A Positivity-preserving Strategy for Entropy Stable Discretizations of the Compressible Euler and Navier-Stokes equations

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SIAM TXLA, Nov 2022

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High order discontinuous Galerkin methods for PDEs

- Physical phenomena governed by PDE: aerospace engineering, nuclear engineering

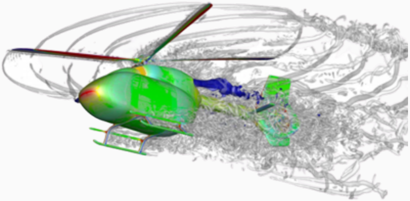

Figure 1: Vortex structures from a helicopter simulation

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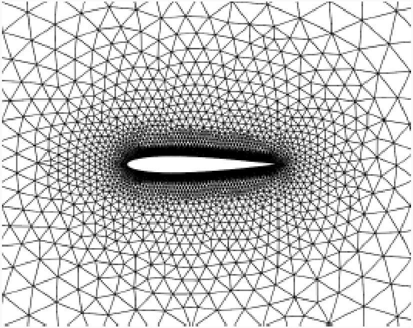

Figure 1: Unstructured mesh for NACA 0012 foil

High order discontinuous Galerkin methods for PDEs

- Physical phenomena governed by PDE: aerospace engineering, nuclear engineering
- High accuracy computational fluid dynamics on complex geometries
- More accurate per degrees of freedom than low order methods (for smooth solutions)

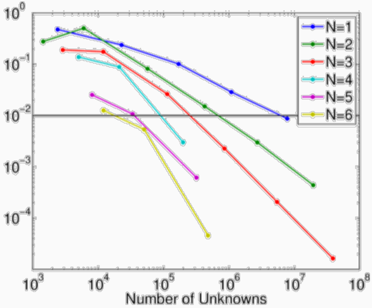

Figure 1: high order methods achieve better accuracy more efficiently

Compressible Euler and Navier-Stokes equations

- Compressible Euler and Navier-Stokes equations

$$\frac{\partial \boldsymbol{U}}{\partial t} + \underbrace{\sum_{i=1}^{3} \frac{\partial \boldsymbol{f}_i(\boldsymbol{U})}{\partial \boldsymbol{x}_i}}_{\text{inviscid flux}} = \underbrace{\sum_{i=1}^{3} \frac{\partial \boldsymbol{g}_i(\boldsymbol{U})}{\partial \boldsymbol{x}_i}}_{\text{viscous flux}}$$

- Entropy variables symmetrizes the viscous fluxes:

$$\sum_{i=1}^{d} \frac{\partial \boldsymbol{g}_i}{\partial x_i} = \sum_{i,j=1}^{d} \frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial \boldsymbol{v}}{\partial x_j}\right),$$

$$K = \begin{bmatrix} K_{11} & \dots & K_{1d} \\ \vdots & \ddots & \vdots \\ K_{d1} & \dots & K_{dd} \end{bmatrix} = K^T, \qquad K \succeq 0$$

Continuous Entropy Balance

- With convex entropy η, entropy variable $\boldsymbol{v} = \frac{\partial \eta(\boldsymbol{u})}{\partial \boldsymbol{u}}$ and entropy potential ψ_i. We can derive an entropy balance

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$$\int_\Omega \frac{\partial \eta(\boldsymbol{u})}{\partial t} + \sum_{i=1}^d \int_{\partial\Omega} n_i \left(F_i(\boldsymbol{u}) - \frac{1}{c_v T} \kappa \frac{\partial T}{\partial x_i} \right) = - \int_\Omega \sum_{i,j=1}^d \left(\frac{\partial \boldsymbol{v}}{\partial x_i} \right)^T \left(K_{ij} \frac{\partial \boldsymbol{v}}{\partial x_j} \right)$$

Integration by parts and chain rule

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Periodic

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- Loss of chain rule at discrete level (discrete effects, inexact quadrature) $\Longrightarrow$ Loss of entropy stability

High order entropy stable DG discretization

- Discretize the variational form of invscid term

$$\int_{\widehat{D}} \frac{\partial \boldsymbol{f}}{\partial x} \vec{l} \quad \xRightarrow{\text{Flux Differencing}} \quad 2\left(\mathsf{Q} \circ \mathsf{F}_S\right) \mathbf{1}, \quad \left(\mathsf{F}_S\right)_{ij} = \boldsymbol{f}_S\left(\boldsymbol{u}_i, \boldsymbol{u}_j\right)$$

Summation-by-parts $\quad \mathsf{Q} = \mathsf{M}\mathsf{D}, \quad \mathsf{Q} + \mathsf{Q}^T = \mathsf{B}, \quad \mathsf{Q}\mathbf{1} = 0$

Entropy conservation $\quad \left(\boldsymbol{v}_L - \boldsymbol{v}_R\right)^T \boldsymbol{f}_S\left(\boldsymbol{u}_L, \boldsymbol{u}_R\right) = \psi\left(\boldsymbol{u}_L\right) - \psi\left(\boldsymbol{u}_R\right)$

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- Discretize the symmetrized viscous term

$$\frac{\partial \boldsymbol{g}}{\partial x} = \frac{\partial}{\partial x}\left(K \frac{\partial \boldsymbol{v}}{\partial x}\right) \quad \xRightarrow{\text{Discretize}} \quad \begin{cases} \left(\boldsymbol{\Theta}, \varphi\right)_\Omega = \left(\frac{\partial \boldsymbol{v}}{\partial x}, \varphi\right)_\Omega + \langle [\![\boldsymbol{v}]\!] n_i, \varphi\rangle_{\partial\Omega} \\ \left(\boldsymbol{\sigma}, \eta\right)_\Omega = \left(K\boldsymbol{\Theta}, \eta\right)_\Omega \\ \left(\boldsymbol{G}_{\text{visc}}, \psi\right)_\Omega = -\left(\boldsymbol{\sigma}, \frac{\partial \psi}{\partial x}\right)_\Omega + \langle \{\{\boldsymbol{\sigma}\}\} n_i, \psi\rangle_{\partial\Omega} \end{cases}$$

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- The scheme is entropy stable

$$\sum_k \left(\frac{\partial \eta\left(\mathbf{u}\right)}{\partial t}, \mathbf{1}\right)_{D^k} = \sum_k \sum_{i,j=1}^{d} -\left(K_{ij}\boldsymbol{\Theta}_j, \boldsymbol{\Theta}_i\right)_{D^k} \leq 0$$

Current work: Positivity Limiting for nodal ESDG

- The entropy is well-defined only if densities and pressures are positive.

$$v_1 = (\gamma + 1 - s) - \frac{(\gamma - 1) E}{p}, \qquad s = \log\left(\frac{p}{\rho^\gamma}\right)$$

Current work: Positivity Limiting for nodal ESDG

- Strong shock forms - Negative densities

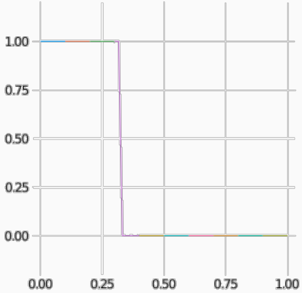

Figure 2: Exact solution

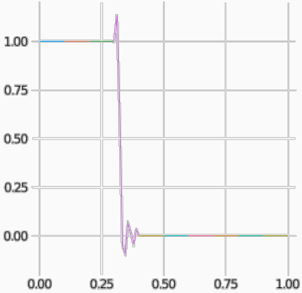

Figure 3: Solution in polynomial basis

- Oscillation by Gibbs phenomenon leads to negative density

Limiting strategy

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$$\frac{\boldsymbol{m}_i}{\tau}\left(\boldsymbol{u}_i^{L,n+1} - \boldsymbol{u}_i^n\right) + \boldsymbol{r}^{\mathrm{L},i} = 0$$
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  - $l_i = 1 \implies$ recovers ESDG.
    $l_i = 0 \implies$ recovers low order positivity-preserving scheme.

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- Elementwise limiting parameter

$$l = \min_{i \in D^k} l_i$$

Positivity preserving discretization

- Low order positivity preserving method could be written as

$$\underbrace{\boldsymbol{m}_i \frac{\partial \boldsymbol{u}}{\partial t} + \sum \boldsymbol{Q}_{ij} \left(\boldsymbol{f}(\boldsymbol{u}_j) - \boldsymbol{\sigma}_j \right)}_{\text{low order nodal DG on LGL nodes}} - \underbrace{\sum d_{ij} (\boldsymbol{u}_j - \boldsymbol{u}_i)}_{\text{graph viscosity}} = 0$$

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$$d_{ij} = \max \left\{ \beta(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{n}_{ij}) \|\boldsymbol{Q}_{ij}\|, \beta(\boldsymbol{u}_j, \boldsymbol{u}_i, \boldsymbol{n}_{ji}) \|\boldsymbol{Q}_{ji}\| \right\}, \boldsymbol{n}_{ij} = \boldsymbol{Q}_{ij} / \|\boldsymbol{Q}_{ij}\|$$

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- Zhang's positivity preserving flux

$$\beta\left(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{\sigma}_i, \boldsymbol{\sigma}_j, \boldsymbol{n}_{ij}\right) = |\boldsymbol{n} \cdot \boldsymbol{u}| + \frac{1}{2\rho^2 e}\left(\sqrt{\rho^2 \left(\boldsymbol{q} \cdot \boldsymbol{n}\right)^2 + 2\rho^2 e \left\| \boldsymbol{n} \cdot \boldsymbol{\tau} - p\boldsymbol{n} \right\|} + \rho \left| \boldsymbol{q} \cdot \boldsymbol{n} \right| \right)$$

Positivity preservation property

- Zhang's positivity preserving flux: positive substates

$$\beta \boldsymbol{u} \pm (\boldsymbol{f} - \boldsymbol{\sigma}) \cdot \boldsymbol{n}$$

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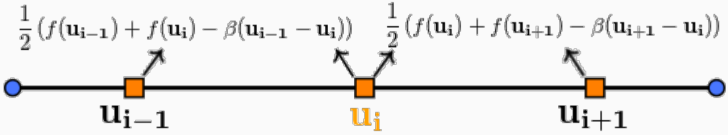
- Positivity preserving under the CFL condition:

$$\tau \leq \frac{\mathbf{m}_i}{2 \sum d_{ij}}$$

Positivity preserving discretization - Tensor product elements

- Interpretation: subcell Lax-Friedriches type dissipation



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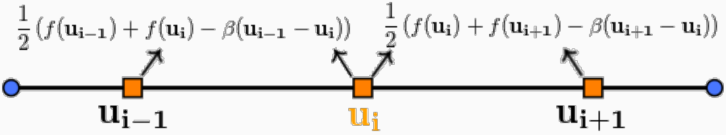
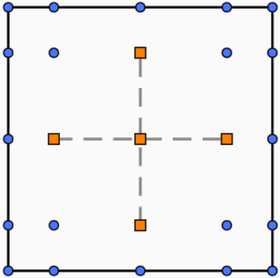
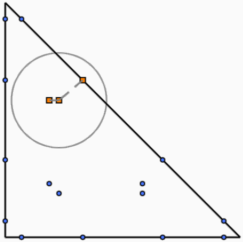


- Extension to tensor product elements



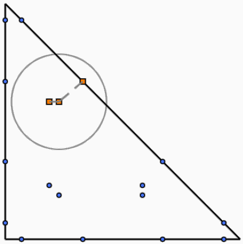
Positivity preserving discretization - Simplex elements

- Build connectivity graph



Positivity preserving discretization - Simplex elements

- Build connectivity graph



- Generalized sparse low order SBP operator

$$
\begin{aligned}
&\mathsf{Q}_r^{\mathrm{L}}\mathbf{1} = 0 \\
\text{s.t.} \quad &\left(\frac{\mathsf{Q}_r^{\mathrm{L}} - \left(\mathsf{Q}_r^{\mathrm{L}}\right)^T}{2}\right)_{ij} = \begin{cases} 0 & \text{if } \mathsf{A}_{ij} = 0 \\ \boldsymbol{\psi}_j - \boldsymbol{\psi}_i & \text{otherwise} \end{cases}.
\end{aligned}
$$

$$
\mathsf{Q}_r^{\mathrm{L}} = \frac{\mathsf{Q}_r^{\mathrm{L}} - \left(\mathsf{Q}_r^{\mathrm{L}}\right)^T}{2} + \frac{1}{2}\mathsf{E}^T\mathsf{B}\mathsf{E}, \qquad \boldsymbol{\psi}^T\mathbf{1} = 0
$$

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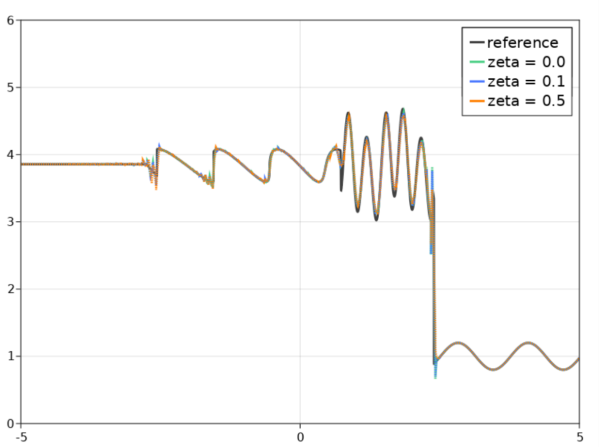
- Shock capturing: replace l with a shock indicator.

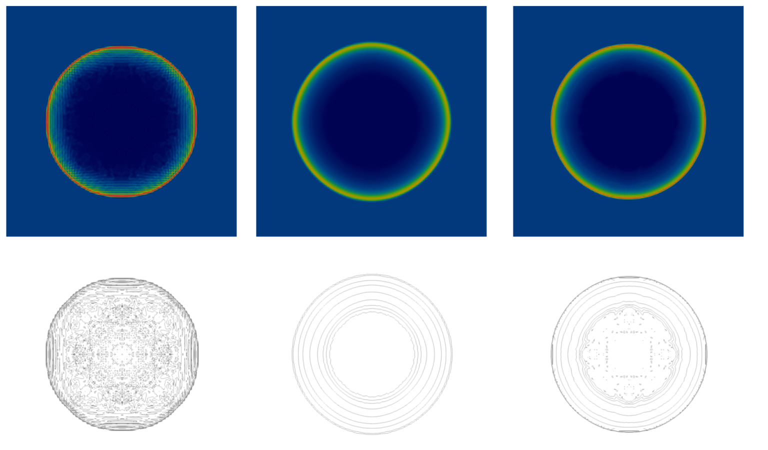
Shu-Osher shocktube

- $N = 3,\ 128$ elements, $T = 0.2$, limiting with the nodal bound $\rho > \zeta\rho^{\mathrm{L}}, \rho e > \zeta\left(\rho e\right)^{\mathrm{L}}$



Sedov blast wave

- $N = 3,\ 100 \times 100$ elements, limiting with the nodal bound $\rho > \zeta \rho^{\mathrm{L}}, \rho e > \zeta \left(\rho e\right)^{\mathrm{L}}$



$\zeta = 0.1$, without shock capturing $\quad$ $\zeta = 0.1$, with shock capturing $\quad$ $\zeta = 0.5$, without shock capturing

Double Mach Reflection - Compressible Euler

- $N = 3,\ 1000 \times 250$ elements, $T = 0.2$, limiting with the nodal bound $\rho > \zeta \rho^{\mathrm{L}}, \rho e > \zeta \left(\rho e\right)^{\mathrm{L}}$

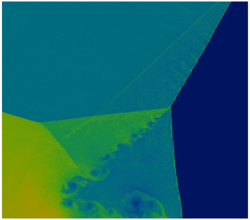


Figure 4: $\zeta = 0.1$ without shock capturing

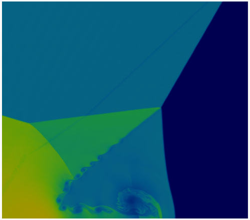


Figure 5: $\zeta = 0.1$ with shock capturing

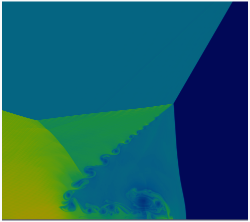


Figure 6: $\zeta = 0.5$ without shock capturing

Double Mach Reflection - Compressible Euler

- $N = 3,\ 1000 \times 250$ elements, $T = 0.2$, limiting with the nodal bound $\rho > \zeta \rho^{\mathrm{L}}, \rho e > \zeta \left(\rho e\right)^{\mathrm{L}}$

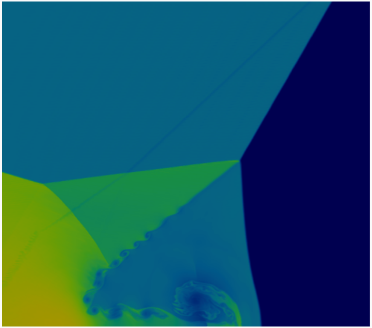


Figure 4: (ESDG) $\zeta = 0.1$ with shock capturing

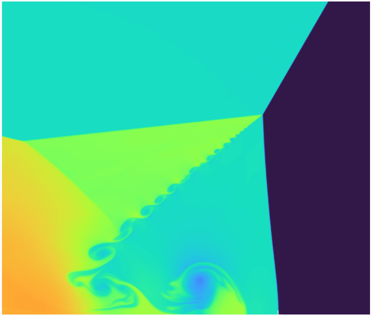


Figure 5: (Pazner, Sprase IDP, enforced minimum entropy principle) $N = 3, 2400 \times 600$ elements, $T \approx 0.275$

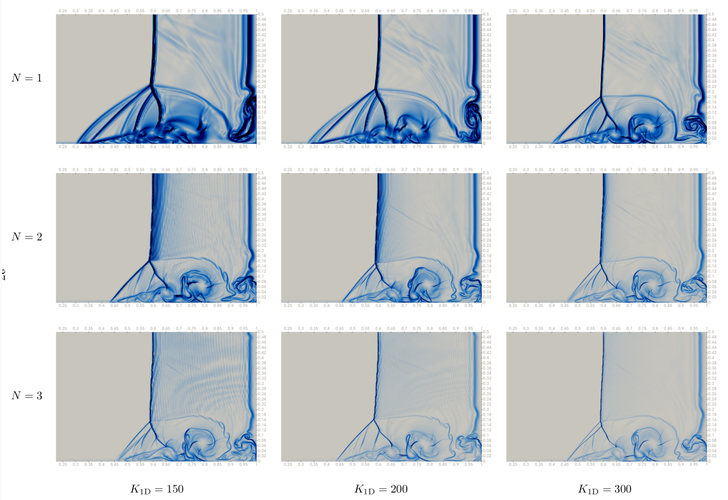


Figure 6: $Re = 1000$, uniform quad mesh, $\eta = 0.1$ without shock capturing

Daru-Tenaud shocktube - Compressible Navier-Stokes

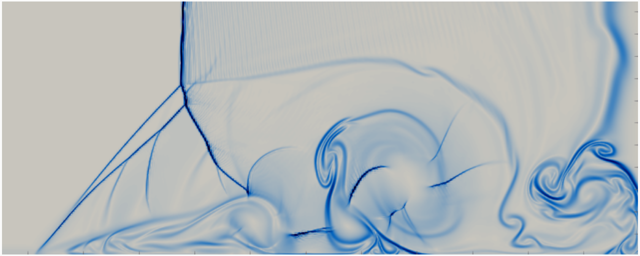


Figure 6: $Re = 1000, T = 1.0$ Result: $N = 3,300 \times 150$ uniform quad elements without shock capturing

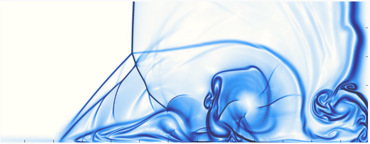


Figure 7: Invariant domain discretization, 2048×1024 elements

Figure 8: WENO5-RK4, 1000×500 grid points

Daru-Tenaud shocktube - Compressible Navier-Stokes

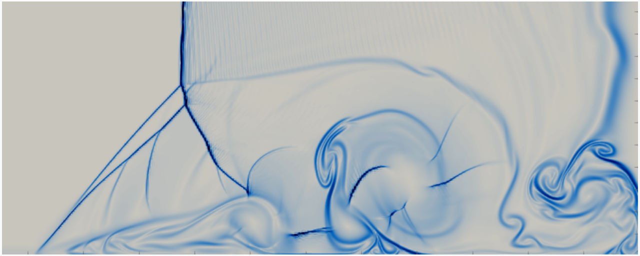
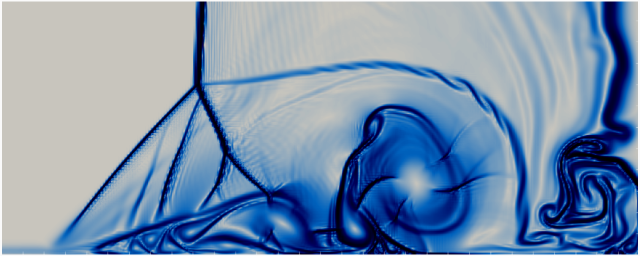


Figure 6: $Re = 1000, T = 1.0$ Result: $N = 3, 300 \times 150$ uniform quad elements without shock capturing



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Summary and future works

- We present a positivity limiting strategy for nodal ESDG based on graph viscosity.
- Future work: Positivity limiting for modal ESDG. Implicit timestepping.

Thank you!