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

Numerical Analysis group

Matthias Möller  m.moller@tudelft.nl

7th DIAM onderwijs- en onderzoeksdag, 5th November 2014
Outline

1 Motivation
   Finite elements in a nutshell

2 Introduction to B-splines
   Knot insertion ($h$-refinement)
   Order elevation ($p$-refinement)
   Geometric mapping
   Definition of ansatz spaces
   Properties of B-splines

3 Constrained data projection
   Numerical examples

4 Constrained transport
   Numerical examples
Finite elements in a nutshell

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

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

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

\[
\int_{\Omega} w[\mathcal{L}u - f] \, dx = 0 \quad \forall w \in W
\]

- **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

\[ \int_{\Omega_h} \phi_i [L u_h - f] \, dx = 0 \quad \forall i = 1, \ldots, \dim(W_h) \]

- neglecting complications due to bc’s this yields

\[ \sum_j \left[ \int_{\Omega_h} \phi_i L \varphi_j \, dx \right] u_j = \int_{\Omega_h} \phi_i f \, dx \quad \forall i = 1, \ldots, \dim(W_h) \]
Problem

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

$L_2$-projection

convective transport
Problem

- Poor approximation of discontinuities/steep gradients if standard Galerkin methods are used with proper stabilization.
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

- 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 ... ;-) mostly for $P_1$ and $Q_1$ finite elements ;-(

M. Möller (NA group)
AFC for B-Spline based FEM
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** \( \Xi = (\xi_1, \xi_2, \ldots, \xi_{n+p+1}) \) 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 \( i = 1, 2, \ldots, n + p + 1 \)
- \( p \) is the polynomial order of the B-splines
- \( n \) is the number of B-spline functions

**Cox-de Boor recursion formula for** \( N_{i,p} : \Omega_0 \rightarrow \mathbb{R} \)

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

\[
p > 0 : \quad N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi)
\]
Knot insertion ($h$-refinement)

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

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

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

\[ \Xi = (0, 0, 1, 1), \ p = 1 \]

\[ \Xi = (0, 0, 0, 1, 1, 1), \ p = 2 \]

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

4\textsuperscript{th}-order B-spline functions

\[ \Xi = (0, 0, 0, 0, 0, \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3}, 1, 1, 1, 1, 1) \]

\( \Xi \) has discontinuity at \( 0, 0, 0, 0, 0 \), \( C^3 \) continuity at \( \frac{1}{3}, \frac{2}{3}, \frac{2}{3}, \frac{2}{3} \), and discontinuity at \( 1, 1, 1, 1, 1 \).
Nonuniform continuity at element boundaries

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

$$\Xi = (0, 0, 0, 0, 0, 1/3, 2/3, 2/3, 2/3, 1, 1, 1, 1, 1)$$

- discontinuity
- $C^3$
- $C^1$
- discontinuity
Geometric mapping

- Define mapping between parameter space \( \Omega_0 = [0, 1] \) and the computational domain \( \Omega \) using control points \( p_i \in \mathbb{R}^d, d = 1, 2, 3 \)

\[
G : \Omega_0 \leftrightarrow \Omega, \quad G(\xi) = \sum_{i=1}^{n} N_{i,p}(\xi)p_i
\]

- Examples:

\[
G : [0, 1] \leftrightarrow [a, b] \subset \mathbb{R} \quad \text{(linear mapping)}
\]

\[
G : [0, 1] \leftrightarrow \text{curve in } \mathbb{R}^2 \text{ or } \mathbb{R}^3 \quad \text{(work in progress)}
\]
Ansatz spaces

- Construct ansatz space from B-spline basis functions

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

- 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.,

\[ v(x)u(x) \approx (vu)_h(x) = \sum_{i=1}^{n} \varphi_i(x)(v_iu_i), \quad x \in \Omega \]
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

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

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

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

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]**

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

\[ Q_{i}^\pm = \max_{j \neq i} \min(0, u_i^L - u_j^L), \quad P_{i}^\pm = \max_{j \neq i} \min(0, f_{ij}) \]

3. Nodal and edge-wise limiting coefficients

\[ R_{i}^\pm = \frac{m_{i} Q_{i}^\pm}{P_{i}^\pm}, \quad \alpha_{ij} = \begin{cases} 
  \min(R_i^+, R_j^-), & \text{if } f_{ij} > 0 \\
  \min(R_j^+, R_i^-), & \text{if } f_{ij} < 0 
\end{cases} \]
Test case: Semi-ellipse of McDonald

\[ p = 1, \ n = 32 \]

\[ ||u^H - u||_1 = 0.0653 \]
\[ ||u^L - u||_1 = 0.0684 \]
\[ ||u^* - u||_1 = 0.0606 \]

\[ ||u^H - u||_2 = 0.1774 \]
\[ ||u^L - u||_2 = 0.1686 \]
\[ ||u^* - u||_2 = 0.1677 \]
Test case: semi-ellipse of McDonald

\[ p = 2, \ n = 32 \]

\[ L_1-/L_2\text{-errors} \]

\[
\begin{align*}
| |u^H - u||_1 &= 0.0351 \\
| |u^L - u||_1 &= 0.0568 \\
| |u^* - u||_1 &= 0.0352 \\
| |u^H - u||_2 &= 0.0748 \\
| |u^L - u||_2 &= 0.1121 \\
| |u^* - u||_2 &= 0.0892
\end{align*}
\]
Test case: semi-ellipse of McDonald

\[ p = 3, \ n = 32 \]
Test case: semi-ellipse of McDonald

\[ p = 4, \quad n = 32 \]

\[ \begin{align*}
    \| u^H - u \|_1 & = 0.0480 \\
    \| u^L - u \|_1 & = 0.0896 \\
    \| u^* - u \|_1 & = 0.0608 \\
    \| u^H - u \|_2 & = 0.1014 \\
    \| u^L - u \|_2 & = 0.1505 \\
    \| u^* - u \|_2 & = 0.1252
\end{align*} \]
Thought experiment: What are ideal knots?

\begin{figure}
\centering
\includegraphics[width=\textwidth]{knot_graph.png}
\end{figure}

• Deduce ideal knots from nodal correction factors or residual $\Xi = (0, 0, 0, 0, 0.1, 0.2, 0.2, 0.2, 0.2, 0.3, 1, 1, 1)$. 
• Use smoothness indicator [8] to avoid peak clipping.
Thought experiment: What are ideal knots?

### $L_1$-$L_2$-errors

\[
\begin{align*}
\|u^H - u\|_1 &= 0.0037 \\
\|u^* - u\|_1 &= 0.0220 \\
\|u^H - u\|_2 &= 0.0091 \\
\|u^* - u\|_2 &= 0.0615
\end{align*}
\]

- Deduce ideal knots from nodal correction factors or residual
  \[\Xi = (0, 0, 0, 0, 0.1, 0.2, 0.2, 0.2, 0.3, 0.4, 0.4, 0.4, 0.4, 0.5, 0.6, 0.6, 0.6, 0.6, 0.7, 0.7, 0.7, 0.8, 0.8, 0.8, 0.8, 0.9, 1, 1, 1, 1)\]

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

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

Galerkin scheme

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

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

Discrete upwind scheme

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

High-resolution TVD-type scheme [11]

$$\sum_{j=1}^{n} (k_{ij} + d_{ij} + s_{ij})u^*_j + \sum_{j \neq i} \alpha_{ij}f_{ij} = 0, \quad f_{ji} = -f_{ij}$$
Test case: steady convection-diffusion $\frac{v}{d} = 100$

$p = 1, n = 16$

$p = 2, n = 16$

$p = 3, n = 16$

$\| u^H - u \|_1 = 0.0325$

$\| u^L - u \|_1 = 0.0056$

$\| u^* - u \|_1 = 0.0028$

$\| u^H - u \|_1 = 0.0415$

$\| u^L - u \|_1 = 0.0061$

$\| u^* - u \|_1 = 0.0031$

$\| u^H - u \|_1 = 0.0365$

$\| u^L - u \|_1 = 0.0059$

$\| u^* - u \|_1 = 0.0029$
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 $G : \Omega_0 \mapsto \Omega$
- Extension to multi-dimensions by tensor-product construction

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

- 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)

\[ \Omega \quad \Omega_h \]

- 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 (?)
References I


D. Kuzmin.
Linearity-preserving flux correction and convergence acceleration for constrained Galerkin schemes.

D. Kuzmin and Y. Gorb.
A flux-corrected transport algorithm for handling the close-packing limit in dense suspensions.
References III


D. Kuzmin and F. Schieweck.
A parameter-free smoothness indicator for high-resolution finite element schemes.

D. Kuzmin, M.J. Shashkov, and D. Svyatskiy.
A constrained finite element method satisfying the discrete maximum principle for anisotropic diffusion problems.
*Journal of Computational Physics, 228(9):3448 – 3463, 2009.*

D. Kuzmin and S. Turek.
Flux correction tools for finite elements.
**D. Kuzmin and S. Turek.**
High-resolution FEM-TVD schemes based on a fully multidimensional flux limiter.

**M. Möller.**
Algebraic flux correction for nonconforming finite element discretizations of scalar transport problems.