# Algebraic flux correction schemes for B-spline based finite elements

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# Outline

#### 1 Motivation

#### 2 Mathematical building blocks

Introduction to isogeometric analysis Principles of Algebraic Flux Correction

#### **3** Applications

Constrained data projection Constrained transport Human brain development

### 4 Outlook

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# Vision

Unified simulation and design optimization toolkit

#### Multi-physics simulation

- complex coupled processes
- different models and scales
- different discretizations
- different resolutions

Multi-objective optimization

- (mutually excluding) goals
- adjoint based-optimization
- derivative-free methods
- hierarchical optimization

#### Commonalities

- one common multi-component master geometry
- amount of data requires parallel/distributed computing
- problem complexity requires HPC programming techniques







# Multiple problems, one master geometry



full scale optimization needs de-featuring

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# Axial turbine blade geometry generation<sup>1</sup>



<sup>1</sup>T. Verstraete. "CADO: a Computer Aided Design and Optimization Tool for Turbomachinery Applications". In: *Proc. of the 2nd International Conference on Engineering Optimization*. 2010.

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# Axial turbine blade geometry generation<sup>1</sup>



- direct control of parameters in k-dimensional design space
- moderate number of design parameters in optimization procedure

<sup>1</sup>T. Verstraete. "CADO: a Computer Aided Design and Optimization Tool for Turbomachinery Applications". In: *Proc. of the 2nd International Conference on Engineering Optimization*. 2010.

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### **Isogeometric Analysis** The solution to all our problems?

Vision of the inventors<sup>2</sup>: Full CAD-CAE integration

- Create analysis-suitable geometry in CAD tool (using NURBS, B-splines, T-splines, hierarchical splines, ...)
- 2 Apply established FEA-tools using the same spline basis functions as test and trial functions in the variational form
- Series Perform automatic design optimization on the control points of the CAD geometry or, at best, in the design parameter space

<sup>2</sup>T.J.R. Hughes, J.A. Cottrell, and Y. Bazilevs. "Isogeometric Analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement". In: *Computer Methods in Applied Mechanics and Engineering* 194 (2005), pp. 4135–4195.

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# **Isogeometric Analysis**

A practical solution to some problems.

After 10 years of practical experience ...

- solid theoretical basis has been established
- succesfull application in fluid and solid mechanics, FSI, ...
- early-adoption in open-source and commercial codes (LSDYNA)

However, ...

- (manual) post-processing of CAD geometries is still required
- assembly of system matrices is more costly than in standard FEA
- global higher continuity in multi-patch scenario is challenging
- very little research pursued on efficient solution techniques
- even less research pursued on IgA for compressible flows

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# Isogeometric Analysis

A promising concept with large research potential!

IgA for convection-dominated and compressible flows

- algebraic stabilization methods based on matrix manipulations
- efficient assembly based on Fletcher's group formulation
- positivity-preserving time-stepping methods, e.g., SSP-RK

Efficient solution techniques

- outer discontinuous Galerkin multi-patch approach
- multi-level iterative solution algorithms

Heterogeneous HPC

- optimized single-patch compute-kernels for different platforms
- exploit compute-intensity and tensor-product construction of IgA

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### Spline space $\mathcal{S}(\Omega_0, p, \mathcal{M}, \mathcal{P})$

• Polynomial space of degree p over interval  $\Omega_0 := [a, b] \subset \mathbb{R}$ 

$$\Pi^{p}([a,b]) := \{q(x) \in \mathcal{C}^{\infty}([a,b]) : q(x) = \sum_{i=0}^{p} c_{i} x^{i}, c_{i} \in \mathbb{R}\}$$

• Polynomial spline of degree p defined as  $s : \Omega_0 \mapsto \mathbb{R}$  if

$$s|_{[x_i, x_{i+1}]} \in \Pi^p([x_i, x_{i+1}]), \quad i = 1, \dots, k$$
$$\frac{d^j}{dx^j} s_{j-1}(x_i) = \frac{d^j}{dx^j} s_i(x_i), \quad i = 2, \dots, k, \ j = 0, \dots, p - m_i$$

for partition  $\mathcal{P} := \{a = x_1 < \cdots < x_{p+1} = b\}$  of the interval  $\Omega_0$ and a set of positive integers  $\mathcal{M} := \{1 \le m_i \le p+1\}$ 

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# **B-splines**

• Knot vector is sequence of non-decreasing coordinates  $\xi_i \in [a,b] \subset \mathbb{R}$  in the parameter space  $\Omega_0 = [a,b]$ 

 $\Xi = (\xi_1, \xi_2, \dots, \xi_{n+p+1}), \quad \text{where} \quad$ 

- $\xi_i \in \mathbb{R}$  is the  $i^{\text{th}}$  knot with knot index i
- p is the polynomial order of the B-splines
- *n* is the number of B-spline functions
- Open knot vector for  $(\Omega_0, p, \mathcal{P}, \mathcal{M})$  is defined as

$$\Xi = (\underbrace{a, \dots, a}_{p+1 \text{ times}}, \dots, \underbrace{x_i, \dots, x_i}_{m_i \text{ times}}, \dots, \xi_n, \underbrace{b, \dots, b}_{p+1 \text{ times}})$$

### B-splines, cont'd

• **B-splines** of order p yield a basis of the spline space

$$\mathcal{S}(\Omega_0, p, \mathcal{M}, \mathcal{P}) = \mathcal{S}(\Xi, p) := \operatorname{span}\{N_{i,p}(\xi), i = 1, \dots, n\}$$

Cox-de Boor recursion formula

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

with ,, 
$$\frac{0}{0} := 0$$

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# B-splines, cont'd

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• **Derivative** of B-spline of order p is a B-spline of order p-1

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

• Expression for  $\mathbf{k}^{\mathrm{th}}$  derivative of B-spline of order p

$$\frac{d^k}{d^k\xi} N_{i,p}(\xi) = \frac{p!}{(p-k)!} \sum_{j=0}^k \alpha_{k,j} N_{i+j,p-k}(\xi)$$

with recursively defined coefficients  $\alpha_{k,j}^{3}$ 

<sup>3</sup>L. Piegl and W. Tiller. *The NURBS book*. Second edition. Springer, 1997. **TUDelft** 

# Nonuniform continuity at element boundaries

 $4^{th}$ -order B-spline functions



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# Nonuniform continuity at element boundaries

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



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### **Properties of B-splines**

• B-splines form a partition of unity

For each 
$$\xi \in [a, b]$$
:  $\sum_{i=1}^{n} N_{i,p}(\xi) = 1 \implies \sum_{i=1}^{n} N'_{i,p}(\xi) = 0$ 

B-splines of order p have compact support

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

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

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



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# **Knot insertion**



Equivalent to classical h-refinement for knot insertion with  $m_{\rm new} = p$ 

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# Knot insertion, cont'd



Enables continuity reduction(!) for knot insertion with  $m_{\text{new}} > p$ 

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# Order elevation



No negative values as with Lagrange basis functions for  $p \ge 2$ 

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# **B-spline curves**

• **B-spline curves**: geometric mapping  $\mathbf{G}: \Omega_0 \mapsto \Omega$ 

 $\mathbf{G}(\xi) = \sum_{i=1}^{n} N_{i,p}(\xi) \mathbf{p}_i$  with control points  $\mathbf{p}_i \in \mathbb{R}^d, d \ge 1$ 



• **B-spline surfaces:** geometric mapping  $\mathbf{G}: \Omega_0 \mapsto \Omega$ 

$$\mathbf{G}(\xi) = \sum_{i=1}^n N_{i,p}(\xi) \mathbf{p}_i$$
 with control points  $\mathbf{p}_i \in \mathbb{R}^d, d \geq 1$ 

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# **B-spline surfaces**

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• Multi-variate B-spline basis for  $\Omega_0 = [a,b] \times [c,d]$ 

$$\mathcal{S}(\Xi,\mathcal{H},p,q) = \operatorname{span}\{N_{i,p}(\xi)N_{j,q}(\eta), i = 1..n, j = 1..m\}$$

• Geometric mapping  $\mathbf{G}:\Omega_0\mapsto\Omega$ 

$$\mathbf{G}(\xi,\eta) = \sum_{i=1}^{n} \sum_{j=1}^{m} N_{i,p}(\xi) N_{j,q}(\eta) \mathbf{p}_{ij}, \quad \mathbf{p}_{ij} \in \mathbb{R}^{d}, d \ge 2$$

• Global basis functions (e.g., line-wise numbering)

$$N_a(\xi, \eta) = N_{i,p}(\xi)N_{j,q}(\eta), \quad a = n(j-1) + i$$

• Canonical generalization to higher dimensions including partition of unity, local support and strict positivity property

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# Multi-patch B-spline surfaces



- Possibility for different p/q and n/m-values per patch
- Use, e.g., Z-ordering for improved locality of DoFs
- Consider only single-patch domains in this talk

#### 

### Ansatz spaces

• Construct ansatz space from B-spline basis functions

$$V_h = \operatorname{span} \{ \varphi_a(\mathbf{x}) = N_a \circ \mathbf{G}^{-1}(\mathbf{x}), \, \mathbf{x} \in \Omega \}$$

Approximate the solution the standard way

$$u(\mathbf{x},t) \approx u_h = \sum_{a=1}^N \varphi_a(\mathbf{x}) u_a(t)$$

Approximate fluxes by Fletcher's group formulation

$$f(u(\mathbf{x},t)) \approx f_h = \sum_{a=1}^N \varphi_a(\mathbf{x}) f_a(t), \quad f_a(t) = f(u_a)$$

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### **Principles of Algebraic Flux Correction**

- Discrete diffusion operators  $^4$  are symmetric  $N\times N$  matrices with zero row and column sums

$$D = \{d_{ab}\}, \quad d_{ab} = d_{ba}, \quad d_{aa} := -\sum_{b \neq a} d_{ab}$$

Decomposition into edge-contributions

$$[Du]_a = \sum_b d_{ab}u_b = d_{aa}u_a + \sum_{b \neq a} d_{ab}u_b = \sum_{b \neq a} f_{ab}$$
$$[Du]_b = \sum_{a \neq b} f_{ba}, \quad f_{ba} = -f_{ab}, \quad f_{ab} = d_{ab}(u_b - u_a)$$

#### <sup>4</sup>KT2002.

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### Row-sum mass lumping

Consistent mass matrix

$$M = \{m_{ab}\}, \qquad m_{ab} = \int_{\Omega} \varphi_a(\mathbf{x}) \varphi_b(\mathbf{x}) d\mathbf{x}$$

Row-sum lumped mass matrix

$$M_l := \mathsf{diag}(m_a), \qquad m_a = \sum_b m_{ab}$$

• Discrete mass diffusion operator

$$D = M - M_l, \qquad d_{ab} = m_{ab}, \quad d_{aa} := -\sum_{b \neq a} m_{ab}$$

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# Principles of Algebraic Flux Correction, cont'd

• Generic discrete system (strong imposition of bc's)

$$\begin{bmatrix} A_{\Omega} & A_{\Gamma} \\ 0 & I \end{bmatrix} \begin{bmatrix} u_{\Omega} \\ u_{\Gamma} \end{bmatrix} = \begin{bmatrix} B_{\Omega} & B_{\Gamma} \\ 0 & I \end{bmatrix} \begin{bmatrix} g_{\Omega} \\ g_{\Gamma} \end{bmatrix}$$

with matrix coefficients

$$a_{aa} > 0, \forall a \quad a_{ab} \le 0, \forall a, b \ne a \quad b_{ab} \ge 0, \forall a, b$$
 (1)

Local discrete maximum principle (proof<sup>5</sup>)

$$(\ref{eq:ab}) \wedge \sum_{b} a_{ab} = \sum_{b} b_{ab} \quad \Rightarrow \quad u_a^{\min} \le u_a \le u_a^{\max}$$

#### <sup>5</sup>K2012a.

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# Principles of Algebraic Flux Correction, cont'd

• Generic discrete system as before with matrix coefficients

$$a_{aa} > 0, \forall a \quad a_{ab} \le 0, \forall a, b \ne a \quad b_{ab} \ge 0, \forall a, b$$
 (2)

and strictly or irreducibly diagonally dominant matrix A. (3)

Then A is an **M-Matrix**, i.e.  $A^{-1} \ge 0$ .

• Global discrete maximum principle (proofs<sup>6</sup>)

$$(\ref{eq:ab}) \land (3) \land \sum_{b} a_{ab} = \sum_{b} b_{ab}, \forall a \quad \Rightarrow \quad \min g \le u \le \max g$$

#### <sup>6</sup>K2012a.

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Constrained data projection Constrained transport Human brain development

### 4 Outlook



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# Constrained data projection<sup>7</sup>

• High-order predictor: consistent L<sub>2</sub>-projections

$$\sum_{b} m_{ab} u_b^H = \int_{\Omega} \varphi_a f \, d\mathbf{x}$$

• Low-order predictor: lumped L<sub>2</sub>-projections

$$m_a u_a^L = \int_\Omega \varphi_a f \, d\mathbf{x}$$

• Prelimited raw antidiffusive flux  $(f_{ba} = -f_{ab})$ 

$$f_{ab} = \begin{cases} m_{ab}(u_a^H - u_b^H), & \text{if } (u_a^H - u_b^H)(u_a^L - u_b^L) > 0 \\ 0, & \text{otherwise} \end{cases}$$

<sup>7</sup>D. Kuzmin et al. "Failsafe flux limiting and constrained data projections for equations of gas dynamics". In: Journal of Computational Physics 229.23 (2010), pp. 8766-8779. ISSN: 0021-9991. DOI: http://dx.doi.org/10.1016/j.jcp.2010.08.009. URL: http://www.sciencedirect.com/science/article/pii/S0021999110004468. **TUDelft** 

# Constrained data projection, cont'd

• Bounds and antidiffusive increments

$$Q_a^{\pm} = \max_{\substack{b \neq a}}^{\max} (0, u_a^L - u_b^L), \qquad P_a^{\pm} = \sum_{b \neq a} \max_{\min} (0, f_{ab})$$

Nodal and edge-wise limiting coefficients

$$R_{a}^{\pm} = \frac{m_{a}Q_{a}^{\pm}}{P_{a}^{\pm}}, \qquad \alpha_{ab} = \begin{cases} \min(R_{a}^{+}, R_{b}^{-}), & \text{if } f_{ab} > 0\\ \min(R_{b}^{+}, R_{a}^{-}), & \text{if } f_{ab} < 0 \end{cases}$$

• Corrector: constrained L<sub>2</sub>-projection

$$u_a^{\star} = u_a^L + \frac{1}{m_a} \sum_{b \neq a} \alpha_{ab} f_{ab}, \quad 0 \le \alpha_{ab} = \alpha_{ba} \le 1$$



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### Test case: Semi-ellipse of McDonald

p = 1, n = 32 $L_1$ -/ $L_2$ -errors  $||u^H - u||_1 = 0.0653$ 0.8  $||u^L - u||_1 = 0.0684$ 0.6  $||u^{\star} - u||_1 = 0.0606$ 0.4 0.2  $||u^H - u||_2 = 0.1774$  $||u^L - u||_2 = 0.1686$ 0  $||u^{\star} - u||_2 = 0.1677$ 0.2 0.4 0.6 0.8 0

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### Test case: semi-ellipse of McDonald



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### Test case: semi-ellipse of McDonald



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### Test case: semi-ellipse of McDonald



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# Thought experiment: What are ideal knots?



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# Thought experiment: What are ideal knots?



Deduce ideal knots from nodal correction factors or residual

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

• Smoothness indicator is used to avoid peak clipping.

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### **Constrained transport**

Stationary convection-diffusion equation

$$\begin{aligned} \nabla \cdot (\mathbf{v} u) - d\Delta u &= 0 \quad \text{in } \Omega \\ u &= g \quad \text{on } \Gamma_D \\ \nabla u \cdot \mathbf{n} &= 0 \quad \text{on } \Gamma_N \end{aligned}$$

• High-order Galerkin scheme:  $(K+S)u^H = 0$ 

$$K = \{ \mathbf{v}_b \cdot \int_{\Omega} \varphi_a \nabla \varphi_b \, d\mathbf{x} \}, \quad S = \{ d \int_{\Omega} \nabla \varphi_a \cdot \nabla \varphi_b \, d\mathbf{x} \}$$

• Low-order scheme:  $(K + D + S)u^L = 0$ 

$$D = \{d_{ab}\}, \quad d_{ab} := -\max\{k_{ab}, 0, k_{ba}\}$$

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### Constrained transport, cont'd

- High-resolution scheme:  $(K + D + S)u^* + \lim(-Du) = 0$
- Raw antidiffusive flux  $f_{ab} = d_{ab}(u_b u_a) = -f_{ba}$
- Bounds and antidiffusive increments

$$Q_{a/b}^{\pm} = \sum_{b \neq a} \max_{\min} (0, -/+f_{ab}), \qquad P_a^{\pm} = \sum_{b \neq a} \max_{\min} (0, f_{ab})$$

Nodal and edge-wise limiting coefficients

$$R_a^{\pm} = \min\{1, \frac{Q_a^{\pm}}{P_a^{\pm}}\}, \qquad \alpha_{ab} = \begin{cases} R_a^+, & \text{if } f_{ab} > 0\\ R_a^-, & \text{if } f_{ab} < 0 \end{cases}$$



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



 $||u^{H} - u||_{1} = 0.0325$   $||u^{H} - u||_{1} = 0.0415$   $||u^{H} - u||_{1} = 0.0365$  $||u^{L} - u||_{1} = 0.0056$   $||u^{L} - u||_{1} = 0.0061$   $||u^{L} - u||_{1} = 0.0059$  $||u^{\star} - u||_{1} = 0.0028$   $||u^{\star} - u||_{1} = 0.0031$   $||u^{\star} - u||_{1} = 0.0029$ 

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### Test case: convection-diffusion

- Configuration:  $\Omega = (0, 1)^2$ , d = 0.001,  $\mathbf{v} = \frac{1}{\sqrt{2}}(1, 1)^\top$  MSc-project by Andrzej Jaeschke using <u>GfSMO</u>, (JKU, Linz)



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### Test case: convection-diffusion

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### Test case: convection-diffusion

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### Human brain development<sup>8</sup>

• Gray-Scott reaction-diffusion model

$$\begin{aligned} \partial_t u + u \partial_t \log \sqrt{g_t} - d_1 \Delta_{\mathcal{M}_t} u &= f(1-u) - uv^2 \qquad \text{(inhibitor u)}\\ \partial_t v + v \partial_t \log \sqrt{g_t} - d_2 \Delta_{\mathcal{M}_t} v &= uv^2 - (f+k)v \qquad \text{(activator v)} \end{aligned}$$

with determinant  $\sqrt{g_t}$  of the surface parameterization

Surface evolution model (morphogen-driven evolution)

$$\partial_t \mathcal{M} = h(u, v)\mathbf{n},$$
 e.g.,  $h(u, v) = Kv$ 

MSc-project by Jochen Hinz using Nutils (TU/e)

<sup>8</sup>J. Lefèvre and J.-F. Mangin. "A Reaction-Diffusion Model of Human Brain Development". In: *PLoS Computational Biology* 6.4 (2009).

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# 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<sup>9</sup>

<sup>9</sup>D. Kuzmin and F. Schieweck. "A parameter-free smoothness indicator for high-resolution finite element schemes". In: *Central European Journal of Mathematics* 11.8 (2013), pp. 1478–1488.

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### Current and future research

- Theoretical analysis of AFC principles for
  - arbitrary geometric mappings, NURBS basis functions, and
  - weakly imposed boundary conditions/multi-patch coupling
- Realization of more schemes of the AFC-type family
  - transport with highly anisotropic diffusion
- Implementation of an HPC IgA-framework in C++-11
  - exploit compute-intensity of high-order methods
  - accelerator support via expression templates for assembly
  - on-demand target-optimized compilation at run time

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