High-Order Compact-Stencil Summation-By-Parts Operators for the Second Derivative with Variable Coefficients

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Abstract: A general framework is presented for deriving compact-stencil, high-order summation-by-parts (SBP) finite-difference operators for the second derivative with variable coefficients for 4^{th} through 6^{th} order accuracy. These second derivative operators are compatible with the first derivative SBP operator, possess the same norm and can therefore be used to construct time stable numerical schemes with simultaneous approximation terms to weakly impose boundary conditions. The derivation of these operators leads to various free parameters which can be used for optimization of the operator about criteria such as spectral radius and truncation error. The choice of a particular operator is dictated by the PDE being discretized and the solution strategy. This paper is thus concerned with operators optimized for the compressible Navier-Stokes equations, the discretization of which is solved within a Newton-Krylov solution strategy. Numerical tests on the compressible Navier-Stokes equations using the method of manufactured solutions as well as external aerodynamic flows over several airfoils are used for verification and characterization studies.

Keywords: Numerical Algorithms, Computational Fluid Dynamics, Summation-By-Parts.

The main difficulty in implementing higher-order methods arises from the boundary treatment. Summation-by-Parts (SBP) operators present a systematic means of deriving higher-order finite-difference operators with suitably high-order boundary treatments. In conjunction with Simultaneous-Approximation-Terms (SATs) impose boundary conditions weakly, SBP operators naturally give rise to multi-block schemes that have low communication overhead, and allow for a straightforward means of proving time-stability (see proof for the linearized Navier-Stokes equations [1]). The disadvantage of SBP operators is that while the interior scheme is $2p$ accurate the boundary treatment is p accurate and thus the global order of accuracy is $p+1$. However, [2] has shown that an additional degree of accuracy is obtained and so the method is formally $p+2$ accurate for $2p > 2$, while [3] has shown that if the formulation is dual consistent then integrated quantities retain the order of accuracy of the interior scheme. Compact-stencil operators have been shown to have various numerical advantages over non-compact operators [1]; they have lower global error, and are more dissipative of high wavenumber modes. Moreover, they have smaller bandwidth and thus require less computational resources, particularly if one is interested in adjoint-based optimization or error estimation for which the Jacobian of the PDE must be constructed. Finally, although one can apply the first derivative operator twice, doing so with SBP operators reduces the order of accuracy by one order.

The primary contribution of this paper is the derivation and optimization of high-order compact-stencil SBP operators for the second derivative with variable coefficients that substantially simplifies those previously in the literature (see [4] for up to 5^{th} order accuracy). The resultant system of non-linear equations emanating from the discretization procedure is large and we take advantage of symmetries in this system to reduce the number of equations that need to be solved, as well as decoupling of equations and simplification of the boundary closures to allow solution without resorting to removing degrees of freedom. The derivation of these operators results in various free parameters which can be used to optimize the operator for specific properties. It is hoped that providing a simple and rigorous method for derivation and optimization will increase the popularity of such SBP schemes, which have numerous advantages, in the CFD community

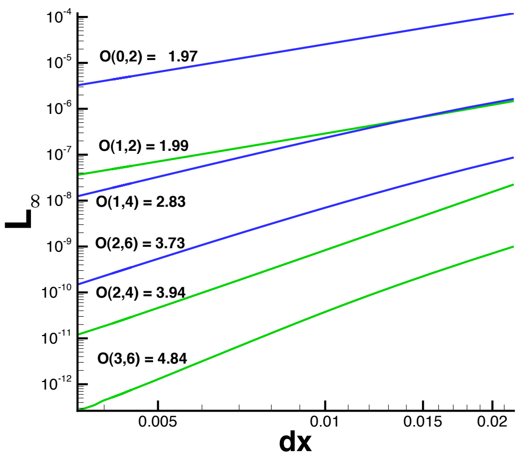

Figure 1: Convergence rates for the 1D linear convection-diffusion equation of the compact (green) and non-compact (blue) operators. For the compact operator we have O(p,2p), and for the non-compact operator we have O($p-1$,2p), where O refers to the order of convergence. The first number in the brackets is the order of accuracy of the operator at the boundary while the second number refers to the order of accuracy of the operator in the interior. Theoretical global accuracy is $p+2$ for the compact and $p+1$ for the non-compact operators, with the exception of the $p=1$ methods which are both second-order accurate.

The SBP property is mimetic of $\int_a^b Q\partial_x Q dx$ for the first derivative, and $\int_a^b Q\partial_x(b\partial_x(Q))dx$, for the second derivative with variable coefficients, leading to the following definition

Definition 1 (SBP Second Derivative)**.** *The matrix $D_2(b) \in R^{n\times n}$ is an SBP operator for the second derivative, with variable coefficients $b > 0$, if it is of the form, $D_2(b) = H^{-1}\{-M + EBD\}$, where H is a diagonal positive-definite (PD) matrix called the norm, $E = Diag(-1, 0, ..., 0, 1)$, $B = diag(b_1, b_2, ..., b_{n-1}, b_n)$, D_b is an approximation to the first derivative, $M = D^T HBD + R$ and both M and R are positive semi-definite (PSD).*

The dissipative term, R_{p+2} for the $p+2$ order operator, and the internal stencil have the general form,

$$R_{p+2} = \sum_{i=p+1}^{2p}(\Delta x)^{2i-1}\alpha_i(D_i)^T C_i B D_i,\ D_2^{(2p)}(b)_{\text{int}} = -\left\{(D^{(2p)})^T b D^{(2p)} + \sum_{p+1}^{2p}(\Delta x)^{2(i-1)}\alpha_i(D_i^{(2)})^T b D_i^{(2)}\right\},$$

where D_i is an approximation to the i^{th} derivative that is a second-order accurate centred difference approximation in the interior, is first-order accurate at $2p$ points at the left and right boundaries, has the same number of nodes as the compact first derivative in the interior, C_i is a diagonal PD matrix, Δx is the grid spacing, and the α_i are coefficients chosen to satisfy the accuracy requirements. Constructed thus, the operator is guaranteed to be PSD, so long as $b > 0$. Figure 1 demonstrates that the compact stencil not only has a higher order of convergence but that the global error is several magnitudes smaller than the non-compact form.

In the final paper we will present in detail the proposed framework for deriving and optimizing the compatible second derivative with variable coefficients and extending the order of accuracy to 6^{th} order. We will present some specific examples of optimized operators for the compressible Navier-Stokes equations, solved using a Newton-Krylov method, and characterize their properties with the method of manufactured solutions as well as for aerodynamic flows.

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