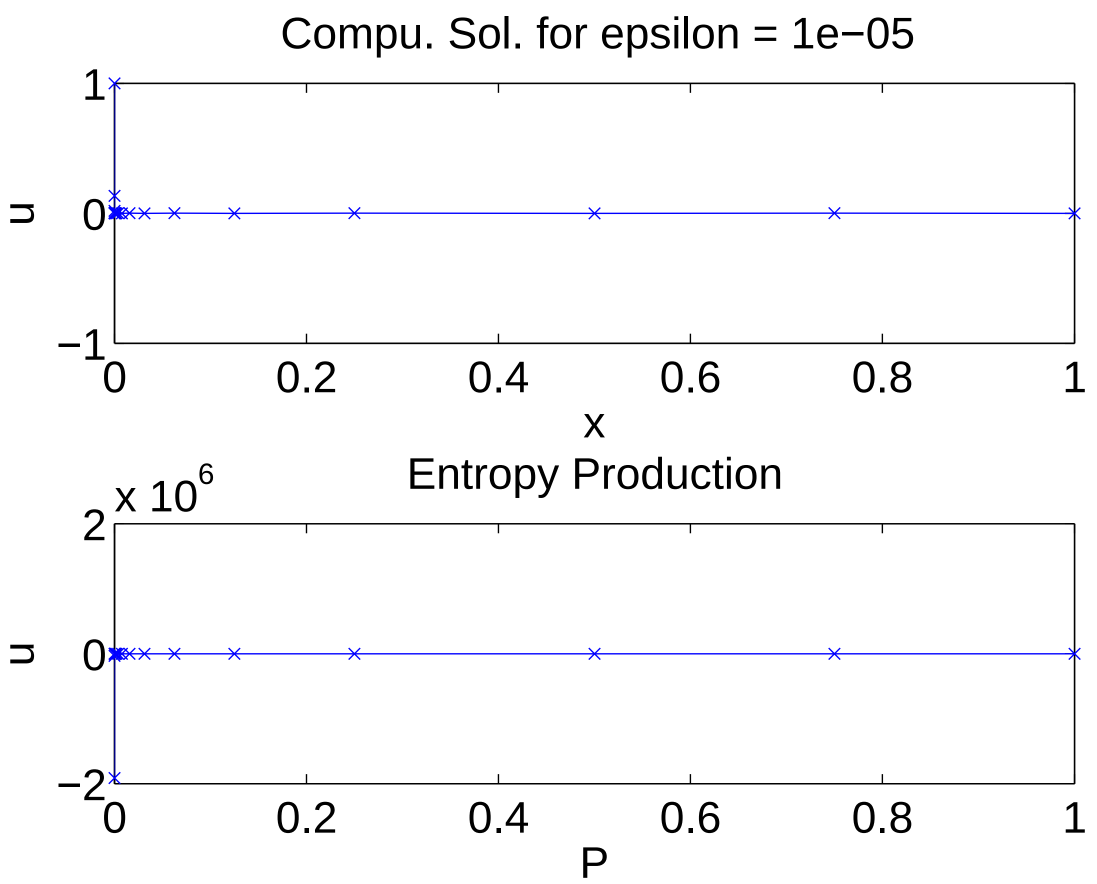
Entropy production at the boundaries points

we introduce a ghost point say x_0 at the left of the node x_L and x_{n+1} on the right of the node x_R, then we calculate

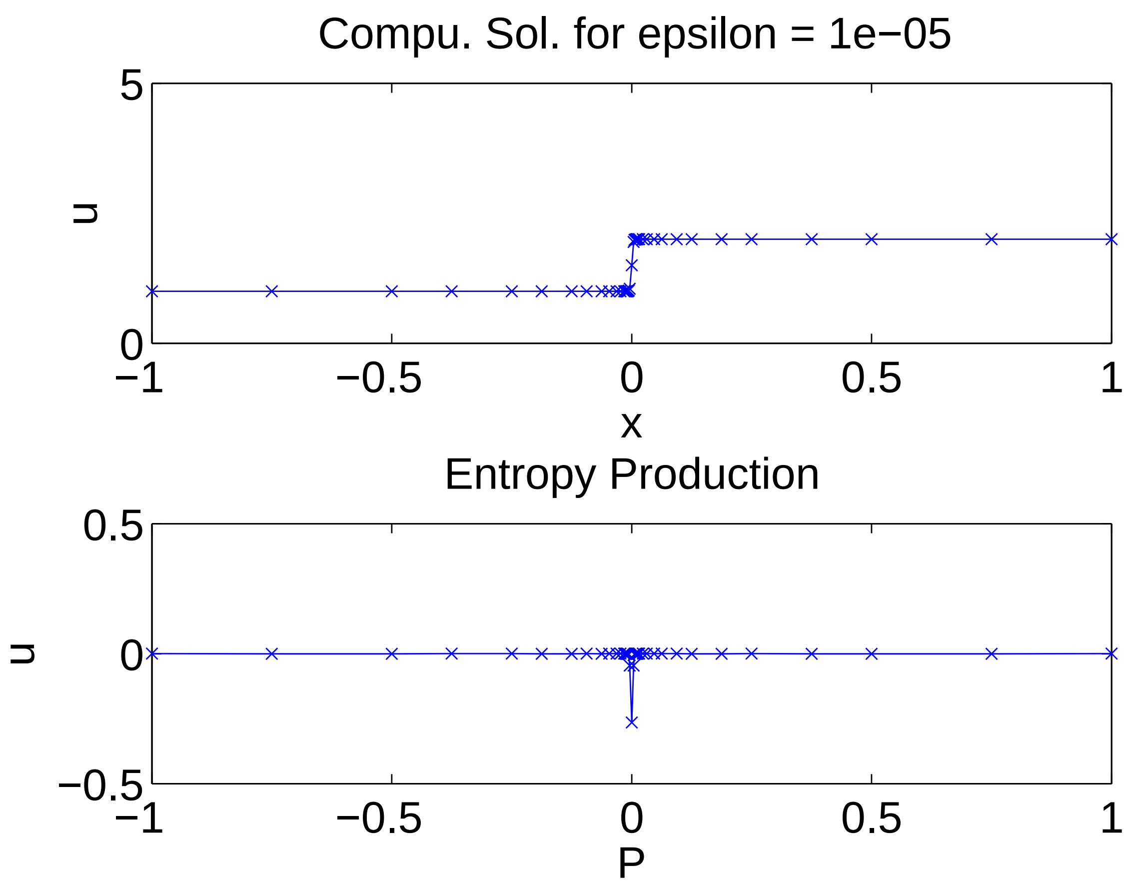
$$\begin{aligned} -\epsilon\delta^2 u_1 - a_1 D^0 u_1 + b_1 u_1 &= f_1 \\ -\epsilon\delta^2 u_n - a_n D^0 u_n + b_n u_n &= f_n \end{aligned}$$

As we already know the computed values of u_1, u_2 and then we calculate u_0 at the ghost point x_0 . Then we can find the entropy at the node x_L as usual. Similarly we can calculate the entropy at the right boundary node x_R.

Results for B.L. on the left



Results with interior layer



Turning point problem with B.L. at both ends

We consider 1D linear convection-diffusion problem with turning point as

$$-\epsilon u'' + 2(2x-1)u' + 4u = 0; x \in (0,1), 0 < \epsilon << 1,$$

with boundary conditions

$$u(0) = 1 \text{ and } \quad u(1) = 1;$$

The exact solution is

$$u = \exp(\frac{-2x(1-x)}{\epsilon}).$$

Results

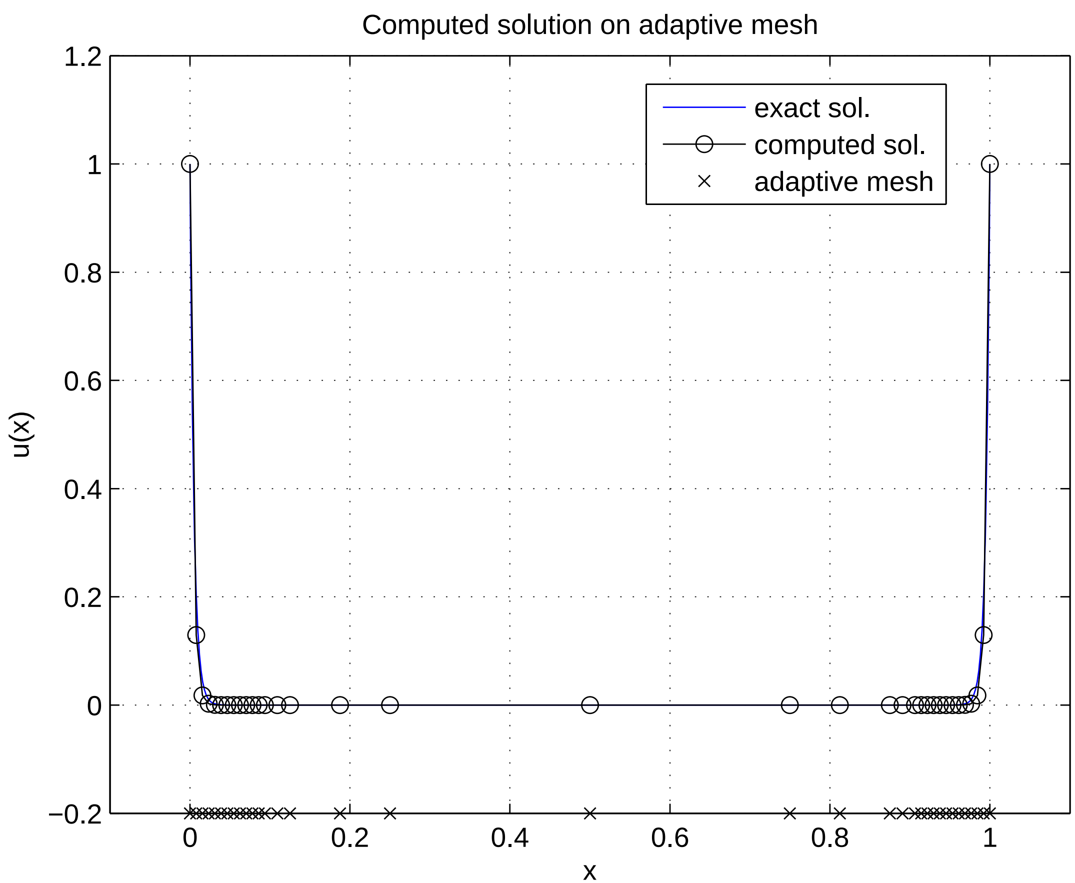


Figure 2: For $\epsilon = 10^{-2}$ with $N_a = 35$ adaptive mesh points

Results

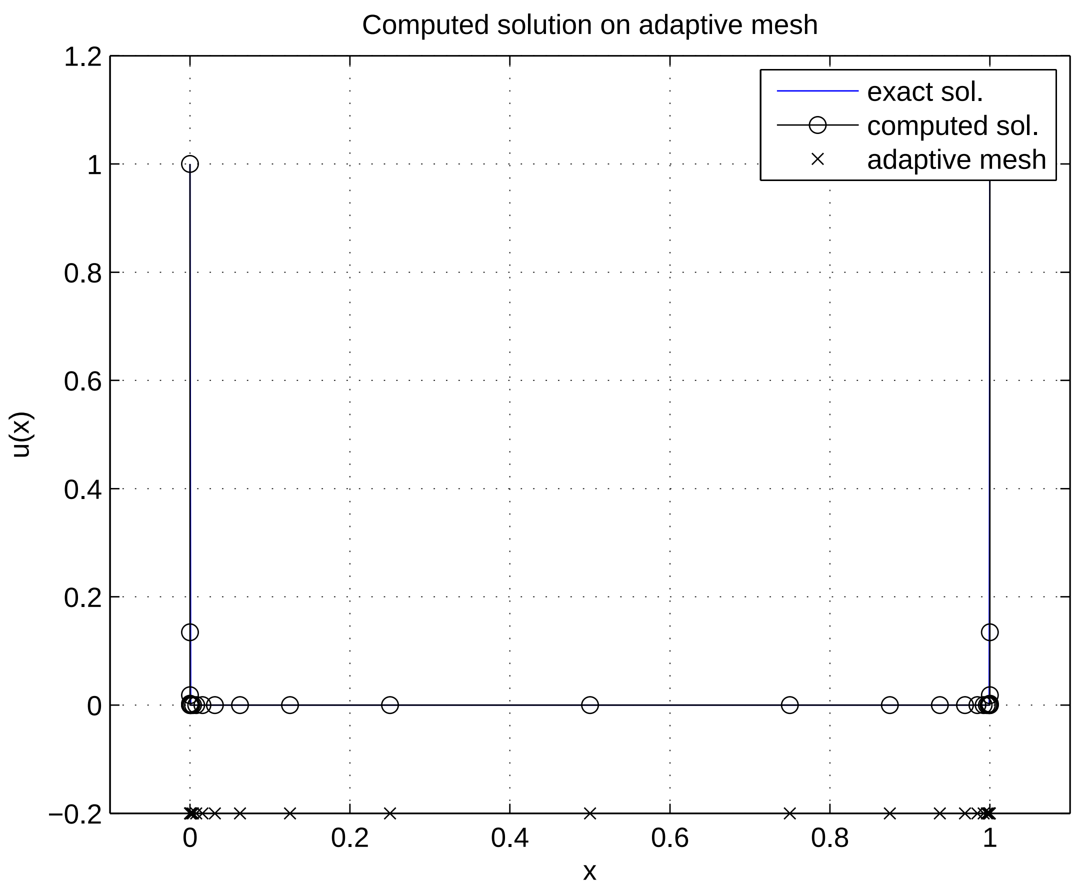


Figure 3: For $\epsilon = 10^{-5}$ with $N_a = 55$ adaptive mesh points

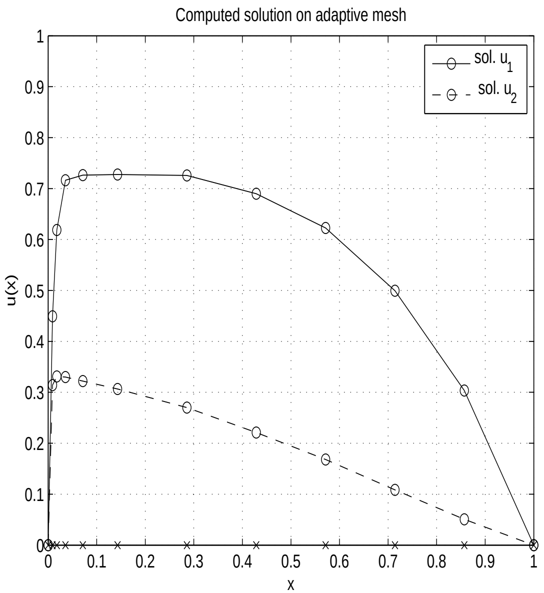
System of coupled equations

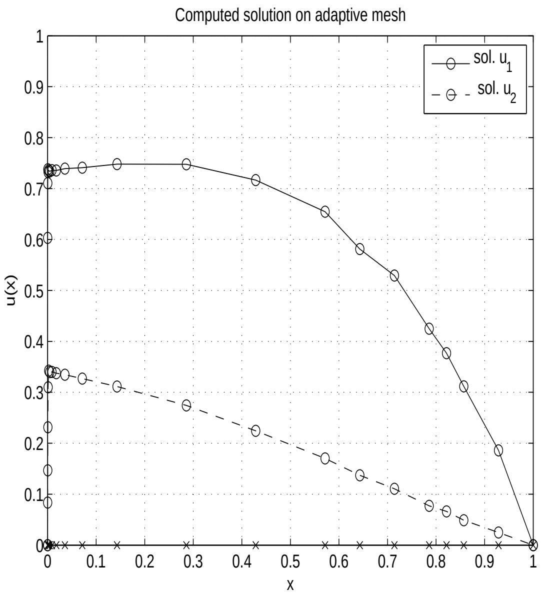
We consider system of coupled convection-diffusion problem as

$$\begin{aligned} -\epsilon_1 u_1'' - u_1' + 2u_1 - u_2 &= e^x, u_1(0) = 0, u_1(1) = 0 \\ -\epsilon_2 u_2'' - 2u_2' + 4u_2 - u_1 &= \cos(x), u_2(0) = 0, u_2(1) = 0 \end{aligned}$$

which shows two overlapping layers near x = 0. The exact solution of this equation is not known. The results for various values of ϵ_1 and ϵ_2 for adaptive meshes have been shown. In the figure, we have generated the adaptive mesh by taking maximum of the entropies S_1, S_2.

Results of coupled equations

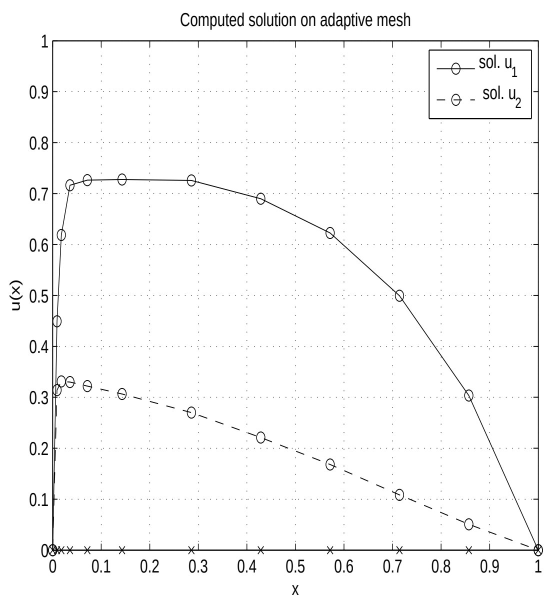




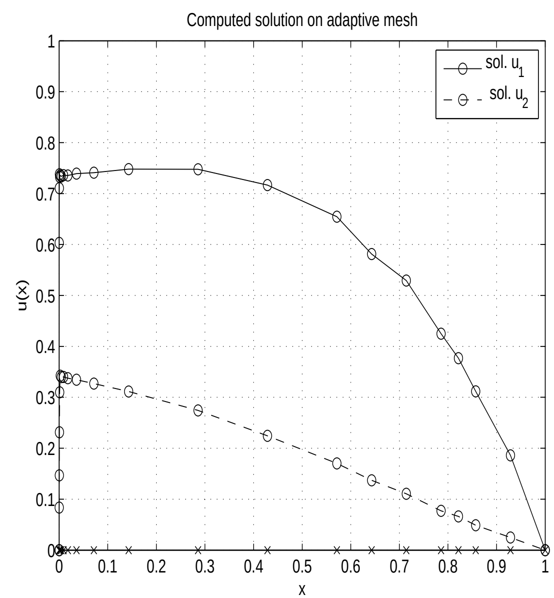
(a) Adaptive mesh points $N_a = 12$ for $\epsilon_1 = .01$ and $\epsilon_2 = .01$

(b) Adaptive mesh points $N_a = 22$ for $\epsilon_1 = .0001$ and $\epsilon_2 = .001$

Results of coupled equations



(c) Adaptive mesh points $N_a = 12$ for $\epsilon_1 = .01$ and $\epsilon_2 = .01$



(d) Adaptive mesh points $N_a = 22$ for $\epsilon_1 = .0001$ and $\epsilon_2 = .001$

Figure 4: Results for coupled case with starting unifrom mesh for N=8, using minimum entropy condition.

Non Linear Case

We also consider the nonlinear singularly perturbed boundary value problem

$$-\epsilon u''(x) - u(x)(u'(x) - 1) = 0 \in (0, 1), u(a) = \alpha, u(b) = \beta; a \leq x \leq b$$

The resulting finite difference equations give a system of non-linear equations. We use Newton-Raphson iterations to determine the solution of the non-linear system. The initial guess for the solution is the approximate solution given by

$$u(x) = x - \bar{x} + w_0 \tanh(w_0(x - \bar{x})/(2\epsilon))$$

where

$$\bar{x} = 0.5(a + b - \alpha - \beta), w_0 = 0.5(a - b + \beta - \alpha).$$

This problem shows an interior layer at $x = 0.25$ for $a = 0, b = 1, \alpha = -1$ and $\beta = 1.5$.

Non Linear Case

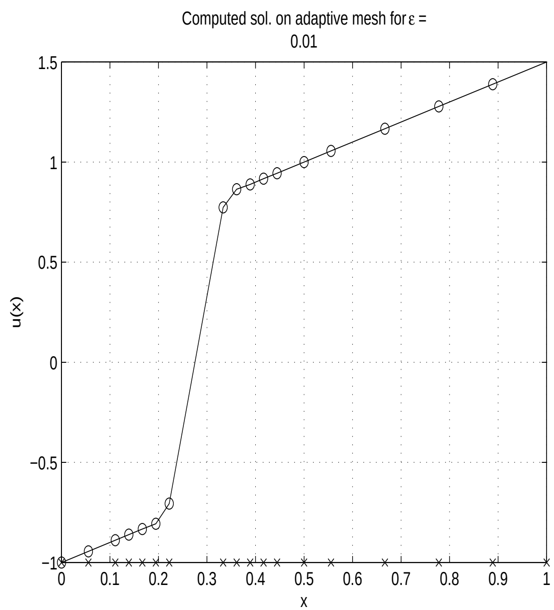
Its conservative form can be written as

$$-\epsilon u''(x) - (\frac{u^2(x)}{2})' + u(x) = 0 \in (0,1), u(a) = \alpha, u(b) = \beta; a \leq x \leq b$$

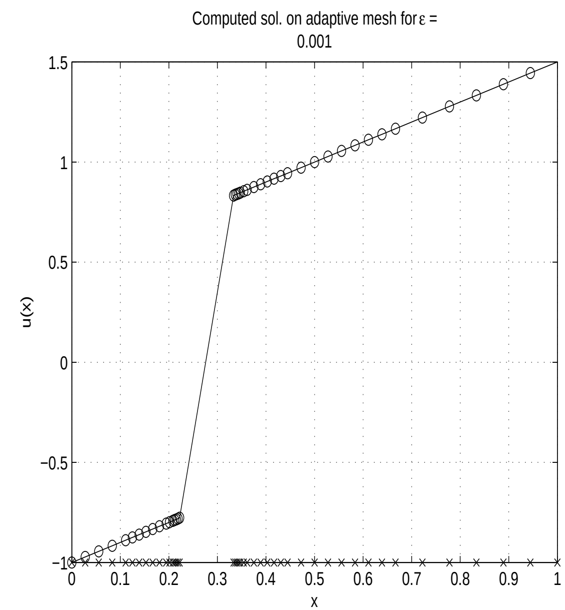
There are several choices for the entropy production equation. Again, in analogy to the entropy equation in hyperbolic conservation laws, we use the conservative of the entropy equation which can be obtained as

$$-\epsilon S''(x) - (\frac{2u^3(x)}{3})' + 2S(x) = -2\epsilon(u'(x))^2$$

Non Linear Case



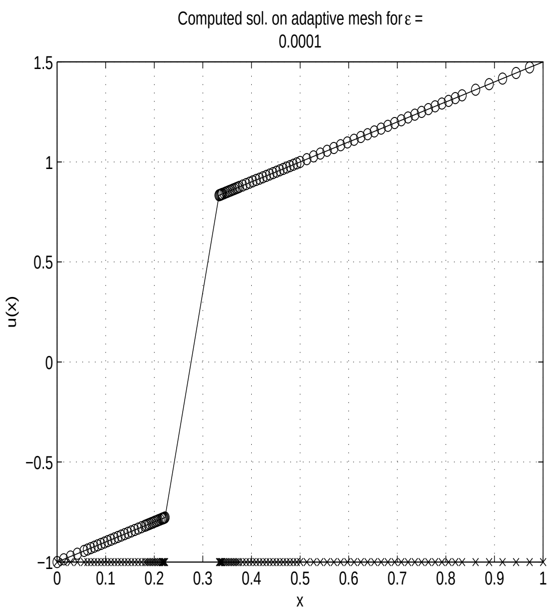
(a) Adaptive mesh points $N_a = 18$ for $\epsilon = .01$



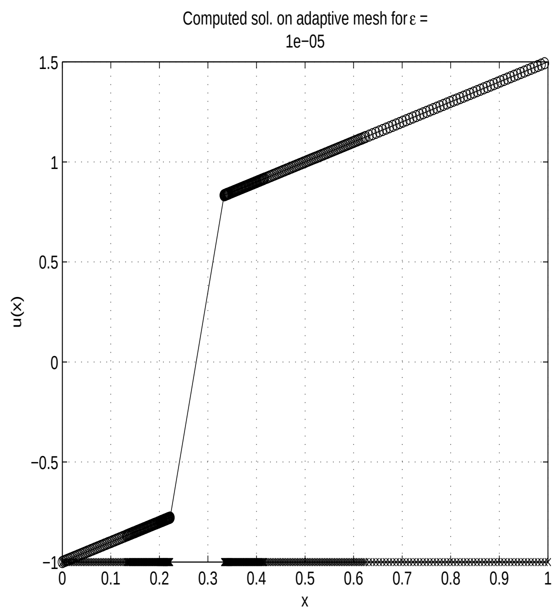
(b) Adaptive mesh points $N_a = 44$ for $\epsilon = .001$

Figure 5: Results for nonlinear case with starting uniform mesh with N=10.

Non Linear Case



(a) Adaptive mesh points $N_a = 100$ for $\epsilon = .0001$



(b) Adaptive mesh points $N_a = 272$ for $\epsilon = .00001$

Figure 6: Results for nonlinear case with starting uniform mesh with N=10.

2D elliptic Problems

$$-\epsilon\Delta u(x,y) + a(x,y)u_x + b(x,y)u_y + c(x,y)u = f(x,y),$$

$$S = u^2 \;\; ; S_x = 2uu_x \;\; ; S_y = 2uu_y$$

$$P = -\epsilon\Delta S + aS_x + bS_y - 2uf = -2\epsilon(u_x^2 + u_x^2) - 2cS \leq 0 \;\; (\text{ for } c \geq 0).$$

Let us take example

$$-\epsilon\Delta u - (x - \frac{1}{2})u_x = 0; (x,y) \in ((0,1)\times(0,1)), 0 < \epsilon << 1,$$

with boundary conditions

$$u(0,y) = 1; \;\; u(1,y) = 2; \text{ and } u(x,0) = u(x,1) = 0.$$

2D Results

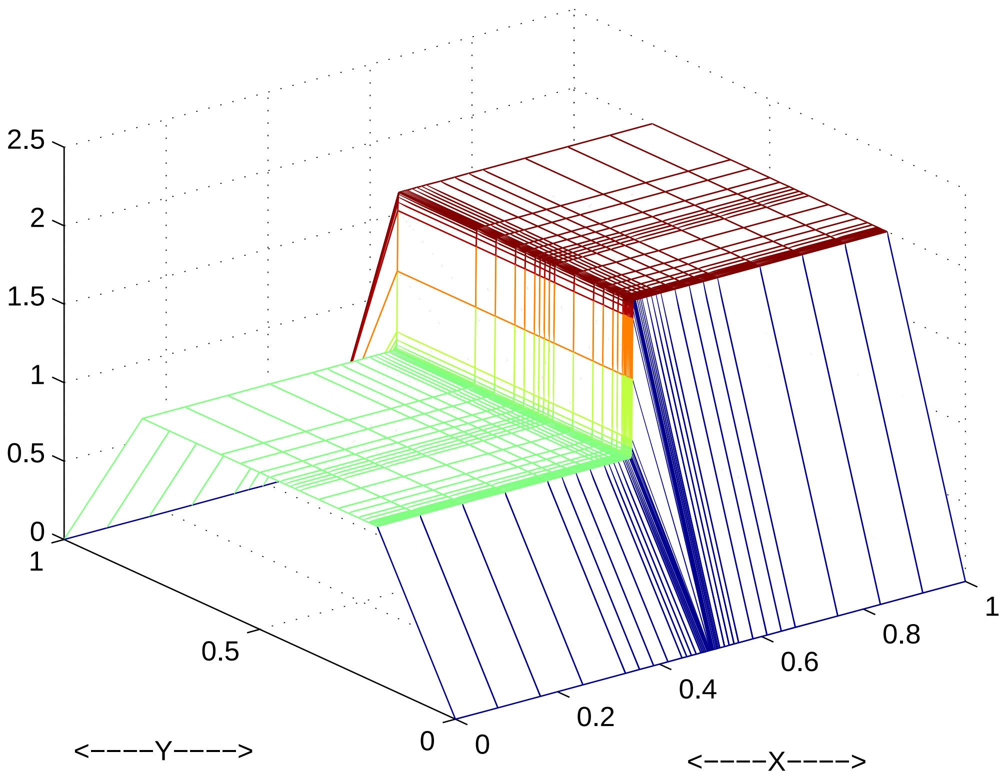


Figure 7: For $\epsilon = 10^{-6}$ with adaptive mesh

Parabolic Problems

$$u_t(x,t) + a(x)u_x(x,t) + b(x)u(x,t) - f(x,t) = \epsilon u_{xx}(x,t),$$

$$S = u^2 \;\; ; S_t = 2uu_t \;\; ; S_x = 2uu_x$$

$$2uu_t = 2u(\epsilon u_{xx} - au_x - bu) + 2uf,$$

which, on expanding, can be written as

$$2uu_t = \epsilon 2uu_{xx} - a2uu_x - b2uu + 2uf.$$

$$S_t = \epsilon(S_{xx} - 2u_x^2) - aS_x - 2bS + 2uf.$$

$$P = S_t - \epsilon S_{xx} + aS_x - 2uf = -2\epsilon u_x^2 - 2bS \leq 0 \;\; (\text{ for } b \geq 0).$$

Parabolic Example

$$u_t + (1 + x(1-x))u_x - f(x,t) = \epsilon u_{xx}; (x,t) \in (0,1) \times (0,1], 0 < \epsilon << 1,$$

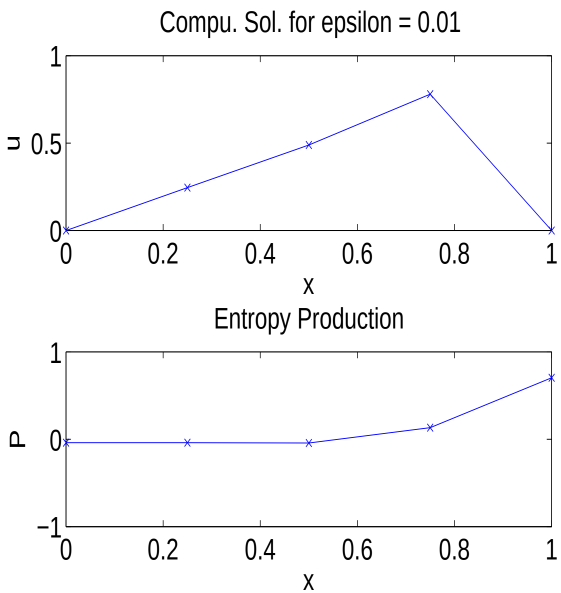
with boundary conditions are given as

$$u(0,t) = 0 \text{ and } \quad u(1,t) = 0;$$

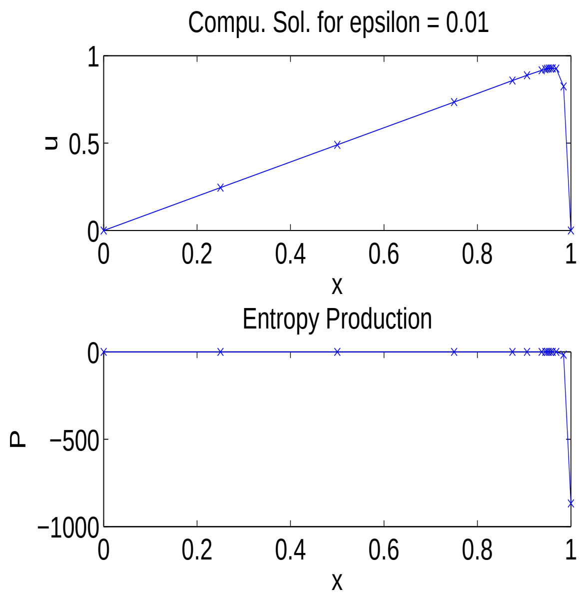
The exact solution is

$$u(x,t) = e^{-t}[e^{-1/\epsilon} + (1 - e^{-1/\epsilon})x - e^{-(1-x)/\epsilon}].$$

Parabolic Results



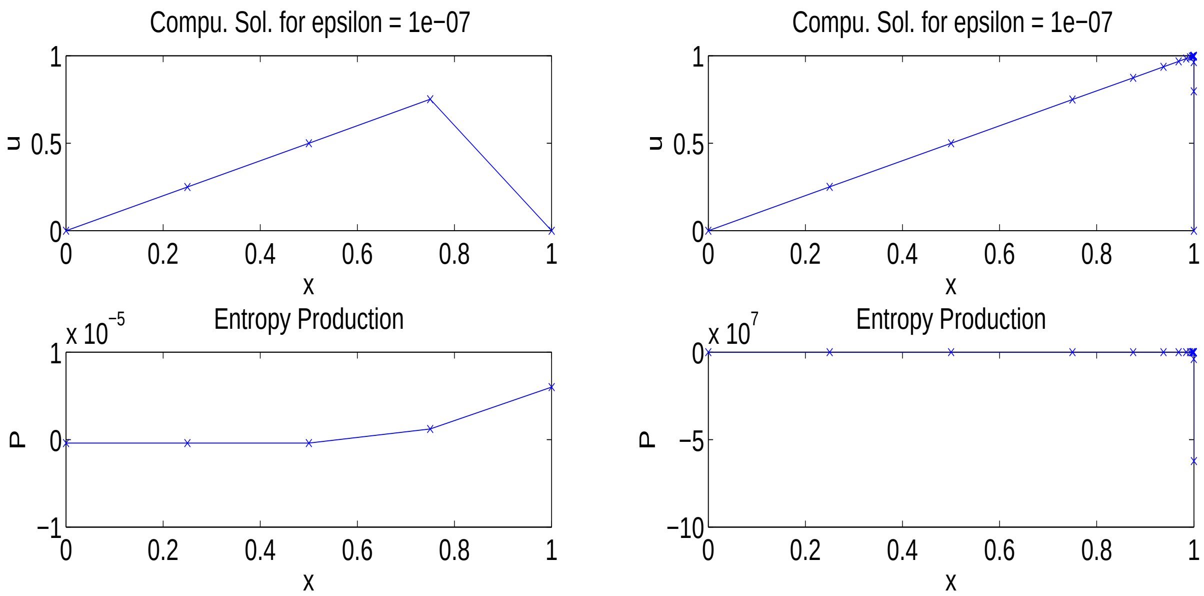
(a) Computed sol. and the corresponding entrophy for initial unifrom mesh



(b) Computed sol. and the corresponding entrophy for adaptive mesh

Figure 8: Results for $\epsilon = 10^{-2}$.

Parabolic Results

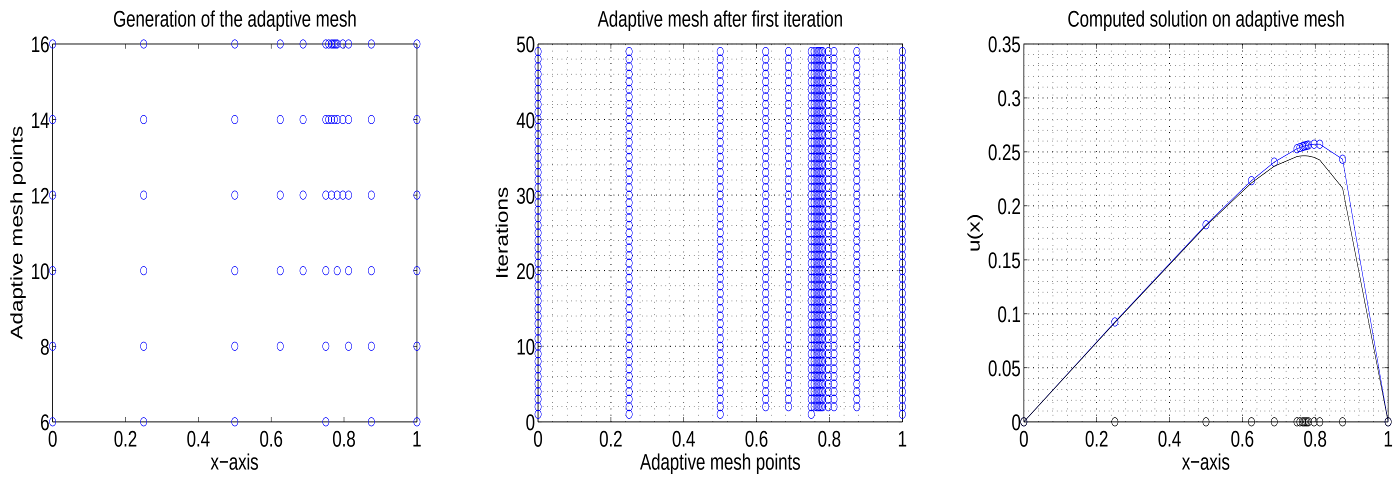


(a) Computed sol. and the corresponding entropy for initial unifrom mesh

(b) Computed sol. and the corresponding entropy for adaptive mesh

Figure 9: Results for $\epsilon = 10^{-7}$

Parabolic Results



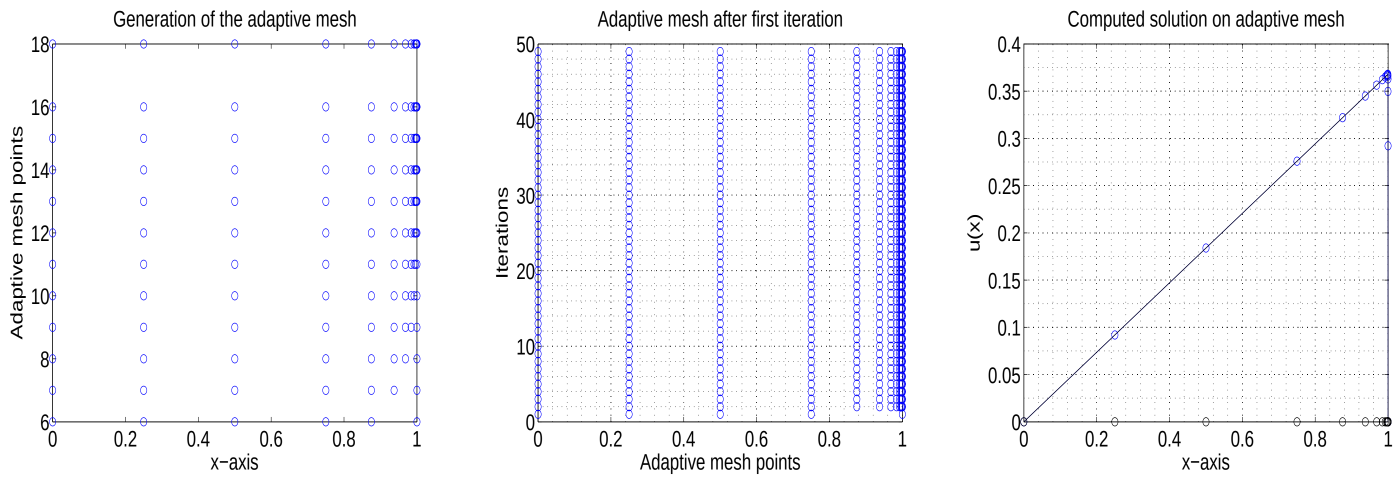
(a) Location of the adaptive mesh points

(b) Adaptive mesh as the time moves forward

(c) Computed sol. verses exact sol.

Figure 10: Results for $\epsilon = 10^{-1}$.

Parabolic Results



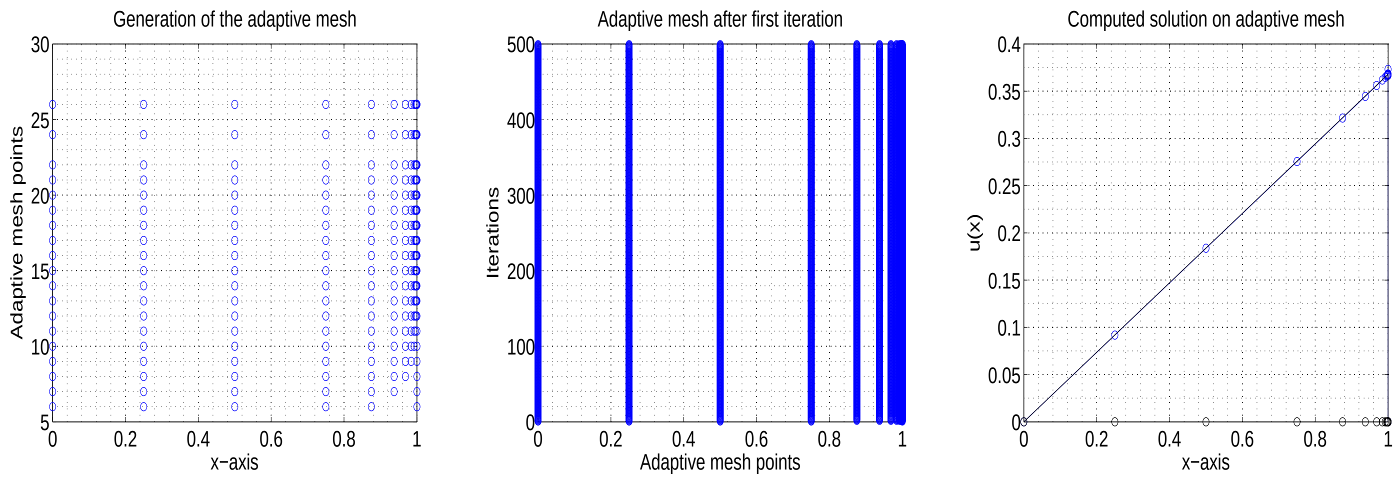
(a) Location of the adaptive mesh points

(b) Adaptive mesh as the time moves forward

(c) Computed sol. verses exact sol.

Figure 11: Results for $\epsilon = 10^{-4}$

Parabolic Results



(a) Location of the adaptive mesh points

(b) Adaptive mesh as the time moves forward

(c) Computed sol. verses exact sol.

Figure 12: Results for $\epsilon = 10^{-6}$

Error estimation

Let N_a be the proposed adaptive mesh which is completely arbitrary in nature. Let us assume that x_i is the i^{th} mesh point and

$$h_f = x_{i+1} - x_i, \;\; h_b = x_i - x_{i-1}$$

be the right hand and left hand side mesh points with distances h_f and h_b. Since we are working with the Crank Nicholson (CN) scheme, which is second order in time and space for a uniform mesh, we can claim that the proposed method is of $O(h_f - h_b, \triangle t^2)$.

Crank Nicolson

We use fully implicit Crank Nicolson (CN) scheme because it is unconditionally stable and also ensures that the time step remains fixed. Let we represent $u(x_i, t_j) = u_i^j$, the CN scheme can be written as

$$\begin{aligned} \frac{u_i^{n+1} - u_i^n}{\triangle t/2} &= \epsilon(\delta^2 u_i^n + \delta^2 u_i^{n+1}) - (a_i^n D_0^n u_i^n + a_i^{n+1} D_0^{n+1} u_i^{n+1}) \\ &- (b_i^n u_i^n + b_i^{n+1} u_i^{n+1}) + f_i^n + f_i^{n+1} \;; \;\; 1 \leq i \leq N_a - 1. \end{aligned}$$

$$r_{i-1}^{j+1} u_{i-1}^{j+1} + r_i^{j+1} u_i^{j+1} + r_{i+1}^{j+1} u_{i+1}^{j+1} = r_{i-1}^j u_{i-1}^j + r_i^j u_i^j + r_{i+1}^j u_{i+1}^j + \frac{(f_i^{j+1} + f_i^j)}{2}$$

Crank Nicolson

$$
\begin{aligned}
r_{i-1}^{j+1} &= \frac{-\epsilon}{(x_i - x_{i-1})(x_{i+1} - x_{i-1})} - \frac{a_i}{2(x_{i+1} - x_{i-1})} \\
r_{i}^{j+1} &= \frac{1}{\triangle t} + \frac{\epsilon}{(x_i - x_{i-1})(x_{i+1} - x_{i})} + \frac{b_i}{2} \\
r_{i+1}^{j+1} &= \frac{-\epsilon}{(x_{i+1} - x_{i})(x_{i+1} - x_{i-1})} + \frac{a_i}{2(x_{i+1} - x_{i-1})} \\
r_{i-1}^{j} &= -r_{i-1}^{j+1} \\
r_{i}^{j} &= \frac{1}{\triangle t} - \frac{\epsilon}{(x_i - x_{i-1})(x_{i+1} - x_{i})} - \frac{b_i}{2} \\
r_{i+1}^{j} &= -r_{i+1}^{j+1}.
\end{aligned}
$$

The above equations can be written as a system

$$AU^{j+1} = BU^{j} + F$$

Stability

Now we show the stability in the norm $\|x\|_{2,\Delta x} = (\sum_{i=1}^{N-1} x_i^2 \Delta x)^{1/2}$. Here we take $\Delta x =$ maximum step size in our adaptive mesh N_a. Rewritten as (considering $f(x,t) = 0$)

$$r_i^{j+1} u_i^{j+1} - r_i^j u_i^j = r_{i-1}^j u_{i-1}^j - r_{i-1}^{j+1} u_{i-1}^{j+1} + r_{i+1}^j u_{i+1}^j - r_{i+1}^{j+1} u_{i+1}^{j+1},$$

$$\begin{aligned} \frac{1}{\triangle t}(u_i^{j+1} - u_i^j) &= r_{i-1}^j (u_{i-1}^j + u_{i-1}^{j+1}) + r_{i+1}^j (u_{i+1}^j + u_{i+1}^{j+1}) \\ &- \left(\frac{\epsilon}{(x_i - x_{i-1})(x_{i+1} - x_i)} + \frac{b_i}{2}\right)(u_i^{j+1} + u_i^j) \text{ for } 1 \le x \le N_a - 1 \\ u_0^{n+1} &= u_0^n = 0,\ \ u_{N_a}^{n+1} = u_{N_a}^n = 0 \text{ (B.C)} . \end{aligned}$$

Stability

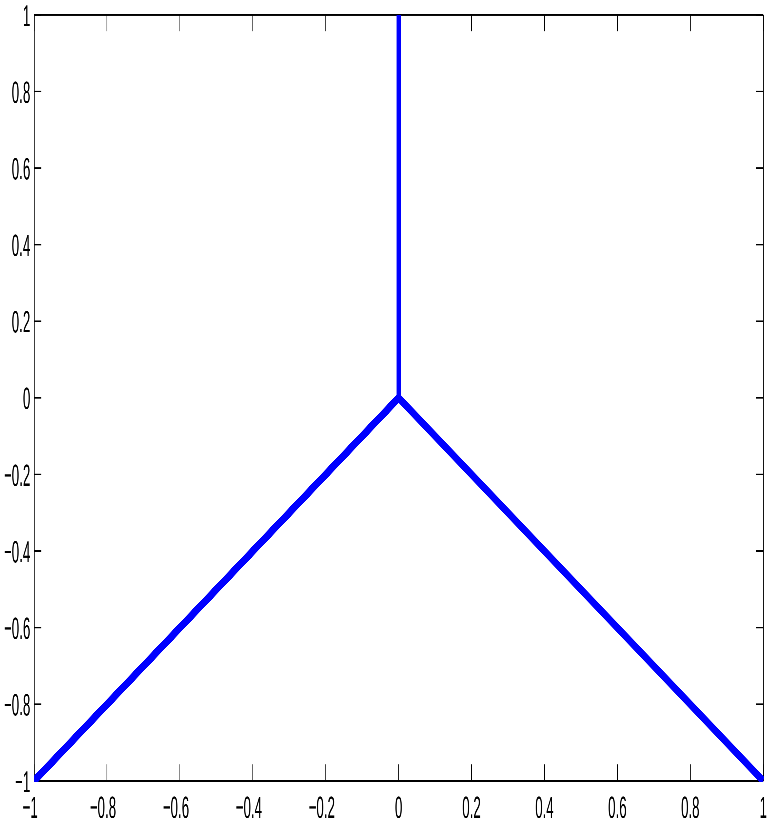
$$\|U^{j+1}\|^2_{2,\Delta x} - \|U^j\|^2_{2,\Delta x} \leq \triangle t \Delta x T[-\Sigma_{i=1}^{N_a-1}(B_i - B_{i+1})^2 - B_1^2] \leq 0,$$

provided $T > 0$. Finally we get

$$\|U^{j+1}\|^2_{2,\Delta x} \leq \|U^j\|^2_{2,\Delta x}$$

which shows that the scheme is stable under the norm $\|x\|_{2,\Delta x} = (\sum_{i=1}^{N-1} x_i^2 \Delta x)^{1/2}$.

Graph Topology



SPP on graph

We consider linear convection-diffusion problem as

$$-\epsilon_i u_i'' + u_i' = 1; k = 1, 2, 3$$

with boundary conditions as $u_k(0) = 0$. We have continuity condition

$$u_1(1) = u_2(1) = u_3(1) = z(say)$$

and Kirchhoff's law at the coupling node

$$\sum_{k=1}^{3} \epsilon_k u_k'(1) = 0$$

We solve it with central finite difference scheme. We introduce ghost points near the boundary $x = 1$. Using Kirchhoff's condition at $x = 1$

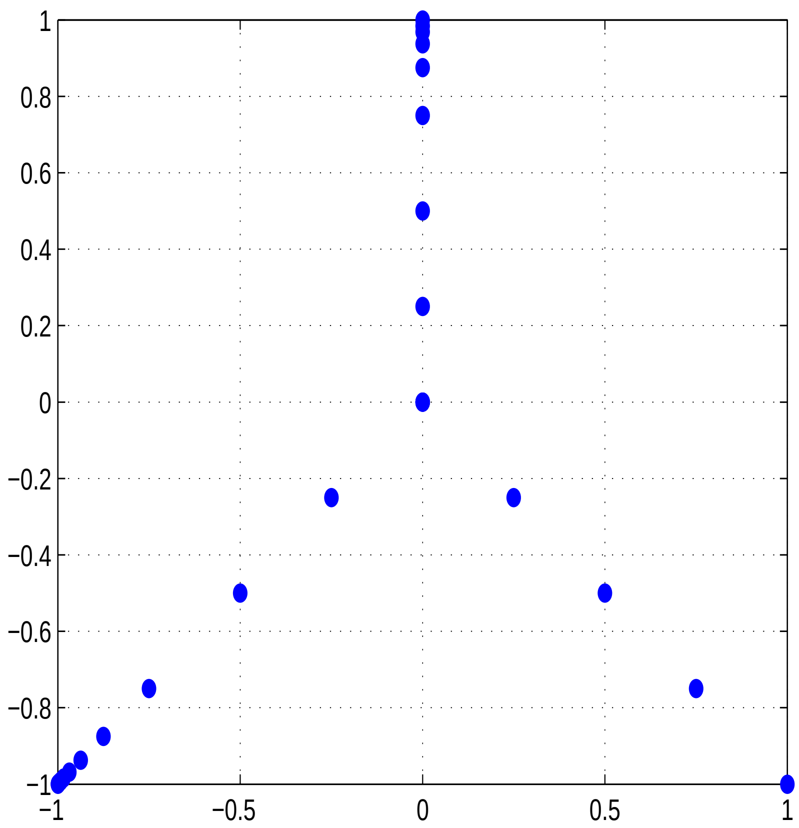
$$\sum_{k=1}^{3} \epsilon_k (u_{k,n_{k+1}} - u_{k,n_{k-1}})/2h_k = 0$$

and the differential operator at $x = 1$,

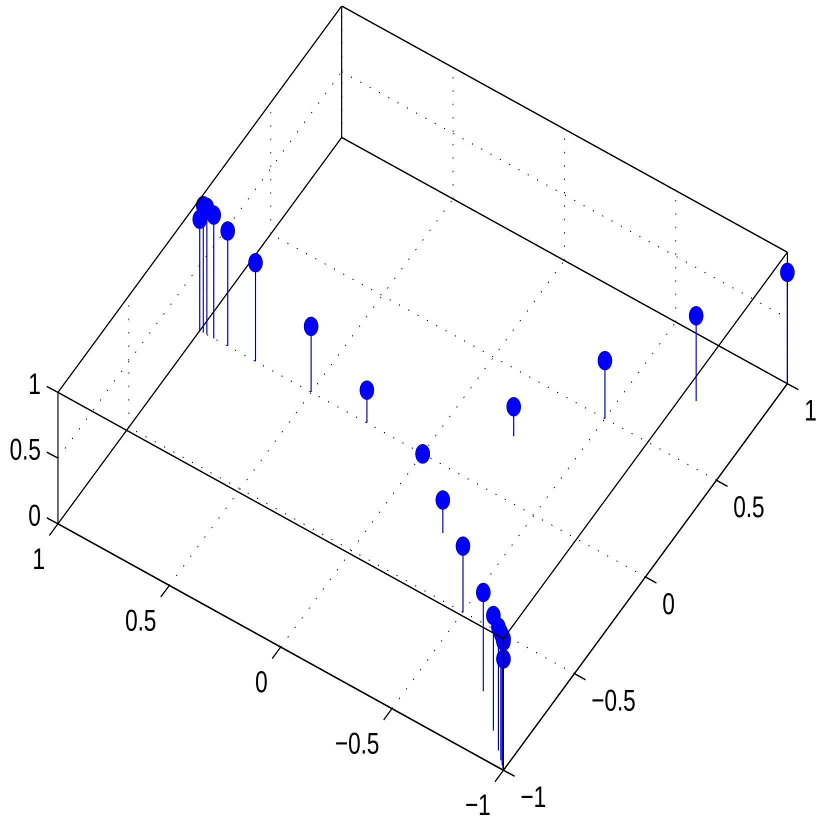
$$-\epsilon_k \delta^2 u_k + D^0 u_k = 1$$

we are able to find the value of z and the solution at the ghost points.

Adaptive mesh on Graph



Solution on Graph



References

- Vivek Kumar, Balaji Srinivasan *An adaptive mesh strategy for singularly perturbed convection diffusion problems*, Applied Mathematical Modelling 39 (2015) 2081-2091.
- Balaji Srinivasan, Vivek Kumar *The versatility of an entropy inequality for the robust computation of convection dominated problems*, Procedia Computer Science 108C (2017) 887-896.