

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

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SIAM Conference on Computational Science and Engineering (CSE23)
1st March 2023

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



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1 Algebraic Stabilisation Schemes

2 A Posteriori Error Analysis

2.1 Residual Based Approach

3 Adaptive Grids

3.1 Implementation

4 Numerical Studies

5 Conclusions and Outlook

- 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

$$\left(c(\mathbf{x}) - \frac{1}{2} \nabla \cdot \mathbf{b}(\mathbf{x}) \right) \geq \sigma_0 > 0$$

- 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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- Alternate approach: Adaptive grids
- Idea: Combine both the approaches

- Variational problem for AFC scheme¹

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 ($V_h \subset V$)

¹Barrenechea, John, Knobloch: arXiv : 2204.07480, 2022

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- 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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- Energy norm

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

¹Barrenechea, John, Knobloch: arXiv : 2204.07480, 2022

Theorem (Global a posteriori error estimate)

A global a posteriori error estimate for the energy norm is given by¹

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

where

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

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

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

¹J.: CAMWA, 97(1), 86–99, 2021

- Standard strategy for solving

SOLVE → **ESTIMATE** → **MARK** → **REFINE**

¹Xu, Zikatanov: MC, 68(228), 1429-1446, 1999

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- **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

¹Xu, 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}

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

¹Gräser : PhD Thesis, FU Berlin 2011

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Theorem

Let $\{\mathcal{T}_0, \dots, \mathcal{T}_j\}$ 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 by¹

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

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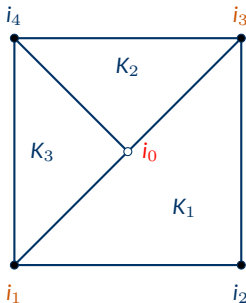
- Satisfaction of DMP
 - DMP is satisfied if¹

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

where a_{ij} is in the stiffness matrix

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

- Consider the sample patch



- Initial assembly

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

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- Conforming test space and continuity of the hanging node

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

- Algebraic stabilisation schemes
 - Algebraic Flux Correction (AFC) schemes
 - Kuzmin limiter¹
 - 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 limiter¹
 - BJK limiter^{2,3}
 - Monotone Upwind-type Algebraically Stabilized (MUAS) method⁴
 - Drops symmetric condition on α_{ij}
 - AFC system is modified

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

where

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

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

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 - Global satisfaction of DMP

$$\text{OSC}_{\max}(u_h) := \max_{(x,y) \in \bar{\Omega}} u_h(x,y) - 1 - \min_{(x,y) \in \bar{\Omega}} u_h(x,y)$$

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- Smearing of internal layer¹

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- For MUAS method neglect η_3

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- **Iterative solver**

- Matrix formulation of the algebraic stabilised schemes^{1,2}

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

- **Fixed point right-hand side**

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

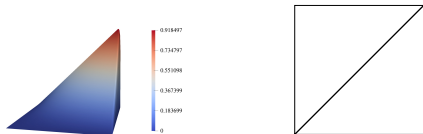
where $\omega > 0$ is a dynamic damping parameter

¹J.John: BAIL 2018 (135), 2020

²J.,John: CAMWA (78), 3117-3138, 2019

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

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



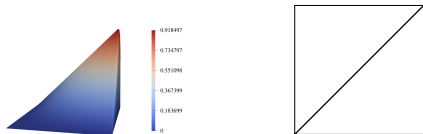
- stop of the non linear iteration²
 - 10000 iterations
 - $\|\text{residual}\|_2 \leq \sqrt{\#\text{dof}} 10^{-10}$

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

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

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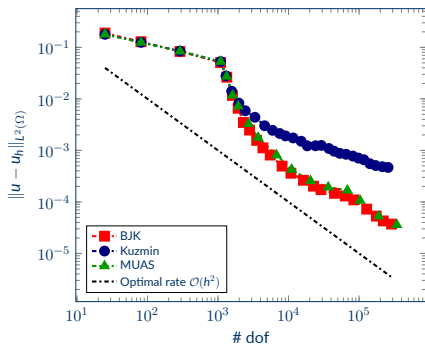
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- stop of the adaptive algorithm
 - $\eta \leq 10^{-3}$
 - $\#\text{dof} \approx 10^6$

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

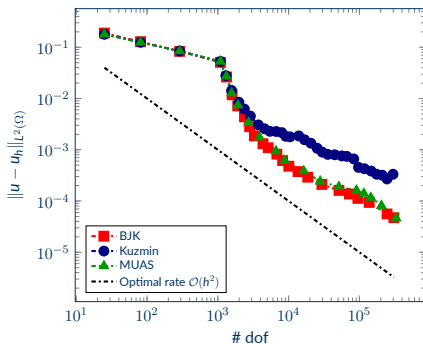
² J., John: CAMWA (78), 3117–3138, 2019

• $L^2(\Omega)$ Error

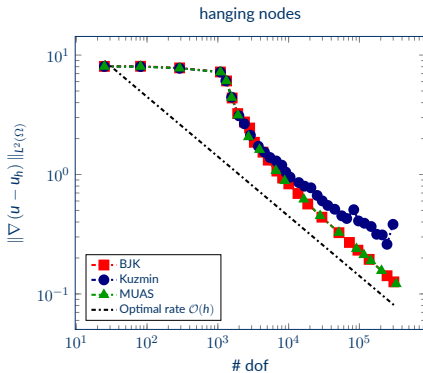
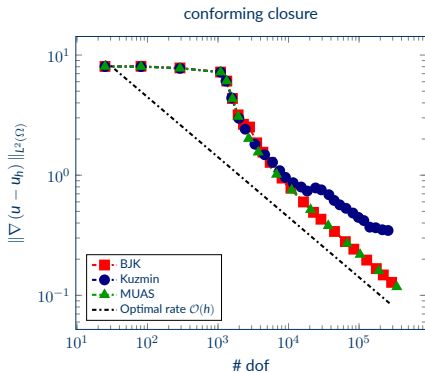
conforming closure



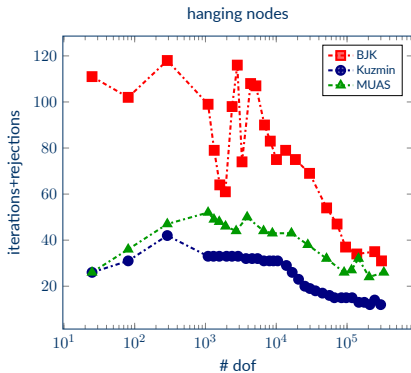
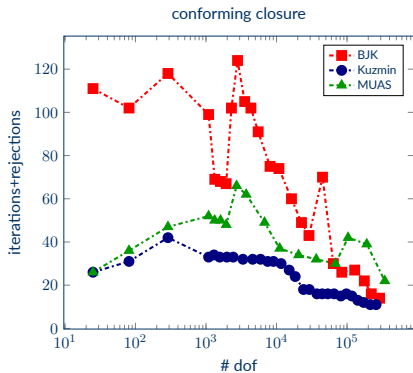
hanging nodes



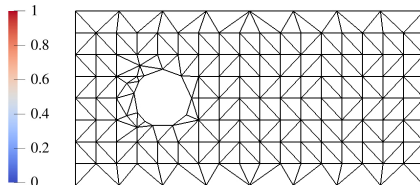
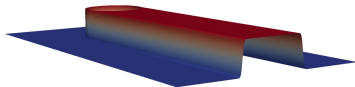
- $L^2(\Omega)$ Error of the gradient



● Efficiency



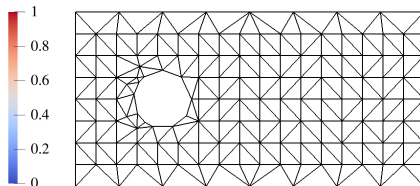
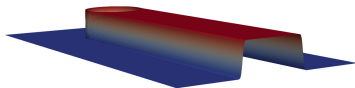
- Hemker problem¹
- $\epsilon = 10^{-4}$, $\mathbf{b} = (1, 0)^T$, $\mathbf{c} = \mathbf{f} = 0$



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

¹Hemker: JCAM 76, 277-285, 1996

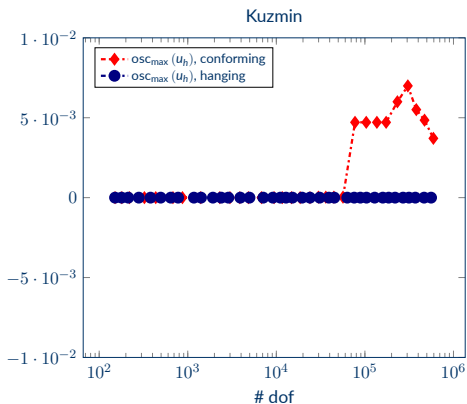
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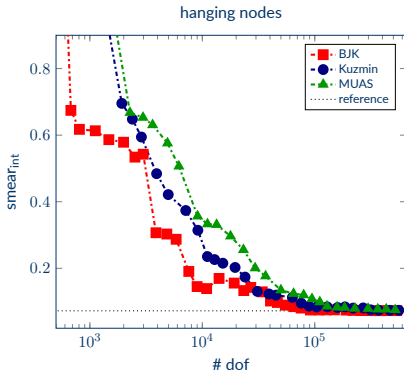
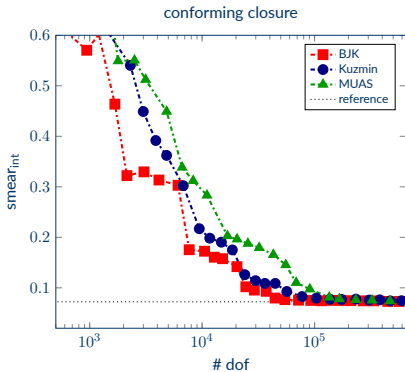
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- Satisfaction of Global DMP



Smearing of internal layer



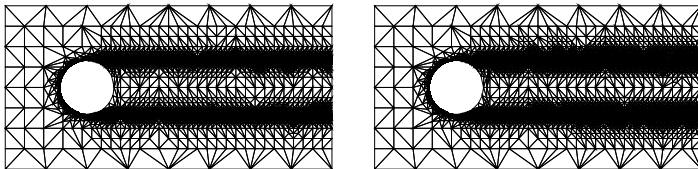
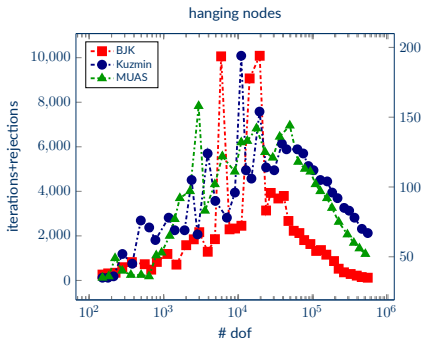
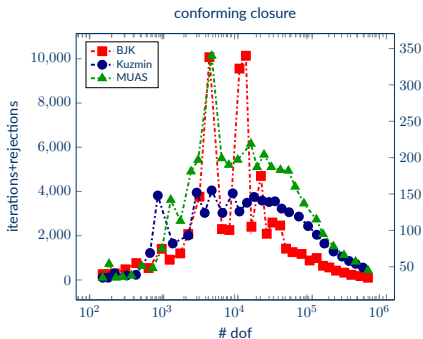


Figure 1: Adaptively refined conforming grids with $\approx 25,000$ #dof, AFC method and Kuzmin limiter (left), MUAS method (right)

● Efficiency



- **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

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

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 - AFC+ **Kuzmin limiter** and the **MUAS method**² most efficient

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 - **Satisfaction** of DMP
 - 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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- **MUAS method most promising**

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²J.,John: CAMWA (78), 3117-3138, 2019

- Outlook

- Development of estimators for **MUAS method**
- Numerical studies in 3D
- Comparison with **Monolithic Convex Limiter**¹²

¹ Kuzmin: CMAME (361), 112804, 2020

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