Algebraic Flux Correction Schemes for High-Order B-Spline Based Finite Element Approximations

Numerical Analysis group

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Outline

Finite elements in a nutshell

- **Strong problem:** find $u \in C^k(\Omega)$ such that

$$\mathcal{L}u = f \quad \text{in } \Omega \quad + \quad \text{bc's}$$

- **Weighted residual formulation:** find $u \in V$ such that

$$\int_\Omega w[\mathcal{L}u - f]\,\mathrm{d}\mathbf{x} = 0 \quad \forall w \in W$$

- Boundary conditions:
  - V (trial) and W (test spaces) contain essential bc's
  - natural bc's are incorporated via integration by parts

Finite elements in a nutshell, cont'd

- **Galerkin finite elements:** choose finite-dimensional spaces

$$V_h := \{\varphi_j\} \approx V \quad \text{and} \quad W_h := \{\phi_i\} \approx W$$

and find $u_h = \sum_j u_j \varphi_j \in V_h$ such that

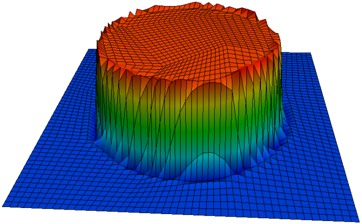
$$\int_{\Omega_h} \phi_i [\mathcal{L} u_h - f] \,\mathrm{d}\mathbf{x} = 0 \quad \forall i = 1, \dots, \dim(W_h)$$

- neglecting complications due to bc's this yields

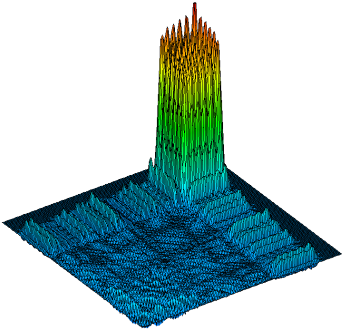
$$\sum_j \left[\int_{\Omega_h} \phi_i \mathcal{L} \varphi_j \,\mathrm{d}\mathbf{x} \right] u_j = \int_{\Omega_h} \phi_i f \,\mathrm{d}\mathbf{x} \quad \forall i = 1, \dots, \dim(W_h)$$

Problem

- Poor approximation of discontinuities/steep gradients if standard Galerkin methods are used without proper stabilization



L_2-projection



convective transport

Problem

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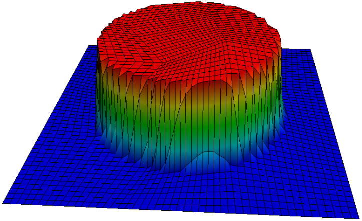
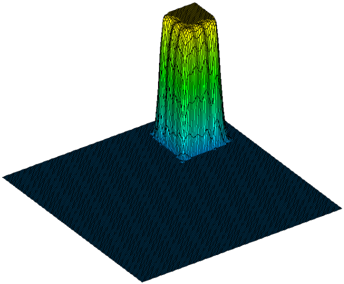


L_2-projection



convective transport

Algebraic Flux Correction

Methodology based on algebraic design criteria to derive robust and accurate **high-resolution finite element schemes** for

- Constrained data projection [5]
- Convection-dominated transport processes [3, 5, 6, 7, 10, 11]
- Anisotropic diffusion processes [3, 9]
- Processes with maximum-packing limit [4]
- ...

Many 'success stories' published . . . ;-)

Algebraic Flux Correction

Methodology based on algebraic design criteria to derive robust and accurate **high-resolution finite element schemes** for

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Many 'success stories' published ... ;-)

mostly for P_1 and Q_1 finite elements ;-(

Algebraic Flux Correction, cont'd

Extension of AFC to

- $\tilde{P}_1/\tilde{Q}_1$ elements [12]:

  > *CR-FE satisfy the necessary prerequisites [...] fail completely [...] yielding overdiffusive approximate solutions. RT-FE provides an accurate resolution [...] if the integral mean value based variant is adopted.*

- P_2 elements [2]:

  > *In summary, algebraic flux correction for quadratic finite elements seems to be feasible but gives rise to many challenging open problems.*

Objective: to extend AFC to **high-order B-spline basis** functions

B-splines in a nutshell

Define **knot vector** $\Xi = (\xi_1, \xi_2, \dots, \xi_{n+p+1})$ as a sequence of non-decreasing coordinates in the parameter space $\Omega_0 = [0, 1]$:

- $\xi_i \in \mathbb{R}$ is the i^{th} knot with index $i = 1, 2, \dots, n + p + 1$
- p is the polynomial order of the B-splines
- n is the number of B-spline functions

Cox-de Boor recursion formula for $N_{i,p} : \Omega_0 \to \mathbb{R}$

$$p = 0: \ N_{i,0}(\xi) = \begin{cases} 1 & \text{if } \xi_i \leq \xi < \xi_{i+1} \\ 0 & \text{otherwise} \end{cases} \qquad \text{define } \frac{0}{0} = 0$$

$$p > 0: \ N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$

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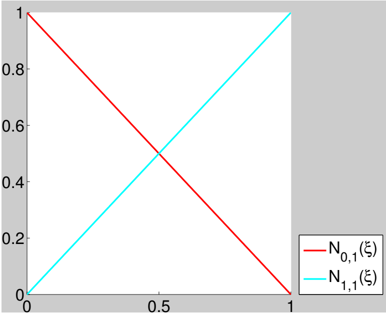
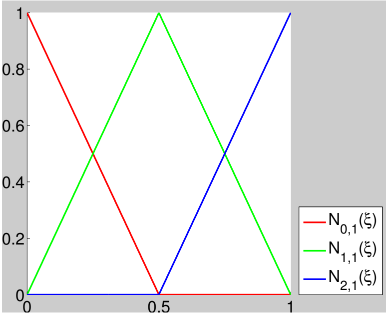
Knot insertion (h-refinement)

$\Xi = (0, 0, 1, 1)$, $p = 1$



one element

$\Xi = (0, 0, 0.5, 1, 1)$, $p = 1$

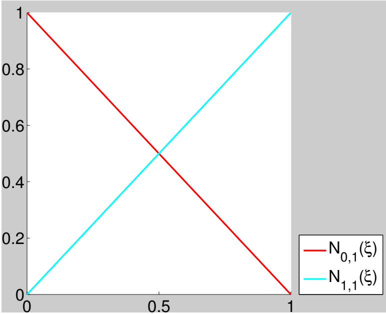


two elements, C^0-continuity

In general we have C^{p-m_i}-continuity across element boundaries, where m_i is the multiplicity of the value of ξ_i in the knot vector.

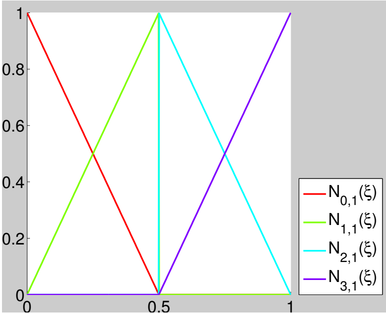
Knot insertion, cont'd

$\Xi = (0, 0, 1, 1)$, $p = 1$



one element

$\Xi = (0, 0, 0.5, 0.5, 1, 1)$, $p = 1$

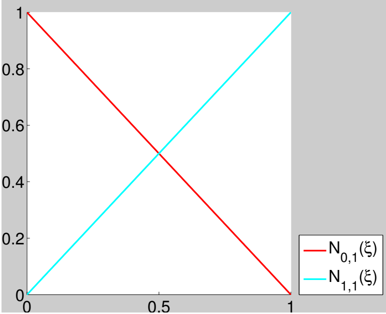


two elements, discontinuity

In general we have C^{p-m_i}-continuity across element boundaries, where m_i is the multiplicity of the value of ξ_i in the knot vector.

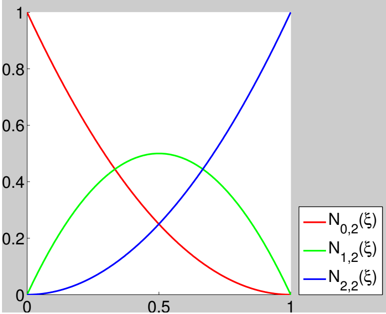
Order elevation

$\Xi = (0,0,1,1)$, $p = 1$



one element

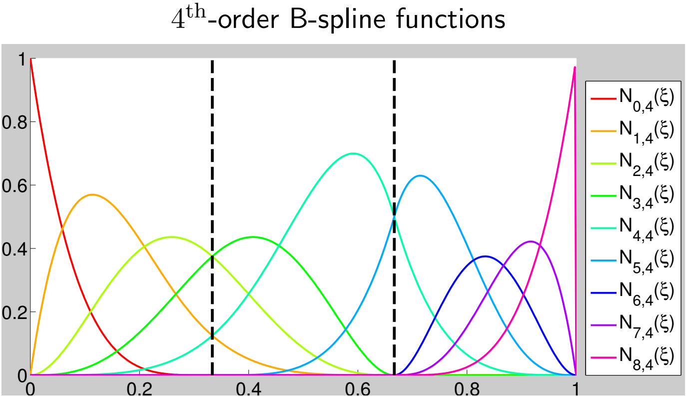
$\Xi = (0,0,0,1,1,1)$, $p = 2$



one element

In contrast to standard Lagrange finite element basis functions, the B-spline functions never become negative over their support.

Nonuniform continuity at element boundaries



$$\Xi = (\underbrace{0,0,0,0,0}_{\text{discontinuity}},\underbrace{1/3}_{C^3},\underbrace{2/3,2/3,2/3}_{C^1},\underbrace{1,1,1,1,1}_{\text{discontinuity}})$$

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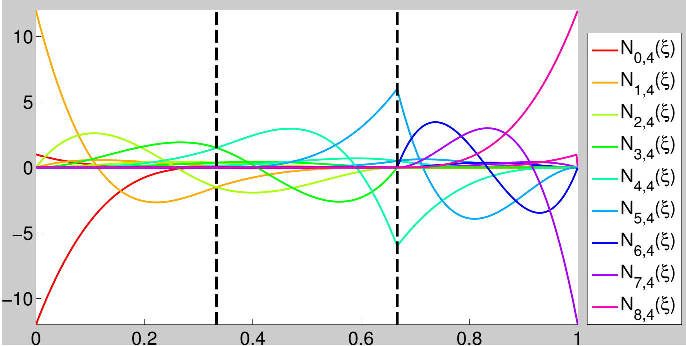
Nonuniform continuity at element boundaries

First derivatives of 4^{th}-order B-spline functions



$$\Xi = (\underbrace{0,0,0,0,0}_{\text{discontinuity}}, \underbrace{1/3}_{C^3}, \underbrace{2/3,2/3,2/3}_{C^1}, \underbrace{1,1,1,1,1}_{\text{discontinuity}})$$

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Geometric mapping

- Define mapping between parameter space $\Omega_0 = [0, 1]$ and the computational domain Ω using control points $\mathbf{p}_i \in \mathbb{R}^d$, $d = 1, 2, 3$

$$\mathbf{G} : \Omega_0 \mapsto \Omega, \qquad \mathbf{G}(\xi) = \sum_{i=1}^{n} N_{i,p}(\xi)\mathbf{p}_i$$

- Examples:

$$\mathbf{G} : [0, 1] \mapsto [a, b] \subset \mathbb{R} \qquad \text{(linear mapping)}$$

$$\mathbf{G} : [0, 1] \mapsto \text{curve in } \mathbb{R}^2 \text{ or } \mathbb{R}^3 \qquad \text{(work in progress)}$$

Ansatz spaces

- Construct ansatz space from B-spline basis functions

$$V_h(\Omega_0, p, \Xi, \mathbf{G}) = \mathsf{span}\{\varphi_i(x) = N_{i,p} \circ \mathbf{G}^{-1}(x)\}$$

- Approximate the solution the standard way

$$u(x) \approx u_h(x) = \sum_{i=1}^{n} \varphi_i(x) u_i, \quad x \in \Omega$$

- Approximate fluxes by Fletcher's group formulation, e.g.,

$$v(x)u(x) \approx (vu)_h(x) = \sum_{i=1}^{n} \varphi_i(x)(v_i u_i), \quad x \in \Omega$$

Properties of B-splines

- Derivative of p^{th} order B-spline is a B-spline of order $p-1$

$$N'_{i,p}(\xi) = \frac{p}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) - \frac{p}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)$$

- B-splines form a partition of unity. That is, for all $\xi \in [a, b]$

$$\sum_{i=1}^{n} N_{i,p}(\xi) = 1 \quad \Rightarrow \quad \sum_{i=1}^{n} N'_{i,p}(\xi) = 0$$

AFC-1: Edge-wise flux decomposition

$$c_{ij} = \int_a^b \varphi_i \varphi'_j \, dx, \quad \sum_{j=1}^{n} c_{ij} = 0 \quad \Rightarrow \quad \sum_{j=1}^{n} c_{ij} u_j = \sum_{j \neq i} c_{ij}(u_j - u_i)$$

Properties of B-splines, cont'd

- B-splines of order p have compact support

$$\text{supp } N_{i,p}(\xi) = [\xi_i, \xi_{i+p+1}), \quad i = 1, \dots, n$$

- B-splines are strictly positive over the interior of their support

$$N_{i,p}(\xi) > 0 \quad \text{for } \xi \in (\xi_i, \xi_{i+p+1}), \quad i = 1, \dots, n$$

AFC-2: positive consistent and lumped mass matrices

$$m_{ij} = \int_a^b \varphi_i \varphi_j \, dx > 0 \quad \Rightarrow \quad m_i = \sum_{j=1}^{n} m_{ij} > 0$$

Constrained data projection

Find $u \in L^2([a,b])$ s.t. $\int_a^b w(u-f)dx = 0 \quad \forall w \in L^2([a,b])$

Consistent L_2-projection

$$\sum_{j=1}^{n} m_{ij} u_j^H = \int_a^b \varphi_i f \, dx$$

Lumped L_2-projection

$$m_i u_i^L = \int_a^b \varphi_i f \, dx$$

Constrained L_2-projection [5]

$$u_i^\star = u_i^L + \frac{1}{m_i} \sum_{j \neq i} \alpha_{ij} f_{ij}^H, \quad 0 \leq \alpha_{ij} = \alpha_{ji} \leq 1, \quad f_{ji}^H = -f_{ij}^H$$

Symmetric flux limiting algorithm [5]

1. Prelimited raw antidiffusive fluxes

$$f_{ij}^H = \begin{cases} m_{ij}(u_i^H - u_j^H), & \text{if } (u_i^H - u_j^H)(u_i^L - u_j^L) > 0 \\ 0, & \text{otherwise (!)} \end{cases}$$

2. Bounds and antidiffusive increments

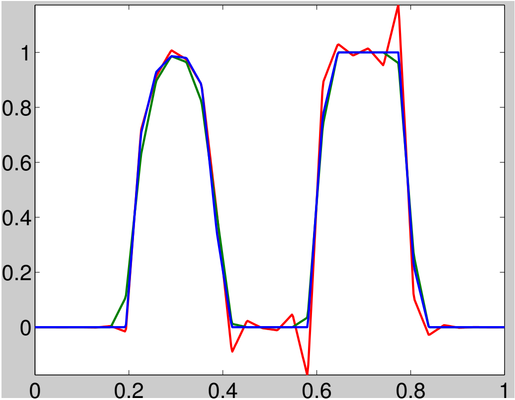
$$Q_i^\pm = \max_{j \neq i}\min (0, u_i^L - u_j^L), \qquad P_i^\pm = \max_{j \neq i}\min (0, f_{ij})$$

3. Nodal and edge-wise limiting coefficients

$$R_i^\pm = \frac{m_i Q_i^\pm}{P_i^\pm}, \qquad \alpha_{ij} = \begin{cases} \min(R_i^+, R_j^-), & \text{if } f_{ij} > 0 \\ \min(R_j^+, R_i^-), & \text{if } f_{ij} < 0 \end{cases}$$

Test case: Semi-ellipse of McDonald

$p = 1, \, n = 32$



L_1-/L_2-errors

$||u^H - u||_1 = 0.0653$

$||u^L - u||_1 = 0.0684$

$||u^\star - u||_1 = 0.0606$

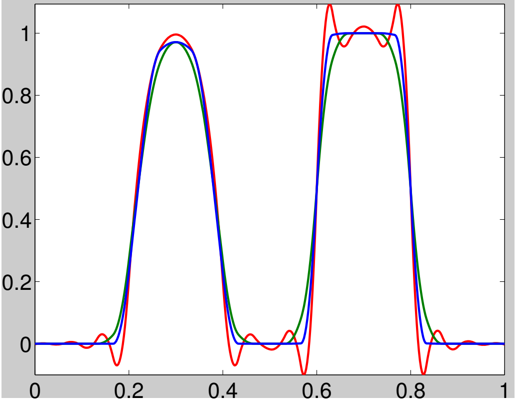
$||u^H - u||_2 = 0.1774$

$||u^L - u||_2 = 0.1686$

$||u^\star - u||_2 = 0.1677$

Test case: semi-ellipse of McDonald

$p = 2,\ n = 32$



L_1-/L_2-errors

$||u^H - u||_1 = 0.0351$

$||u^L - u||_1 = 0.0568$

$||u^\star - u||_1 = 0.0352$

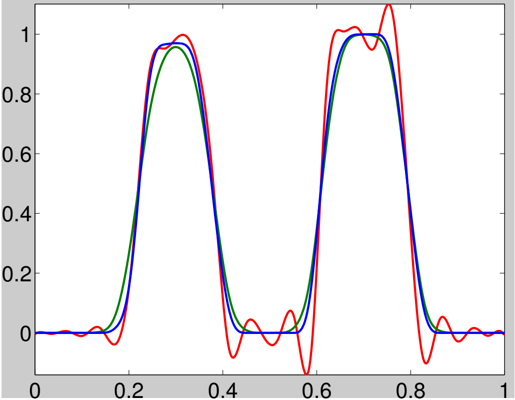
$||u^H - u||_2 = 0.0748$

$||u^L - u||_2 = 0.1121$

$||u^\star - u||_2 = 0.0892$

Test case: semi-ellipse of McDonald

$p = 3,\ n = 32$



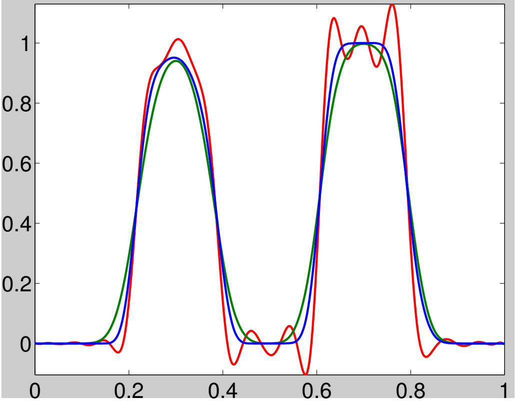
L_1-/L_2-errors

$$||u^H - u||_1 = 0.0595$$
$$||u^L - u||_1 = 0.0788$$
$$||u^\star - u||_1 = 0.0615$$

$$||u^H - u||_2 = 0.1213$$
$$||u^L - u||_2 = 0.1435$$
$$||u^\star - u||_2 = 0.1317$$

Test case: semi-ellipse of McDonald

$p = 4, \; n = 32$



L_1-/L_2-errors

$||u^H - u||_1 = 0.0480$

$||u^L - u||_1 = 0.0896$

$||u^\star - u||_1 = 0.0608$

$||u^H - u||_2 = 0.1014$

$||u^L - u||_2 = 0.1505$

$||u^\star - u||_2 = 0.1252$

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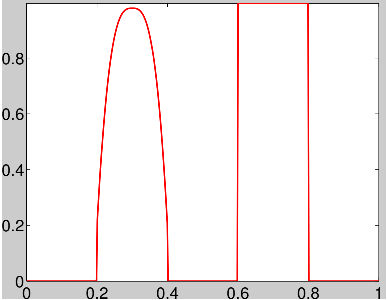
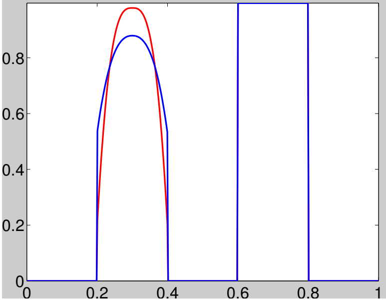
Thought experiment: What are ideal knots?



Thought experiment: What are ideal knots?



L_1-/L_2-errors

$$||u^H - u||_1 = 0.0037$$
$$||u^\star - u||_1 = 0.0220$$

$$||u^H - u||_2 = 0.0091$$
$$||u^\star - u||_2 = 0.0615$$

- Deduce ideal knots from nodal correction factors or residual

$$\Xi = (0,0,0,0,0.1,0.2,0.2,0.2,0.2,0.3,0.4,0.4,0.4,0.4,0.5,\\ 0.6,0.6,0.6,0.6,0.7,0.7,0.7,0.8,0.8,0.8,0.8,0.9,1,1,1,1)$$

- Use smoothness indicator [8] to avoid peak clipping.

Constrained transport

Find $u \in H^1_D([a,b])$ s.t. $\int_a^b w(vu)_x + dw_x u_x dx = 0 \quad \forall w \in H^1_0([a,b])$

Galerkin scheme

$$\sum_{j=1}^{n} (k_{ij} + s_{ij}) u_j^H = 0$$

Discrete upwind scheme

$$\sum_{j=1}^{n} (k_{ij} + d_{ij} + s_{ij}) u_j^L = 0$$

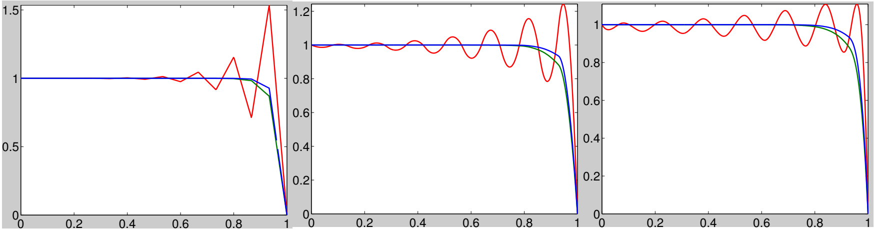
$$k_{ij} = v_j \int_a^b \varphi_i \varphi_j' dx, \quad s_{ij} = d \int_a^b \varphi_i' \varphi_j' dx, \quad d_{ij} = -\max(k_{ij}, 0, k_{ji})$$

High-resolution TVD-type scheme [11]

$$\sum_{j=1}^{n} (k_{ij} + d_{ij} + s_{ij}) u_j^\star + \sum_{j \neq i} \alpha_{ij} f_{ij} = 0, \quad f_{ji} = -f_{ij}$$

Test case: steady convection-diffusion $\frac{v}{d} = 100$

$p = 1,\ n = 16$ | $p = 2,\ n = 16$ | $p = 3,\ n = 16$



$||u^H - u||_1 = 0.0325$ | $||u^H - u||_1 = 0.0415$ | $||u^H - u||_1 = 0.0365$

$||u^L - u||_1 = 0.0056$ | $||u^L - u||_1 = 0.0061$ | $||u^L - u||_1 = 0.0059$

$||u^\star - u||_1 = 0.0028$ | $||u^\star - u||_1 = 0.0031$ | $||u^\star - u||_1 = 0.0029$

Summary

- Algebraic flux correction concept has been generalized to higher-order approximations based on B-spline bases
- Original lowest-order approximation is naturally included
- Nodal correction factors/residual provide information to locally reduce 'inter-element' continuity by increasing knot multiplicity
- Peak clipping at smooth extrema is prevented by locally deactivating the flux limiter using the smoothness indicator [8]

Current and future research

- Analysis for general geometric mappings $\mathbf{G} : \Omega_0 \mapsto \Omega$
- Extension to multi-dimensions by tensor-product construction

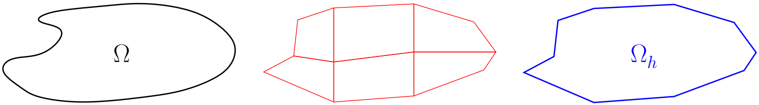
$$\mathbf{G}(\xi, \eta, \zeta) = \sum_{i=1}^{n} \sum_{j=1}^{m} \sum_{k=1}^{l} N_{i,p}(\xi) N_{j,q}(\eta) N_{k,r}(\zeta) \mathbf{p}_{ijk}$$

- Embed local B-spline based AFC-scheme into global outer Galerkin method with unstructured quad/hexa macro mesh
- Exploit potential of fully structured data per macro element

- A. Jaeschke (COSSE-MSc), S-R. Janssen (DD: AM-LR)

Outlook: Isogeometric Analysis [1]

- Poor approximation of curved boundaries (with low-order FEs)



- IgA approach adopts the same (hierarchical) B-spline, NURBS, etc. basis functions for the approximate solution $u_h \approx u$ and for *exactly* representing the geometry $\Omega_h = \Omega$

Our activities in IgA:

- bi-weekly PhD-seminar (participants from LR)
- PhD-candidate in CSC-15 and/or EU-project (?)

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