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

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High order discontinuous Galerkin methods for PDEs

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

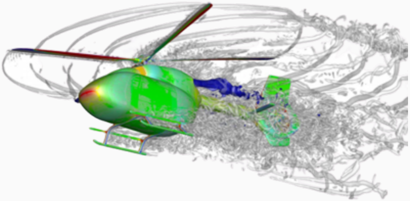

Figure 1: Vortex structures from a helicopter simulation

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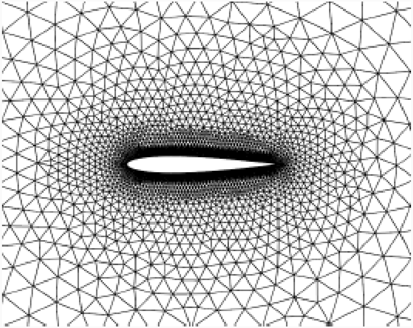

Figure 1: Unstructured mesh for NACA 0012 foil

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)

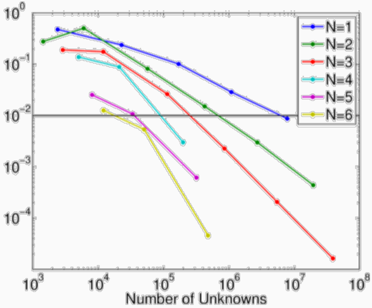

Figure 1: high order methods achieve better accuracy more efficiently

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

Discretization of the inviscid term - Nodal ESDG

- Entropy conservative numerical flux

$$\boldsymbol{f}_S(\boldsymbol{u},\boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{u}), \qquad \boldsymbol{f}_S(\boldsymbol{u}_L,\boldsymbol{u}_R) = \boldsymbol{f}_S(\boldsymbol{u}_R,\boldsymbol{u}_L)$$

$$(\boldsymbol{v}_L - \boldsymbol{v}_R)^T \boldsymbol{f}_S(\boldsymbol{u}_L,\boldsymbol{u}_R) = \psi(\boldsymbol{u}_L) - \psi(\boldsymbol{u}_R)$$

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- Flux differencing technique

$$\frac{\partial \boldsymbol{f}(\boldsymbol{u}(x))}{\partial x} = 2\left.\frac{\partial \boldsymbol{f}_S(\boldsymbol{u}(x),\boldsymbol{u}(y))}{\partial x}\right|_{y=x}$$

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- Collocation on Lobatto quadrature nodes gives summation-by-parts (SBP) operator

$$\mathsf{Q}=\mathsf{M}\mathsf{D}, \qquad \mathsf{Q}+\mathsf{Q}^T=\mathsf{B}, \qquad \mathsf{Q}\mathbf{1}=0$$

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- Discretize the variational form

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

Viscous term discretization

- We write the system differently:

$$\frac{\partial g}{\partial x} = \frac{\partial}{\partial x}\left(K\frac{\partial v}{\partial x}\right) \quad \xRightarrow{\text{Rewrite}} \quad \begin{cases} \boldsymbol{\Theta} = \frac{\partial v}{\partial x} \\ \boldsymbol{\sigma} = K\boldsymbol{\Theta} = g \\ G_{\mathrm{visc}} = \frac{\partial \sigma}{\partial x} \end{cases}$$

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

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- Viscous term dissipates entropy

$$\sum_k (G_{\text{visc}}, \boldsymbol{v})_{D^k} = \sum_k \sum_{i,j=1}^{d} -\left(K_{ij}\boldsymbol{\Theta}_j, \boldsymbol{\Theta}_i\right)_{D^k} \le 0$$

Current work: Positivity Limiting for nodal ESDG

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

$$\boldsymbol{v}_1 = (\gamma + 1 - s) - \frac{(\gamma - 1)\, E}{p}, \qquad s = \log\left(\frac{p}{\rho^\gamma}\right)$$

Current work: Positivity Limiting for nodal ESDG

- Strong shock forms - Negative densities

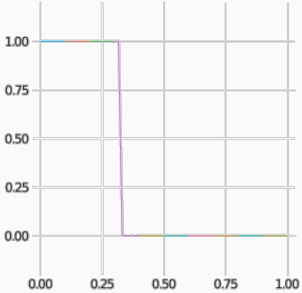

Figure 2: Exact solution

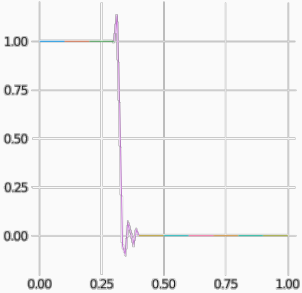

Figure 3: Solution in polynomial basis

- Oscillation by Gibbs phenomenon leads to negative density

Limiting strategy

- Step 1. Compute high order target scheme (nodal ESDG)

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  - Low order positivity-preserving and ESDG in algebraic flux form:

$$
\begin{aligned}
\frac{\boldsymbol{m}_i}{\tau}(\boldsymbol{u}_i^{L,n+1} - \boldsymbol{u}_i^n) + \sum \mathsf{F}_{ij}^{L,n} = 0 \\
\frac{\boldsymbol{m}_i}{\tau}(\boldsymbol{u}_i^{H,n+1} - \boldsymbol{u}_i^n) + \sum \mathsf{F}_{ij}^{H,n} = 0
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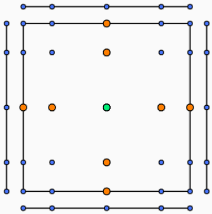
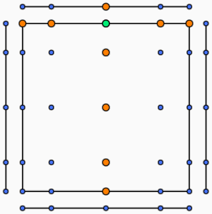
  - High order algebraic flux

$$\mathsf{F}_{ij}^{\mathrm{H}} = \left(\mathsf{Q} - \mathsf{Q}^T\right)_{ij}\left[f_S\left(\mathsf{u}_i, \mathsf{u}_j\right) - \frac{\boldsymbol{\sigma}_i + \boldsymbol{\sigma}_j}{2}\right]$$

Limiting strategy

- Choose suitable parameter $l_{ij} \in [0, 1]$ to satisfy positivity

$$m_i u_i^{n+1} = m_i u_i^{L,n+1} + \sum \tau l_{ij} (\mathsf{F}_{ij}^{L,n} - \mathsf{F}_{ij}^{H,n})$$

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- Find largest possible l_{ij} that satisify positivity.

Convex Limiting

- Limited solution as a convex combination of substates

$$u_i^{n+1} = u_i^{L,n+1} + \sum \tau \frac{l_{ij}}{\mathrm{m}_i}(\mathsf{F}_{ij}^{L,n} - \mathsf{F}_{ij}^{H,n})$$

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- Solutions with positive density and internal energy (pressure) is a convex set

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\mathcal{A} := \{ u = (\rho, \rho u, E) \mid \rho(u) > 0, \rho e(u) > 0 \}
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- Solving for l_{ij} is a simple quadratic solve

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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- Weighted differentiation matrix $\boldsymbol{Q}$ is a sparse low order (SBP) operator:

$$\begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & 0 & 0 & \dots & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & \dots & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

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- Low order algebraic flux

$$\mathrm{F}_{ij}^{\mathrm{L}} = \frac{1}{2} \left(\mathrm{Q}^{\mathrm{L}} - \left(\mathrm{Q}^{\mathrm{L}} \right)^T \right)_{ij} \left[f(\mathrm{u}_i) + f(\mathrm{u}_j) - (\sigma)_i - (\sigma)_j \right] - d_{ij} \left(\mathrm{u}_j - \mathrm{u}_i \right)$$

Graph viscosity coefficients

$$\mathsf{Q} = \begin{bmatrix} -\frac{1}{2} & \frac{1}{2} & 0 & 0 & \dots & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} & 0 & \dots & 0 \\ 0 & -\frac{1}{2} & 0 & \frac{1}{2} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}$$

- Define the graph viscosity coefficients:

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

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- Compressible Euler - Maximum wavespeed (Lax-Friedrichs flux)

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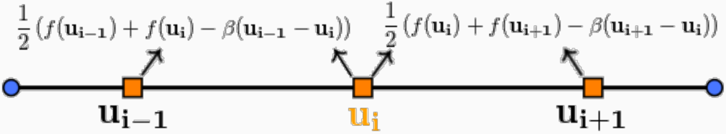
- Compressible Navier-Stokes - Zhang's positivity preserving flux

$$\beta\left(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{n}_{ij}\right) = \epsilon_0 + |\boldsymbol{n}\cdot\boldsymbol{u}| + \frac{1}{2\rho^2 e}\left(\sqrt{\rho^2\left(\boldsymbol{q}\cdot\boldsymbol{n}\right)^2 + 2\rho^2 e\,\|\boldsymbol{n}\cdot\boldsymbol{\tau} - p\boldsymbol{n}\|} + \rho\,|\boldsymbol{q}\cdot\boldsymbol{n}|\right)$$

Positivity preserving discretization - Tensor product elements

- Interpretation: subcell Lax-Friedriches type dissipation



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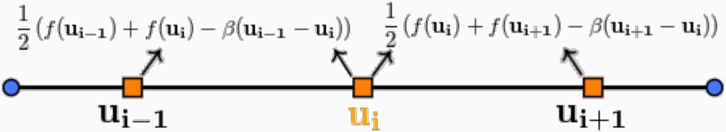
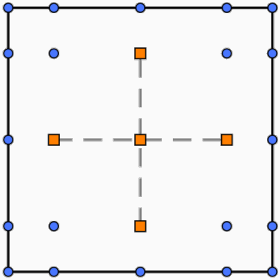
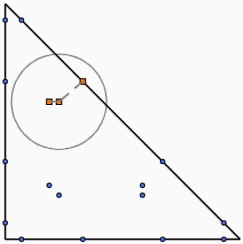


- Extension to tensor product elements



Positivity preserving discretization - Simplex elements

- Build connectivity graph



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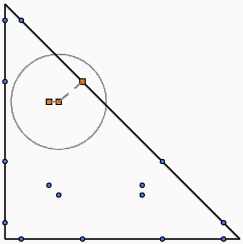


- Generalized sparse low order SBP operator

$$\mathsf{Q}_r^{\mathrm{L}}\mathbf{1} = 0$$

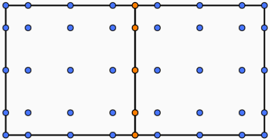
$$\text{s.t.} \quad \left(\frac{\mathsf{Q}_r^{\mathrm{L}} - \left(\mathsf{Q}_r^{\mathrm{L}}\right)^T}{2}\right)_{ij} = \begin{cases} 0 & \text{if } \mathsf{A}_{ij} = 0 \\ \boldsymbol{\psi}_j - \boldsymbol{\psi}_i & \text{otherwise} \end{cases}.$$

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

Modifications of interface fluxes

- The limited solution is

$$\mathsf{m}_i \mathsf{u}_i^{n+1} = \mathsf{m}_i \mathsf{u}_i^{\mathrm{L},n+1} + \tau \left(\sum_{j \in \mathcal{I}(i)} l_{ij} \left(\mathsf{F}_{ij}^{\mathrm{L}} - \mathsf{F}_{ij}^{\mathrm{H}} \right) + \sum_{j \in \mathcal{B}(i)} l_{ij} \left(\mathsf{F}_{ij}^{\mathrm{B,L}} - \mathsf{F}_{ij}^{\mathrm{B,H}} \right) \right)$$



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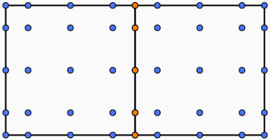

- Modify interface fluxes

$$\mathsf{F}_{ij}^{\mathrm{B,H}} = \mathsf{F}_{ij}^{\mathrm{B,L}} = \sum_{k=1}^{2} \frac{1}{2} \left(\mathsf{E}^T \mathsf{B}_k \mathsf{E} \right)_{ii} \left[\boldsymbol{f}_k \left(\mathsf{u}_i \right) + \boldsymbol{f}_k \left(\mathsf{u}_j \right) \right] - \left(\boldsymbol{\lambda}_k \right)_i \left(\mathsf{u}_j - \mathsf{u}_i \right).$$

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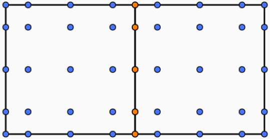

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- Low order positive $+$ High order entropy stable $\not\Rightarrow$ positivity-preserving and entropy stable limited solution

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$$l = \min \left\{ l_{ij}, \quad i, j \text{ in the same element} \right\}$$

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$$

$$
l = \min \left\{ l_{ij}, \quad i, j \text{ in the same element} \right\}
$$

- The limited solution is both positivity-preserving and entropy stable.

$$
\mathbf{u}_i^{n+1} = (1 - l)\, \mathbf{u}_i^{\mathrm{L},n} + l \mathbf{u}_i^{\mathrm{H},n}
$$

Entropy stable and positivity-preserving limited solution

- (Euler) Local Lax-Friedrichs flux dissipates entropy

$$\psi - \mathbf{v}^T \boldsymbol{f}_{\text{LF}} \leq 0$$

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$$\boldsymbol{v}^T \mathsf{M} \frac{\partial \boldsymbol{u}}{\partial t} \leq \mathbf{1}^T \mathsf{B} \left(\psi - \boldsymbol{v}^T \boldsymbol{f}^* \right) \quad \Longleftrightarrow \quad \int_D \frac{\partial \eta\left(\boldsymbol{u}\right)}{\partial t} \leq \int_{\partial D} \boldsymbol{n} \left(\psi - \boldsymbol{v}^T \boldsymbol{f}^* \right)$$

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- Discrete entropy balance (Navier-Stokes)

$$\beta\left(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{n}_{ij}\right) = \max\left\{\lambda_{\max}\left(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{n}_{ij}\right), \boldsymbol{\alpha}\left(\boldsymbol{u}_i, \boldsymbol{u}_j, \boldsymbol{n}_{ij}\right)\right\}$$

$$\boldsymbol{v}^T \mathsf{M} \frac{\partial \boldsymbol{u}}{\partial t} \leq \mathbf{1}^T \mathsf{B} \left(\boldsymbol{\psi} - \boldsymbol{v}^T \boldsymbol{f}^*\right) - \boldsymbol{v}^T \mathsf{M} \boldsymbol{G}_{\mathrm{visc}}$$

$$\Longleftrightarrow \quad \int_D \frac{\partial \eta\left(\boldsymbol{u}\right)}{\partial t} \leq \int_{\partial D} \boldsymbol{n} \left(\boldsymbol{\psi} - \boldsymbol{v}^T \boldsymbol{f}^*\right) - \int_D \left(\frac{\partial \boldsymbol{v}}{\partial x}\right)^T \left(\mathsf{K} \frac{\partial \boldsymbol{v}}{\partial x}\right)$$

Numerical results: LeBlanc shocktube

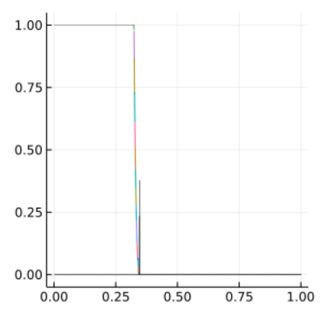

Figure 4: LeBlanc shocktube, N = 2, K = 800

K	L1 error	Rate
50	0.09403	
100	0.02240	2.07
200	0.00905	1.31
400	0.00348	1.38
800	0.00182	0.93
1600	0.00072	1.34

Numerical results: 1D viscous shocktube

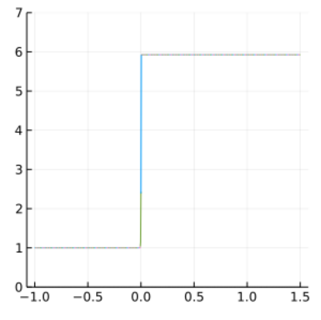

Figure 5: Viscous shocktube, N = 2, K = 400

K	L1 error	Rate
50	0.03278	
100	0.01852	0.82
200	0.00856	1.11
400	0.00241	1.83
800	0.00042	2.52
1600	0.00006	2.80

Double Mach Reflection - Compressible Euler

- $N = 3,\ 1000 \times 250$ elements, $T = 0.2$, element-wise and node-wise limiting

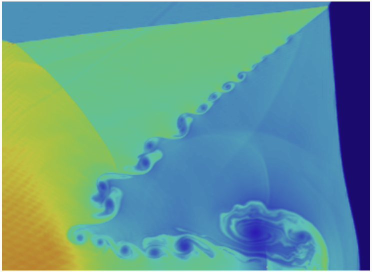

Figure 6: Element-wise

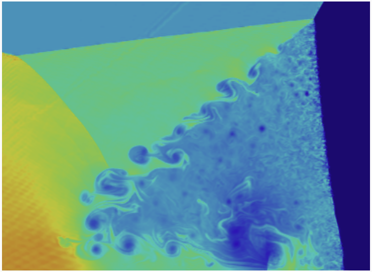

Figure 7: Node-wise

Double Mach Reflection - Compressible Euler

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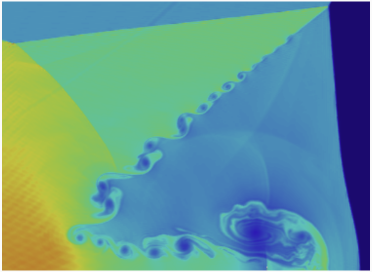

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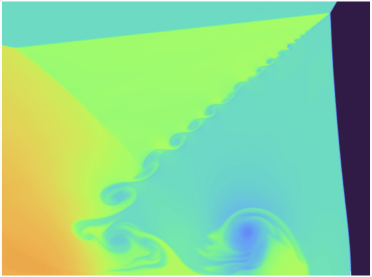

Figure 7: (Pazner) $N = 3, 2400 \times 600$ elements, $T \approx 0.275$

Double Mach Reflection - Compressible Navier-Stokes

- $N = 3,\ 250 \times 750, Re = 500$ elements, element-wise and node-wise limiting

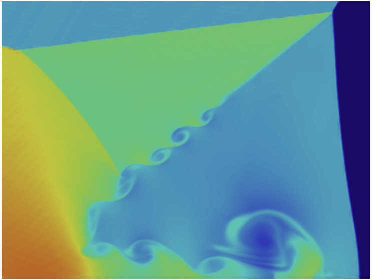

Figure 8: Element-wise

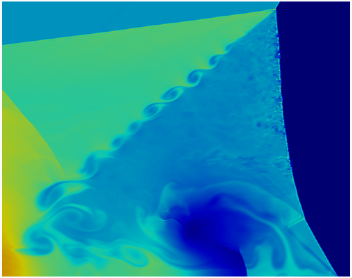

Figure 9: Node-wise

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!