Adaptive Grids for Algebraic Stabilizations of Convection-Diffusion-Reaction Equations

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Joint work with Volker John (WIAS, Berlin) and Petr Knobloch (Charles University, Prague)

Outline

- Steady-state convection-diffusion-reaction equation

$$\begin{aligned} -\varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu &= f && \text{in } \Omega, \\ u &= u_b && \text{on } \Gamma_D, \\ -\varepsilon\nabla u\cdot\mathbf{n} &= g && \text{on } \Gamma_N \end{aligned}$$

  - Ω – bounded polyhedral Lipschitz domain in $\mathbb{R}^d$, $d \in \{2,3\}$
  - $\mathbf{n}$ – outward pointing unit normal
  - Assume

$$\left(c(x) - \frac{1}{2}\nabla\cdot\mathbf{b}(x)\right) \geq \sigma > 0$$

  - Interested in convection-dominated regime, $\varepsilon \ll \|\mathbf{b}\|_{L^\infty(\Omega)} L$
  - L – Characteristic length of the problem

- Ideal discretization
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- Because of 2^{nd} property: Algebraic stabilised schemes very well suited for applications
- Alternate approach: Adaptive grids
- Idea: Combine both the approaches

- Derivation
  - Galerkin FEM (Algebraic form)

$$\sum_{j=1}^{N} a_{ij} u_j = f_i, \quad i = 1, \ldots, M,$$
$$u_i = u_i^b, \quad i = M+1, \ldots, N$$

  - Artificial diffusion matrix D

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

  - Anti-diffusive fluxes

$$f_{ij} = d_{ij}(u_j - u_i), \quad f_{ij} = -f_{ji}, \quad i, j = 1, \ldots, N$$

- Derivation (cont.)
  - Solution-dependent coefficients

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

with

$$\alpha_{ij} \in [0,1]$$

  - Final scheme

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

- Variational problem for AFC scheme
  Find $u_h \in V_h$ such that

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

  - $V_h -$ finite element space with homogeneous Dirichlet boundary conditions $(V_h \subset V)$
  - stabilization

$$d_h(w; z, v) = \sum_{i,j=1}^{N} (1 - \alpha_{ij}(w)) d_{ij}(z_j - z_i) v_i \quad \forall\, w, v, z \in V_h$$

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- Another representation of stabilization for $w, v, z \in V_h$,[1]

$$d_h(w; z, v) = \sum_{E \in \mathcal{E}_h} (1 - \alpha_E(w)) d_E h_E \left(\nabla z \cdot \mathbf{t}_E, \nabla v \cdot \mathbf{t}_E \right)$$

[1] Barrenechea, John, Knobloch, Rankin: SeMA Journal (75), 655–685, 2018

- AFC norm

$$\|u_h\|_{\mathrm{AFC}}^2 = \|u_h\|_a^2 + d_h(u_h, u_h, u_h) \quad \forall u_h \in V_h$$

  - where $\|u_h\|_a^2 = \varepsilon |u_h|_1^2 + \sigma \|u_h\|_0^2$

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- Let $I_h u$ denote the Scott-Zhang interpolation operator. Galerkin orthogonality arguments

$$\begin{aligned}\|u - u_h\|_{\mathrm{AFC}}^2 &= \langle f, u - I_h u\rangle + \langle g, u - I_h u\rangle_{\Gamma_N} - a_h(u_h, u - I_h u) \\ &\quad + d_h(u_h; u, I_h u - u_h)\end{aligned}$$

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- Standard residual a posteriori error bound [1]

$$\begin{aligned} &\langle f, u - I_h u\rangle + \langle g, u - I_h u\rangle_{\Gamma_N} - a_h(u_h, u - I_h u) \\ &= \sum_{K \in \mathcal{T}_h} (R_K(u_h), u - I_h u)_K + \sum_{F \in \mathcal{F}_h} \langle R_F(u_h), u - I_h u\rangle_F \end{aligned}$$

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with

$$R_K(u_h) := f + \varepsilon \Delta u_h - \mathbf{b} \cdot \nabla u_h - c u_h|_K,$$

$$R_F(u_h) := \begin{cases} -\varepsilon [|\nabla u_h \cdot \mathbf{n}_F|]_F & \text{if } F \in \mathcal{F}_{h,\Omega}, \\ g - \varepsilon(\nabla u_h \cdot \mathbf{n}_F) & \text{if } F \in \mathcal{F}_{h,N}, \\ 0 & \text{if } F \in \mathcal{F}_{h,D} \end{cases}$$

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$$

- Using interpolation estimates, Cauchy-Schwarz, and Young's inequality

$$
\begin{aligned}
&\|u-u_h\|_a^2 + \frac{C_Y}{C_Y-1} d_h(u_h; u-u_h, u-u_h) \\
\leq\ & \frac{C_Y^2}{2(C_Y-1)} \sum_{K\in\mathcal{T}_h} \min\left\{\frac{C_I^2}{\sigma}, \frac{C_I^2 h_K^2}{\varepsilon}\right\} \|R_K(u_h)\|_{L^2(K)}^2 \\
&+ \frac{C_Y^2}{2(C_Y-1)} \sum_{F\in\mathcal{F}_h} \min\left\{\frac{C_F^2 h_F}{\varepsilon}, \frac{C_F^2}{\sigma^{1/2}\varepsilon^{1/2}}\right\} \|R_F(u_h)\|_{L^2(F)}^2 \\
&+ \frac{C_Y}{C_Y-1} d_h(u_h; u, I_h u - u_h)
\end{aligned}
$$

- Linearity of $d_h(\cdot;\cdot,\cdot)$,

$$d_h(u_h; u, I_h u - u_h) = d_h(u_h; u - u_h, I_h u - u_h) + d_h(u_h; u_h, I_h u - u_h)$$

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- Using interpolation estimates, Cauchy-Schwarz, trace inequality, inverse estimate, and Young's inequality

$$\begin{aligned} d_h(u_h; u_h, I_h u - u_h) \quad & \leq \quad \frac{C_Y}{2} \sum_{E \in \mathcal{E}_h} \min\left\{ \frac{\kappa_1 h_E^2}{\varepsilon}, \frac{\kappa_2}{\sigma} \right\} (1 - \alpha_E)^2 |d_E|^2 h_E^{1-d} \\ & \quad \times \|\nabla u_h \cdot \mathbf{t}_E\|_{L^2(E)}^2 + \frac{1}{C_Y} \|u - u_h\|_a^2, \end{aligned}$$

where

$$\begin{aligned} \kappa_1 &= C_{\text{edge,max}} \left(1 + (1 + C_I)^2\right), \\ \kappa_2 &= C_{\text{inv}}^2 C_{\text{edge,max}} \left(1 + (1 + C_I)^2\right). \end{aligned}$$

Theorem (Global a posteriori error estimate)

A global a posteriori error estimate for the energy norm is given by[1]

$$\|u - u_h\|_a^2 \leq \eta_1^2 + \eta_2^2 + \eta_3^2,$$

where

$$\eta_1^2 = \sum_{K\in\mathcal{T}_h} \min\left\{\frac{4C_I^2}{\sigma}, \frac{4C_I^2 h_K^2}{\varepsilon}\right\} \|R_K(u_h)\|_{L^2(K)}^2,$$

$$\eta_2^2 = \sum_{F\in\mathcal{F}_h} \min\left\{\frac{4C_F^2 h_F}{\varepsilon}, \frac{4C_F^2}{\sigma^{1/2}\varepsilon^{1/2}}\right\} \|R_F(u_h)\|_{L^2(F)}^2,$$

$$\eta_3^2 = \sum_{E\in\mathcal{E}_h} \min\left\{\frac{4\kappa_1 h_E^2}{\varepsilon}, \frac{4\kappa_2}{\sigma}\right\} (1-\alpha_E)^2 |d_E|^2 h_E^{1-d} \|\nabla u_h \cdot \mathbf{t}_E\|_{L^2(E)}^2$$

[1] J.: CAMWA, 97(1), 86–99, 2021

- Standard strategy for solving

SOLVE → ESTIMATE → MARK → REFINE

[1] Xu, Zikatanov: MC, 68(228), 1429–1446, 1999

Hanging Nodes

- Standard strategy for solving

SOLVE → ESTIMATE → MARK → REFINE

- Hanging nodes
  - Preserves angles after red-refinement
  - Avoids prism and pyramids in 3D mesh refinement
  - *hp* adaptive refinement
- Certain stabilized schemes rely on the property of triangulation [1]

[1] Xu, Zikatanov: MC, 68(228), 1429–1446, 1999

Lemma

Let $\mathcal{T}$ be a non-conforming triangulation of Ω, i.e., $\mathcal{T}$ has hanging nodes. Then, for all $q \in H(\mathcal{T})$ there are coefficients a_{qp} with $p \in N_F(\mathcal{T}) \setminus H(\mathcal{T})$ such that all $v \in V_h$ can be represented as[1 2]

$$v(q) = \sum_{p \in N_F(\mathcal{T}) \setminus H(\mathcal{T})} a_{qp} v(p)$$

[1] Gräser : PhD Thesis, FU Berlin 2011

[2] J.: PhD Thesis, FU Berlin 2020

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Theorem

Let $\{\mathcal{T}_0, \cdots, \mathcal{T}_j\}$ be a grid hierarchy on Ω with $\mathcal{T}_0$ being conforming. Let us denote $\mathcal{T} = \mathcal{T}_j$, i.e., the final refinement level. Then a basis of V_h is given by[1]

$$B(\mathcal{T}) := \left\{ \varphi_p = \varphi_p^{\mathrm{nc}} + \sum_{q \in H(\mathcal{T})} a_{qp} \varphi_q^{\mathrm{nc}} : p \in N_F(\mathcal{T}) \setminus H(\mathcal{T}) \right\}$$

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[1] Gräser : PhD Thesis, FU Berlin 2011

[2] J.: PhD Thesis, FU Berlin 2020

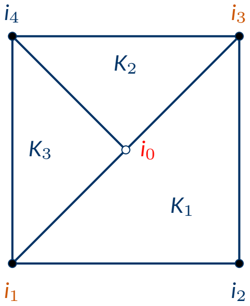
- Satisfaction of DMP
  - DMP is satisfied if[1]

$$\begin{aligned} a_{ii} &> 0, \\ a_{ij} + a_{ji} &\leq 0, \end{aligned}$$

where a_{ij} is in the stiffness matrix

[1] Barrenechea, John, Knobloch: SINUM (54), 2427–2451, 2016

- Consider the sample patch



- Initial assembly

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & a_{03} & a_{04} \\ a_{10} & a_{11} & a_{12} & a_{13} & a_{14} \\ a_{20} & a_{21} & a_{22} & a_{23} & a_{24} \\ a_{30} & a_{31} & a_{32} & a_{33} & a_{34} \\ a_{40} & a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}, \qquad \begin{pmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

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- Conforming test space and continuity of the hanging node

$$\begin{pmatrix} 1 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ a_{10} + \frac{a_{00}}{2} & a_{11} + \frac{a_{01}}{2} & a_{12} + \frac{a_{02}}{2} & a_{13} + \frac{a_{03}}{2} & a_{14} + \frac{a_{04}}{2} \\ a_{20} & a_{21} & a_{22} & a_{23} & a_{24} \\ a_{30} + \frac{a_{00}}{2} & a_{31} + \frac{a_{01}}{2} & a_{32} + \frac{a_{02}}{2} & a_{33} + \frac{a_{03}}{2} & a_{34} + \frac{a_{04}}{2} \\ a_{40} & a_{41} & a_{42} & a_{43} & a_{44} \end{pmatrix}, \quad \begin{pmatrix} 0 \\ b_1 + \frac{b_0}{2} \\ b_2 \\ b_3 + \frac{b_0}{2} \\ b_4 \end{pmatrix}$$

- Conforming ansatz space

$$\begin{pmatrix} 1 & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 \\ 0 & a_{11} + \frac{a_{01}}{2} + \frac{a_{10}}{2} + \frac{a_{00}}{4} & a_{12} + \frac{a_{02}}{2} & a_{13} + \frac{a_{03}}{2} + \frac{a_{10}}{2} + \frac{a_{00}}{4} & a_{14} + \frac{a_{04}}{2} \\ 0 & a_{21} + \frac{a_{20}}{2} & a_{22} & a_{23} + \frac{a_{20}}{2} & a_{24} \\ 0 & a_{31} + \frac{a_{01}}{2} + \frac{a_{30}}{2} + \frac{a_{00}}{4} & a_{32} + \frac{a_{02}}{2} & a_{33} + \frac{a_{03}}{2} + \frac{a_{30}}{2} + \frac{a_{00}}{4} & a_{34} + \frac{a_{04}}{2} \\ 0 & a_{41} + \frac{a_{40}}{2} & a_{42} & a_{43} + \frac{a_{40}}{2} & a_{44} \end{pmatrix}$$

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- Increases the matrix stencil by few elements

- Algebraic stabilisation schemes
  - Algebraic Flux Correction (AFC) schemes
    - Kuzmin limiter[1]
    - BJK limiter[2][3]

[1] Kuzmin: in Proc. Int. Conf. Comput. Meth. for Coupled Problems in Science and Engineering, CIMNE, 2007

[2] Barrenechea, John, Knobloch: M3AS (27), 525–548, 2017

[3] Barrenechea, John, Knobloch: arXiv: 2204.07480, 2022

[4] John, Knobloch: arXiv: 2111.08697, 2021

- Algebraic stabilisation schemes
  - Algebraic Flux Correction (AFC) schemes
    - Kuzmin limiter[1]
    - BJK limiter[2][3]
  - Monotone Upwind-type Algebraically Stabilized (MUAS) method[4]
    - Drops symmetric condition on α_{ij}
    - AFC system is modified

$$(A + D)\, U = F + (D - B)\, U,$$

where

$$b_{ij} = \max\left\{ \left(1 - \overline{\alpha_{ij}}(u)\right) a_{ij}, 0, \left(1 - \overline{\alpha_{ji}}(u)\right) a_{ji} \right\}$$

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- Comparison of results:
  - Accuracy of solution
    - $\|\cdot\|_{L^2(\Omega)}$
    - $\|\nabla(\cdot)\|_{L^2(\Omega)}$

[1] Augustin, Caiazzo, Fiebach, Fuhrmann, John, Linke, Umla : CMAME (200), 3395 - 3409, 2011

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  - Efficiency of the scheme
  - Global satisfaction of DMP

$$\mathrm{osc}_{\max}(u_h) := \max_{(x,y)\in\overline{\Omega}} u_h(x,y) - 1 - \min_{(x,y)\in\overline{\Omega}} u_h(x,y)$$

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  - Adaptive grids
    - Conforming closure
    - Hanging nodes

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- For MUAS method neglect η_3

[1] Augustin, Caiazzo, Fiebach, Fuhrmann, John, Linke, Umla : CMAME (200), 3395 - 3409, 2011

- Iterative solver
  - Matrix formulation of the algebraic stabilised schemes[1,2]

$$(A + D)\, U = F + (D - B(U))\, U$$

  - Fixed point right-hand side

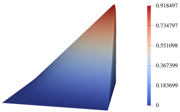
$$\begin{aligned}(A + D)\, \tilde{U}^{\mu} &= F + (D - B(U^{\mu}))\, U^{\mu}, \\ U^{\mu+1} &= \omega \tilde{U}^{\mu} + (1 - \omega) U^{\mu},\end{aligned}$$

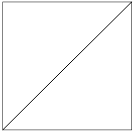
where $\omega > 0$ is a dynamic damping parameter

[1] J.John: BAIL 2018 (135), 2020
[2] J.,John: CAMWA (78), 3117-3138, 2019

- Example with corner boundary layer[1]
- $\Omega = (0,1)^2$, $\varepsilon = 10^{-2}$, $\mathbf{b} = (2,3)^T$, $c = 1$, $u_b = 0$, $g = 0$, and f such that

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





- stop of the non linear iteration [2]
  - 10000 iterations
  - $\|\text{residual}\|_2 \leq \sqrt{\#\text{dof}}10^{-10}$

[1] John, Knobloch, Savescu: CMAME (200), 2916–2929, 2011

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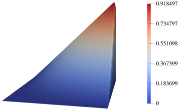
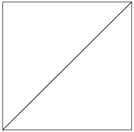
$$u(x,y) = xy^2 - y^2 \exp\left(\frac{2(x-1)}{\varepsilon}\right) - x\exp\left(\frac{3(y-1)}{\varepsilon}\right) + \exp\left(\frac{2(x-1)+3(y-1)}{\varepsilon}\right)$$





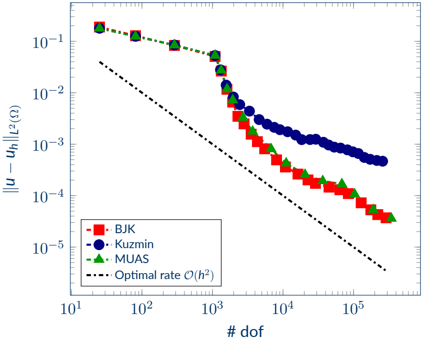
- stop of the non linear iteration [2]
  - 10000 iterations
  - $\|\text{residual}\|_2 \leq \sqrt{\#\text{dof}}\,10^{-10}$
- stop of the adaptive algorithm
  - $\eta \leq 10^{-3}$
  - $\#\text{dof} \approx 10^6$

[1] John, Knobloch, Savescu: CMAME (200), 2916–2929, 2011

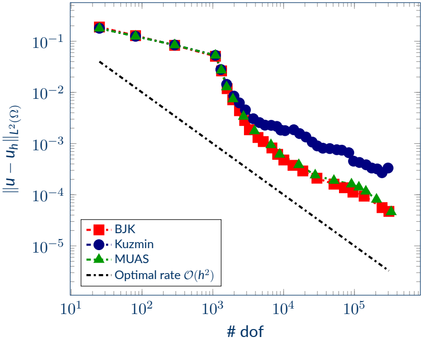
[2] J.,John: CAMWA (78), 3117-3138, 2019

- $L^2(\Omega)$ Error

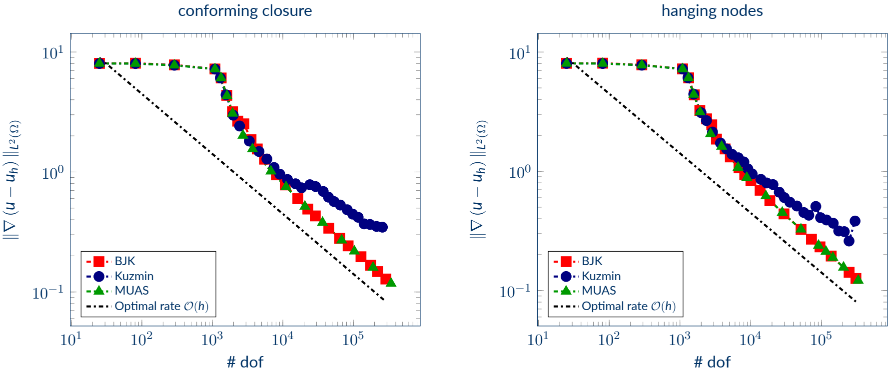
conforming closure



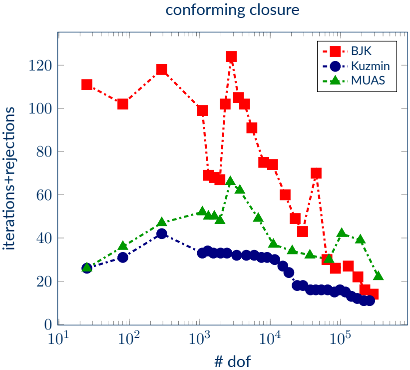
hanging nodes

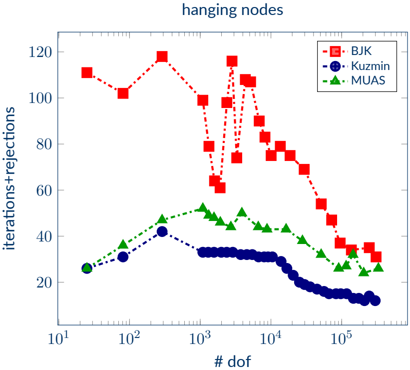


- $L^2(\Omega)$ Error of the gradient



- Efficiency


conforming closure
BJK
Kuzmin
MUAS
iterations+rejections
0
20
40
60
80
100
120
10^1
10^2
10^3
10^4
10^5
dof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20
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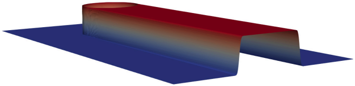
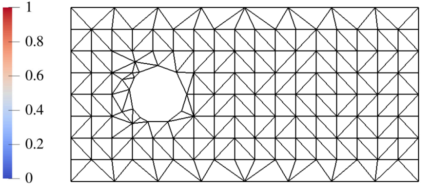
10^5
dof

- Hemker problem[1]
- $\varepsilon = 10^{-4}, \mathbf{b} = (1,0)^T, c = f = 0$





- stop of the non linear iteration
  - 10000 iterations
  - $\|\text{residual}\|_2 \leq \sqrt{\#\text{dof}}10^{-8}$

[1] Hemker: JCAM 76, 277-285, 1996

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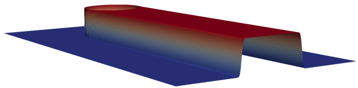

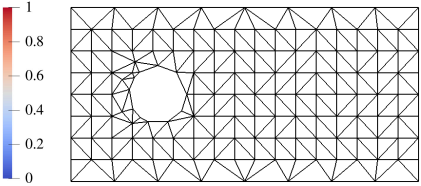

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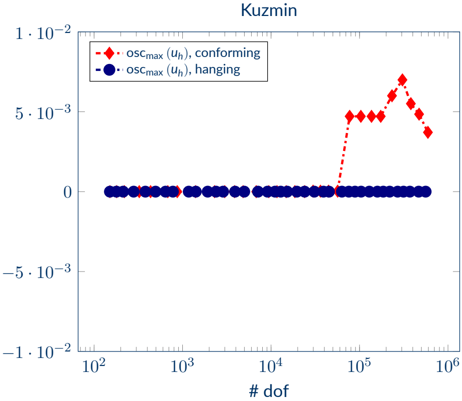
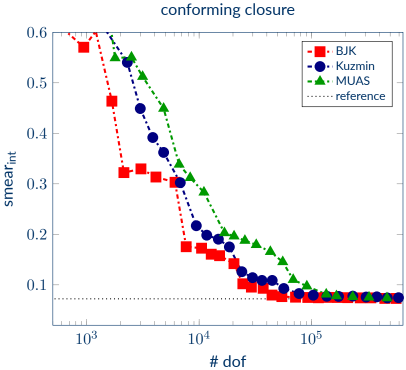
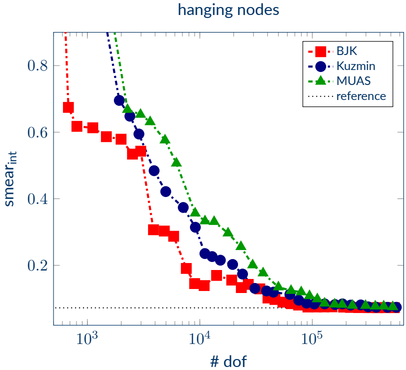
[1] Hemker: JCAM 76, 277-285, 1996

- Satisfaction of Global DMP



- Smearing of internal layer





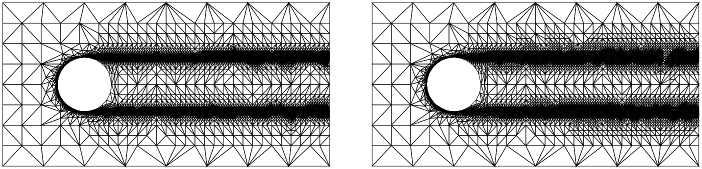
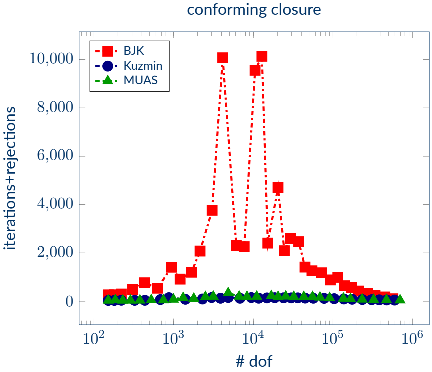
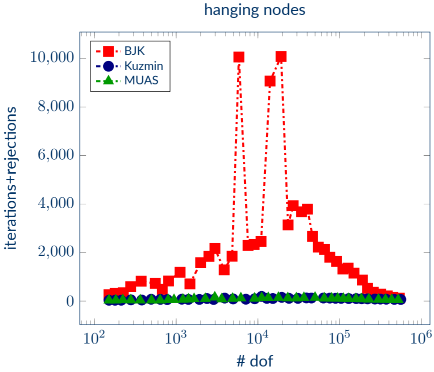


Figure 1: Adaptively refined conforming grids with $\approx 25,000$ #dof, AFC method and Kuzmin limiter (left), MUAS method (right)

- Efficiency


conforming closure
BJK
Kuzmin
MUAS
iterations+rejections
10,000
8,000
6,000
4,000
2,000
0
10^2
10^3
10^4
10^5
10^6
dof


hanging nodes
BJK
Kuzmin
MUAS
iterations+rejections
10,000
8,000
6,000
4,000
2,000
0
10^2
10^3
10^4
10^5
10^6
dof

- Conclusions[1]
  - Accuracy of solution
    - AFC + BJK limiter and MUAS method converge on all grids
    - AFC + Kuzmin limiter does not converge on adaptively refined grids if solution becomes (locally) diffusion-dominated

[1] J.,John, Knobloch: arXiv : 2007.08405 , 2022

[2] J.,John: CAMWA (78), 3117-3138, 2019

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    - Global DMP satisfied on grids with hanging nodes
    - AFC+ Kuzmin limiter did not satisfy on conformally closed grids

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    - AFC + BJK limiter sharpest layer
    - For fine grids, all values close to reference value

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[1] J.,John, Knobloch: arXiv : 2007.08405 , 2022

[2] J.,John: CAMWA (78), 3117-3138, 2019

- Outlook
  - Development of estimators for MUAS method
  - Numerical studies in 3D
  - Comparison with Monolithic Convex Limiter[1][2]

[1] Kuzmin: CMAME (361), 112804, 2020

[2] J., Partl, Ahmed, Kuzmin: JNUM, 10.1515/jnma-2021-0123, 2022