Analysis of algebraic flux correction schemes

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joint work with

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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
- examples of limiters
- numerical results

Stabilization

Problem for a PDE containing a wide range of scales

$\Rightarrow$ Galerkin FEM fails unless all scales are resolved.

Resolution of all scales typically not affordable.

Remedy: modification of the Galerkin FEM (stabilization)

1) in the integral form

2) on the algebraic level (goal: conservation & DMP)

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

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

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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

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

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

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

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Assumption (A1):

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

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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 $i = 1, \dots, M$:

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

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

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 $i \in \{1,\ldots,M\}$. 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

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

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

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

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

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Lemma Denoting

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

one has

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

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

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

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

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

Kuzmin's limiter

Zalesak (1979), Kuzmin (2007)

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

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

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

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

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

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

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

BJK limiter

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

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

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

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Assumption (A2) always satisfied

$\Rightarrow$ DMP guranteed for arbitrary 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

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

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Improved error estimate on special meshes

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

Example 1 (polynomial solution)

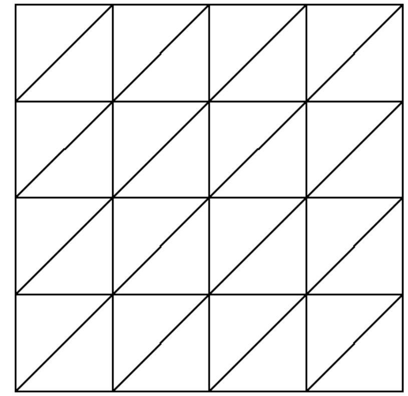
$$\Omega = (0,1)^2\,, \qquad \mathbf{b} = (3,2)\,, \qquad c = 1\,, \qquad u_b = 0\,.$$

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

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

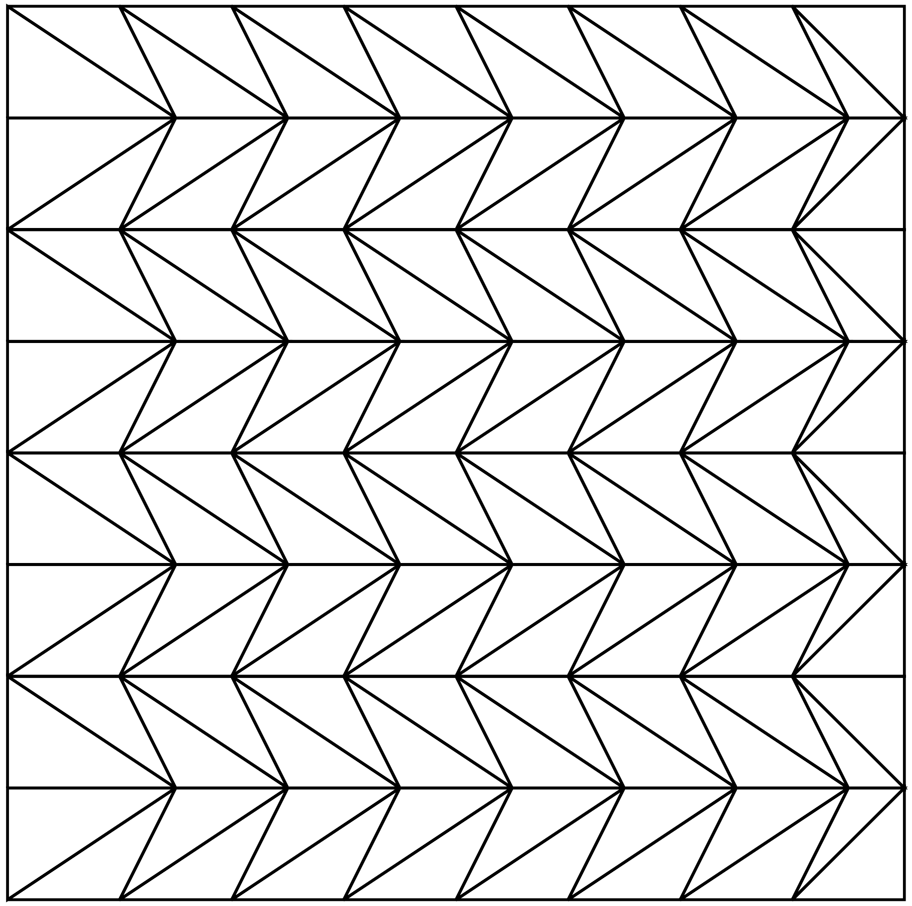
is the exact solution.

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



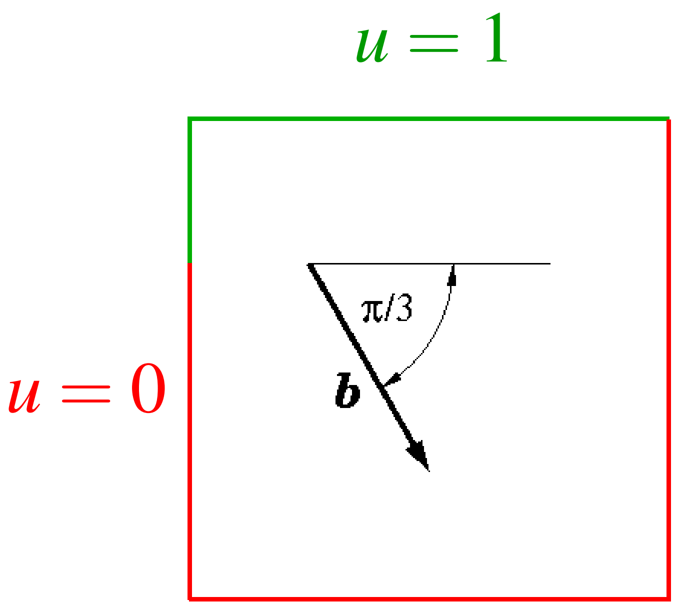
Example 1, Kuzmin's limiter, $\varepsilon = 10$ (non-Delaunay mesh)

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 2 (interior layer and exponential boundary layers)



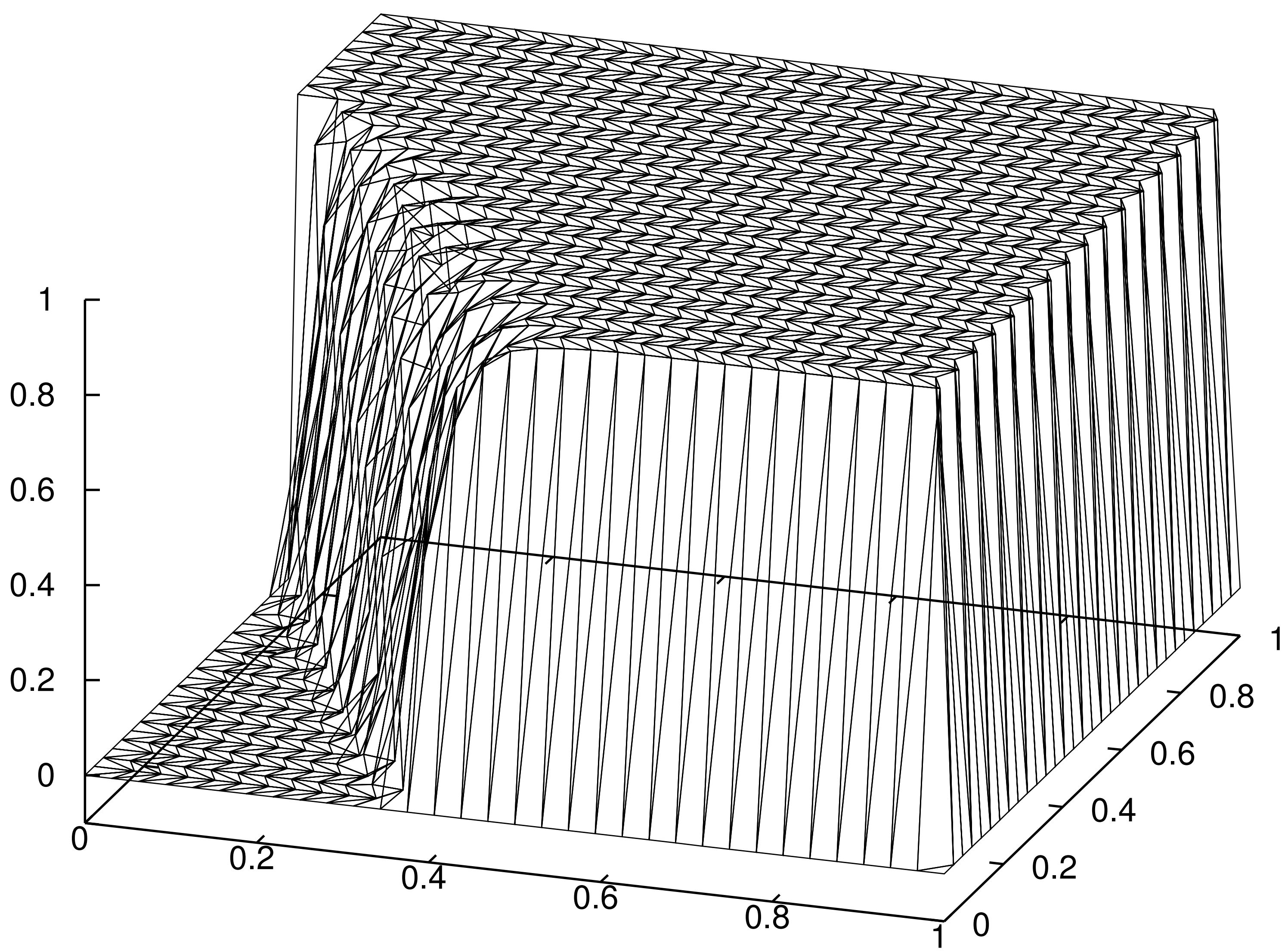
$$\varepsilon = 10^{-8}$$

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

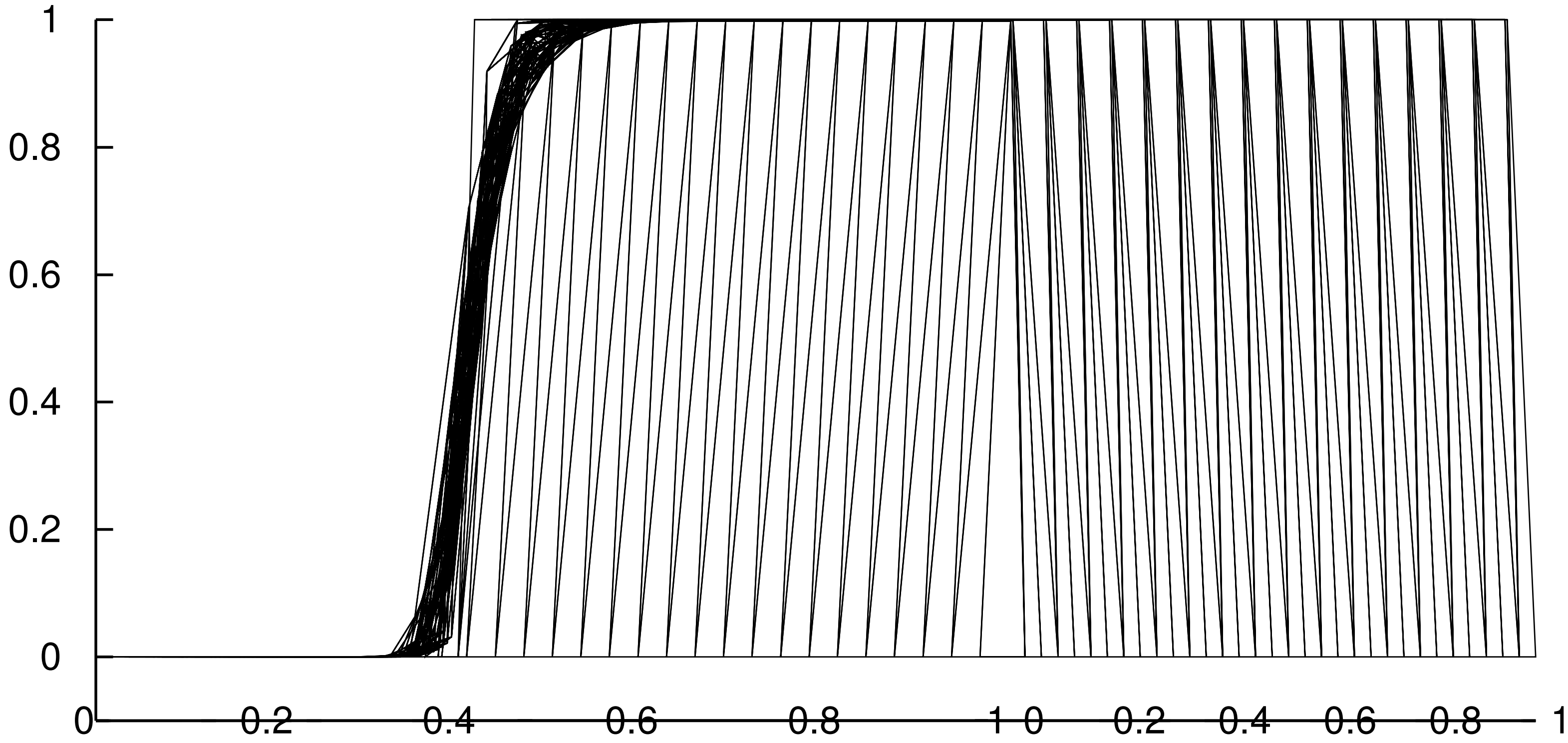
$$c = 0$$

$$f = 0$$

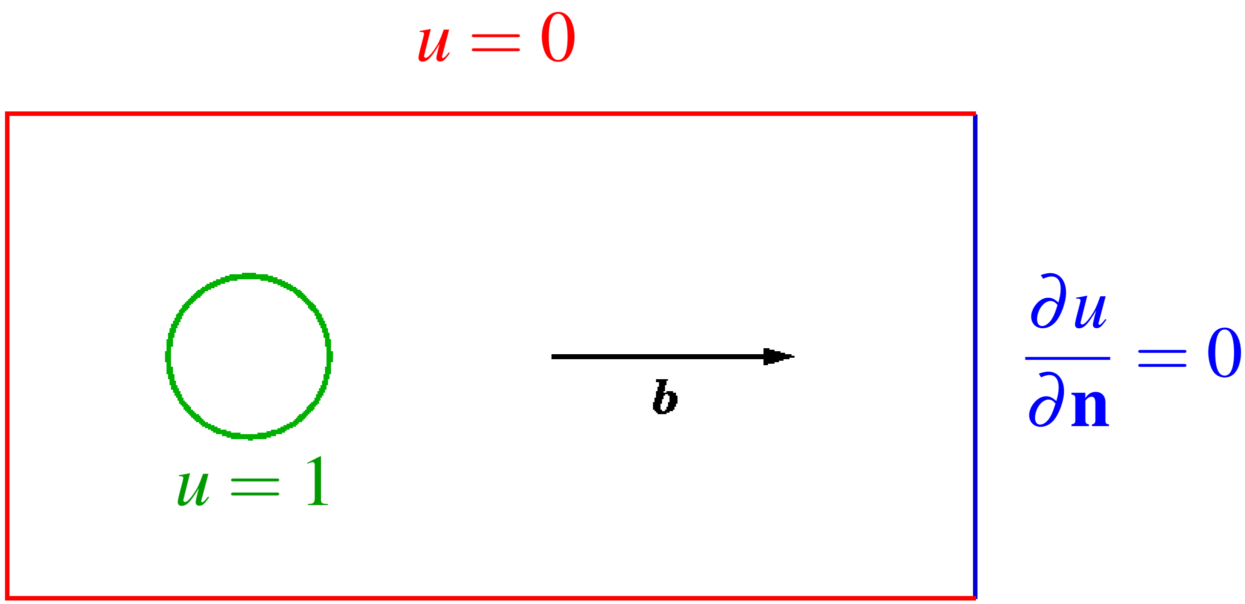
Example 2, BJK limiter



Example 2, BJK limiter



Example 3 (P. Hemker's problem)



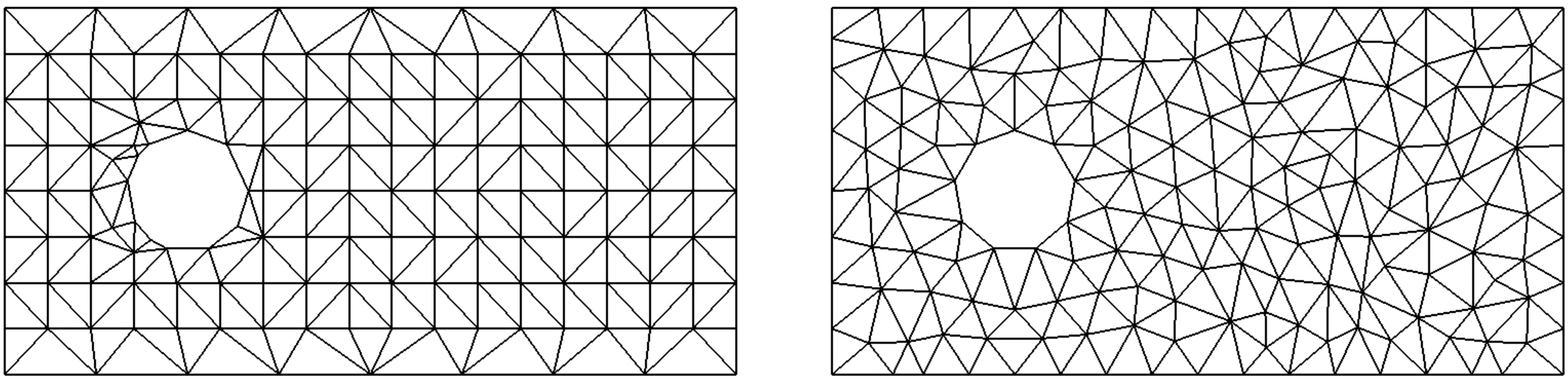
$$\varepsilon = 10^{-4}$$

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

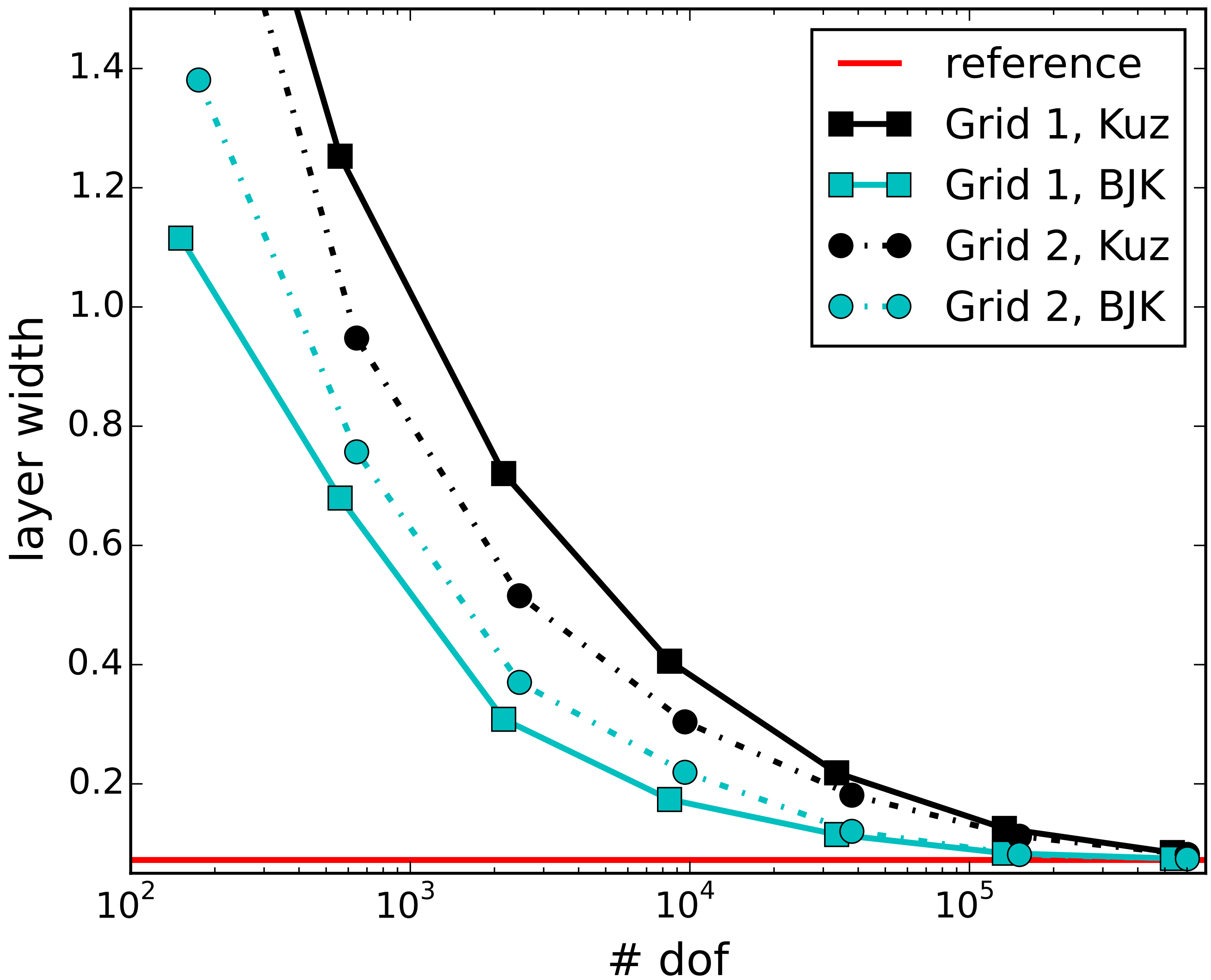
$$c = 0$$

$$f = 0$$

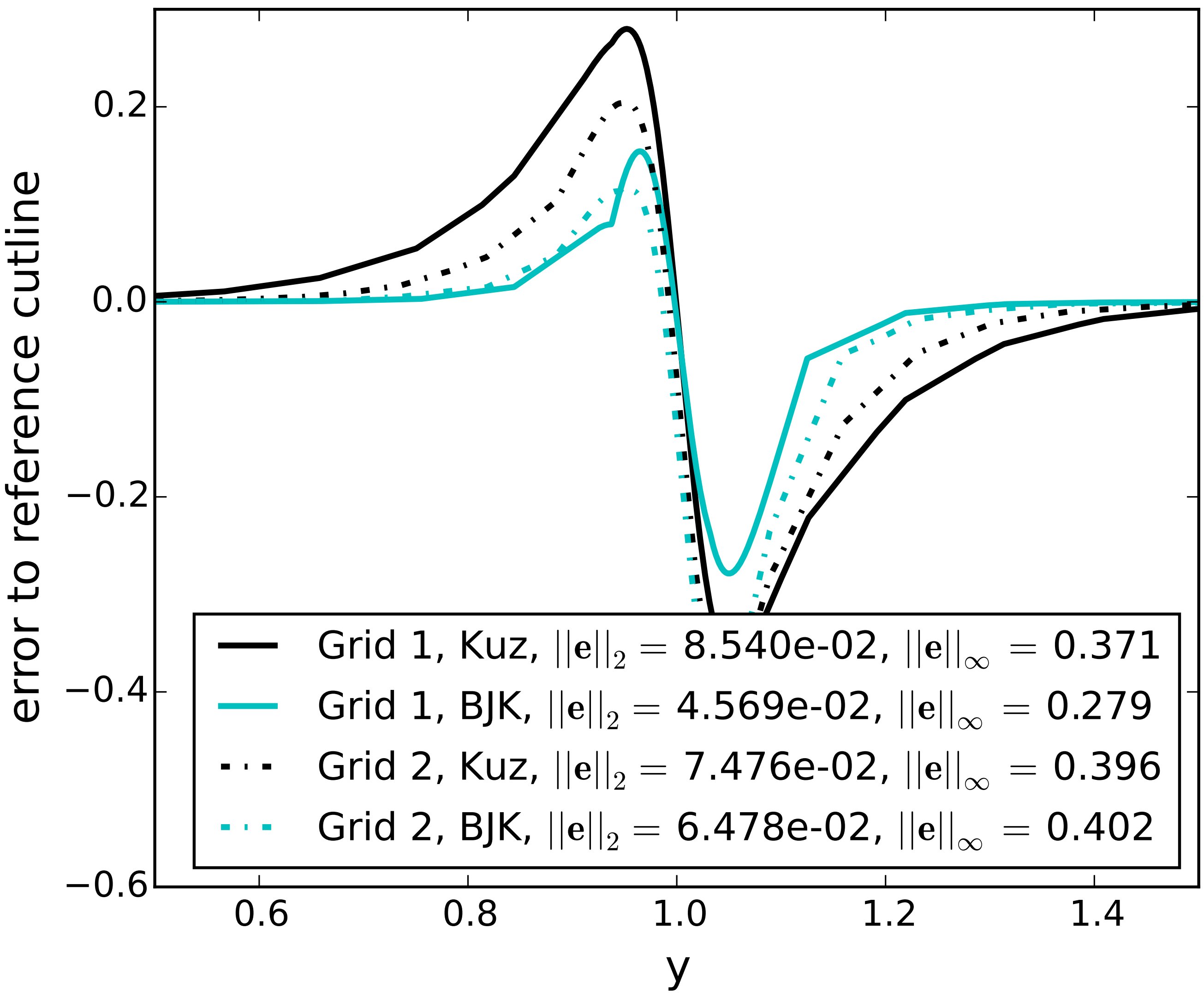
Example 3, Grid 1 (left) and Grid 2 (right), both level 0



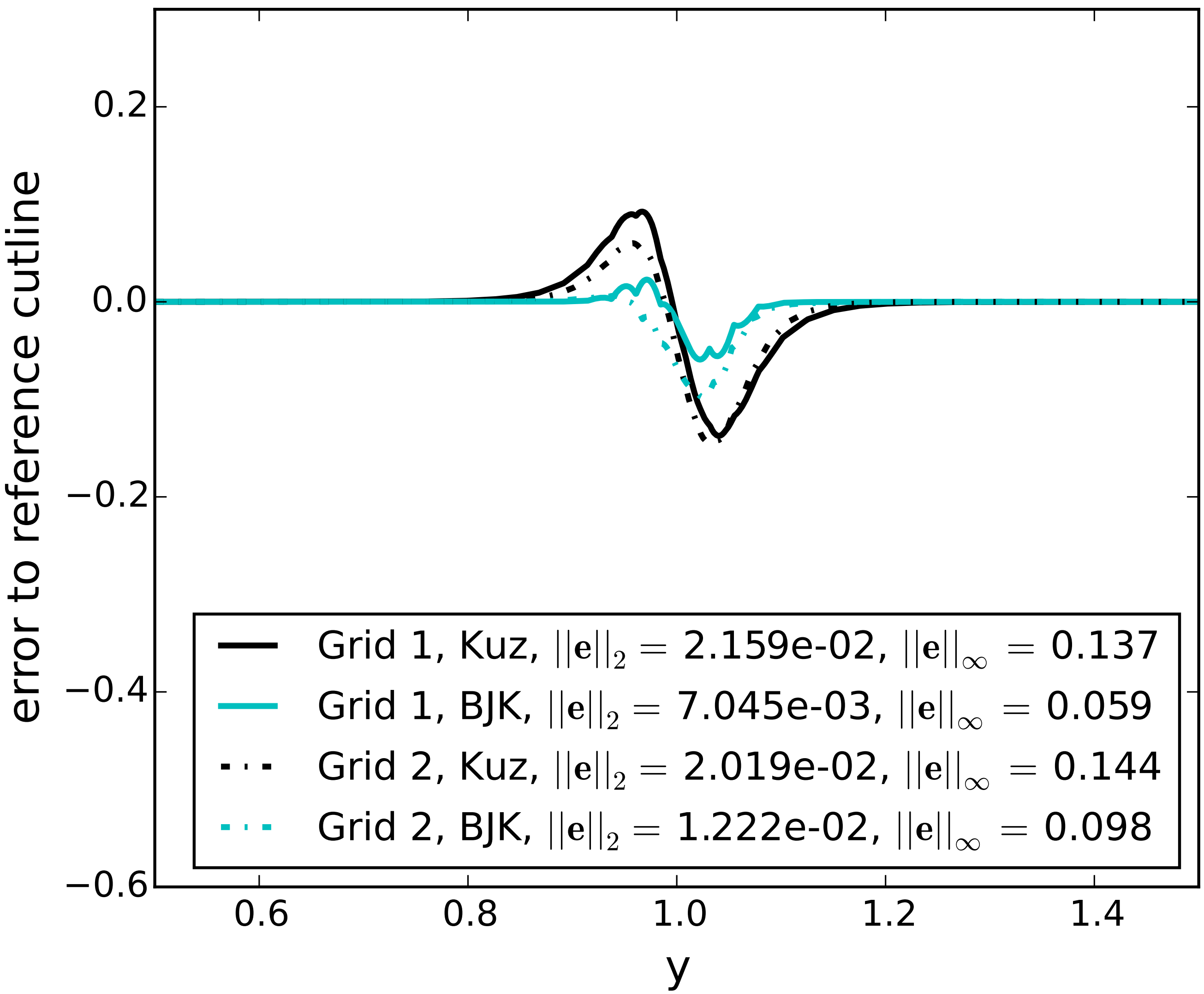
Example 3, width of the interior layer at $x = 4$



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



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



Conclusions

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

– theory applicable to various limiters

– properties of the limiters illustrated by numerical results