Algebraic flux correction for convection–diffusion problems

Petr Knobloch

Charles University, Prague

joint work with

Gabriel R. Barrenechea (Glasgow)

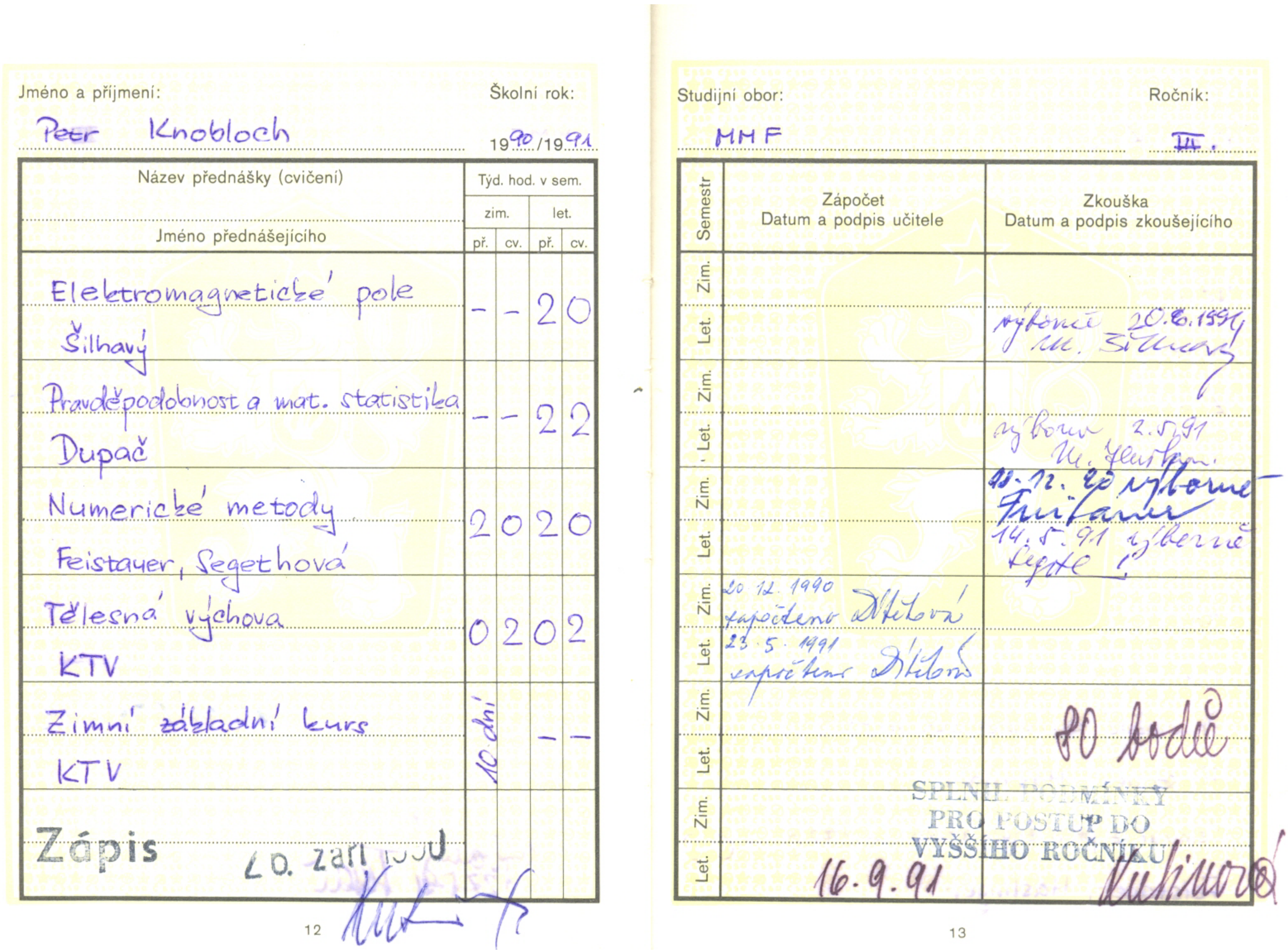
Volker John (Berlin)

Special seminar devoted to Professor Miloslav Feistauer

Institute of Mathematics of the Czech Academy of Sciences

Prague, February 8, 2019

My first meeting with Sláva Feistauer



Jméno a příjmení: Peter Knobloch

Školní rok: 1990/1991

Název přednášky (cvičení) / Jméno přednášejícího	Týd. hod. v sem. zim. př.	zim. cv.	let. př.	let. cv.
Elektromagnetické pole / Šilhavý	–	–	2	0
Pravděpodobnost a mat. statistika / Dupač	–	–	2	2
Numerické metody / Feistauer, Segethová	2	0	2	0
Tělesná výchova / KTV	0	2	0	2
Zimní základní kurs / KTV	10 dní		–	–
Zápis 20. září 1990				

12

Studijní obor: MMF

Ročník: II.

Semestr	Zápočet Datum a podpis učitele	Zkouška Datum a podpis zkoušejícího
Zim.		
Let.		výborně 20.6.1991 M. Šilhavý
Zim.		
Let.		výborně 2.5.91 [illegible]
Zim.		20.12.90 výborně Feistauer
Let.		14.5.91 výborně [illegible]
Zim.	20.12.1990 započteno [illegible]	
Let.	23.5.1991 započteno [illegible]	
Zim.		80 bodů
Let.		
Zim.		SPLNIL PODMÍNKY PRO POSTUP DO VYŠŠÍHO ROČNÍKU
Let.	16.9.91	[illegible]

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Outline

– algebraic flux correction scheme for a steady-state convection–diffusion–reaction equation

– formulation as edge-based stabilization

– theoretical analysis under general assumptions: solvability, discrete maximum principle, error estimates

– example of a limiter

– numerical results

Algebraically stabilized schemes

Boris, Book (1973), Zalesak (1979) – basic philosophy of flux-corrected transport

Arminjon, Dervieux (1989), Selmin (1987),
Löhner, Morgan, Peraire, Vahdati (1987) – FEM-FCT

Kuzmin et al. (2001–now) – algebraic flux correction
– algebraic stabilizations for linear boundary value problems

first rigorous theoretical analysis of the AFC method:

Barrenechea, John, K. (IMAJNA 2015, SINUM 2016, M3AS 2017)

a unified framework:

Barrenechea, John, K., Rankin (SeMA 2018)

Steady-state convection–diffusion–reaction equation

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

with constant $\varepsilon > 0$ and

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

FE discretization

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

$$a(u_h, v_h) = (f, v_h) \qquad \forall\, v_h \in V_h\,,$$

where

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

$$a(u_h, v_h) = \varepsilon\,(\nabla u_h, \nabla v_h) + (\mathbf{b}\cdot\nabla u_h, v_h) + (c\,u_h, v_h)\,.$$

Algebraic problem

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

$$u_i = u_i^b\,, \qquad i = M+1,\ldots,N\,.$$

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$$\sum_{j=1}^{N} a_{ij} u_j = f_i \,, \qquad i = 1, \ldots, M \,,$$
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Properties: $(a_{ij})_{i,j=1}^{M}$ is positive definite,

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

Algebraic flux correction schemes

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

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

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

Symmetric artificial diffusion matrix $\mathbb{D}$:

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

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Stabilized problem: $(\mathbb{A}\,\mathrm{U})_i + (\mathbb{D}\,\mathrm{U})_i = f_i\,, \qquad i = 1, \dots, M,$

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Limiting: limit the diffusive fluxes f_{ij} to reduce smearing

$$(\mathbb{A}\,\mathrm{U})_i + \sum_{j\neq i} \beta_{ij}\, f_{ij} = f_i\,, \qquad i = 1,\dots,M, \quad \beta_{ij} \in [0,1]\,.$$

Algebraic flux correction scheme

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

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

where $\beta_{ij}(\mathrm{U}) \in [0,1]$ and

$$\beta_{ij} = \beta_{ji}\,, \qquad i,j = 1,\dots,N\,.$$

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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

$$a(u_h,v_h) + d_h(u_h;u_h,v_h) = (f,v_h) \qquad \forall\, v_h \in V_h\,,$$

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

Edge-based formulation of the AFC scheme

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

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

where $\qquad a_h(z; v, w) = a(v, w) + d_h(z; v, w) \qquad$ and

$$d_h(z; v, w) = \sum_{E \in \mathscr{E}_h} \beta_E(z)\, |d_E|\, (v(x_{E,1}) - v(x_{E,2}))(w(x_{E,1}) - w(x_{E,2}))\,.$$

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One has

$$d_h(z;v,w) = \sum_{E\in\mathscr{E}_h} \beta_E(z)\,|d_E|\,h_E\,(\nabla v\cdot\mathbf{t}_E\,,\nabla w\cdot\mathbf{t}_E)_E \qquad \forall\, v,w \in W_h\,.$$

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Assumption (A1):

For any $E \in \mathscr{E}_h$, the function $\beta_E(u_h)(\nabla u_h)|_E \cdot \mathbf{t}_E$ is a continuous function of $u_h \in V_h$.

Edge-based formulation of the AFC scheme

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

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Theorem For any $\beta_E \in [0,1]$ satisfying Assumption (A1), the edge-based AFC scheme has a solution.

Discrete maximum principle

Local sets for $i = 1,\dots,M$:

$S_i = \{j \in \{1,\dots,N\} \setminus \{i\}\,;\ x_i \text{ and } x_j \text{ are endpoints of the same edge}\}$

$\Delta_i = \bigcup \{K \in \mathscr{T}_h\,;\ x_i \in K\}$

Assumption (A2):

Consider any $u_h \in W_h$ and any $i \in \{1,\dots,M\}$. If $u_h(x_i)$ is a strict local extremum of u_h on Δ_i, i.e.,

$$u_h(x_i) > u_h(x) \quad \forall\, x \in \Delta_i \setminus \{x_i\}$$

or

$$u_h(x_i) < u_h(x) \quad \forall\, x \in \Delta_i \setminus \{x_i\}\,,$$

then

$$a_h(u_h; \varphi_j, \varphi_i) \le 0 \qquad \forall\, j \in S_i\,.$$

Local discrete maximum principle

Let $u_h \in W_h$ be a solution of the AFC scheme with limiters β_E satisfying Assumption (A2). Consider any $i \in \{1,\dots,M\}$. Then

$$f \le 0 \ \text{ in } \Delta_i \quad \Rightarrow \quad \max_{\Delta_i} u_h \le \max_{\partial\Delta_i} u_h^+ \,,$$

$$f \ge 0 \ \text{ in } \Delta_i \quad \Rightarrow \quad \min_{\Delta_i} u_h \ge \min_{\partial\Delta_i} u_h^- \,,$$

where $u_h^+ = \max\{0, u_h\}$ and $u_h^- = \min\{0, u_h\}$. If, in addition, $c = 0$ in Δ_i, then

$$f \le 0 \ \text{ in } \Delta_i \quad \Rightarrow \quad \max_{\Delta_i} u_h = \max_{\partial\Delta_i} u_h \,,$$

$$f \ge 0 \ \text{ in } \Delta_i \quad \Rightarrow \quad \min_{\Delta_i} u_h = \min_{\partial\Delta_i} u_h \,.$$

Global discrete maximum principle

Let $u_h \in W_h$ be a solution of the AFC scheme with limiters β_E satisfying Assumptions (A1) and (A2). Then

$$f \le 0 \ \text{ in } \Omega \quad \Rightarrow \quad \max_{\overline{\Omega}} u_h \le \max_{\partial\Omega} u_h^+ \,,$$

$$f \ge 0 \ \text{ in } \Omega \quad \Rightarrow \quad \min_{\overline{\Omega}} u_h \ge \min_{\partial\Omega} u_h^- \,.$$

If, in addition, $c = 0$ in Ω, then

$$f \le 0 \ \text{ in } \Omega \quad \Rightarrow \quad \max_{\overline{\Omega}} u_h = \max_{\partial\Omega} u_h \,,$$

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A priori error estimates

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

Theorem Let $u \in H^2(\Omega)$ and $\sigma_0 > 0$. Then

$$\|u-u_h\|_h \le C\big(\varepsilon + \sigma_0^{-1}\{\|\mathbf{b}\|_{0,\infty,\Omega}^2 + \|c\|_{0,\infty,\Omega}^2\,h^2\}\big)^{1/2} h\,|u|_{2,\Omega} + d_h(u_h;i_hu,i_hu)^{1/2}\,.$$

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Lemma Denoting

$$A_h = \max_{E \in \mathscr{E}_h}\left(|d_E|\,h_E^{2-d}\right),$$

one has

$$d_h(u_h; i_h u, i_h u) \leq C A_h\,|i_h u|^2_{1,\Omega} \qquad \forall\, u_h \in W_h,\, u \in C(\overline{\Omega})\,.$$

If, in particular, d_E are defined as at the beginning, then

$$d_h(u_h; i_h u, i_h u) \leq C\,(\varepsilon + \|\mathbf{b}\|_{0,\infty,\Omega}\,h + \|c\|_{0,\infty,\Omega}\,h^2)\,|i_h u|^2_{1,\Omega}\,.$$

An improved estimate

Assumption (A3):

The limiters β_E possess the linearity-preservation property, i.e.,

$$\beta_E(u_h) = 0 \qquad \text{if } \ u_h|_{\omega_E} \in P_1(\omega_E) \qquad \forall\, E \in \mathscr{E}_h\,.$$

Assumption (A4):

For any $E \in \mathscr{E}_h$ with endpoints x_i and x_j, the function $\beta_E(u_h)(\nabla u_h)|_E \cdot \mathbf{t}_E$ is Lipschitz continuous in the sense that

$$\left|\beta_E(u_h)(\nabla u_h)|_E \cdot \mathbf{t}_E - \beta_E(v_h)(\nabla v_h)|_E \cdot \mathbf{t}_E\right| \leq C \sum_{E' \in \mathscr{E}_i \cup \mathscr{E}_j} \left|(\nabla(u_h - v_h))|_{E'} \cdot \mathbf{t}_{E'}\right|.$$

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Lemma Under Assumptions (A3) and (A4) one has

$$d_h(u_h; i_h u, i_h u) \le \frac{\varepsilon}{2}\,|u_h - i_h u|^2_{1,\Omega} + C\,\frac{A_h^2}{\varepsilon}\,|i_h u|^2_{1,\Omega} + \varepsilon\, h^2\,|u|^2_{2,\Omega}\,.$$

Example of a limiter Kuzmin (2012), Barrenechea, John, K. (2017)

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

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

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

$$f_{ij} = d_{ij}\,(u_j - u_i)$$

$$\alpha_{ij} := \begin{cases} R_i^+ & \text{if } f_{ij} > 0\,, \\ 1 & \text{if } f_{ij} = 0\,, \\ R_i^- & \text{if } f_{ij} < 0\,, \end{cases}$$

$$\beta_E := 1 - \min\{\alpha_{ij}, \alpha_{ji}\}.$$

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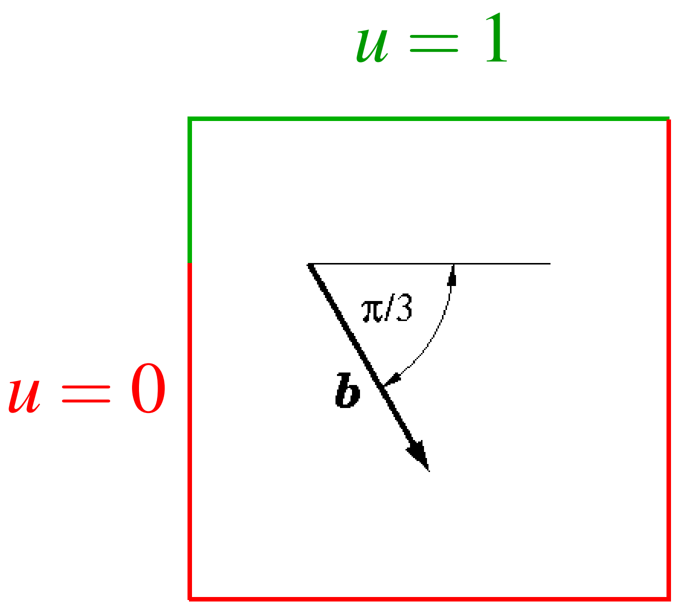
$$\beta_E := 1 - \min\{\alpha_{ij}, \alpha_{ji}\}.$$

Assumption (A2) always satisfied

$\Rightarrow$ DMP guranteed for arbitrary meshes!

Example (interior layer and exponential boundary layers)



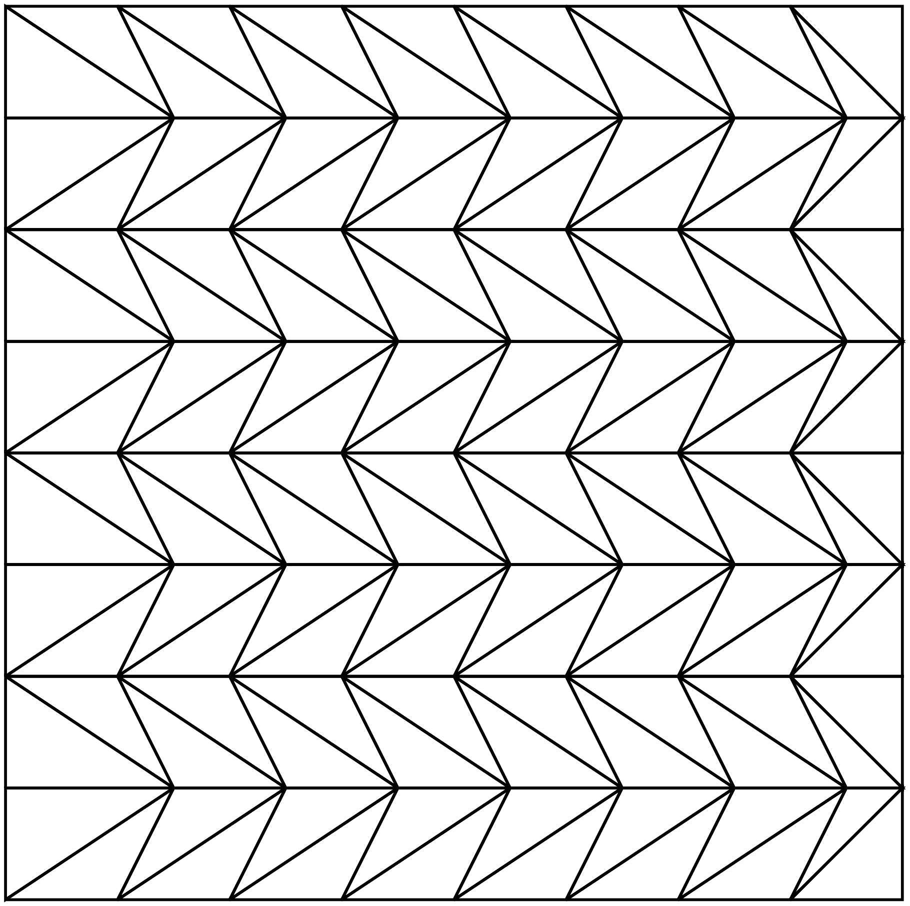
$$\varepsilon = 10^{-8}$$

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

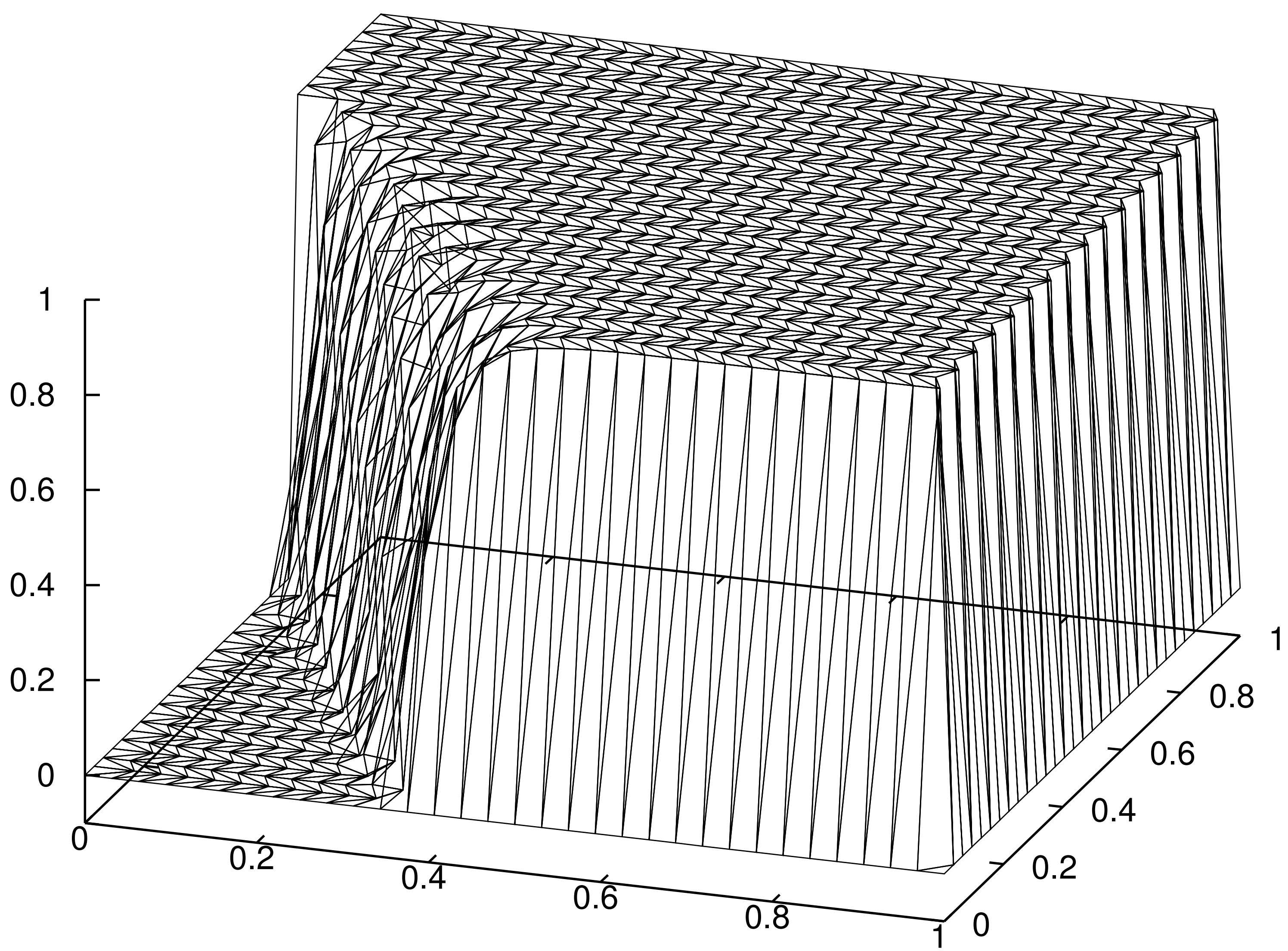
$$c = 0$$

$$f = 0$$

Non-Delaunay meshes



Solution of the AFC scheme



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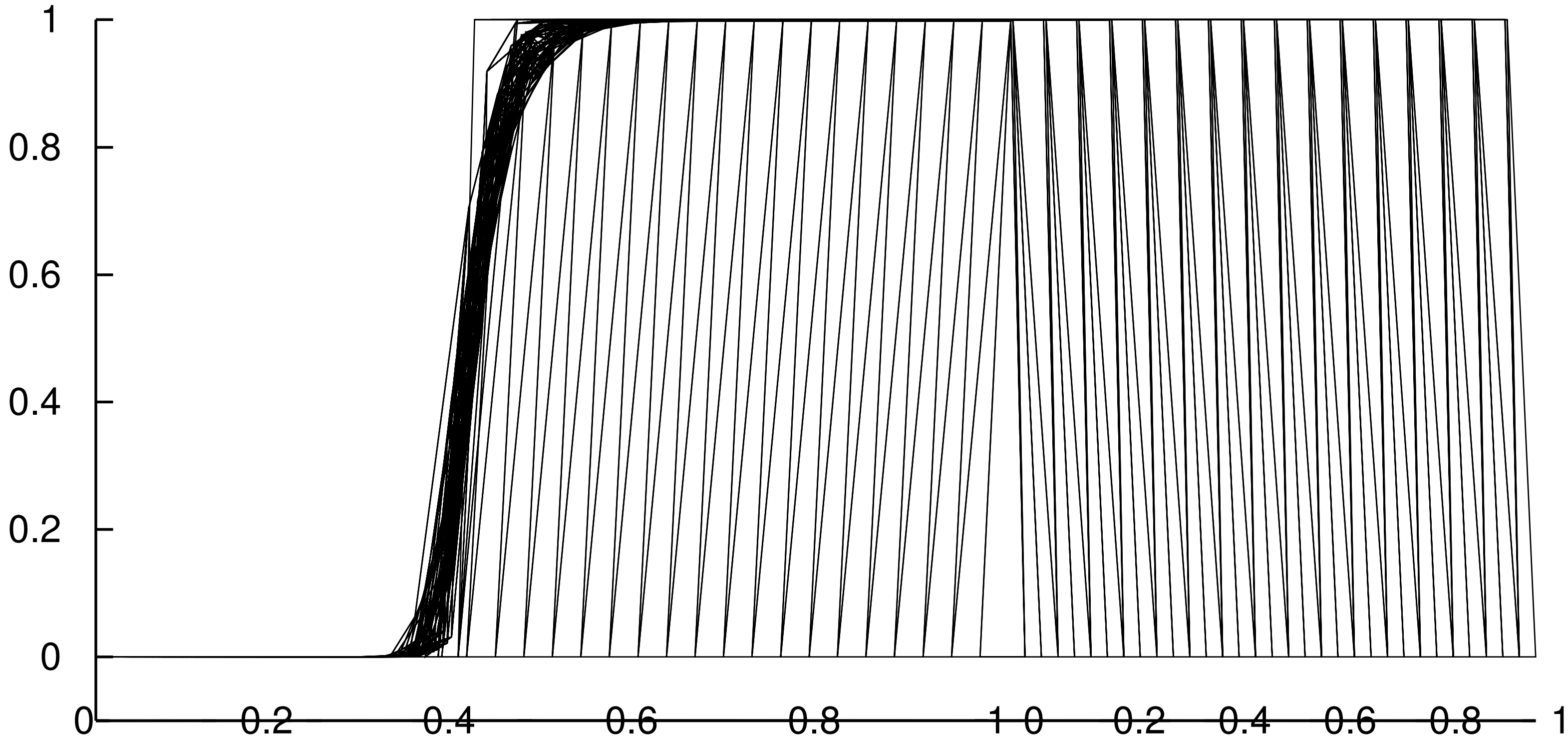

Conclusions

– unified theoretical analysis for algebraic flux correction schemes applied to convection–diffusion–reaction equations

– theory applicable to various limiters

– oscillation-free solutions can be computed without smearing the layers

I wish you, Sláva,

many further brilliant mathematical results

and a happy birthday!!!

Kuzmin's limiter

Zalesak (1979), Kuzmin (2007)

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

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

$$f_{ij} = d_{ij}(u_j - u_i)$$

$$\alpha_{ij} := \begin{cases} R_i^+ & \text{if } f_{ij} > 0, \\ 1 & \text{if } f_{ij} = 0, \\ R_i^- & \text{if } f_{ij} < 0, \end{cases} \qquad \beta_E := \begin{cases} 1 - \alpha_{ij} & \text{if } a_{ji} \le a_{ij}, \\ 1 - \alpha_{ji} & \text{else.} \end{cases}$$

Kuzmin's limiter

Zalesak (1979), Kuzmin (2007)

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Assumption (A2) satisfied if $\min\{a_{ij}, a_{ji}\} \le 0 \quad \forall\, i, j \in \{1, \ldots, N\}$

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$\Rightarrow$ DMP guranteed for Delaunay meshes for lumped react. term

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

Validity of Assumption (A3) (linearity preservation)

Kuzmin's limiter: only for $\mathbf{b} =$ const. and special meshes (e.g., Friedrichs–Keller)

BJK limiter: for arbitrary meshes if

$$\gamma_i = \frac{\max\limits_{x_j \in \partial\Delta_i} |x_i - x_j|}{\operatorname{dist}(x_i, \partial\Delta_i^{\text{conv}})}, \qquad i = 1, \dots, M$$

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Improved error estimate on special meshes

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

Example 1 (polynomial solution)

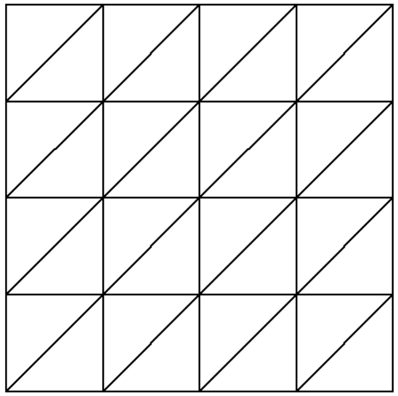
$$\Omega = (0,1)^2\,, \qquad \mathbf{b} = (3,2)\,, \qquad c = 1\,, \qquad u_b = 0\,.$$

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

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

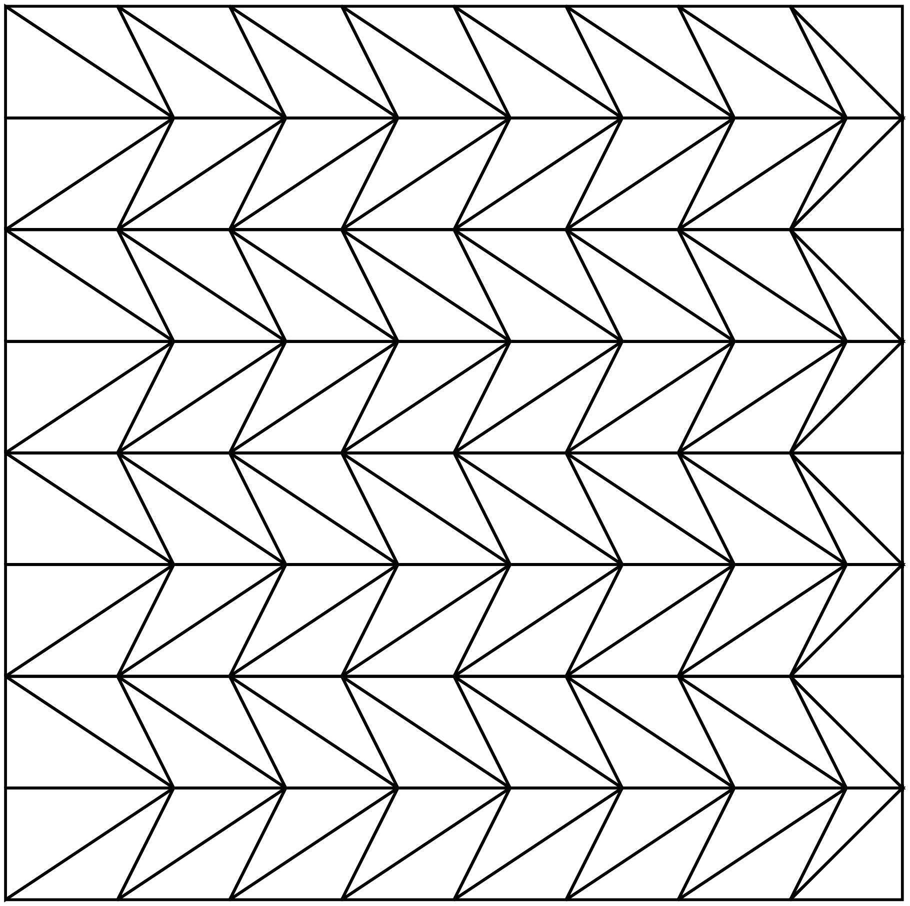
is the exact solution.

Example 1, Kuzmin's limiter, $\varepsilon = 10^{-8}$



ne	$\|e_h\|_{0,\Omega}$	ord.	$\|e_h\|_{1,\Omega}$	ord.	$d_h^{1/2}(u_h)$	ord.
32	5.457e−3	1.85	2.287e−1	1.10	1.163e−2	2.11
64	1.408e−3	1.95	1.074e−1	1.09	2.683e−3	2.12
128	3.493e−4	2.01	5.113e−2	1.07	6.410e−4	2.07
256	8.652e−5	2.01	2.546e−2	1.01	1.633e−4	1.97
512	2.152e−5	2.01	1.321e−2	0.95	4.099e−5	1.99
1024	5.357e−6	2.01	6.822e−3	0.95	1.018e−5	2.01

Non-Delaunay meshes



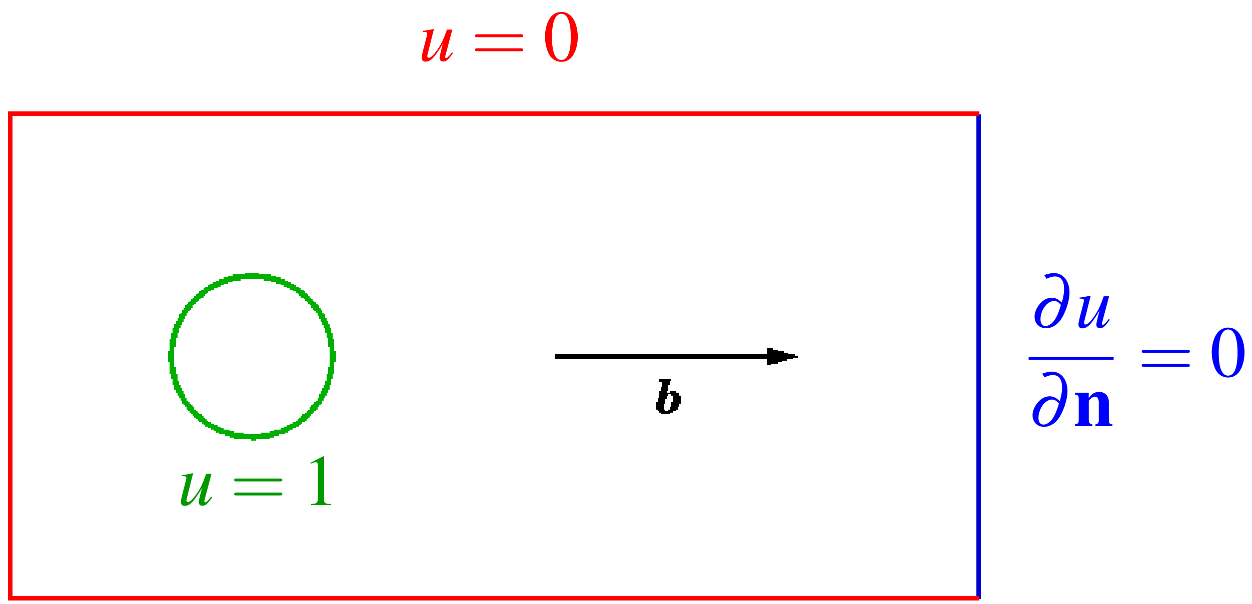
Example 1, Kuzmin's limiter, $\varepsilon = 10$ (non-Delaunay mesh)

ne	$\|e_h\|_{0,\Omega}$	ord.	$\|e_h\|_{1,\Omega}$	ord.	$\|e_h\|_h$	ord.
16	5.637e−2	0.22	6.741e−1	0.41	2.626e+0	0.24
32	5.385e−2	0.07	5.908e−1	0.19	2.437e+0	0.11
64	5.332e−2	0.01	5.661e−1	0.06	2.380e+0	0.03
128	5.321e−2	0.00	5.593e−1	0.02	2.363e+0	0.01
256	5.319e−2	0.00	5.575e−1	0.00	2.358e+0	0.00
512	5.320e−2	0.00	5.570e−1	0.00	2.356e+0	0.00

Example 1, BJK limiter, $\varepsilon = 10$ (non-Delaunay mesh)

ne	$\|e_h\|_{0,\Omega}$	ord.	$\|e_h\|_{1,\Omega}$	ord.	$\|e_h\|_h$	ord.
16	1.786e−2	1.74	4.726e−1	0.87	1.522e+0	0.88
32	4.218e−3	2.08	2.404e−1	0.98	7.633e−1	1.00
64	1.016e−3	2.05	1.213e−1	0.99	3.841e−1	0.99
128	2.545e−4	2.00	6.082e−2	1.00	1.924e−1	1.00
256	6.439e−5	1.98	3.045e−2	1.00	9.632e−2	1.00
512	1.628e−5	1.98	1.524e−2	1.00	4.819e−2	1.00

Example 3 (P. Hemker's problem)



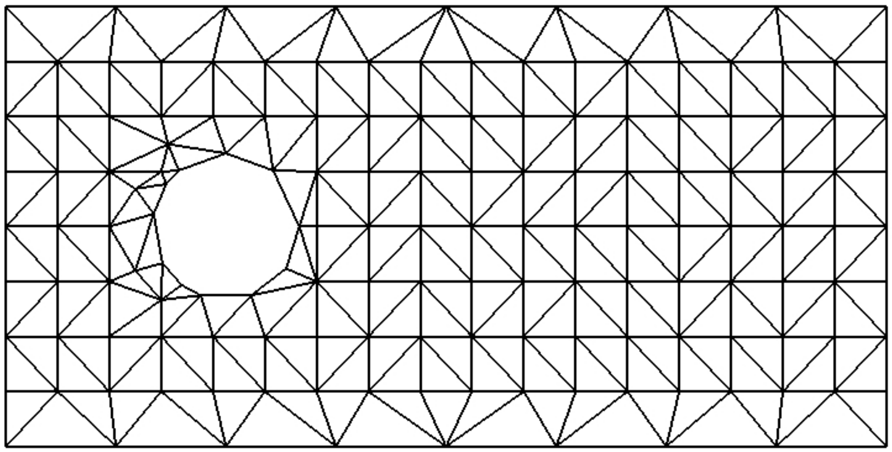
$\varepsilon = 10^{-4}$

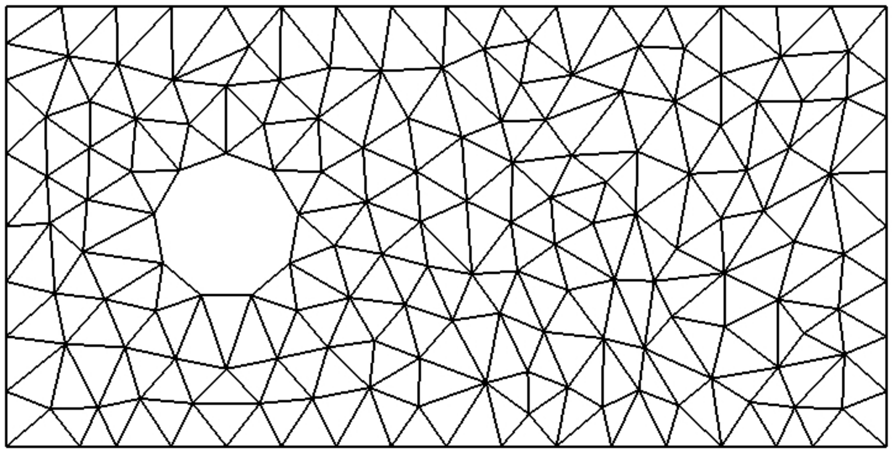
$|\mathbf{b}| = 1$

$c = 0$

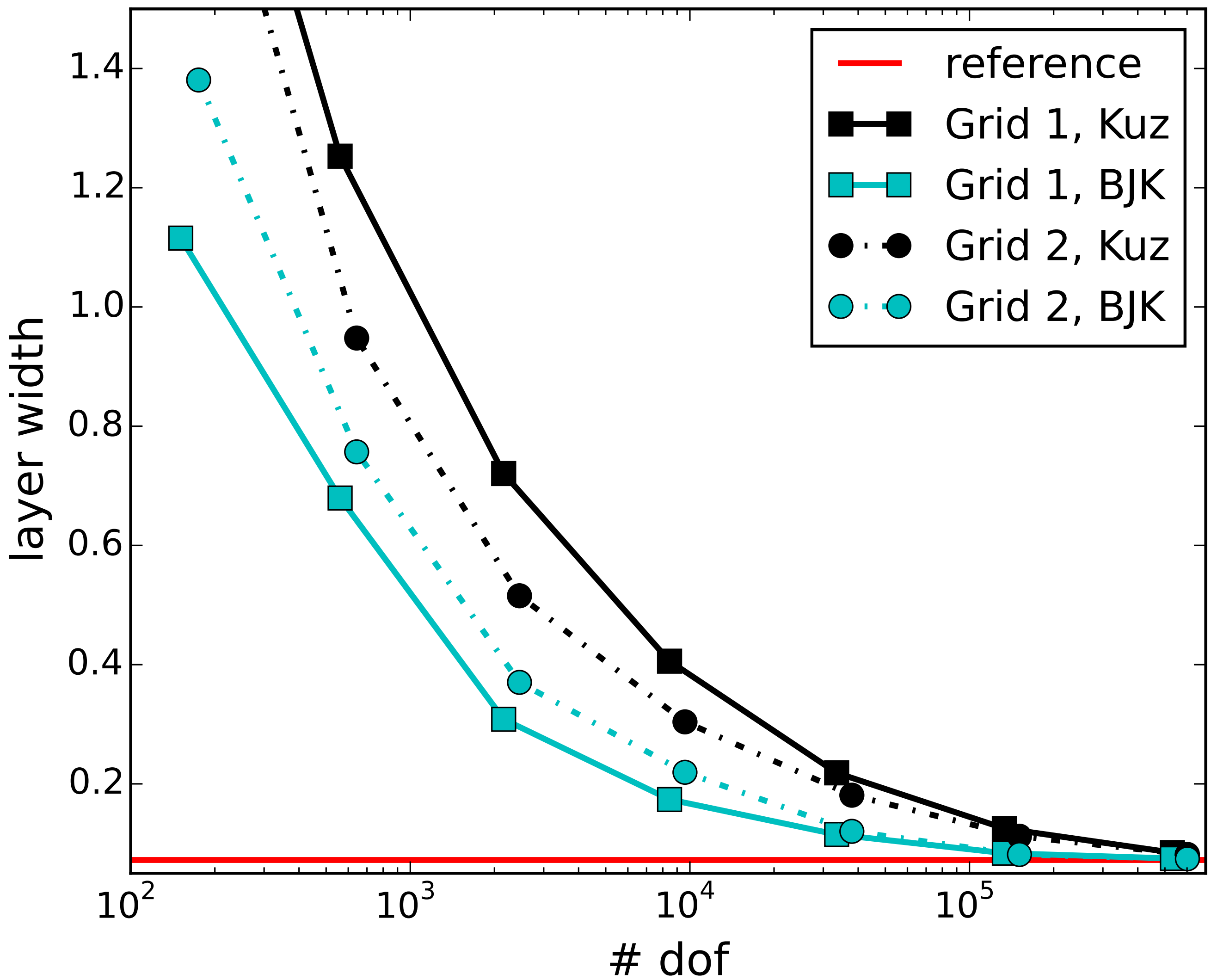
$f = 0$

Example 3, Grid 1 (left) and Grid 2 (right), both level 0

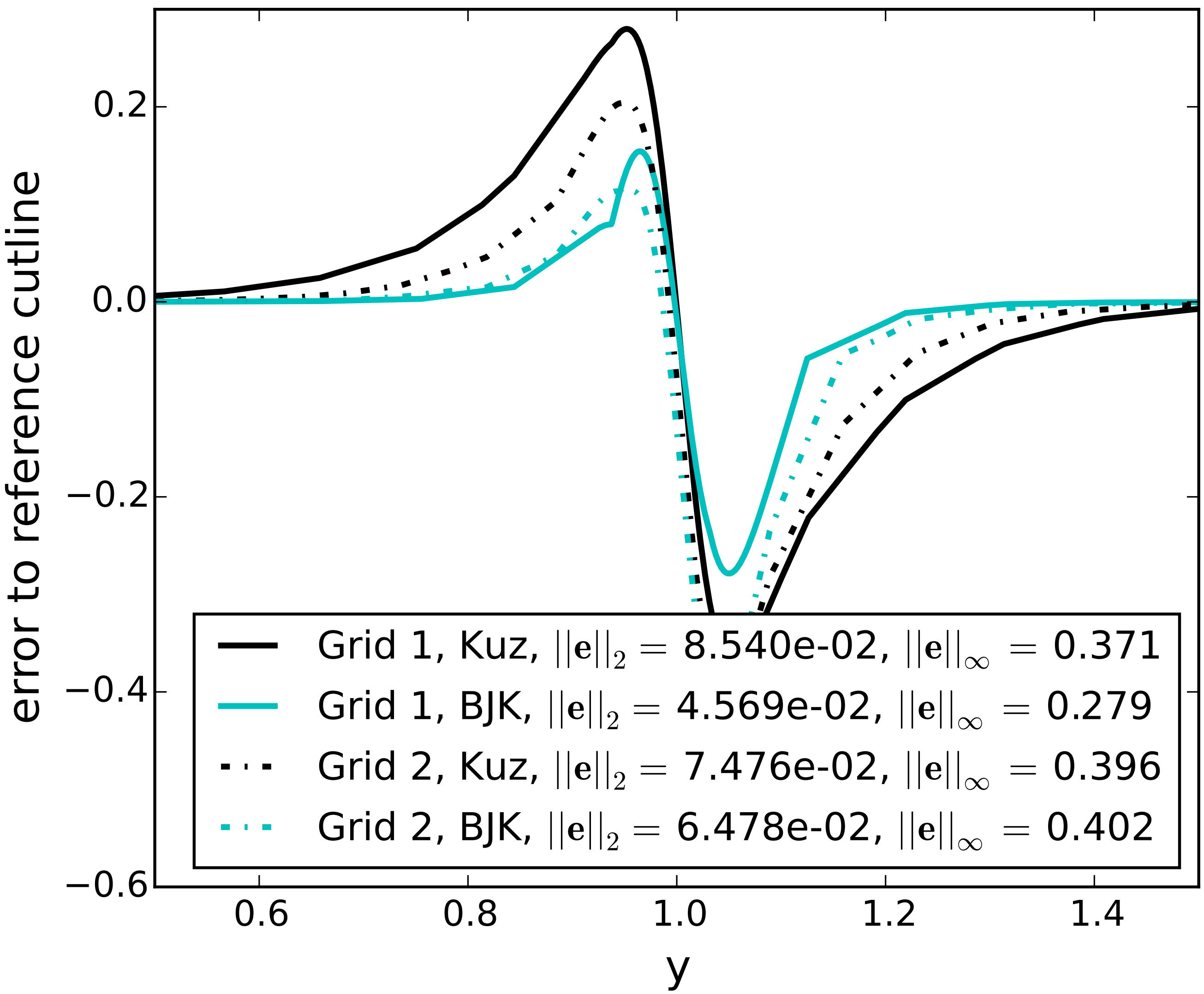




Example 3, width of the interior layer at $x = 4$



Example 3, level 3 (~ 10000 dofs), errors along $x = 4$



Example 3, level 5 (~ 150000 dofs), errors along $x = 4$