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

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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

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

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

Viscous term discretization

- We write the system differently:

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

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

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- Viscous term dissipates entropy

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

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

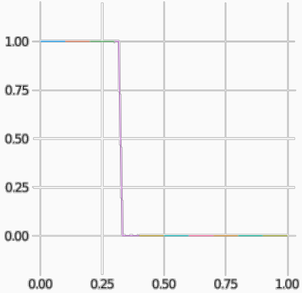

Figure 1: Exact solution

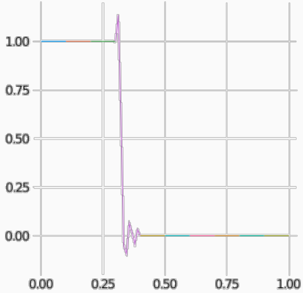

Figure 2: Solution in polynomial basis

- Oscillation by Gibbs phenomenon leads to negative density

Limiting strategy

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

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

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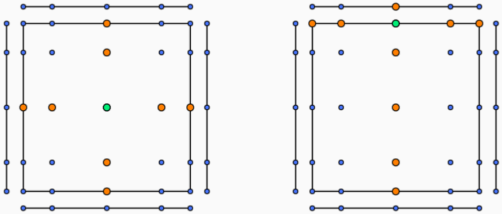
  - High order algebraic flux

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



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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  $l_{ij} = 0 \implies$ recovers low order positivity-preserving scheme.

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

Convex Limiting

- Limited solution as a convex combination of substates

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

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

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\mathcal{A} \coloneqq \{\boldsymbol{u} = (\rho, \rho u, E) \mid \rho(\boldsymbol{u}) > 0, \rho e(\boldsymbol{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

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

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

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- Low order algebraic flux

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

Graph viscosity coefficients

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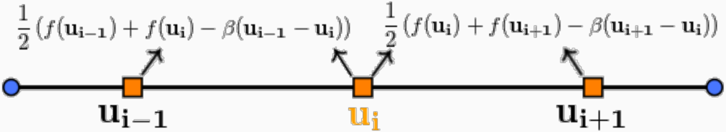
- Compressible Navier-Stokes - Zhang's positivity preserving flux

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

Positivity preserving discretization - Tensor product elements

- Interpretation: subcell Lax-Friedriches type dissipation



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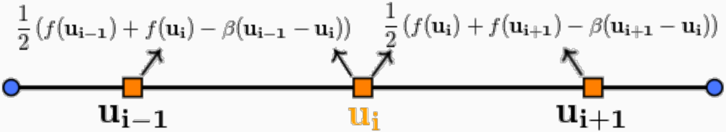
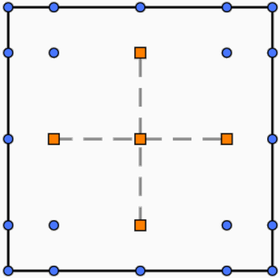
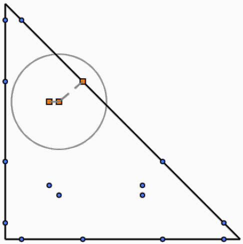


- Extension to tensor product elements



Positivity preserving discretization - Simplex elements

- Build connectivity graph



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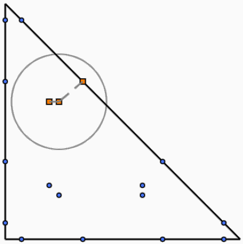

- Generalized sparse low order SBP operator

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

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

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

Modifications of interface fluxes

- The limited solution is

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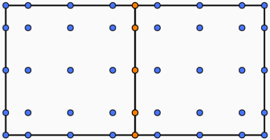

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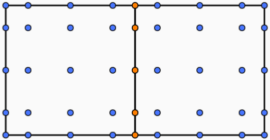

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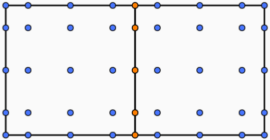

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- Compressible Navier-Stokes:

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

Numerical results: Isentropic vortex

- Elementwise limiting is only low order accurate for smooth solutions

	$N=3$		$N=4$	
K	L^1 error	Rate	L^1 error	Rate
2	2.834×10^{0}		1.494×10^{0}	
4	9.281×10^{-1}	1.61	7.104×10^{-1}	1.07
8	3.239×10^{-1}	1.52	3.193×10^{-1}	1.15
16	8.068×10^{-2}	2.01	8.047×10^{-2}	1.99
32	7.469×10^{-3}	3.43	1.148×10^{-2}	2.64

Table 1: Quad mesh

	$N=3$		$N=4$	
K	L^1 error	Rate	L^1 error	Rate
2	2.055×10^{0}		1.332×10^{0}	
4	7.907×10^{-1}	1.38	1.161×10^{0}	0.20
8	3.527×10^{-1}	1.16	9.058×10^{-1}	0.36
16	1.247×10^{-1}	1.50	6.115×10^{-1}	0.57
32	3.578×10^{-2}	1.80	3.915×10^{-1}	0.64

Table 2: Simplicial mesh

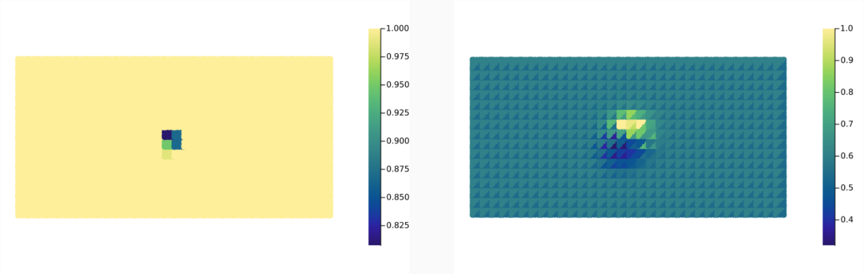

Figure 3: Limiting parameters

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- Option 1: positivity detector

$$l^k = 1 \quad \text{if} \quad \mathbf{u}_i^{\mathrm{H}} \in \mathcal{A} \text{ for all } i \in D^k$$

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- Option 2: Zhang-Shu type limiter

$$l^k = \max\left\{ l \in [0,1] \mid \mathbf{u}_i = \mathbf{u}_i^{\mathrm{L},n+1} + l \frac{\tau}{\mathbf{m}_i} \sum_{j \in \mathcal{I}(i)} \left(\mathbf{F}_{ij}^{\mathrm{L}} - \mathbf{F}_{ij}^{\mathrm{H}} \right) \in \mathcal{A}, i \in D^k \right\},$$

Numerical results: Isentropic vortex

- Positivity detector recovers high order accuracy

	$N=1$		$N=4$	
K_{1D}	L^1 error	Rate	L^1 error	Rate
2	3.336×10^{0}		1.588×10^{0}	
4	8.625×10^{-1}	1.95	4.891×10^{-1}	1.70
8	1.676×10^{-1}	2.36	9.222×10^{-2}	2.41
16	2.107×10^{-2}	2.99	7.355×10^{-3}	3.65
32	1.758×10^{-3}	3.58	1.312×10^{-4}	5.81

Table 1: Quad mesh

	$N=3$		$N=4$	
K_{1D}	L^1 error	Rate	L^1 error	Rate
2	2.516×10^{0}		1.512×10^{0}	
4	6.611×10^{-1}	1.93	5.415×10^{-1}	1.48
8	1.776×10^{-1}	1.90	8.944×10^{-2}	2.60
16	2.935×10^{-2}	2.89	7.943×10^{-3}	3.49
32	2.883×10^{-3}	3.66	2.341×10^{-4}	5.08

Table 2: Simplicial mesh

Figure 3: Limiting parameters

Double Mach Reflection - Compressible Euler

- $N = 3,\ 1000 \times 250$ elements, $T = 0.2$, element-wise with positivity detection, Zhang-Shu type and node-wise limiting

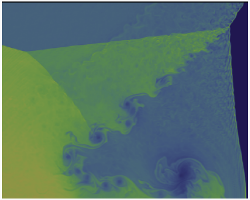

Figure 4: Elementwise

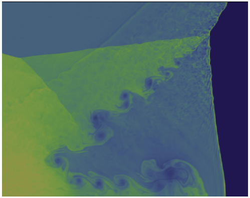

Figure 5: Zhang-Shu type

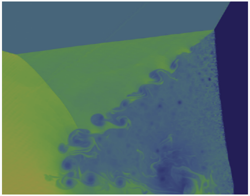

Figure 6: Nodewise

Double Mach Reflection - Compressible Euler

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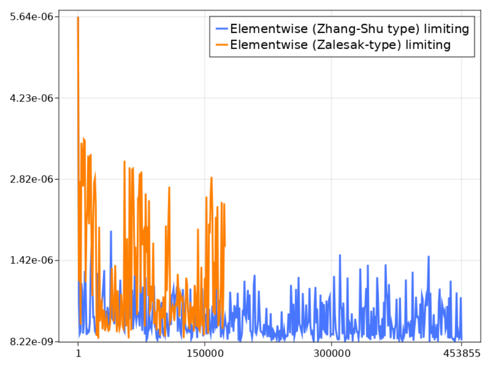

Figure 4: Timestep history

Double Mach Reflection - Compressible Navier-Stokes

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

Figure 5: Elementwise

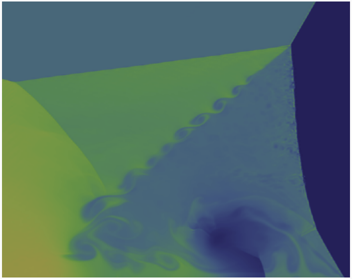

Figure 6: Nodewise

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!