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Development and Investigation of Efficient High-Order Generalized Summation-By-Parts Operators for Computational Fluid Dynamics

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International High Performance Computing Summer School June 25-30 2017

Computational fluid dynamics (CFD) algorithms constructed using high-order operators can potentially provide higher accuracy at a lower computational cost compared to numerical schemes developed using low-order methods. Recently, generalized summation-by-parts (GSBP) operators have been introduced as a means of constructing numerical methods that are arbitrarily high-order, conservative, and provably stable. One advantage of the GSBP framework is that it can potentially offer more freedom compared to other popular methods, for example, the discontinuous Galerkin approach, as a result of not requiring basis functions. The purpose of the present work is to develop a CFD solver to investigate novel computationally efficient high-order GSBP operators with respect to their accuracy and efficiency in the numerical solution of the compressible Navier-Stokes equations. Presently, the University of Toronto Computational Aerodynamics Group employs a parallel implicit Newton-Krylov flow solver called Diablo, which uses classical summation-by-parts operators in combination with simultaneous approximation terms to solve the compressible Navier-Stokes equations on multi-block structured grids. The current flow solver will be extended using existing and newly constructed GSBP operators; and an extensive sequence of test cases will be performed to verify the efficiency of the constructed operators. This work is part of a larger research program focused on the multi-disciplinary high-fidelity design and optimization of aircraft using novel CFD algorithms, motivated by the need to reduce fuel consumption and emissions.

Background

Motivation

- Using numerical methods to solve problems in fluid dynamics is computationally expensive
- High-order methods can provide higher accuracy at a lower computational cost compared to low-order methods
- The potential for high-order methods to enable the construction of efficient algorithms motivates their further development

Definition

Summation-by-parts (SBP) operator for the first derivative: *A matrix operator*, $\mathsf{D}_\xi \in \mathbb{R}^{N\times N}$, *is an SBP operator that approximates the derivative* $\frac{\partial}{\partial \xi}$, *on the nodal distribution* $\boldsymbol{\xi} = [\xi_L, \xi_R]$, *of degree* p *if* [1]

1. $\mathsf{D}_\xi \boldsymbol{\xi}^k = \mathsf{H}_\xi^{-1}\mathsf{Q}_\xi \boldsymbol{\xi}^k = \mathsf{H}_\xi^{-1}\left(\mathsf{S}_\xi + \frac{1}{2}\mathsf{E}_\xi\right)\boldsymbol{\xi}^k = k\boldsymbol{\xi}^{k-1}, \quad k = 0, 1, \ldots, p;$
2. H_ξ, *the norm matrix, is symmetric and positive definite;*
3. $\mathsf{E}_\xi = \mathsf{E}_\xi^{\mathrm{T}}$, $\mathsf{S}_\xi = -\mathsf{S}_\xi^{\mathrm{T}}$, *therefore,* $\mathsf{Q}_\xi + \mathsf{Q}_\xi^{\mathrm{T}} = \mathsf{E}_\xi$; *and*
4. $\left(\boldsymbol{\xi}^i\right)^{\mathrm{T}} \mathsf{E}_\xi \boldsymbol{\xi}^j = \xi_R^{i+j} - \xi_L^{i+j}, \quad i,\ j = 0, 1, \ldots, p.$

To impose boundary conditions using simultaneous approximation terms, it is useful to construct E_ξ in the following manner:

$$\mathsf{E}_\xi = \mathbf{t}_{\xi_R}\mathbf{t}_{\xi_R}^{\mathrm{T}} - \mathbf{t}_{\xi_L}\mathbf{t}_{\xi_L}^{\mathrm{T}}, \quad \text{where} \quad \mathbf{t}_{\xi_L}^{\mathrm{T}}\boldsymbol{\xi}^k = \xi_L^k, \quad \mathbf{t}_{\xi_R}^{\mathrm{T}}\boldsymbol{\xi}^k = \xi_R^k, \quad k = 0, 1, \ldots, p.$$

[1] D.C. Del Rey Fernández, P.D. Boom, and D.W. Zingg.
A Generalized Framework for Nodal First Derivative Summation-By-Parts Operators.
Journal of Computational Physics, 266:214–239, 2014.

Traditional (or block) operator example

- Repeated interior point operator
- Uniform nodal distribution
- Boundary nodes included

For diagonal H_ξ, the classical degree one SBP operator is given by

$$\mathrm{D}_\xi = \frac{1}{2\Delta\xi}\begin{bmatrix} -2 & 2 & & & \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ & & & -2 & 2 \end{bmatrix}.$$

Projection operators for matrix derivative operators that include boundary nodes:

$$\mathbf{t}_{\xi_L} = [1, 0, 0, \ldots, 0]^{\mathrm{T}}$$
$$\mathbf{t}_{\xi_R} = [0, 0, \ldots, 0, 1]^{\mathrm{T}}$$

Element-type operator example

Legendre-Gauss quadrature nodes: do not include boundary nodes and are found by solving $P_n = 0$, where P_n is the n^{th} Legendre polynomial and is given by ($\xi \in [-1, 1]$)

$$P_n(\xi) = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}^2(\xi-1)^{n-k}(\xi+1)^k.$$

A degree two element-type SBP operator constructed on the Legendre-Gauss quadrature nodes $\boldsymbol{\xi} = [-\sqrt{15}/5, 0, \sqrt{15}/5]^{\mathrm{T}}$ is given by

$$\mathrm{D}_\xi = \begin{bmatrix} -\frac{1}{2}\sqrt{15} & \frac{2}{3}\sqrt{15} & -\frac{1}{6}\sqrt{15} \\ -\frac{1}{6}\sqrt{15} & 0 & \frac{1}{6}\sqrt{15} \\ \frac{1}{6}\sqrt{15} & -\frac{2}{3}\sqrt{15} & \frac{1}{2}\sqrt{15} \end{bmatrix}.$$

Projection operators:

$$\mathbf{t}_{\xi_L} = [(5+\sqrt{15})/6, -2/3, (5-\sqrt{15})/6]^{\mathrm{T}}$$
$$\mathbf{t}_{\xi_R} = [(5-\sqrt{15})/6, -2/3, (5+\sqrt{15})/6]^{\mathrm{T}}$$

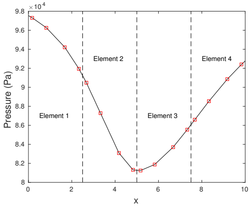
- GSBP operators can be derived using a variety of nodal distributions including the following nodal distributions: Legendre-Gauss-Lobatto (LGL), Legendre-Gauss (LG), Hybrid-Gauss-Trapezoidal-Lobatto (HGTL), Hybrid-Gauss-Trapezoidal (HGT).

Subsonic Converging-Diverging Nozzle

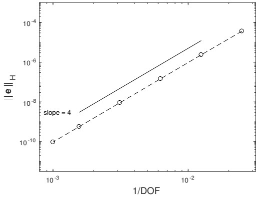
- Quasi-one-dimensional Euler equations
- Steady solution
- Element-type operators

} Problem summary

Legendre-Gauss ($p = 3$)



Exact ($-$) and numerical ($\square$) solutions

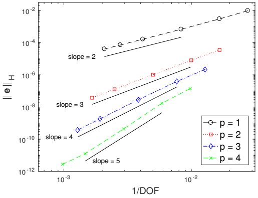


H norm of the solution error versus 1/Degrees Of Freedom

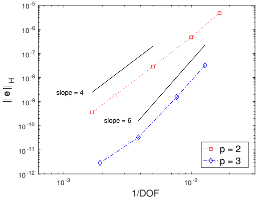
- For the classical operators (CSBP), the dense norm version converges at a higher rate compared to the diagonal norm version

- This is because, while both versions have interior operators of order $2p$, the boundary operators decrease to orders p and $2p - 1$ for the diagonal and dense norm cases, respectively

Classical



Diagonal norm operator: $p + 1$ convergence



Dense norm operator: $2p$ convergence

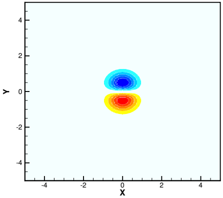
Vertex Transport by Uniform Flow

- Two-dimensional Euler equations
- Unsteady solution
- Fourth-order Runge-Kutta time marching
- Mach $= 0.5$, degree $= 2$

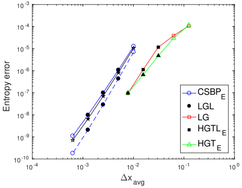
All operators achieve at least approximately $p + 1$ convergence

Operator	CSBP_E	LGL	LG	HGTL_E	HGT_E
Convergence	3.3906	3.4740	2.8031	3.4827	3.8556

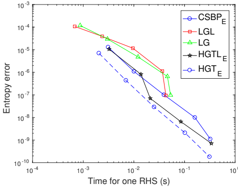
Note: The subscript E denotes element-type refinement



u-momentum after one period



Error versus grid spacing



Error versus time

Conclusion: Non-uniform nodal distributions can potentially lead to more efficient operators

Future Work

- Artificial dissipation - not known how existing models apply to generalized SBP operators
- High-order meshing - high-order approximation of curved geometries required to get high-order accuracy
- Preconditioning - required to efficiently solve the linear system of equations that arises at each time step
- Flexibility of GSBP approach - exploit to develop novel operators with optimized efficiency