

Algebraic flux correction for convection–diffusion problems

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joint work with

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Outline

- algebraic flux correction scheme for a steady-state convection–diffusion–reaction equation
- theoretical analysis: error estimate, discrete maximum principle
- examples of limiters
- linearity preservation
- approximation of boundary layers
- difficulties caused by non-vanishing right-hand side
- numerical results

Steady-state convection–diffusion–reaction equation

$$-\varepsilon \Delta u + \mathbf{b} \cdot \nabla u + cu = f \quad \text{in } \Omega, \quad u = u_b \quad \text{on } \partial\Omega$$

with constant $\varepsilon > 0$ and

$$\nabla \cdot \mathbf{b} = 0, \quad c \geq \sigma_0 \geq 0 \quad \text{in } \Omega.$$

FE discretization

Find $u_h \in W_h$ such that $u_h(x_i) = u_b(x_i)$, $i = M + 1, \dots, N$, and

$$a_h(u_h, v_h) = (f, v_h) \quad \forall v_h \in V_h,$$

where

$$W_h = \{v_h \in C(\overline{\Omega}); v|_K \in P_1(K) \forall K \in \mathcal{T}_h\}, \quad V_h = W_h \cap H_0^1(\Omega),$$

$$a_h(u_h, v_h) = \varepsilon (\nabla u_h, \nabla v_h) + (\mathbf{b} \cdot \nabla u_h, v_h) + \sum_{i=1}^M (c, \varphi_i) u_i v_i.$$

Algebraic problem

$$\sum_{j=1}^N a_{ij} u_j = f_i, \quad i = 1, \dots, M,$$

$$u_i = u_i^b, \quad i = M + 1, \dots, N.$$

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Properties: $(a_{ij})_{i,j=1}^M$ is positive definite,

$$\sum_{j=1}^N a_{ij} \geq 0 \quad \forall i = 1, \dots, M$$

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Algebraic flux correction Kuzmin et al. (2001–now)

Aim: manipulate the algebraic system in such a way that the solution satisfies **DMP** and layers are **not smeared**.

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$(a_{ij})_{i,j=1}^N$... FE matrix for homogeneous natural b.c.

$(d_{ij})_{i,j=1}^N$... symmetric artificial diffusion matrix:

$$d_{ij} = -\max\{a_{ij}, 0, a_{ji}\} \quad \forall i \neq j, \quad d_{ii} = -\sum_{j \neq i} d_{ij}.$$

Algebraic flux correction scheme

$$\sum_{j=1}^N a_{ij} u_j + \sum_{j=1}^N (1 - \alpha_{ij}) d_{ij} (u_j - u_i) = f_i, \quad i = 1, \dots, M,$$

$$u_i = u_i^b, \quad i = M + 1, \dots, N,$$

where $\alpha_{ij} = \alpha_{ij}(u_1, \dots, u_N) \in [0, 1]$,

$$\alpha_{ij} = \alpha_{ji}, \quad i, j = 1, \dots, N.$$

and $\alpha_{ij}(U)(u_i - u_j)$ are continuous functions of $U = (u_1, \dots, u_N)$.

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Theoretical analysis:

Barrenechea, John, K., IMAJNA (2015)

Barrenechea, John, K., SINUM (2016)

Barrenechea, John, K., M3AS (2017)

Variational form of the AFC scheme

Find $u_h \in W_h$ such that $u_h(x_i) = u_b(x_i)$, $i = M + 1, \dots, N$, and

$$a_h(u_h, v_h) + d_h(u_h; u_h, v_h) = (f, v_h) \quad \forall v_h \in V_h$$

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$$d_h(w_h; z, v) = \sum_{i,j=1}^N (1 - \alpha_{ij}(w_h)) d_{ij} (z(x_j) - z(x_i)) v(x_i).$$

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Error estimate (for $\sigma_0 > 0$)

Natural norm: $\|v_h\|_h = \left(\varepsilon |v|_{1,\Omega}^2 + \sigma_0 \|v\|_{0,\Omega}^2 + d_h(u_h; v_h, v_h) \right)^{1/2}$

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$$\begin{aligned} \Rightarrow \|u - u_h\|_h &\leq C \|u - i_h u\|_h + \sup_{v_h \in V_h} \frac{a(u, v_h) - a_h(i_h u, v_h)}{\|v_h\|_h} \\ &\quad + d_h(u_h; i_h u, i_h u)^{1/2} \end{aligned}$$

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$$+ d_h(u_h; i_h u, i_h u)^{1/2} \leq Ch \|u\|_{2,\Omega} + d_h(u_h; i_h u, i_h u)^{1/2}$$

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Discrete maximum principle

Local index sets: $S_i \supset \{j \in \{1, \dots, N\} \setminus \{i\}; a_{ij} \neq 0 \text{ or } a_{ji} > 0\}$,
 $i = 1, \dots, M$.

Assumption (A):

For any $i \in \{1, \dots, M\}$ and any $U = (u_1, \dots, u_N) \in \mathbb{R}^N$:

$$u_i > u_j \quad \forall j \in S_i \quad \text{or} \quad u_i < u_j \quad \forall j \in S_i \\ \Rightarrow \quad a_{ij} + (1 - \alpha_{ij}(U)) d_{ij} \leq 0 \quad \forall j \in S_i.$$

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Theorem Consider any $i \in \{1, \dots, M\}$. Then

$$f_i \leq 0 \quad \Rightarrow \quad u_i \leq \max_{j \in S_i} u_j^+, \quad f_i \geq 0 \quad \Rightarrow \quad u_i \geq \min_{j \in S_i} u_j^-.$$

If $\sum_{j=1}^N a_{ij} = 0$, then

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Limiter 1

Zalesak (1979), Kuzmin (2007)

$$P_i^+ := \sum_{\substack{j=1 \\ a_{ji} \leq a_{ij}}}^N f_{ij}^+, \quad Q_i^+ := - \sum_{j=1}^N f_{ij}^-, \quad R_i^+ := \min \left\{ 1, \frac{Q_i^+}{P_i^+} \right\},$$

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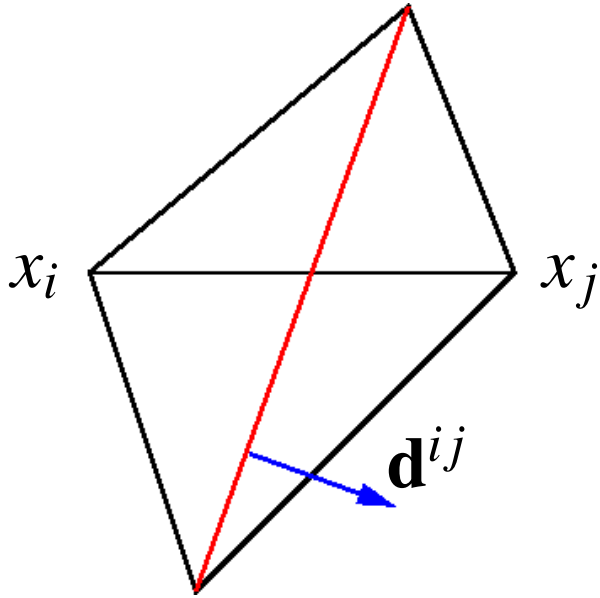
Assumption (A) satisfied if $\min\{a_{ij}, a_{ji}\} \leq 0 \quad \forall i, j \in \{1, \dots, N\}$

\Rightarrow DMP guranteed for Delaunay meshes,

... and often holds on non-Delaunay meshes!!!

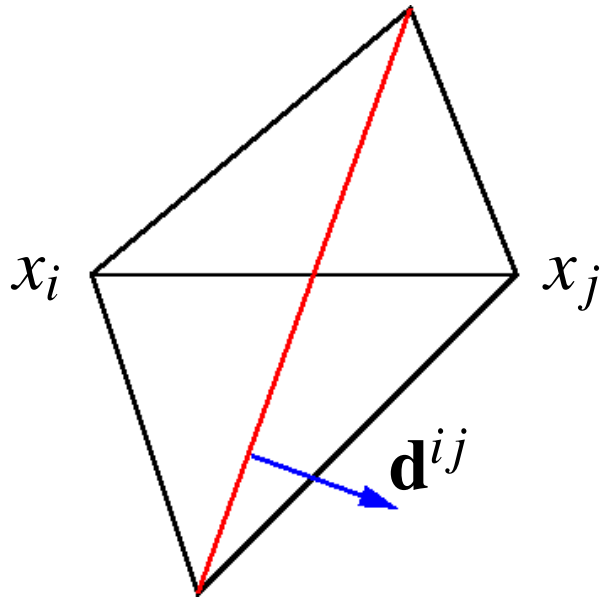
Condition $a_{ji} \leq a_{ij}$ **for constant** \mathbf{b}

$$a_{ji} < a_{ij} \Leftrightarrow \mathbf{b} \cdot \mathbf{d}^{ij} > 0 \quad \text{with} \quad \mathbf{d}^{ij} = \int_{\Omega} \varphi_i \nabla \varphi_j \, dx$$



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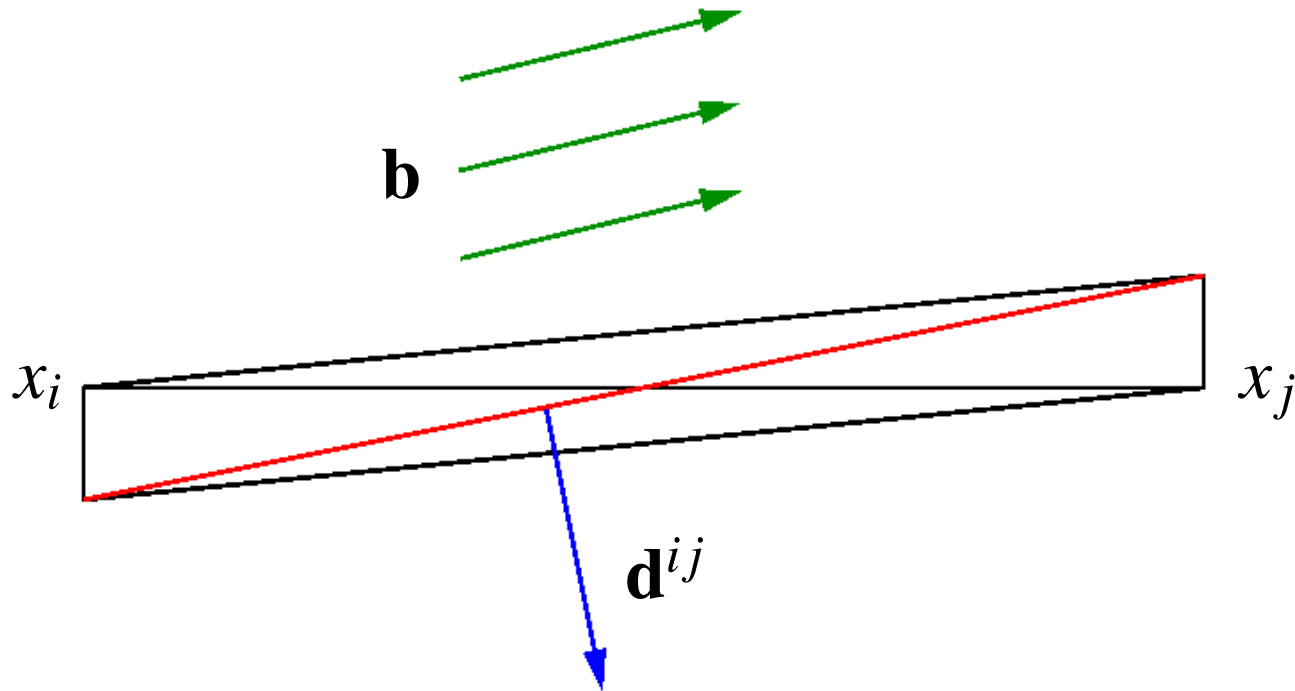
\Rightarrow if $\mathbf{b} \parallel x_i x_j$ or red line $\perp x_i x_j$, then

$a_{ji} < a_{ij} \Leftrightarrow x_i$ is the upwind vertex.

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BUT:



$a_{ji} > a_{ij}$, but x_i is the upwind vertex!

Limiter 2

Kuzmin (2012), Barrenechea, John, K. (2016)

$$u_i^{\max} := \max_{j \in S_i \cup \{i\}} u_j, \quad u_i^{\min} := \min_{j \in S_i \cup \{i\}} u_j, \quad q_i := \gamma_i \sum_{j \in S_i} d_{ij},$$

$$P_i^+ := \sum_{j \in S_i} f_{ij}^+, \quad Q_i^+ := q_i (u_i - u_i^{\max}), \quad R_i^+ := \min \left\{ 1, \frac{Q_i^+}{P_i^+} \right\},$$

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Assumption (A) always satisfied

⇒ DMP guranteed for arbitrary meshes!

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Limiter 2: for **arbitrary meshes** if

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Improved error estimate on Delaunay meshes

Lipschitz-continuity $\Rightarrow d_h(u_h; i_h u, i_h u)$

$$\leq C \|\mathbf{b}\|_{0,\infty,\Omega} h |u - u_h|_{1,\Omega} |i_h u|_{1,\Omega} + C \|\mathbf{b}\|_{0,\infty,\Omega} h^2 |u|_{2,\Omega} |i_h u|_{1,\Omega}$$

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$$\Rightarrow \|u - u_h\|_h \leq Ch \|u\|_{2,\Omega} + C \frac{h}{\sqrt{\varepsilon}} |i_h u|_{1,\Omega}$$

Limiter 3

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$$\tilde{\alpha}_{ij} := \begin{cases} R_i^+ & \text{if } f_{ij} > 0, \\ 1 & \text{if } f_{ij} = 0, \\ R_i^- & \text{if } f_{ij} < 0, \end{cases} \quad \alpha_{ij} = \alpha_{ji} := \begin{cases} \tilde{\alpha}_{ij} & \text{if } a_{ji} \leq a_{ij}, \\ \tilde{\alpha}_{ji} & \text{else.} \end{cases}$$

Limiter 4

$\alpha_{ij} = \alpha_{ji}$ defined as for Limiter 3 if $\min\{a_{ij}, a_{ji}\} \leq 0$ and as for Limiter 2 otherwise.

Example 1 (polynomial solution)

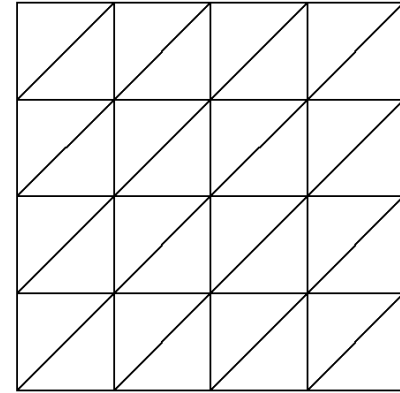
$$\Omega = (0, 1)^2, \quad \mathbf{b} = (3, 2), \quad c = 1, \quad u_b = 0.$$

The right-hand side f is chosen such that, for given ε ,

$$u(x, y) = 100x^2(1-x)^2y(1-y)(1-2y)$$

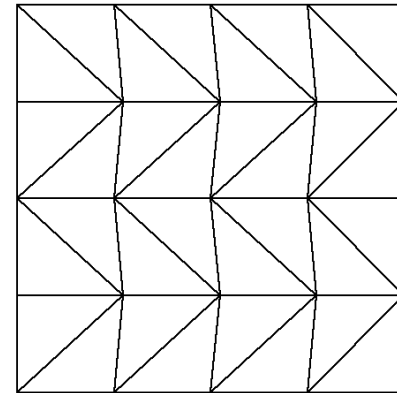
is the exact solution.

Example 1, Limiter 1, $\varepsilon = 10^{-8}$



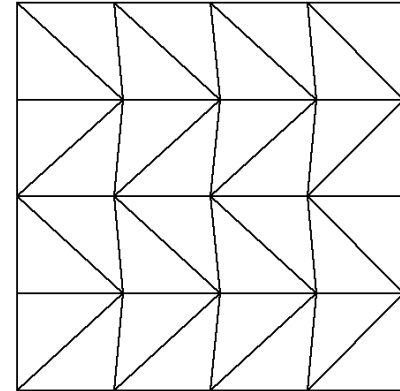
l	$\ e_h\ _{0,\Omega}$	ord.	$ e_h _{1,\Omega}$	ord.	$d_h^{1/2}(u_h)$	ord.
3	5.457e-3	1.85	2.287e-1	1.10	1.163e-2	2.11
4	1.408e-3	1.95	1.074e-1	1.09	2.683e-3	2.12
5	3.493e-4	2.01	5.113e-2	1.07	6.410e-4	2.07
6	8.652e-5	2.01	2.546e-2	1.01	1.633e-4	1.97
7	2.152e-5	2.01	1.321e-2	0.95	4.099e-5	1.99
8	5.357e-6	2.01	6.822e-3	0.95	1.018e-5	2.01

**Example 1, Limiter 1, $\varepsilon = 10$
(non-Delaunay grid)**



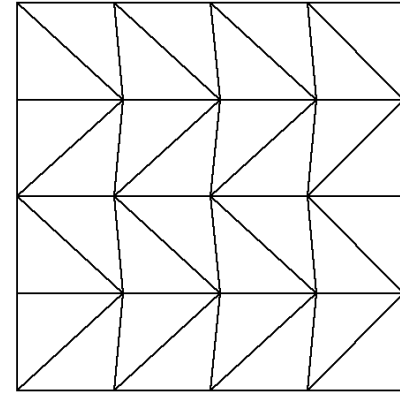
l	$\ e_h\ _{0,\Omega}$	ord.	$ e_h _{1,\Omega}$	ord.	$d_h^{1/2}(u_h)$	ord.
3	1.248e-2	0.48	2.229e-1	0.79	7.211e-1	0.77
4	1.123e-2	0.15	1.558e-1	0.52	5.135e-1	0.49
5	1.090e-2	0.04	1.333e-1	0.22	4.452e-1	0.21
6	1.080e-2	0.01	1.269e-1	0.07	4.259e-1	0.06
7	1.077e-2	0.00	1.252e-1	0.02	4.207e-1	0.02
8	1.076e-2	0.00	1.248e-1	0.00	4.193e-1	0.00

**Example 1, Limiter 4, $\varepsilon = 10$
(non-Delaunay grid)**



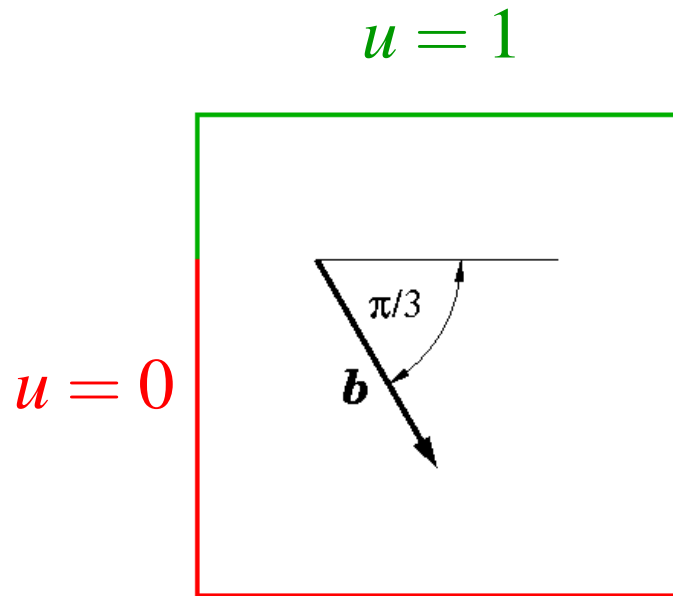
l	$\ e_h\ _{0,\Omega}$	ord.	$ e_h _{1,\Omega}$	ord.	$d_h^{1/2}(u_h)$	ord.
3	2.259e-3	2.01	1.850e-1	0.99	5.850e-1	0.99
4	5.588e-4	2.02	9.278e-2	1.00	2.934e-1	1.00
5	1.391e-4	2.01	4.643e-2	1.00	1.468e-1	1.00
6	3.472e-5	2.00	2.322e-2	1.00	7.343e-2	1.00
7	8.675e-6	2.00	1.161e-2	1.00	3.672e-2	1.00

**Example 1, Limiter 4, $\varepsilon = 10$, $\gamma_i := \gamma_i/10$
(non-Delaunay grid)**



l	$\ e_h\ _{0,\Omega}$	ord.	$ e_h _{1,\Omega}$	ord.	$d_h^{1/2}(u_h)$	ord.
3	1.938e-2	0.40	2.395e-1	0.73	7.741e-1	0.71
4	1.746e-2	0.15	1.749e-1	0.45	5.739e-1	0.43
5	1.679e-2	0.06	1.530e-1	0.19	5.066e-1	0.18
6	1.652e-2	0.02	1.463e-1	0.06	4.859e-1	0.06
7	1.640e-2	0.01	1.442e-1	0.02	4.794e-1	0.02

Example 2 (interior layer and exponential boundary layers)



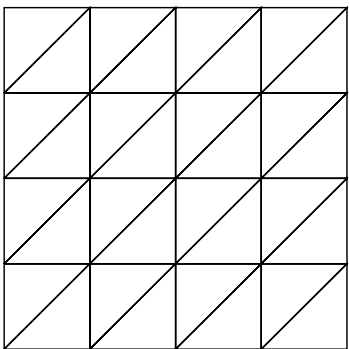
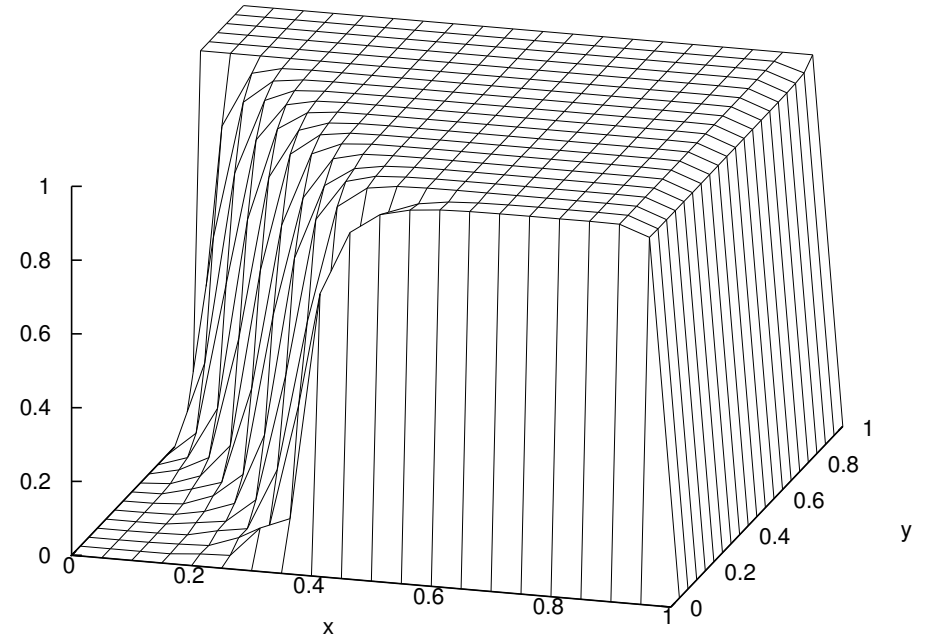
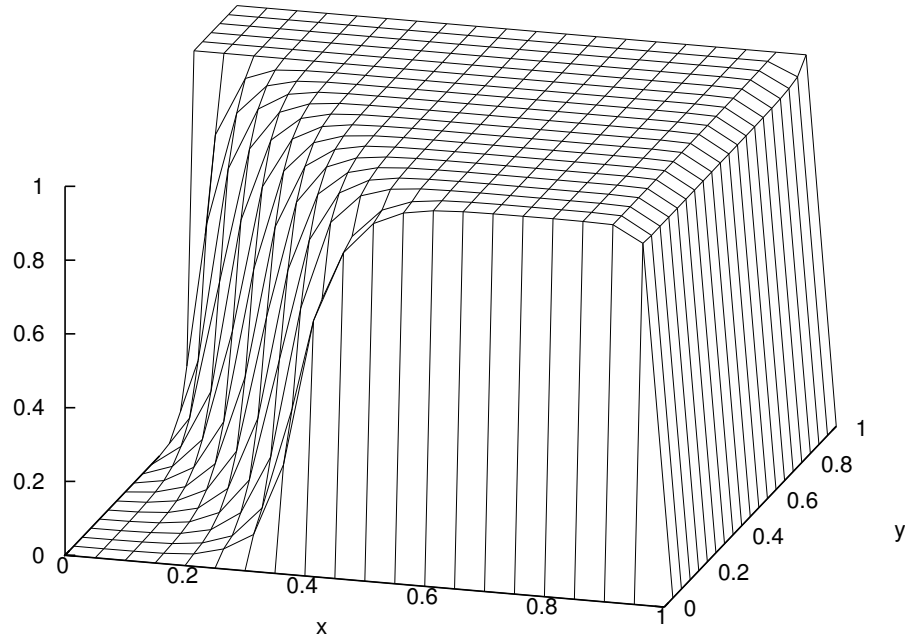
$$\varepsilon = 10^{-8}$$

$$|\mathbf{b}| = 1$$

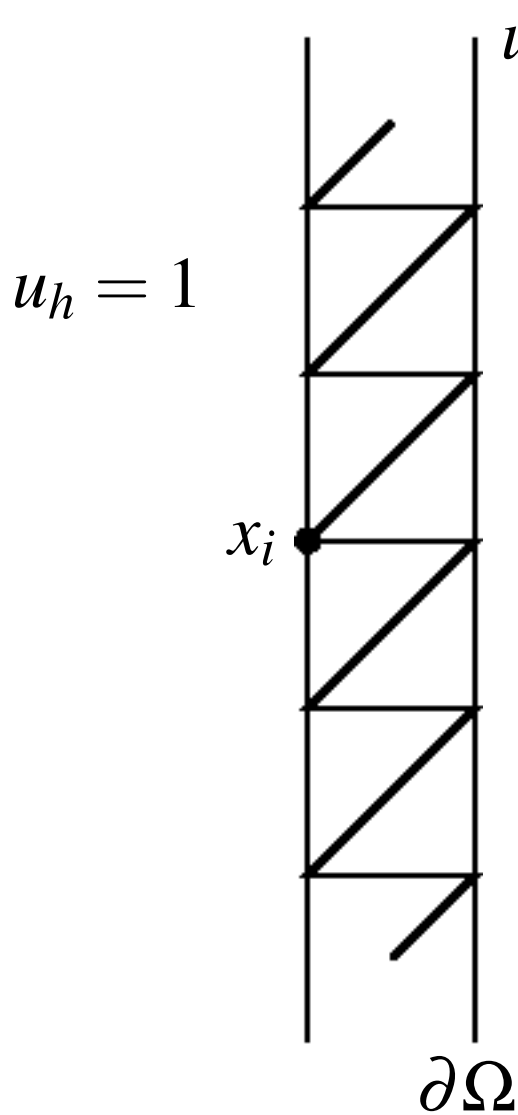
$$c = 0$$

$$f = 0$$

Example 2, Limiter 4, 21x21 mesh, $\gamma_i = 1$ vs. $\gamma_i = 2$



Approximation of boundary layers



Assumption (A) & continuity \Rightarrow

$$[a_{ij} + (1 - \alpha_{ij}(U)) d_{ij}] (u_j - u_i) \geq 0 \quad \forall j \in S_i$$

AFC scheme:

$$\sum_{j \in S_i} [a_{ij} + (1 - \alpha_{ij}(U)) d_{ij}] (u_j - u_i) = 0$$

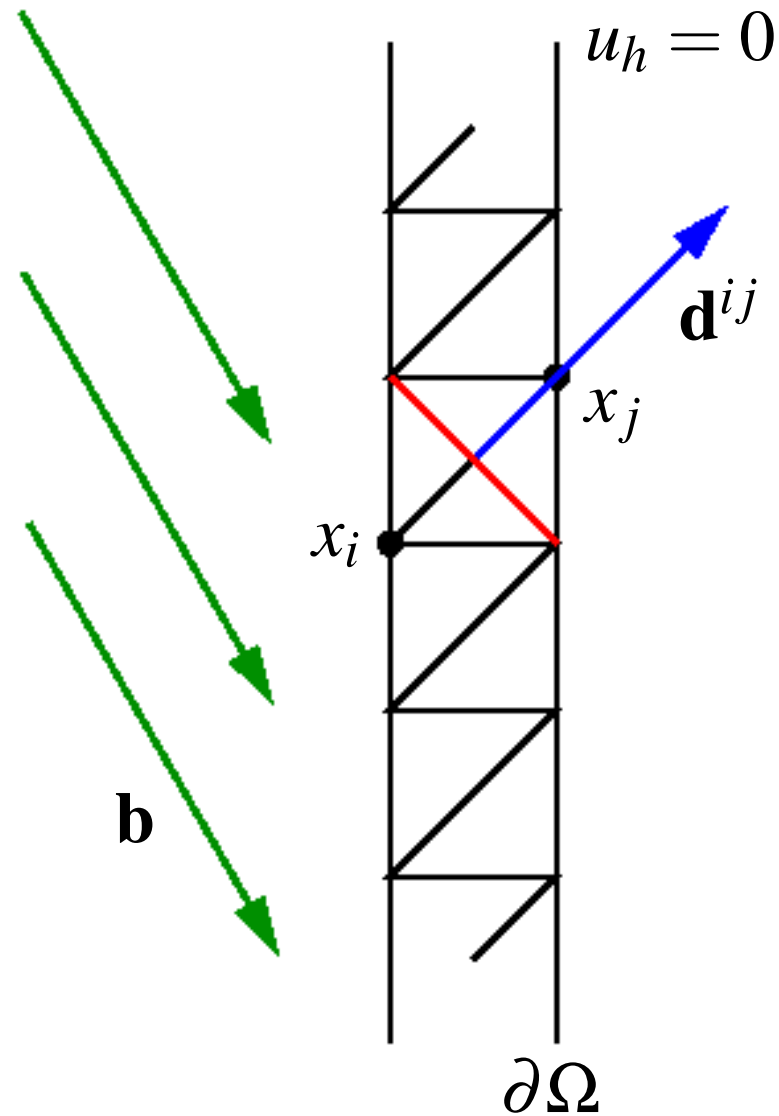
$$\Rightarrow a_{ij} + (1 - \alpha_{ij}(U)) d_{ij} = 0 \quad \forall j \in S_i^{\partial\Omega}$$

$$\Rightarrow a_{ij} \geq 0 \quad \forall j \in S_i^{\partial\Omega} \quad \text{also sufficient!}$$

$$\Rightarrow \mathbf{b} \cdot \mathbf{d}^{ij} \geq 0 \quad \forall j \in S_i^{\partial\Omega}$$

since $a_{ij} = \varepsilon (\nabla \varphi_j, \nabla \varphi_i) + \mathbf{b} \cdot \mathbf{d}^{ij}$

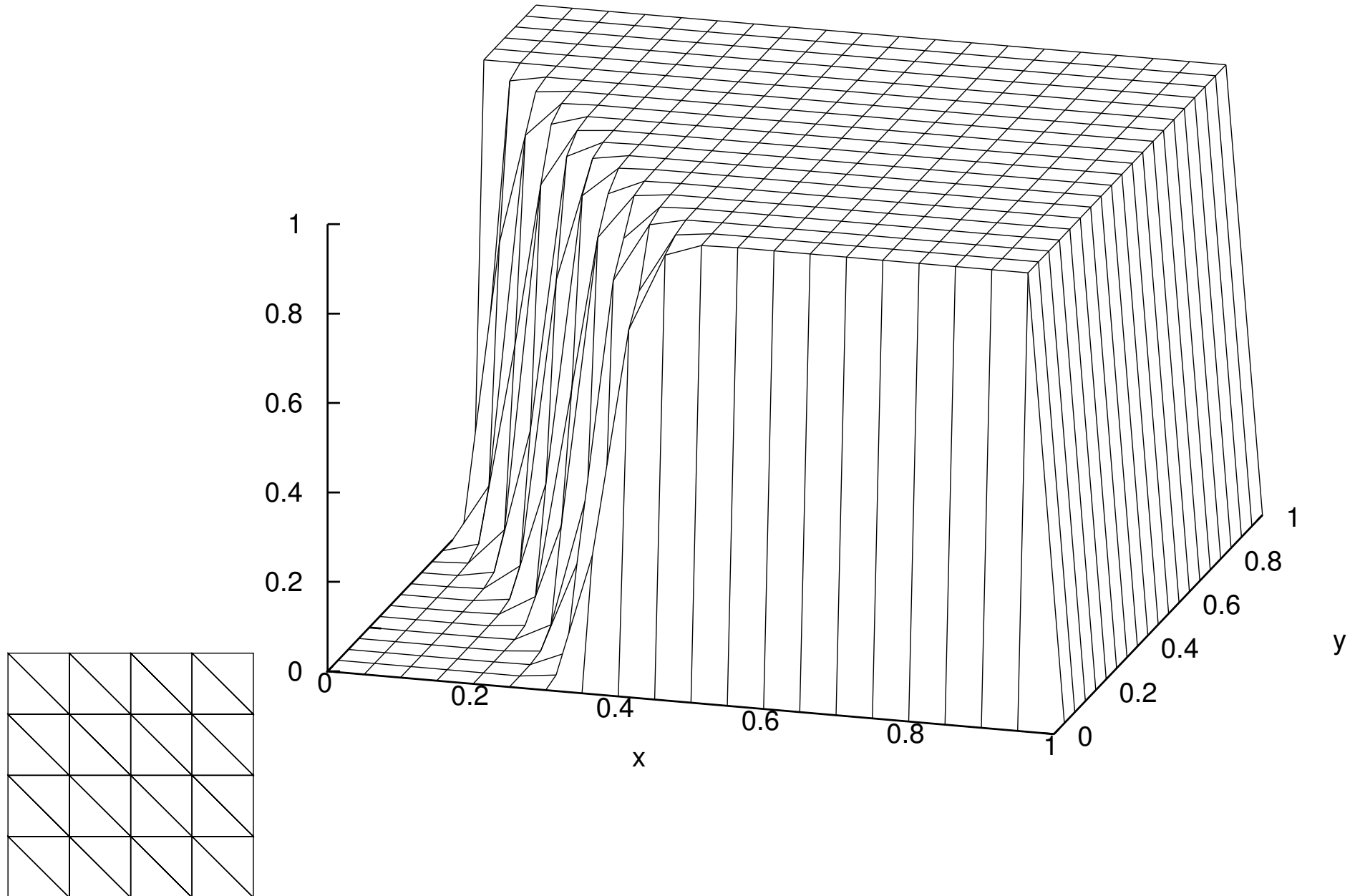
Approximation of boundary layers



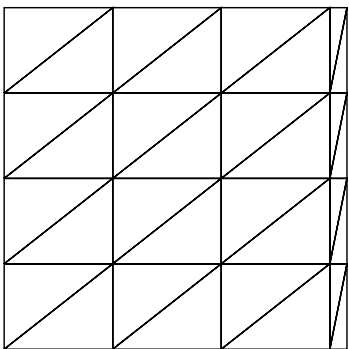
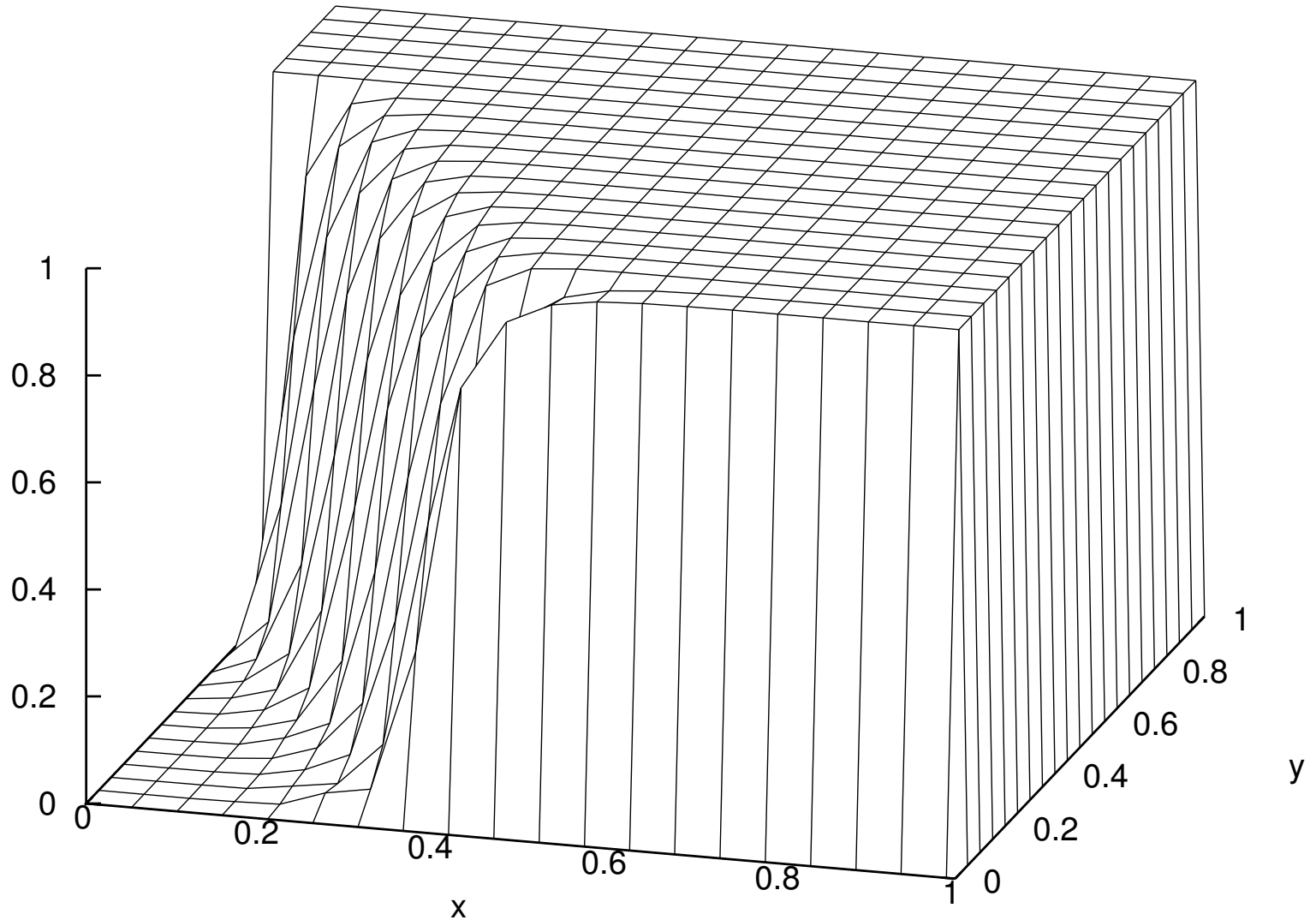
$$\mathbf{b} \cdot \mathbf{d}^{ij} < 0$$

sharp approximation of the boundary layer not possible with any limiter for meshes of this type!!!

Example 2, Limiter 4, 21x21 mesh



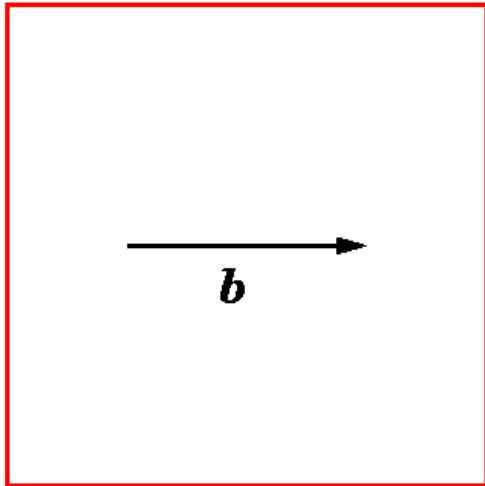
Example 2, Limiter 4, 21x21 mesh



Geometry of the mesh important,
not only the directions of edges!

Example 3 (exponential and parabolic boundary layers)

$$u = 0$$



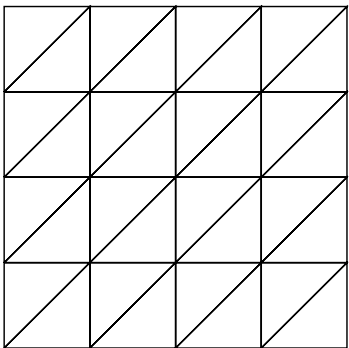
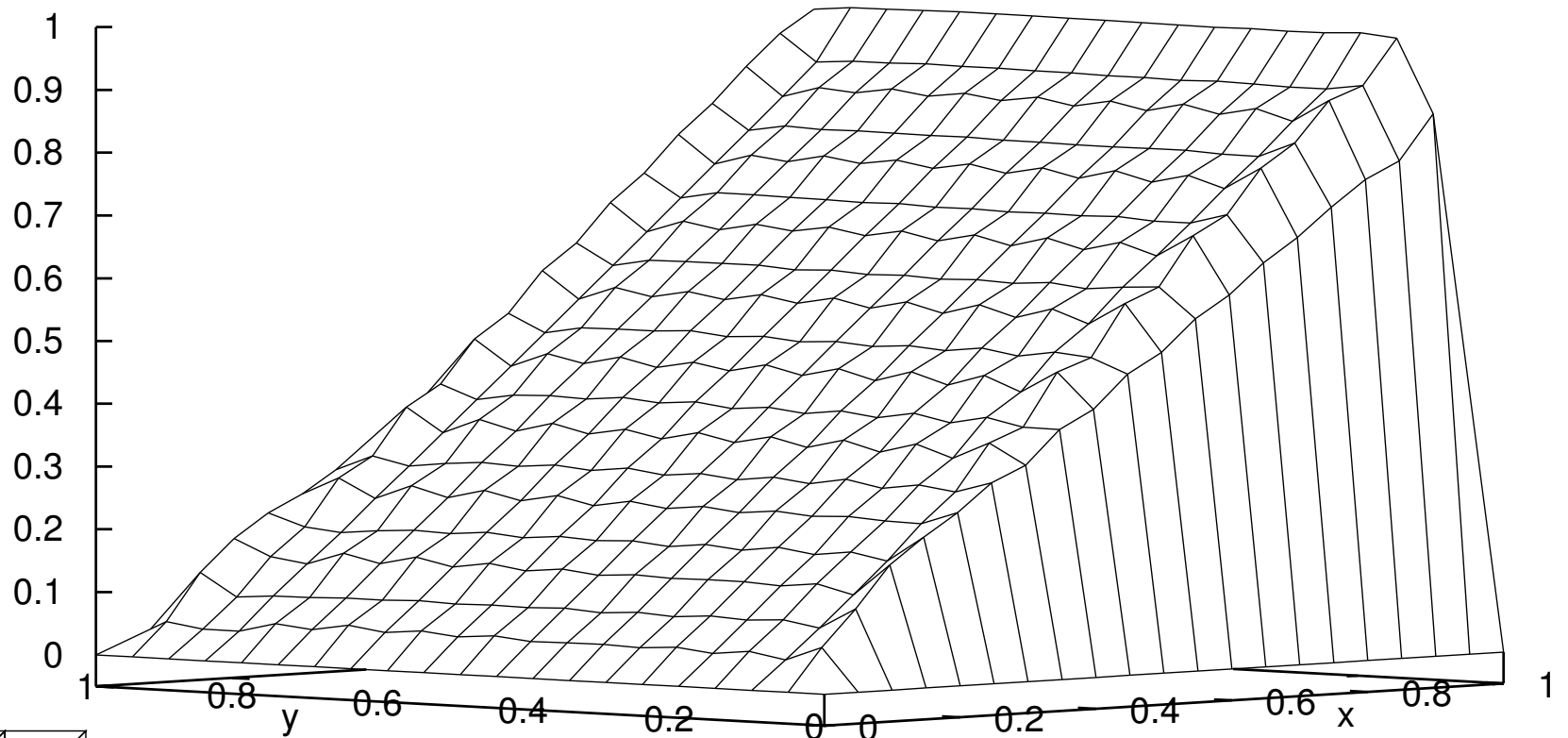
$$\varepsilon = 10^{-8}$$

$$|\mathbf{b}| = 1$$

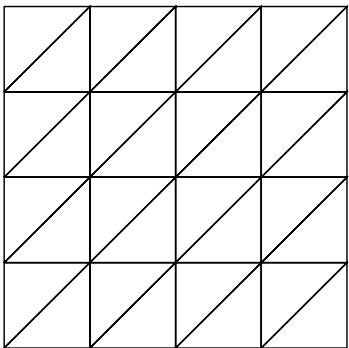
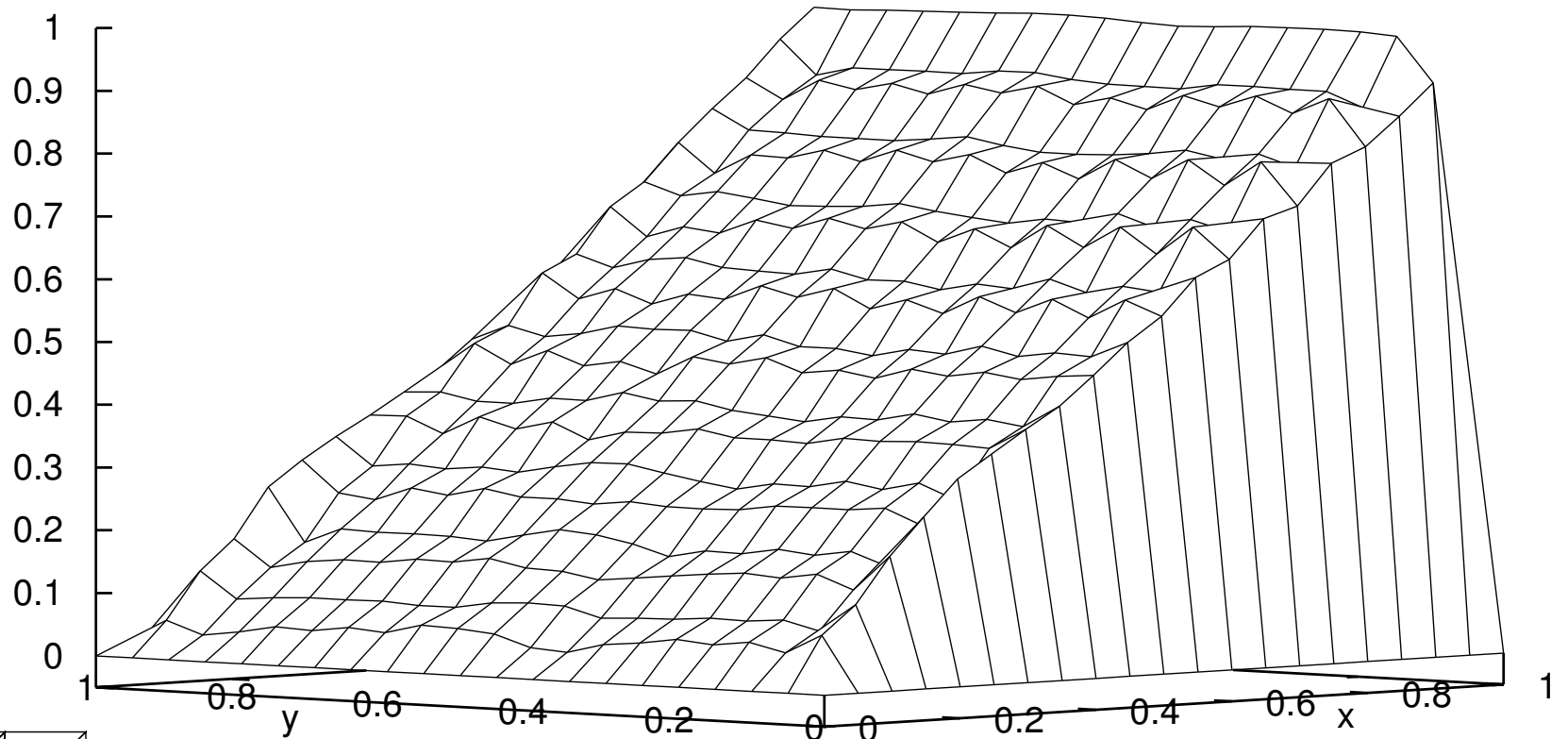
$$c = 0$$

$$f = 1$$

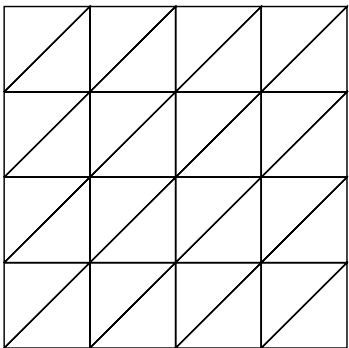
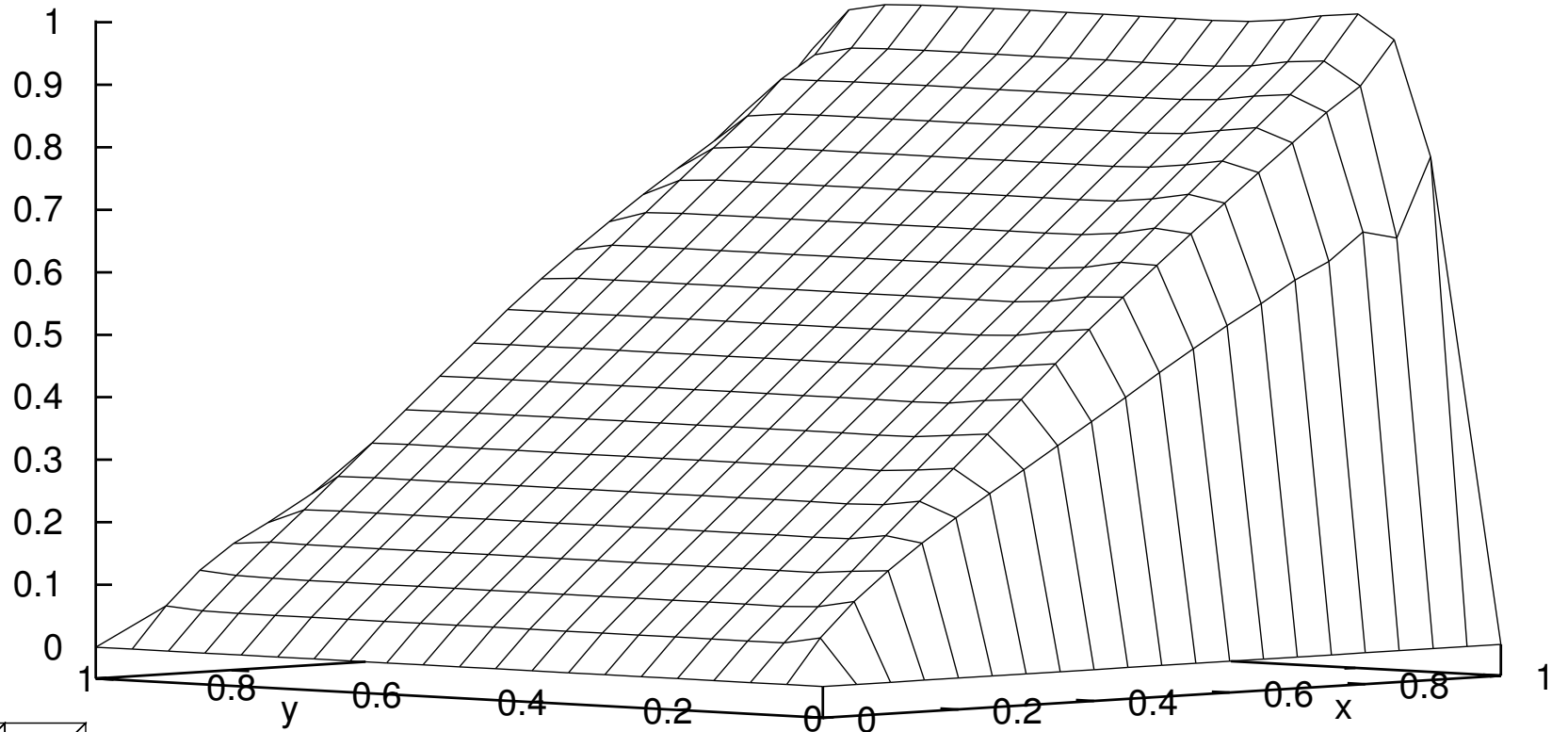
Example 3, Limiter 4, 21x21 mesh, $\gamma_i = 1$



Example 3, Limiter 4, 21x21 mesh, $\gamma_i = 2$



Example 3, Limiter 4, 21x21 mesh, $\gamma_i = 0.5$



Two-step method

The problem

$$\mathcal{L} u := -\varepsilon \Delta u + \mathbf{b} \cdot \nabla u + c u = f \quad \text{in } \Omega, \quad u = u_b \quad \text{on } \partial\Omega$$

is decomposed into two problems:

$$\mathcal{L} u_1 := f \quad \text{in } \Omega, \quad u_1 = u_b \quad \text{on } \Gamma_-, \quad \frac{\partial u_1}{\partial \mathbf{n}} = 0 \quad \text{on } \Gamma_+ \cup \Gamma_0$$

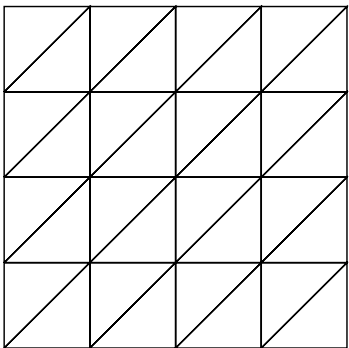
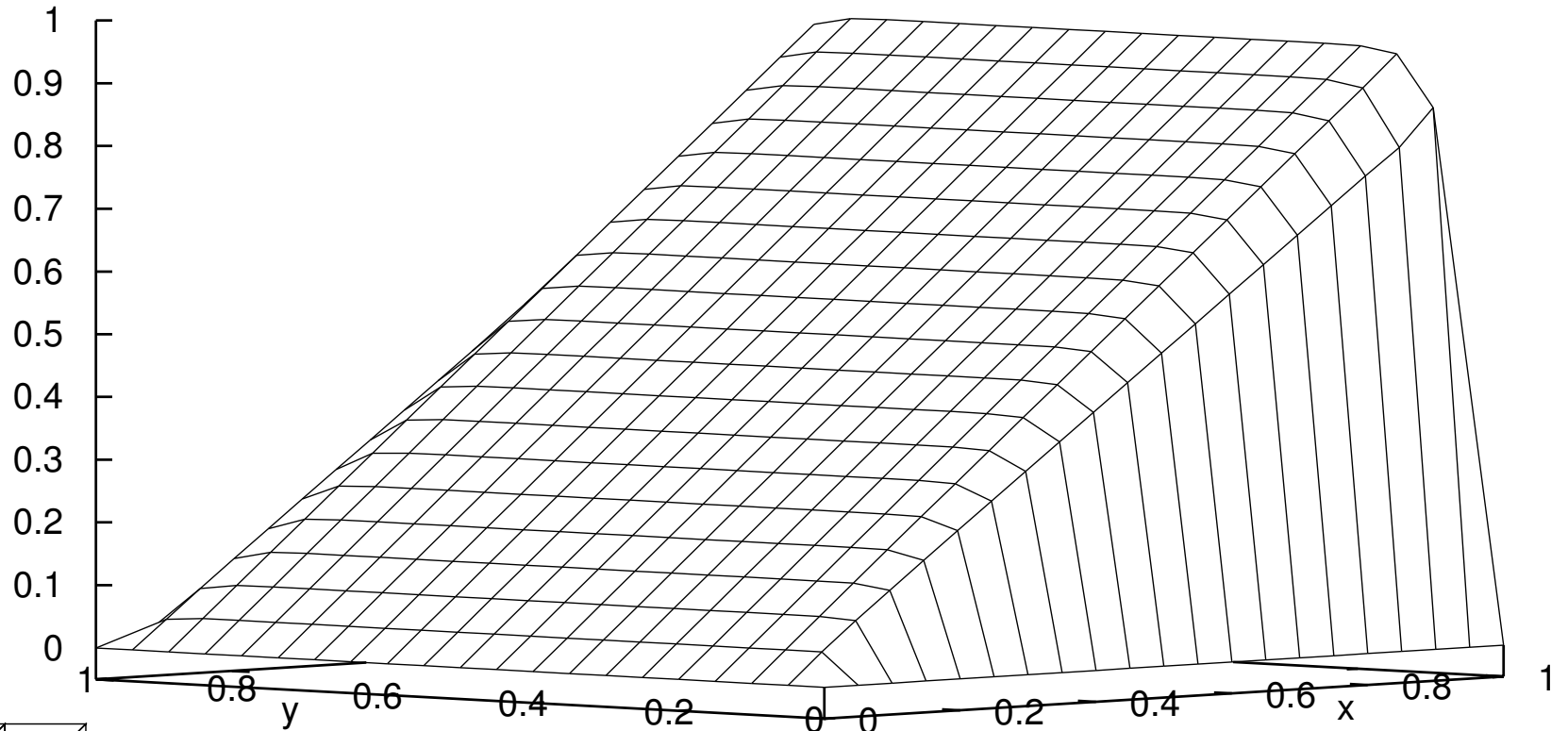
and

$$\mathcal{L} u_2 := 0 \quad \text{in } \Omega, \quad u_2 = u_b - u_1 \quad \text{on } \partial\Omega.$$

Then $u = u_1 + u_2$.

The AFC scheme is applied to each of these subproblems separately.

Example 3, two-step method, Limiter 4, 21x21 mesh, $\gamma_i = 2$



Example 4 (exponential boundary layers)

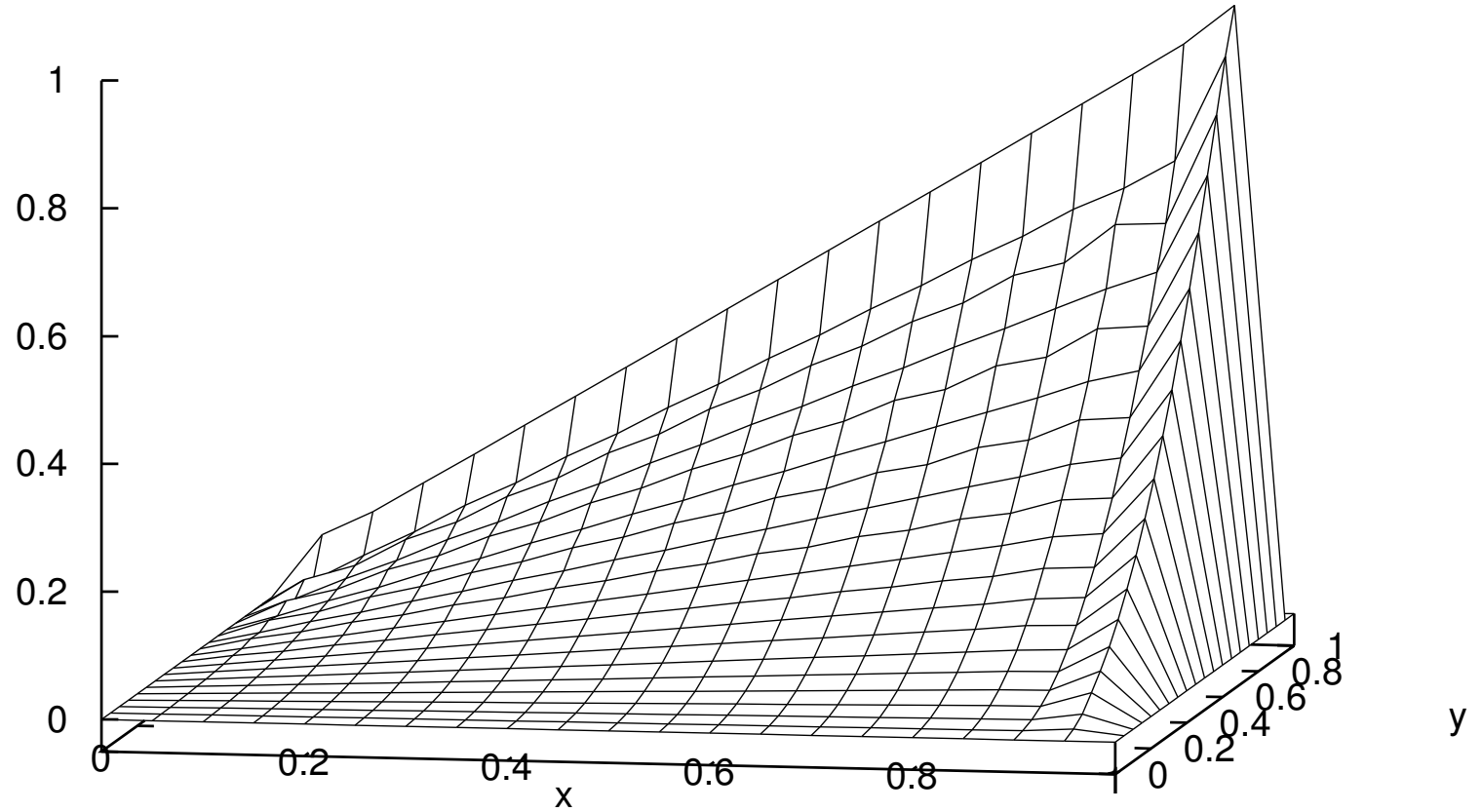
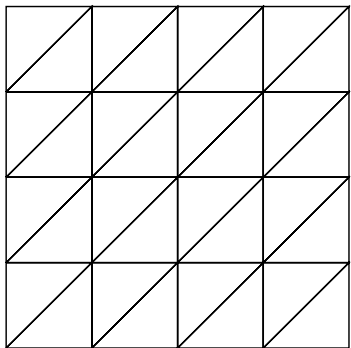
$$\Omega = (0, 1)^2, \quad \varepsilon = 10^{-8}, \quad \mathbf{b} = (2, 3), \quad c = 0.$$

The functions f and u_b are chosen in such a way that

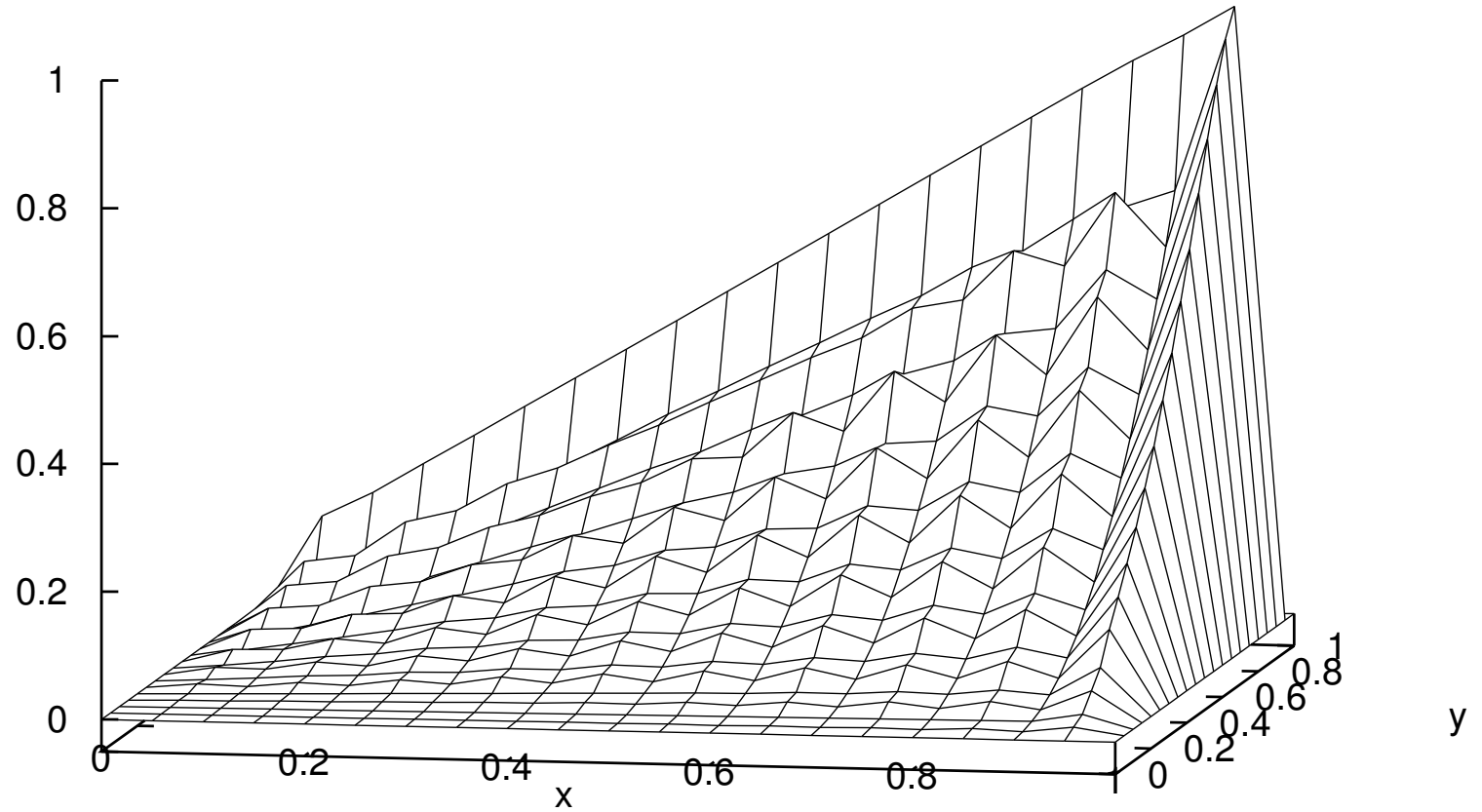
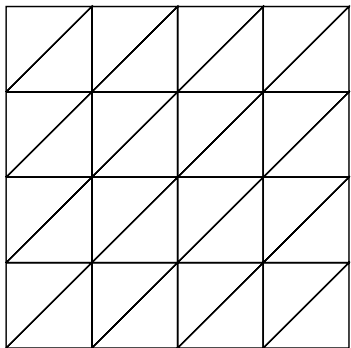
$$u(x, y) = xy^2 - y^2 \exp\left(\frac{2(x-1)}{\varepsilon}\right) - x \exp\left(\frac{3(y-1)}{\varepsilon}\right) + \exp\left(\frac{2(x-1) + 3(y-1)}{\varepsilon}\right)$$

is the exact solution.

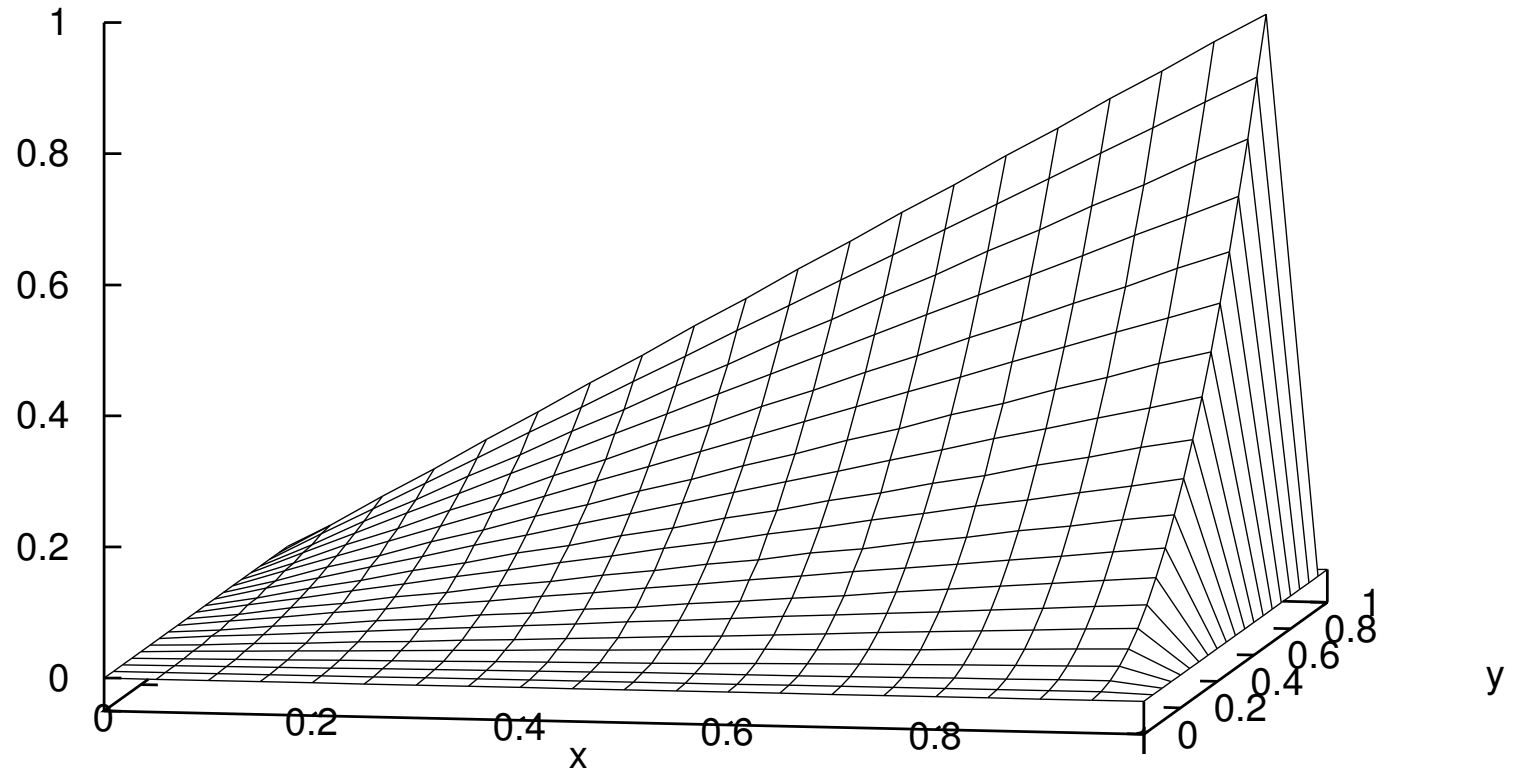
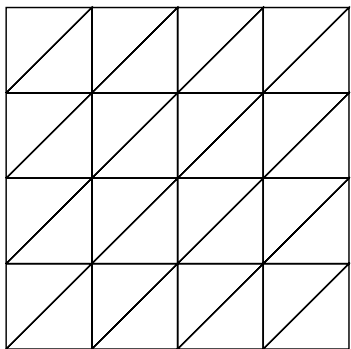
Example 4, Limiter 4, 21x21 mesh, $\gamma_i = 1$



Example 4, Limiter 4, 21x21 mesh, $\gamma_i = 2$



Example 4, two-step method, Limiter 4, 21x21 mesh, $\gamma_i = 2$



Example 4, two-step method, Limiter 4, $N \times N$ mesh, $\gamma_i = 2$

N	$\ e_h\ _{0,\Omega}^*$	$ e_h _{1,\Omega}^*$	$ e_h _{0,\infty,\Omega}^*$	$ e_h _{0,\infty,\Omega}$
6	9.29e-3	1.50e-1	3.01e-2	3.01e-2
11	1.93e-3	7.67e-2	9.25e-3	9.25e-3
21	4.48e-4	3.88e-2	2.12e-3	2.29e-3
41	1.12e-4	1.99e-2	5.43e-4	5.91e-4
81	2.80e-5	1.01e-2	1.37e-4	1.53e-4
ord.	2.00	0.98	1.99	1.95

Conclusions

- general theoretical analysis for algebraic flux correction schemes applied to convection–diffusion–reaction equations
- new limiter of upwind type leading to the discrete maximum principle and linearity preservation on arbitrary meshes
- AFC scheme alone cannot guarantee sharp approximations of boundary layers – the use of appropriate meshes is essential
- two-step method as a remedy for difficulties caused by non-vanishing right-hand side