A Residual based a Posteriori Error Estimators for Algebraic Flux Correction Scheme

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Outline

Applied and Computational Mathematics | RWTH AACHEN UNIVERSITY

- Steady-state convection-diffusion-reaction equation

$$\begin{aligned} -\varepsilon\Delta u + \mathbf{b}\cdot\nabla u + cu &= f && \text{in } \Omega \\ u &= u_b && \text{on } \Gamma_D, \\ -\varepsilon\nabla u\cdot\mathbf{n} &= g && \text{on } \Gamma_N \end{aligned} \tag{1}$$

  - 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
  1. Accurate and sharp layers
     - Many discretizations satisfy this property, e.g., SUPG
     - Reasonably well for AFC schemes

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

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  2. Physically consistent results (no spurious oscillations)
     - Most discretizations violate this property, e.g., SUPG, SOLD schemes
     - Satisfied for AFC schemes

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Algebraic Flux Correction (AFC) Schemes

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  3. Efficient computation of the solutions
     - Satisfied for linear discretizations
     - Usually not satisfied for nonlinear discretizations, like AFC schemes [1]

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  3. Efficient computation of the solutions
     - Satisfied for linear discretizations
     - Usually not satisfied for nonlinear discretizations, like AFC schemes [1]
- Because of 2^{nd} property: AFC schemes very well suited for applications

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

- 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

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

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

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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

Residual Based Approach

- AFC norm

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

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

[1] John, Novo: CMAME (255), 289–305, 2013

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

- 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]

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

[1] John, Novo: CMAME (255), 289–305, 2013

with

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

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

Residual Based Approach

with

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

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

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

Residual Based Approach

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

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

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

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

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

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

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

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

where

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

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

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

- Formal local lower bound for a mesh cell K

$$\eta_K^2 = \eta_{\mathrm{Int},\mathrm{K}}^2 + \sum_{F \in \mathcal{F}_h(K)} \eta_{\mathrm{Face},F}^2 + \sum_{E \in \mathcal{E}_h(K)} \eta_{d_h,E}^2$$

- Formal local lower bound for a mesh cell K

$$\eta_K^2 = \eta_{\text{Int,K}}^2 + \sum_{F \in \mathcal{F}_h(K)} \eta_{\text{Face},F}^2 + \sum_{E \in \mathcal{E}_h(K)} \eta_{d_h,E}^2$$

where

$$\eta_{\text{Int},K}^2 = \min\left\{\frac{4C_I^2}{\sigma}, \frac{4C_I^2 h_K^2}{\varepsilon}\right\} \|R_{K,h}(u_h)\|_{L^2(K)}^2,$$

$$\eta_{\text{Face},F}^2 = \frac{1}{2}\min\left\{\frac{4C_F^2 h_F}{\varepsilon}, \frac{4C_F^2}{\sigma^{1/2}\varepsilon^{1/2}}\right\} \|R_F(u_h)\|_{L^2(F)}^2,$$

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

Residual Based Approach

- Using standard bubble function arguments

$$\eta_{\mathrm{Int},K} \leq C\Bigg(\max\left\{C_K^2 + \frac{C_K h_K}{\varepsilon}\|\mathbf{b}\|_{L^\infty(K)}, \frac{C_K}{\sigma}\|c\|_{L^\infty(K)}\right\}\|u-u_h\|_{a,K} + \frac{h_K}{\varepsilon^{1/2}}C_K\Big(\|f-f_h\|_{0,K} + \|(\mathbf{b}-\mathbf{b}_h)\cdot\nabla u_h\|_{0,K} + \|(c-c_h)u_h\|_{0,K}\Big)\Bigg)$$

Residual Based Approach

- Using standard bubble function arguments

$$\eta_{\mathrm{Int},K} \leq C\Bigg(\max\left\{C_K^2 + \frac{C_K h_K}{\varepsilon}\|\mathbf{b}\|_{L^\infty(K)}, \frac{C_K}{\sigma}\|c\|_{L^\infty(K)}\right\}\|u-u_h\|_{a,K}$$
$$+\frac{h_K}{\varepsilon^{1/2}}C_K\Big(\|f-f_h\|_{0,K} + \|(\mathbf{b}-\mathbf{b}_h)\cdot\nabla u_h\|_{0,K} + \|(c-c_h)u_h\|_{0,K}\Big)\Bigg)$$

and

$$\eta_{\mathrm{Face},F} \leq C\Bigg(\max\left\{C_F + \frac{C_F h_F\|\mathbf{b}\|_{L^\infty(\omega_F)}}{\varepsilon}, \frac{C_F h_F\|c\|_{L^\infty(\omega_F)}}{\varepsilon^{1/2}\sigma^{1/2}}\right\}\|u-u_h\|_{a,\omega_F}$$
$$+\delta_{F\in\mathcal{F}_{h,N}}\frac{h_F^{1/2}}{\varepsilon^{1/2}}\|g-g_h\|_{L^2(F)}$$
$$+\sum_{K\in\omega_F}\Big[\eta_{\mathrm{Int},K} + \frac{h_K}{\varepsilon^{1/2}}\big(\|f-f_h\|_{0,K} + \|(\mathbf{b}-\mathbf{b}_h)\cdot\nabla u_h\|_{0,K}$$
$$+\|(c-c_h)u_h\|_{0,K}\big)\Big]\Bigg)$$

- For the stabilization term, from [1] we get

$$|d_E| \leq C \left(\varepsilon + \|\mathbf{b}\|_{L^\infty(\Omega)} h + \|c\|_{L^\infty(\Omega)} h^2 \right) h_E^{d-2}$$

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

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$$|d_E| \leq C\left(\varepsilon + \|\mathbf{b}\|_{L^\infty(\Omega)} h + \|\mathbf{c}\|_{L^\infty(\Omega)} h^2\right) h_E^{d-2}$$

Hence,

$$\eta_{d_h,E} \leq C \sum_{E\in\mathcal{E}_h} (1-\alpha_E)\left(\varepsilon + \|\mathbf{b}\|_{L^\infty(\Omega)} h + \|\mathbf{c}\|_{L^\infty(\Omega)} h^2\right) \times \frac{h_E^{(3-d)/2}}{\varepsilon^{1/2}} \|\nabla u_h \cdot \mathbf{t}_E\|_{L^2(E)}$$

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

Theorem (Formal local lower bound)

There exists a constant $C > 0$, independent of the size of elements of $\mathcal{T}$, such that, for every $K \in \mathcal{T}$, the following formal local lower bound holds

$$
\begin{aligned}
&\eta_{\mathrm{Int},K} + \sum_{K \in \mathcal{F}_h(K)} \eta_{\mathrm{Face},F} + \sum_{E \in \mathcal{E}_h(K)} \eta_{d_h,E} \\
\leq\ & \max\left\{ C_K^2 + \frac{C_K h_K}{\varepsilon} \|\mathbf{b}\|_{L^\infty(K)}, \frac{C_K}{\sigma} \|c\|_{L^\infty(K)} \right\} \|u - u_h\|_{a,\omega_K} \\
& + C \sum_{K \in \omega_K} \frac{h_K}{\varepsilon^{1/2}} \left(\|f - f_h\|_{0,K} + \|(\mathbf{b} - \mathbf{b}_h) \cdot \nabla u_h\|_{0,K} + \|(c - c_h) u_h\|_{0,K} \right) \\
& + C \sum_{F \in \mathcal{F}_h(K)} \delta_{F \in \mathcal{F}_{h,N}} \frac{h_F^{1/2}}{\varepsilon^{1/2}} \|g - g_h\|_{L^2(F)} \\
& + \sum_{E \in \mathcal{E}_h(K)} h^{1-d/2} \frac{h^{1/2}}{\varepsilon^{1/2}} \left(\varepsilon + \|\mathbf{b}\|_{L^\infty(\Omega)} h + \|c\|_{L^\infty(\Omega)} h^2 \right) \|\nabla u_h \cdot \mathbf{t}_E\|_{L^2(E)}.
\end{aligned}
$$

- The initial solution for the nonlinear loop is the SUPG solution [1]
  - $u_{\text{AFC}} :=$ AFC solution
  - $u_{\text{SUPG}} :=$ SUPG solution
- By triangle inequality

$$\begin{aligned}\|u - u_{\text{AFC}}\|_a^2 &\leq 2\left(\|u - u_{\text{SUPG}}\|_a^2 + \|u_{\text{SUPG}} - u_{\text{AFC}}\|_a^2\right)\\ &\leq 2\left(\|u - u_{\text{SUPG}}\|_{\text{SUPG}}^2 + \|u_{\text{SUPG}} - u_{\text{AFC}}\|_a^2\right)\end{aligned}$$

[1] J.John: BAIL 2018 (135), 2020

[2] John, Novo: CMAME (255), 289-305, 2013

AFC-SUPG Approach

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- Using estimators from [2]

$$\|u - u_{\mathrm{SUPG}}\|_{\mathrm{SUPG}}^2 \leq \eta_{\mathrm{SUPG}}^2$$

[1] J.John: BAIL 2018 (135), 2020

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- Using estimators from [2]

$$\|u - u_{\text{SUPG}}\|_{\text{SUPG}}^2 \leq \eta_{\text{SUPG}}^2$$

and denoting

$$\eta_{\text{AFC}-\text{SUPG}}^2 := \|u_{\text{SUPG}} - u_{\text{AFC}}\|_a^2$$

$\Rightarrow$

$$\|u - u_h\|_a^2 \leq 2\left(\eta_{\text{SUPG}}^2 + \eta_{\text{AFC}-\text{SUPG}}^2\right)$$

[1] J.John: BAIL 2018 (135), 2020

[2] John, Novo: CMAME (255), 289-305, 2013

- Standard strategy for solving

SOLVE → ESTIMATE → MARK → REFINE

- Effectivity index for the estimator

$$\eta_{\text{eff}} = \frac{\eta}{\|u - u_h\|_a}$$

[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, Rankin: SeMA Journal (75), 655–685, 2018

- Standard strategy for solving

SOLVE → ESTIMATE → MARK → REFINE

- Effectivity index for the estimator

$$\eta_{\text{eff}} = \frac{\eta}{\|u - u_h\|_a}$$

- Limiters
  - Monolithic upwind (MU) limiter[1]
  - Linearity preservation (LP) 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, Rankin: SeMA Journal (75), 655–685, 2018

- Comparison of results:
  - On effectivity index (η_{eff})
  - Adaptive grid refinement
  - Behavior of η_{d_h}
  - Behavior of η_{SUPG} and $\eta_{\text{AFC-SUPG}}$
  - Smearing of internal layer[1]

[1] John, Knobloch: CMAME (197), 1997–2014, 2008

- Iterative solver for AFC schemes
  - Matrix formulation of the AFC schemes[1][2]

$$AU + (I - \alpha) DU = F$$

  - Fixed point right-hand side

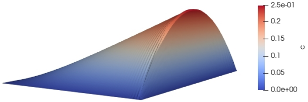
$$(A + D) U^{\nu+1} = F + \omega \alpha D U^{\nu},$$

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

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

- $\Omega = (0,1)^2$, $\varepsilon = 10^{-3}$, $\mathbf{b} = (2,1)^T$, $c = 1$ and f such that

$$u(x,y) = y(1-y)\left(x - \frac{e^{(x-1)/\varepsilon} - e^{-1/\varepsilon}}{1 - e^{-1/\varepsilon}}\right)$$



- proposed in [1]
- $\mathbb{P}_1$ finite elements
- stop of the non linear iteration [2]
  - 25000 iterations
  - $\|\text{residual}\|_2 \leq \sqrt{\#\text{nDOFs}}10^{-10}$

[1] Allendes et. al. : SISC 39(5):A1903-A1927, 2017
[2] J.,John: CAMWA (78), 3117-3138, 2019

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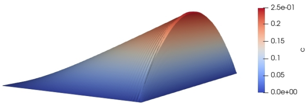
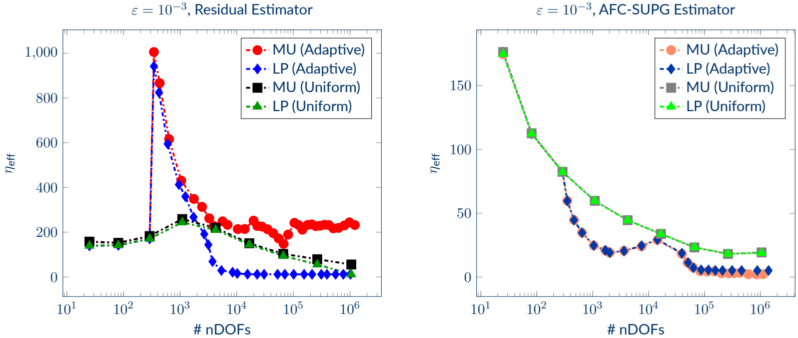


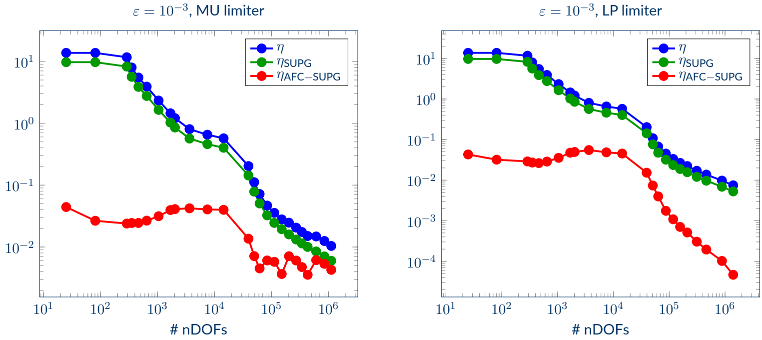
- proposed in [1]
- $\mathbb{P}_1$ finite elements
- stop of the non linear iteration [2]
  - 25000 iterations
  - $\|\text{residual}\|_2 \leq \sqrt{\#\text{nDOFs}}10^{-10}$
- stop of the adaptive algorithm
  - $\eta \leq 10^{-3}$
  - $\#\text{nDOFs} \approx 10^6$

[1] Allendes et. al. : SISC 39(5):A1903-A1927, 2017
[2] J.,John: CAMWA (78), 3117-3138, 2019

- Effectivity index

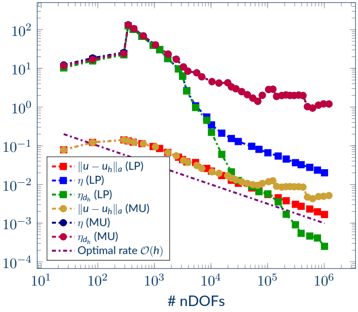


- Comparison of η_{SUPG} and $\eta_{\mathrm{AFC-SUPG}}$

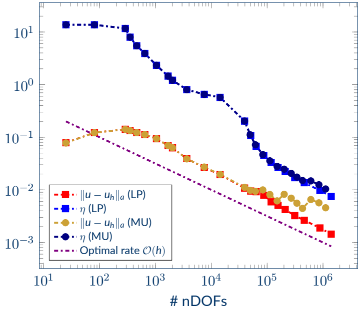


- Errors on adaptive grids

$\varepsilon = 10^{-3}$, Residual Estimator[1]



$\varepsilon = 10^{-3}$, AFC-SUPG Estimator



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

Numerical Studies

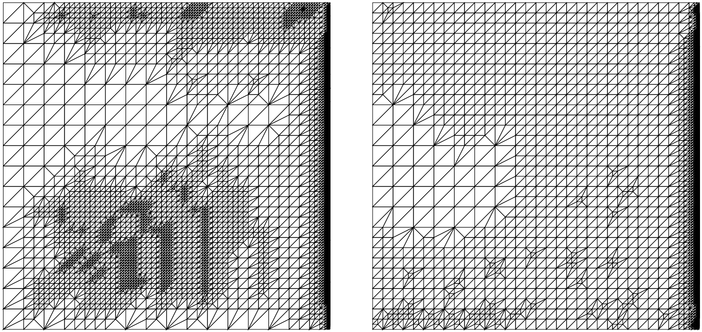
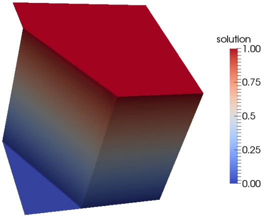


Figure 1: 14^{th} adaptively refined grid with residual estimator. MU limiter (#nDOFs $= 22962$) (left) and LP limiter (#nDOFs $= 23572$) (right)

- Example with interior and boundary layer[1]
- $\Omega = (0,1)^2, \varepsilon = 10^{-4}, \mathbf{b} = (\cos(-\pi/3), \sin(-\pi/3))^T, c = f = 0$

$$u_b = \begin{cases} 1 & (y = 1 \wedge x > 0) \text{ or } (x = 0 \wedge y > 0.7), \\ 0 & \text{else.} \end{cases}$$



[1] Hughes, Mallet, Mizukami: CMAME, 54(3), 341-345, 1986

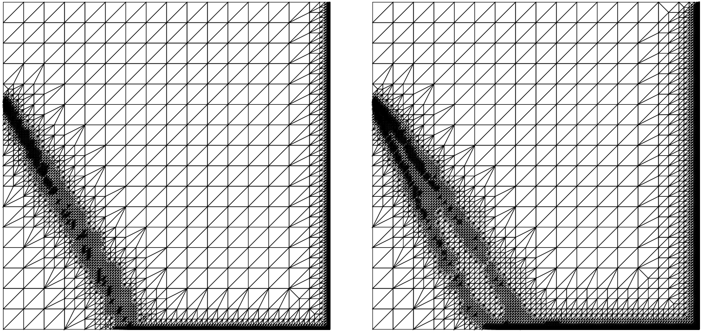
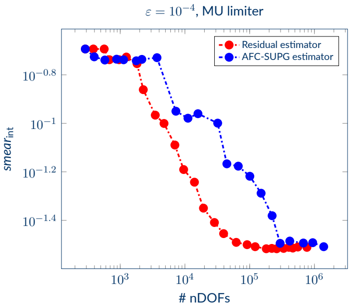
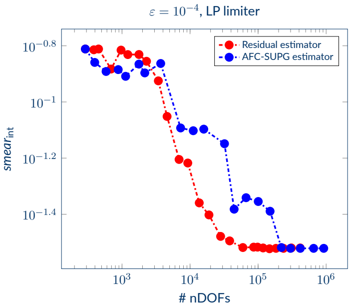


Figure 2: 14^{th} adaptively refined grid for MU limiter. Residual estimator (left) and AFC-SUPG estimator (right)

- Thickness of internal layer





- Conclusions[1]
  - Effectivity index not robust with residual based approach
  - For the AFC-SUPG estimator, the effectivity index was better
  - Choice of limiter did not play a role in AFC-SUPG estimator

[1] Jha: CAMWA, 97(1), 86–99, 2021

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

Conclusions and Outlook

- Conclusions[1]
  - Effectivity index not robust with residual based approach
  - For the AFC-SUPG estimator, the effectivity index was better
  - Choice of limiter did not play a role in AFC-SUPG estimator
  - For the MU limiter with the residual estimator reduced order of convergence
  - η_{d_h} is the dominating term in η for MU limiter if problem becomes locally diffusion-dominated. For LP limiter dominating term in the convection-dominated situation
  - With adaptive grid refinement, problem could become locally diffusion-dominated. Then use LP limiter
  - For a small diffusion coefficient, use MU limiter because nonlinear problems difficult to solve with LP limiter[2]
  - Residual estimator approximates the internal layer better

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[1] Jha: CAMWA, 97(1), 86–99, 2021

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

Outlook

- Outlook
    - Development of robust estimators
    - Numerical studies in 3D
    - Extending the analysis for the local efficiency of the estimator
    - Interplay of hanging nodes and AFC schemes
    - Comparison with monolithic convex limiter[1]

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