Computing SIAC spline coefficients

Jörg Peters

October 2, 2014

Abstract

The Discontinuous Galerkin (DG) method applied to hyperbolic differential equations outputs weakly-linked polynomial pieces. Post-processing these pieces by Smoothness-Increasing Accuracy-Conserving (SIAC) convolution with B-splines can improve the accuracy of the output and yield superconvergence. SIAC convolution is considered optimal if the SIAC kernels, in the form of a linear combinations of B-splines of degree $d$, reproduce polynomials of degree $2d$. This paper derives simple formulas for computing the optimal SIAC spline coefficients.

1 Introduction

The Discontinuous Galerkin (DG) method is widely used to solve hyperbolic partial differential equations (PDEs). The lack of continuity between the elements is appropriate for modeling the weak flux constraints between elements and computationally convenient: the discontinuity allows for a flexible discretization of the PDE that locally adjusts the polynomial degree and element spacing, and the discontinuity increases opportunities for parallelism when stepping forward in a simulation. However, except near jump discontinuities, the inter-element discontinuities do not agree with the smoothness of the expected outcome.

Filtering, in particular Smoothness-Increasing Accuracy-Conserving (SIAC) filtering, has been proposed to smoothly connect elements while maintaining the order of the accuracy of the original DG solution. Remarkably, such post-filtering by convolution applied to approximate DG solutions is not only convenient for downstream applications such as stream line tracing [WRKH09], but improves the accuracy of the resulting output as a solution to hyperbolic partial differential
equations. Already Bramble and Schatz [BS77] showed that, for a wide class of elliptic boundary value problems and uniform subdivision of the domain, averaging of the output can yield superconvergence, i.e. a more accurate approximation to the solution than the degree of the elements suggests. Underlying superconvergence is the fact that certain integral norms, called moment norms [ML78] or negative-order norms, converge faster than expected and can bound the error of the convolved output. In the context of linear hyperbolic PDEs this fact was convincingly demonstrated in [CLSS03].

Starting with [CKRS07], a series of papers has generalized SIAC filtering of DG output from the prototypical case of linear equations with periodic boundary conditions over a uniform mesh to non-uniform scenarios and spatial dimensions two and three, including structured and unstructured bivariate and tetrahedral meshes [MJRK11, MKRK13, MRK14].

SIAC filtering was authoritatively reviewed during the 2014 Icosahom conference, notably in the planary talk by Jennifer Ryan. Newest results were presented in the minisymposium on post-processing DG solutions [MR14], organized by Mirzagar and Ryan. Among the recent advances were simple formulas that allow solving for the optimal coefficients of uniform SIAC B-spline filters (note by contrast that [MRK12] used Gaussian quadrature to determine the entries of the corresponding constraint matrix). Since the SIAC approach has been extended to non-uniform meshes, formulas corresponding to the general case of B-splines with non-uniform knot spacing can improve computational efficiency. The following pages develop such formulas.

Section 2 succinctly reviews B-splines, SIAC filtering and convolution to the extent needed for the result. Section 3 derives the entries of the constraint matrix whose solution yields the optimal coefficients for filters that post-process DG solutions with splines over non-uniform knot sequences.

2 Convolution and B-splines

A succinct but comprehensive treatment of B-splines can be found in Carl de Boor’s summary [dB02] (see also [Sch81]). There are a number of ways to derive or define B-splines, for example as the smoothest class of piecewise polynomials over a given support. The subclass of uniform B-splines additionally admits definitions via convolution that are efficiently carried out in Fourier space. That definition is handy when deriving optimal coefficients of uniform SIAC B-spline filters. For
our purpose, a more convenient definition is via divided differences \( \Delta(t_{i:j})h \).

The notation \( i : j \) is short for the sequence \( i, i+1, \ldots, j-1, j \) and \( t_{i:j} \) stands correspondingly for the sequence of real numbers \( t_i, t_{i+1}, \ldots, t_j \). For a sufficiently smooth univariate real-valued function \( h \) with \( k \)th derivative \( h^{(k)} \), divided differences are defined by

\[
\Delta(t_i)h := h(t_i), \quad \text{and for } j > i
\]

\[
\Delta(t_{i:j})h := \begin{cases} 
(\Delta(t_{i+1:j})h - \Delta(t_{i:j-1})h)/(t_j - t_i), & \text{if } t_i \neq t_j, \\
\frac{h^{(j-i)}(t_i)}{(j-i)!}, & \text{if } t_i = t_j.
\end{cases}
\]

(1)

If \( t_{i:j} \) is a non-decreasing sequence, we call its elements \( t_\ell \) knots and define the B-spline with knot sequence \( t_{i:j} \) as

\[
B(x|t_{i:j}) := (t_j - t_i) \Delta(t_{i:j})(\max\{(x - t), 0\})^d,
\]

(2)

where \( \Delta(t_{i:j}) \) acts on the function \( h : t \to (\max\{(t - x), 0\})^d \) for a given \( x \in \mathbb{R} \). A B-spline is a non-negative piecewise polynomial of degree \( d \) with support on the interval \([t_i, t_j]\). If \( \mu \) is the multiplicity of the number \( t_\ell \) in the sequence \( t_{i:j} \), then \( B(x|t_{i:j}) \) is at least \( d - \mu \) times continuously differentiable at \( t_\ell \).

The goal of SIAC filtering is to smooth out the transitions between polynomial pieces on consecutive intervals \( p_j : [t_j..t_{j+1}) \to \mathbb{R}, j = 0..n \) that are output by DG computations and typically do not join continuously. To this end, we convolve the piecewise output with a linear combination of B-splines. The convolution \( f \ast g \) of a function \( f \) with a function \( g \) is defined as

\[
(f \ast g)(x) := \int_\mathbb{R} f(t)g(x-t)dt,
\]

(3)

for every \( x \) where the integral exists. When \( g \geq 0 \) and \( \int_\mathbb{R} g = 1 \) then the convolution has special, desirable properties: if \( f \) is non-negative, (directionally) monotone or convex then so is \( f \ast g \). Moreover, the graph of \( f \ast g \) is in the convex hull of the graph of \( f \). Convolution is commutative, associative and distributive.

For convolving splines with functions \( g := p_j \), we make use of Peano’s formula:

\[
\frac{1}{k!} \int_\mathbb{R} B(t|t_{0:k})g^{(k)}(t)dt = \Delta(t_{0:k})g.
\]

(4)

The authoritative survey [DB05] advertises the symbol \( \Delta \) for divided differences over alternatives such as \([t_{i:j}]h \) or \( h[t_{i:j}] \).
Here \( g^{(k)} \) denotes the \( k \)th derivative of the univariate function \( g \). To be able to interpret Peano’s formula as a convolution formula for monomials, we select \( g \) so that \( g^{(k)}(t) = (k!)(t - x)^{\delta} \). The choice \( g(t) := (k+\delta)^{-1}(t - x)^{k+\delta} \) accomplishes this. Then (4) implies for the alternating monomial \((-\cdot)^{\delta} : t \rightarrow (-t)^{\delta}\),

\[
(B\cdot|t_{0:k}) \ast (-\cdot)^{\delta})(x) = \int_{\mathbb{R}} B(t|t_{0:k})(-(x-t))^{\delta} dt = \frac{1}{k!} \int_{\mathbb{R}} B(t|t_{0:k}) g^{(k)}(t) dt
\]

(5)

\[
= \binom{k+\delta}{k}^{-1} \Delta t_{0:k}(t - x)^{k+\delta}.
\]

(The divided difference in the last expression applies to the variable \( t \). Therefore \( \Delta t_{0:k}(t - x)^{k+\delta} \) does not depend on \( t \), but only on the sequence \( t_{0:k} \).)

3 Optimal convolution coefficients

A spline SIAC convolution kernel \( K : \mathbb{R} \rightarrow \mathbb{R} \) is a piecewise polynomial of degree \( d \). The function \( K \) is considered optimal if

\[
(K \ast (\cdot)^{\delta})(x) = x^{\delta}, \quad \delta = 0, \ldots, 2d,
\]

i.e. if convolution of \( K \) with monomials reproduces the monomials up to the maximal degree \( 2d \). The choice of interest for SIAC convolution on the interval \([t_0..t_{d+1})\) is \( K(x) := \sum_{\gamma=-d}^{d} c_{\gamma} B(x|t_{\gamma:t_{\gamma+d+1}}) \), a spline of degree \( d \) with leftmost knot \( t_{-d} \). To satisfy the polynomial equations (6), we want to determine the coefficients \( c_{-d}, \ldots, c_d \) so that

\[
\left( \sum_{\gamma=-d}^{d} c_{\gamma} B(\cdot|t_{\gamma:t_{\gamma+d+1}}) \ast (-\cdot)^{\delta} \right)(x) = (-x)^{\delta}, \quad \delta = 0, \ldots, 2d.
\]

(6)

Theorem 3.1 The vector of optimal SIAC convolution coefficients \( c := [c_{-d}, \ldots, c_d]^T \in \mathbb{R}^{2d+1} \) is

\[
c := M_0^{-1} e_1, \quad e_i(\delta) := \begin{cases} 1 & \text{if } \delta = i \\ 0 & \text{else} \end{cases}, \quad M_0 := \left[ \Delta t_{\gamma:t_{\gamma+d+1}} t^{d+1+\delta} \right]_{\delta=0:2d,\gamma=-d:d}.
\]

4
The matrix $M_0$ is of size $(2d + 1) \times (2d + 1)$. Its entries $M_0(k, \ell) \in \mathbb{R}$ in row $k$ and column $\ell$ are defined by $\delta = k - 1$ and $\gamma = \ell - d - 1$ and do not depend on $t$, but on $t_{\gamma; \gamma+d+1}$.

**Proof**  

By (5), the system of polynomial equations (6) in $x$ is equivalent to

$$
M(x)c := \left[ \Delta t_{\gamma; \gamma+d+1}(t - x)^{d+1+\delta} \right]_{\delta=0:2d, \gamma = -d:d} = \left( d + 1 + \delta \atop \delta \right) \left[ (-x)^\delta \right]_{\delta=0:2d}.
$$

(6')

Since (6') has to hold for $x = 0$, setting $x = 0$ in (6') yields the following $2d + 1 \times 2d + 1$ system of equations

$$
\left[ \left( d + 1 + \delta \atop \delta \right)^{-1} \Delta t_{\gamma; \gamma+d+1} t^{d+1+\delta} \right]_{\delta=0:2d, \gamma = -d:d} c = e_1.
$$

(7)

Multiplying, for all $\delta = 0 : 2d$, the equation of the system (7) corresponding to $\delta$ with $\left( d + 1 + \delta \atop \delta \right)$ and noting that, by convention, $\left( d + 1 + \delta \atop \delta \right) = 1$ for $\delta = 0$, we can write the system (7) in the simpler equivalent form $M_0 c = e_1$. Using the fact from [dB05, Sect. 8] that the $k$th divided difference is linked to the the $k$th derivative by $\Delta t_{\gamma; \gamma+d+1} t^{d+1+\delta} = (d + 1 + \delta) \cdots (1 + \delta) \xi^\delta_\gamma$, for distinct $\xi_\gamma \in (t_{\gamma}..t_{\gamma+d+1})$, we see that $M_0$ is a Vandermonde matrix, hence invertible. That is $c := M_0^{-1} e_1$ is well-defined.

To show that $c$ solves the polynomial system (6) for all $x$, not just $x = 0$, we define the $2d + 1$ linearly independent functionals $F_k$, $k = 0, \ldots, 2d$. The functional $F_k$ differentiates (each entry of $M(x)$) $k$-times with respect to $x$ and then evaluates at zero. Applying $F_k$ to both sides of (6') yields the system

$$
M_k c = \left( d - k + \delta \atop d + 1 \right) e_{k+1}, \quad M_k(j, :) := \begin{cases} M_0(j - k, :) & \text{if } j > k, \\ 0 & \text{else}. \end{cases}
$$

(6')

(Here $M_k(j, :)$ denotes the $j$th row of the matrix $M_k$.) Since $M_k c = M_k M_0^{-1} e_1 = e_{k+1}$ and $\left( d - k + \delta \atop d + 1 \right) = 1$ for $\delta = k + 1$, we see that the choice $c := M_0^{-1} e_1$ satisfies all $2d + 1$ systems of equations (6'). This implies that the system of polynomial equations (6) is satisfied by $c$.

If the knots are strictly increasing, we can expand the divided differences of polynomials to make the expression for $M_0$ more explicit.

---

2 Mirzaee et al. [MRK12, p.90] state that systems of type (6) are non-singular and refer to the exposition in [CLSS03] for a a proof of existence and uniqueness of the solution. I was unable to spot it there.
Corollary 3.1 (single knots) If, for \(i = -d : 2d\), \(t_i < t_{i+1}\) then

\[
M_0 = \left[ \sum_{\ell=\gamma}^{\gamma+d+1} \frac{(x-x_\ell)^{d+1+\delta}}{\prod_{j=\gamma,j\neq\ell} (x_j-x_\ell)} \right]_{\delta=0:2d,\gamma=-d:d}.
\] (9)

When the knot spacing is uniform, i.e. \(t_{i+1} - t_i = t_i - t_{i-1}\), then it is good to symmetrize the construction about \(t = 0\). That is, we define the knot sequence to be \(\tau := [-d - \sigma : d - \sigma]\), \(\sigma := \frac{d+1}{2}\). For example, for \(d = 1\), \(\tau = [-2, -1, 0]\) and for \(d = 2\), \(\tau = [-3.5, -2.5, -1.5, -0.5, 0.5]\). Then for \(d = 2\), the first knot subsequence is \([-3.5 : 0.5]\) and, symmetrically, the last knot subsequence is \([0.5 : 3.5]\).

Corollary 3.2 (uniform knots) For uniform knots

\[
M_0 = \left[ \frac{1}{(d+1)!} \sum_{\ell=0}^{d+1} (-1)^\ell \gamma^\ell (\gamma + \ell)^{d+1+\delta} \right]_{\delta=0:2d,\gamma\in\tau}.
\] (10)

For comparison, Mirzagar [MR14] characterizes the symmetric SIAC kernel coefficients by the relations \(\tilde{M}(x)c = [x^\delta]_{\delta=0:2d}\), where

\[
\tilde{M}(x) := \left[ \sum_{\ell=0}^{\delta} (-1)^\ell \gamma^\ell (\delta^\ell)(B(\cdot | 0 : 2d) * (\cdot)^{\delta-\ell})(x) \right]_{\delta=0:2d,\gamma=-d:d}.
\] (11)

The explicit form (10) makes it easy to confirm a conjecture by Kirby and Ryan that the optimal SIAC coefficients in the uniform case are rational numbers: by Cramer’s rule,

\[
c = \frac{\det [e_1 M_0(; 2 : 2d + 1)]}{\det M_0}
\] (12)

and the determinants only contain rational numbers. For example, the optimal symmetric SIAC spline convolution coefficients for degree \(d\) are (omitted entries in slots \(d + 2 : 2d + 1\) indicated by “…” are defined by symmetry):

\[
d = 1 : [-1, 14, -1]/12,
\]

\[
d = 2 : [-37, 388, -2622, 388, -37]/1920,
\]

\[
d = 3 : [-82, 933, -5514, 24446, -5514, 933, -82]/15120,
\]

\[
d = 4 : [-153617, 1983016, -12615836, 54427672, -180179750, \ldots]/92897280,
\]

\[
d = 5 : [-4201, 61546, -437073, 2034000, -7077894, 18830604, \ldots]/7983360.
\]
4 Conclusion

Especially in the presence of non-uniform knots, where pre-tabulation may not be practical, it is good to have explicit formulas for the entries of the SIAC coefficient matrix $M_0$ in terms of divided differences. Numerically stable implementations of divided differences are well-known. The paper may serve as a building block towards addressing the important issue of choosing good non-uniform knot sequences for SIAC post-processing. The author conjectures that the subtle issue of knot selection is also closely related to a classical theorem of spline theory.

Acknowledgement This work was supported in part by NSF grant CCF-1117695 and NIH R01 LM011300-01. Jennifer Ryan, Mahsa Mirzagar, Mike Kirby and Xiaozhou Li introduced me to the topic and patiently answered my questions.

References

[BS77] J. H. Bramble and A. H. Schatz. Higher order local accuracy by averaging in the finite element method. *Mathematics of Computation*, 31(137):94–111, January 1977.

[CKRS07] Sean Curtis, Robert M. Kirby, Jennifer K. Ryan, and Chi-Wang Shu. Postprocessing for the discontinuous Galerkin method over nonuniform meshes. *SIAM J. Scientific Computing*, 30(1):272–289, 2007.

[CLSS03] Bernardo Cockburn, Mitchell Luskin, Chi-Wang Shu, and Endre Süli. Enhanced accuracy by post-processing for finite element methods for hyperbolic equations. *Math. Comput.*, 72(242):577–606, 2003.

[dB02] C.W. de Boor. B-spline Basics. In M. Kim G. Farin, J. Hoschek, editor, *Handbook of Computer Aided Geometric Design*. Elsevier, 2002.

[dB05] C. W. de Boor. Divided differences. *Surveys in Approximation Theory*, 1:46–69, 2005.

[MJRK11] Hanieh Mirzaee, Liangyue Ji, Jennifer K. Ryan, and Robert M. Kirby. Smoothness-increasing accuracy-conserving (SIAC) postpro-
cessing for discontinuous Galerkin solutions over structured triangular meshes. *SIAM J. Numerical Analysis*, 49(5):1899–1920, 2011.

[MRKR13] Hanieh Mirzaee, James King, Jennifer K. Ryan, and Robert M. Kirby. Smoothness-increasing accuracy-conserving filters for discontinuous Galerkin solutions over unstructured triangular meshes. *SIAM J. Scientific Computing*, 35(1), 2013.

[ML78] M.S. Mock and P.D. Lax. The computation of discontinuous solutions of linear hyperbolic equations. *Comm. Pure Appl. Math.*, 31(4):423–430, 1978.

[MR14] Mahsa Mirzargar and Jennifer K. Ryan. Filtering: A unified view from approximation theory to the post-processing of discontinuous Galerkin solutions, 2014. Mini-symposium at Icosahom 2014, Salt Lake City, July 2014.

[MRK12] Hanieh Mirzaee, Jennifer K. Ryan, and Robert M. Kirby. Efficient implementation of smoothness-increasing accuracy-conserving (SIAC) filters for discontinuous Galerkin solutions. *J. Sci. Comput.*, 52(1):85–112, 2012.

[MRK14] Hanieh Mirzaee, Jennifer K. Ryan, and Robert M. Kirby. Smoothness-increasing accuracy-conserving (SIAC) filters for discontinuous Galerkin solutions: Application to structured tetrahedral meshes. *J. Sci. Comput.*, 58(3):690–704, 2014.

[Sch81] L.L. Schumaker. *Spline Functions: Basic Theory*. 1981. Wiley, New York.

[WRKH09] David Walfisch, Jennifer K. Ryan, Robert M. Kirby, and Robert Haimes. One-sided smoothness-increasing accuracy-conserving filtering for enhanced streamline integration through discontinuous fields. *J. Sci. Comput.*, 38(2):164–184, 2009.