Entropy stable schemes for the compressible Navier-Stokes equations: boundary conditions and positivity preserving schemes

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Compressible Navier-Stokes equations

- Compressible 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:

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

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

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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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Discretization of the inviscid term - Nodal ESDG

- Entropy conservative numerical flux

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

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

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- Discretize the variational form

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

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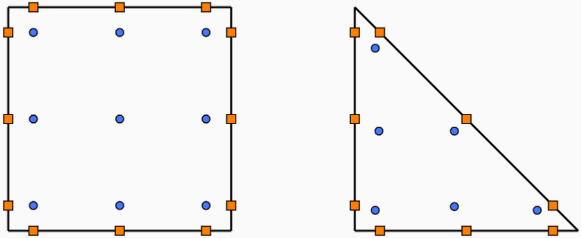
- Modal ESDG allows arbitrary choice of approximation basis and quadrature rules
- Extends nodal ESDG via over-integration



Discretization of the inviscid term - Modal ESDG

- "Hyrbridized" SBP operator

$$\mathsf{Q}_h = \frac{1}{2}\begin{bmatrix} \mathsf{Q} - \mathsf{Q}^T & \mathsf{E}^T\mathsf{B} \\ -\mathsf{B}\mathsf{E} & \mathsf{B} \end{bmatrix}, \qquad \mathsf{Q}_h\mathbf{1} = 0, \qquad \mathsf{Q}_h + \mathsf{Q}_h^T = \begin{bmatrix} 0 & 0 \\ 0 & \mathsf{B} \end{bmatrix}$$

$$\int_{\widehat{D}} u\frac{\partial v}{\partial x} + \int_{\widehat{D}} v\frac{\partial u}{\partial x} = \int_{\partial\widehat{D}} uv\widehat{\mathsf{n}} \xrightarrow{\text{Discretize}} \mathsf{v}^T\mathsf{Q}_h\mathsf{u} + \mathsf{v}^T\mathsf{Q}_h^T\mathsf{u} = \mathsf{v}_f^T\mathsf{B}\mathsf{u}_f$$

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- Entropy projection ensures consistency with respect to the polynomial basis and the entropy conservative flux

$$\mathsf{v}_h = \Pi_N \boldsymbol{v}, \qquad \widetilde{\mathsf{u}} = \boldsymbol{u}\left(\Pi_N \boldsymbol{v}\right)$$

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Discretization of the viscous term

- Usual approach: discretize the viscous term by writing it as a first order system

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

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- Previous enforcement of wall boundary conditions (Dalcin et al.) involve transformations between primitive and entropy variables.
    - Step 1: Enforce boundary conditions on primitive variables $\boldsymbol{w}$, define $\boldsymbol{v}^+, K^+$ accordingly.
    - Step 2: Rotate $\boldsymbol{\Theta}$ to the gradient of primitive variables $\boldsymbol{\Pi}$
    - Step 3: Enforce Neumann boundary conditions on $\boldsymbol{\Pi}$, get $\boldsymbol{\Pi}^+$
    - Step 4: Rotate $\boldsymbol{\Pi}^+$ back to $\boldsymbol{\Theta}^+$

Viscous term discretization

- We write the system differently:

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

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- Viscous term dissipates entropy

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

Simpler enforcement of wall boundary conditions

- Adiabatic no-slip wall boundary condition

$$\begin{cases} u_n & = 0 \\ u_t & = u_{\text{wall}} \\ \kappa \frac{\partial T}{\partial n} \frac{1}{T} & = g(t) \end{cases} \implies \begin{cases} \{\{v_{1+i}\}\} & = -u_{i,\text{wall}} v_4 \\ \{\{\sigma_{4,i}\}\} & = u_{1,\text{wall}} \sigma_{2,i} + u_{2,\text{wall}} \sigma_{3,i} + \frac{g(t) n_i}{c_v v_4} \end{cases}$$

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- Reflective wall boundary condition

$$\begin{cases} u_n & = 0 \\ \sum t_i \sigma_{ij} n_j & = 0 \\ \kappa \frac{\partial T}{\partial n} & = 0 \end{cases} \implies \begin{cases} \{\{\mathbf{v}\}\} = \mathbf{v} - v_n \mathbf{n} \\ \begin{bmatrix} \{\{\sigma_{2,1}\}\} & \{\{\sigma_{2,2}\}\} \\ \{\{\sigma_{3,1}\}\} & \{\{\sigma_{3,2}\}\} \end{bmatrix} \mathbf{n} = \mathbf{n}\mathbf{n}^T \begin{bmatrix} \sigma_{2,1} & \sigma_{2,2} \\ \sigma_{3,1} & \sigma_{3,2} \end{bmatrix} \mathbf{n} \\ \{\{v_4\}\} = v_4, \quad \{\{\sigma_{4,i}\}\} = 0 \end{cases}$$

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- Simplifies the proofs of entropy stability under these wall boundary conditions.

Numerical results: Viscous shocktube

$h \backslash N$	$N = 2$	Rate	$N = 3$	Rate	$N = 4$	Rate
$1/4$	0.0318		0.00566		0.0052	
$1/8$	0.00306	3.376	0.000462	3.616	0.000185	4.814
$1/16$	0.00033	3.213	5.22e-05	3.146	5.18e-06	5.157
$1/32$	4.5e-05	2.874	3.13e-06	4.060	1.81e-07	4.842
$1/64$	5.81e-06	2.952	2.1e-07	3.898	6.24e-09	4.856

(a) L^1 errors

$h \backslash N$	$N = 2$	Rate	$N = 3$	Rate	$N = 4$	Rate
$1/4$	0.0639		0.00916		0.011	
$1/8$	0.00631	3.339	0.00103	3.156	0.000449	4.618
$1/16$	0.000853	2.887	0.000162	2.665	1.38e-05	5.020
$1/32$	0.000132	2.694	9.71e-06	4.062	6.19e-07	4.483
$1/64$	1.73e-05	2.931	6.87e-07	3.821	2.16e-08	4.839

(b) L^2 errors

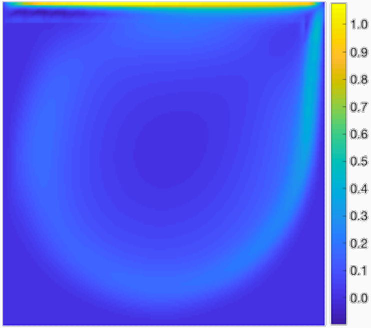
Table 1: L^1 and L^2 errors for the viscous shock tube problem.

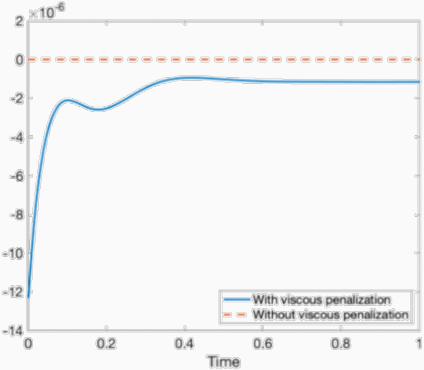
Numerical results: Lid driven cavity

- Evolution of viscous entropy residual $r(t)$

$$r(t) = \sum_{k} \left[\left(\mathbf{G}_{\text{visc}}, \mathbf{v}\right)_{D^k} + \sum_{i,j=1}^{d} \left(\mathbf{K}_{ij}\boldsymbol{\Theta}_j, \boldsymbol{\Theta}_i\right) \right] = \left\langle \frac{g(t)}{c_v}, 1 \right\rangle_{\partial\Omega}$$

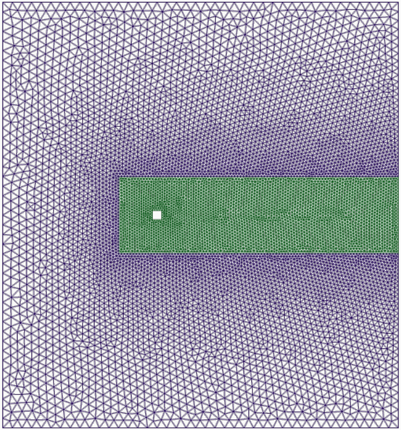
- Lid driven cavity with $Re = 1000$, adiabatic wall boundary condition $g(t) = 0$



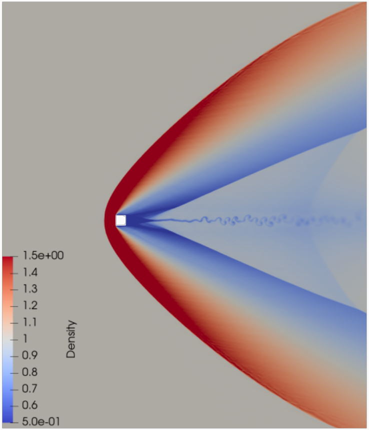


Numerical results: Flow over cylinder

- Supersonic flow over cylinder with $Re = 10^4$, $Ma = 1.5$



(a) Mesh



(b) Zoom of density ρ at $T_{\text{final}} = 100$

Current work: Positivity Limiting for nodal ESDG

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

Current work: Positivity Limiting for nodal ESDG

- Strong shock forms - Negative densities

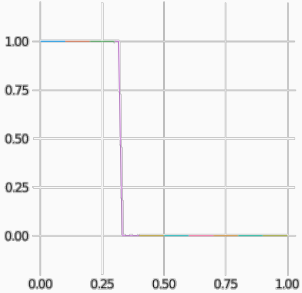


Figure 1: Exact solution

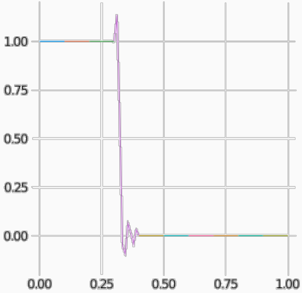


Figure 2: Solution in polynomial basis

- Oscillation by Gibbs phenomenon leads to negative density

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

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

    - $l_{ij} = 1 \implies$ recovers ESDG.
      $l_{ij} = 0 \implies$ recovers low order positivity-preserving scheme.

Limiting strategy

- Step 1. Compute high order target scheme (nodal ESDG)
- Step 2. Compute low order positivity-preserving scheme
- Step 3. Blend two schemes together through convex limiting
  - Low order positivity-preserving and ESDG in algebraic flux form:

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

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

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

  - $l_{ij} = 1 \implies$ recovers ESDG.
    $l_{ij} = 0 \implies$ recovers low order positivity-preserving scheme.
  - Find largest possible l_{ij} that satisify positivity.

Positivity preserving discretization

- Low order positivity preserving method could be written as

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

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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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- 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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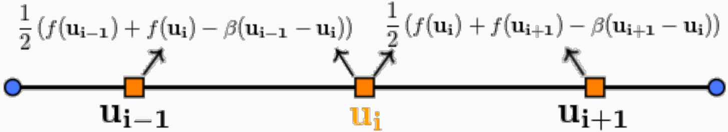
- Compressible Navier-Stokes - Zhang's positivity preserving flux
  Compressible Euler - Maximum wavespeed (Lax-Friedrichs flux)

Positivity preserving discretization

- Interpretation: subcell Lax-Friedriches type dissipation



Positivity preserving discretization

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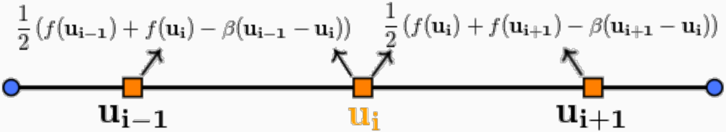
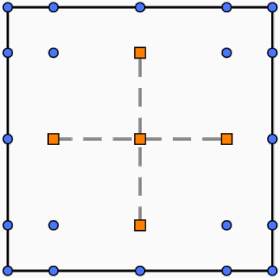
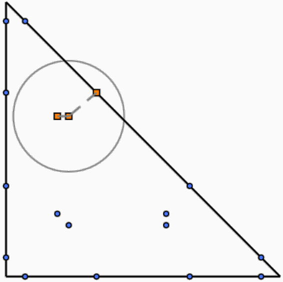


- Extension to 2D (tensor product and simplex elements)





Numerical results: LeBlanc shocktube

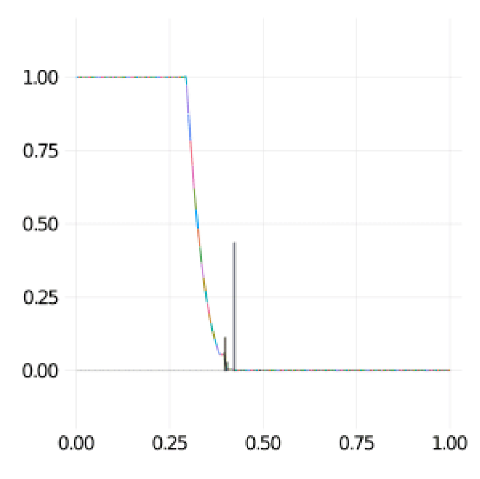


Figure 3: LeBlanc shocktube, N = 3, K = 200

Summary and future works

- We present an entropy stable approach to discretize the viscous term and explicit formulas for entropy stable imposition of no-slip and reflective boundary conditions.
- We briefly preview a positive limiting strategy for nodal ESDG.
- Future work: curvilinear and moving meshes, positivity limiting for modal ESDG.

Thank you!