Various aspects of Entropy stable discontinuous Galerkin Methods

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High order discontinuous Galerkin methods for PDEs

- Physical phenomena governed by PDE: aerospace engineering, biological science

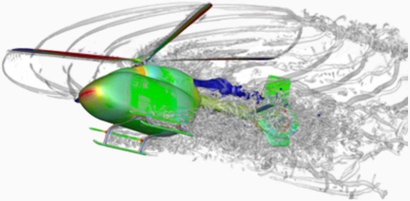

Figure 1: Vortex structures from a helicopter simulation

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- High accuracy computational fluid dynamics on complex geometries

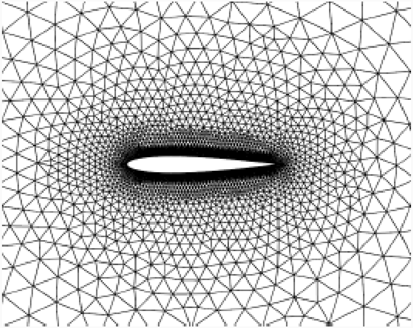

Figure 1: Unstructured mesh for NACA 0012 foil

High order discontinuous Galerkin methods for PDEs

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

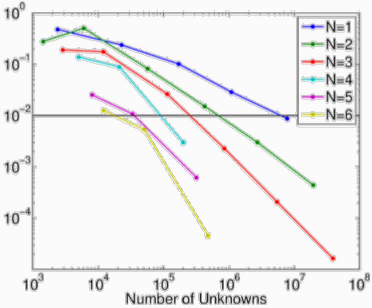

Figure 1: high order methods achieve better accuracy more efficiently

Energy stability for PDEs

- Linear advection equations on the periodic domain $[-1, 1]$

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- Energy stability doesn't work in nonlinear conservation laws

$$\frac{\partial \boldsymbol{u}}{\partial t} + \sum_{i=1}^{d} \frac{\partial \boldsymbol{f}_i(\boldsymbol{u})}{\partial x_i} = 0, \quad \boldsymbol{u}, \boldsymbol{f}_i : \mathbb{R}^n \to \mathbb{R}^n$$

Mathematical entropy

- 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 equality

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

Typical stabilization procedures

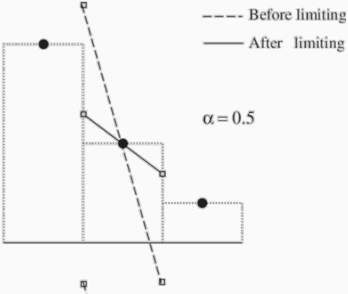

Figure 2: Slope limiting procedure

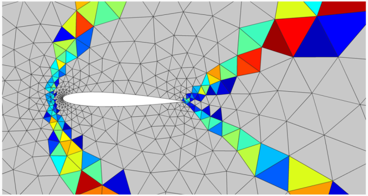

Figure 3: Sub-cell viscosity[1]

- Slope limiting, filtering and artificial viscosity: loses high order accuracy, require heuristic tuning

[1]Persson and Peraire, "Sub-cell shock capturing for discontinuous Galerkin methods".

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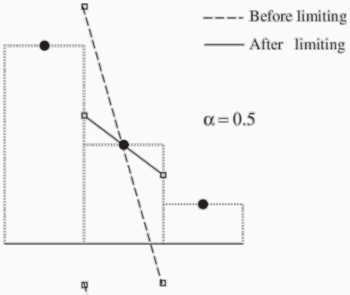

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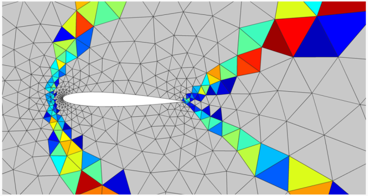

Figure 3: Sub-cell viscosity[1]

- Slope limiting, filtering and artificial viscosity: loses high order accuracy, require heuristic tuning
- Limited theoretical justification

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Robust DG formulation: entropy stable nodal DG

- Collocation nodal DG: matrix vector product

$$\mathsf{M}\frac{\mathrm{d}\mathsf{u}}{\mathrm{d}t} + \mathsf{Q}\boldsymbol{f}(\mathsf{u}) = 0$$

- Entropy stable nodal DG: Hadamard product

$$\mathsf{M}\frac{\mathrm{d}\mathsf{u}}{\mathrm{d}t} + 2(\mathsf{Q} \circ \mathsf{F}_S)\mathbf{1} = 0$$

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- Entropy stable DG is computationally more expensive

1. Entropy Stable DG-Fourier methods

with Jesse Chan

2. Modal ESDG formulation for the compressible Navier-Stokes equation

with Jesse Chan and Tim Warburton

3. Positivity Limiting for nodal ESDG methods

with Jesse Chan, Xinhui Wu and Ignacio Tomas

Discontinuous Galerkin-Fourier methods

- Approximate solutions with Fourier basis in one dimension

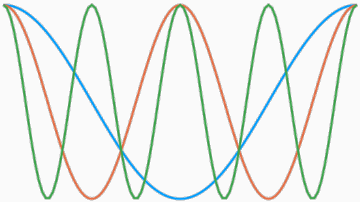


Figure 4: Example of Fourier basis

Discontinuous Galerkin-Fourier methods

- Approximate solutions with Fourier basis in one dimension
- Spectral accuracy for smooth solutions

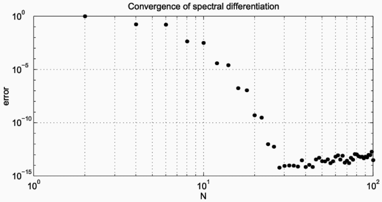


Figure 4: Accuracy of spectral differentiation[2]

[2] Trefethen, *Spectral methods in MATLAB.*

Discontinuous Galerkin-Fourier methods

- Approximate solutions with Fourier basis in one dimension
- Spectral accuracy for smooth solutions
- Only works on periodic domains

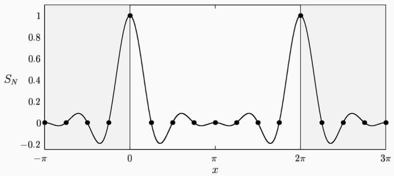


Figure 4: Nodal Fourier basis is periodic

[1] Trefethen, *Spectral methods in MATLAB*.

Discontinuous Galerkin-Fourier methods

- Approximate solutions with Fourier basis in one dimension
- Spectral accuracy for smooth solutions
- Only works on periodic domains
- Suitable for simulating quasi-2D flow

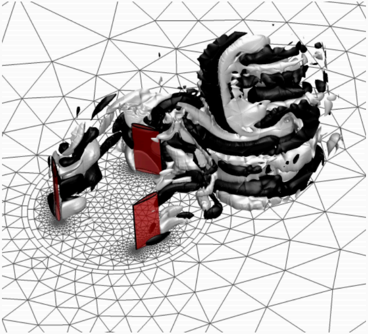


Figure 4: Applications: wind turbine[2]

[2] Ferrer and Willden, “A high order discontinuous Galerkin–Fourier incompressible 3D Navier–Stokes solver with rotating sliding meshes”.

Geometric assumptions

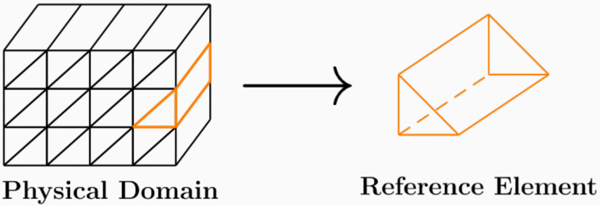


Figure 5: Example physical domain and reference element

- The geometry is homogeneous and periodic in one direction
- Reference element in 3D: wedge

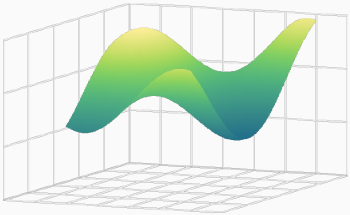


Figure 6: Polynomial basis

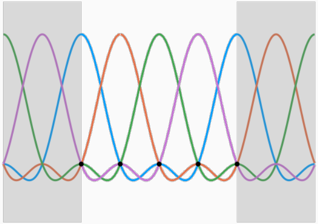
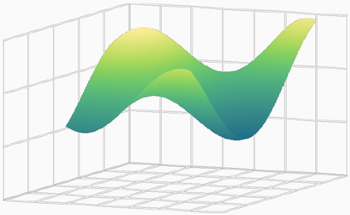


Figure 7: Nodal Fourier basis

- Triangles: polynomial of degree N^{P}
  z-direction: nodal Fourier basis

$$S\left(\hat{z}\right) = \frac{\sin\left(N^{\mathrm{F}}\frac{\hat{z}}{2}\right)}{N^{\mathrm{F}}\tan\left(\frac{\hat{z}}{2}\right)}, \qquad S_i\left(\hat{z}\right) = S\left(\hat{z} - \hat{z}_i\right)$$

Approximation space



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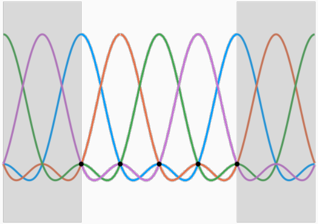

Figure 7: Nodal Fourier basis

- Approximation space: tensor product of polynomial and sinc basis

$$\begin{aligned} V_h\left(\widehat{D}\right) &= P^{N^{\mathrm{P}}}\left(\widehat{D}^{\mathrm{P}}\right) \otimes F^{N^{\mathrm{F}}}\left(\widehat{D}^{\mathrm{F}}\right) \\ &= \left\{\varphi_i\left(\widehat{x},\widehat{z}\right) = p_{k_1,\ldots,k_{d-1}}\left(\widehat{x}\right) S_i\left(\widehat{z}\right), \quad \widehat{x} \in \widehat{D}^{\mathrm{P}}, \widehat{z} \in \widehat{D}^{\mathrm{F}}\right\} \end{aligned}$$

Quadrature rules

- Quadrature on triangles $\left(\widehat{\mathbf{x}}_i, w_i\right)$, $\left(\widehat{\mathbf{x}}_i^f, w_i^f\right)$: degree $2N^{\mathrm{P}}$ volume and surface quadratures

$$\left(\frac{\partial u}{\partial x_n}, v\right)_{\widehat{D}^{\mathrm{P}}} = \langle u, v \rangle_{\partial \widehat{D}^{\mathrm{P}}} - \left(u, \frac{\partial v}{\partial x_n}\right)_{\widehat{D}^{\mathrm{P}}}$$

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- Quadrature rule on the spanwise direction, $h = \frac{2\pi}{N_p^{\mathsf{F}}}$

$$\int_0^{2\pi} f(z)\ \mathrm{d}z \approx h \sum_{i=1}^{N_p^{\mathsf{F}}} f(\widehat{z}_i), \quad \widehat{z}_i = hi, \quad i = 1, \ldots, N_p^{\mathsf{F}}$$

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- Combine through tensor product

$$\left\{(\widehat{\mathsf{x}}_i, \widehat{z}_j), h w_i\right\}_{\substack{i=1\dots N_q^{\mathrm{P}},\\ j=1\dots N^{\mathrm{F}}}} \quad \left\{(\widehat{\mathsf{x}}_i^f, \widehat{z}_j), h w_i^f\right\}_{\substack{i=1\dots N_{f,q}^{\mathrm{P}}\\ j=1\dots N^{\mathrm{F}}}}$$

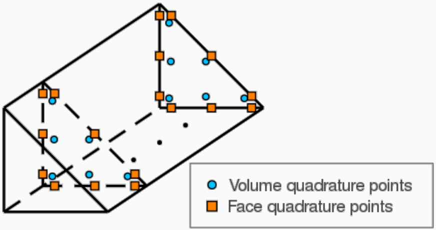
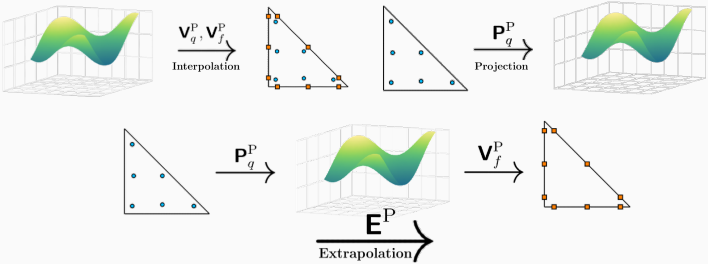


Figure 8: Reference element with quadrature nodes

Quadrature based operators on the reference triangle



- Mass matrix, boundary integration, differentiation

$$\mathsf{M}^{\mathrm{P}} \approx \int_{\widehat{D}^{\mathrm{P}}} p_i(\widehat{x}) p_j(\widehat{x}) \, \mathrm{d}\widehat{x}, \qquad \mathsf{B}_n^{\mathrm{P}} \approx \int_{\partial \widehat{D}^{\mathrm{P}}} u v \widehat{\boldsymbol{n}}_n, \qquad \mathsf{D}_{q,n}^{\mathrm{P}} \approx \frac{\partial}{\partial x} (\Pi_{N^{\mathrm{P}}})$$

- Chan's hybridized SBP operators, $n = 1, 2$

$$\mathsf{Q}_{h,n}^{\mathrm{P}} = \begin{bmatrix} \mathsf{Q}_{q,n}^{\mathrm{P}} - \frac{1}{2} (\mathsf{E}^{\mathrm{P}})^T \mathsf{B}_n^{\mathrm{P}} \mathsf{E}^{\mathrm{P}} & \frac{1}{2} (\mathsf{E}^{\mathrm{P}})^T \mathsf{B}_n^{\mathrm{P}} \\ -\frac{1}{2} \mathsf{B}_n^{\mathrm{P}} \mathsf{E}^{\mathrm{P}} & \frac{1}{2} \mathsf{B}_n^{\mathrm{P}} \end{bmatrix}$$

Quadrature based operators on the reference wedge

- By tensor product structure of approximation space, extend modal operators A:

$$\mathsf{A} = \mathbf{I}_{N^{\mathsf{F}}} \otimes \mathsf{A}^{\mathsf{P}}$$

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$$\int_{\widehat{D}} \varphi\left(\widehat{x}, \widehat{z}\right) = \int_{\widehat{D}^{\mathrm{P}}} p\left(\widehat{x}\right) \int_{\widehat{D}^{\mathrm{F}}} S\left(\widehat{z}\right) \implies \mathsf{T} = h\mathbf{I}_{N^{\mathrm{F}}} \otimes \mathsf{T}^{\mathrm{P}}$$

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- Hybridized operators on x, y directions retain SBP property

$$\begin{aligned} \mathsf{Q}_{h,n} + \left(\mathsf{Q}_{h,n}\right)^T &= h\mathbf{I}_{N^{\mathrm{F}}} \otimes \begin{bmatrix} 0 & \\ & \mathsf{B}_n^{\mathrm{P}} \end{bmatrix}, \qquad n = 1, 2 \\ &\approxeq \int_{\widehat{D}} u \frac{\partial v}{\partial x_n} + \int_{\widehat{D}} v \frac{\partial u}{\partial x_n} = \int_{\partial \widehat{D}} uv \widehat{\mathbf{n}}_n \end{aligned}$$

Quadrature based operators on the reference wedge

- Spectral differentiation matrix D^{F} on z direction

$$\mathsf{D}^{\mathsf{F}} = \begin{bmatrix} 0 & & & -\frac{1}{2}\cot\frac{h}{2} \\ -\frac{1}{2}\cot\frac{h}{2} & \ddots & \ddots & \frac{1}{2}\cot h \\ \frac{1}{2}\cot h & & \ddots & -\frac{1}{2}\cot\frac{3h}{2} \\ \vdots & \ddots & \ddots & \vdots \\ \frac{1}{2}\cot\frac{h}{2} & & & 0 \end{bmatrix}, \quad \mathsf{D}^{\mathsf{F}} + (\mathsf{D}^{\mathsf{F}})^T = 0, \quad \mathsf{D}^{\mathsf{F}}\mathbf{1} = 0$$

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- Hybridized operator on z direction

$$\mathsf{Q}_{h,3} = h\mathsf{D}^{\mathrm{F}} \otimes \begin{bmatrix} \mathsf{W}^{\mathrm{P}} & \\ & \mathbf{0} \end{bmatrix}$$

mimics integration by parts

$$\mathsf{Q}_{h,3} + (\mathsf{Q}_{h,3})^T = 0 \approxeq \int_{\widehat{D}} u\frac{\partial v}{\partial x_3} + \int_{\widehat{D}} v\frac{\partial u}{\partial x_3} = \int_{\partial\widehat{D}} uv\widehat{\mathsf{n}}_3 = 0$$

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Entropy conservative fluxes and flux differencing

- Tadmor's entropy conservative numerical flux:

$$\boldsymbol{f}_S(\boldsymbol{u}, \boldsymbol{u}) = \boldsymbol{f}(\boldsymbol{u}) \qquad \text{(consistency)}$$

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

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

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(\boldsymbol{v}(\boldsymbol{u}_L)-\boldsymbol{v}(\boldsymbol{u}_R))^T\boldsymbol{f}_S(\boldsymbol{u}_L,\boldsymbol{u}_R) &= \psi(\boldsymbol{v}(\boldsymbol{u}_L))-\psi(\boldsymbol{v}(\boldsymbol{u}_R)) \\
&&& \text{(entropy conservation)}
\end{aligned}
$$

- Flux differencing technique

$$
\frac{\partial \boldsymbol{f}(\boldsymbol{u}(\boldsymbol{x}))}{\partial x_i} = 2\frac{\partial \boldsymbol{f}_S(\boldsymbol{u}(\boldsymbol{x}),\boldsymbol{u}(\boldsymbol{y}))}{\partial x_i}\bigg|_{\boldsymbol{x}=\boldsymbol{y}} \approx 2(\mathsf{D}\circ\mathsf{F})\mathbf{1}
$$

Entropy projection

- Recall the first step in proof of entropy inequality

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = 0 \Longrightarrow \int_\Omega \boldsymbol{v}^T \frac{\partial \boldsymbol{u}}{\partial t} + \int_\Omega \boldsymbol{v}^T \frac{\partial \boldsymbol{f}(\boldsymbol{u})}{\partial x} = 0$$

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- Entropy projected variables, approximation of $\Pi_N \boldsymbol{v}$

$$\boldsymbol{v}_h = \mathsf{P}_q \boldsymbol{v}(\mathsf{u}_q)$$

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- Entropy conservation of the numerical flux

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

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- Entropy projected conservative variables, approximation of $\boldsymbol{u}(\Pi_N \boldsymbol{v})$

$$\widetilde{\boldsymbol{u}} = \boldsymbol{u}(\mathsf{V}_h \boldsymbol{v}_h)$$

ESDG-Fourier formulation on the reference element

- DG variational formulation

$$\frac{\partial \boldsymbol{u}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \boldsymbol{f}_i(\boldsymbol{u})}{\partial x_i} = 0$$

ESDG-Fourier formulation on the reference element

- DG variational formulation

$$\frac{\partial \boldsymbol{u}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \boldsymbol{f}_i(\boldsymbol{u})}{\partial x_i} = 0$$

$$\left(\frac{\partial \boldsymbol{u}_N}{\partial t}, \varphi_m\right)_{\widehat{D}} + \sum_{i=1}^{3}\left(\frac{\partial \boldsymbol{f}_i(\boldsymbol{u}_N)}{\partial x_i}, \varphi_m\right)_{\widehat{D}} + \sum_{i=1}^{3}\langle \widehat{\mathsf{n}}_i \cdot (\mathsf{f}_i^* - \boldsymbol{f}_i(\boldsymbol{u}_N)), \varphi_m\rangle_{\partial\widehat{D}} = 0,$$

$$m = 1, \ldots, N_p \qquad \text{(Galerkin approximation)}$$

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$$m = 1, \ldots, N_p \qquad \text{(Galerkin approximation)}$$

- ESDG-Fourier formulation

$$\mathsf{M}\frac{\partial \mathbf{u}_h}{\partial t} = -\mathsf{V}_h^T\left(\sum_{i=1}^{3} 2(\mathsf{Q}_{h,i} \circ \mathsf{F}_i)\mathbf{1}\right) - \mathsf{V}_f^T \sum_{i=1}^{2} \mathsf{B}_i(\mathbf{f}_i^* - \boldsymbol{f}_i(\widetilde{\mathbf{u}}_f))$$

$$(\mathsf{F}_n)_{ij} = \boldsymbol{f}_{n,S}(\widetilde{\mathbf{u}}_i, \widetilde{\mathbf{u}}_j), \quad 1 \le i,j \le N_h$$

Proof of entropy conservation

Theorem (Conservation of entropy)

Let $\boldsymbol{f}_{i,S}$ be an entropy conservative flux. Assuming continuity in time, if $\eta(\mathbf{u}_h)$ is convex, solutions $\mathbf{u}_h$ satisfy a semi-discrete conservation of entropy

$$\mathbf{1}^T \mathsf{W} \frac{\mathrm{d}\eta(\mathbf{u}_q)}{\mathrm{d}t} = \sum_{i=1}^{d-1} \mathbf{1}^T \mathsf{W}_f (\mathrm{diag}(\widehat{\mathbf{n}}_i)(\psi_i(\widetilde{\mathbf{u}}_f) - \widetilde{\mathbf{v}}_f^T \mathbf{f}_i^*))$$

which are the quadrature approximations to the following

$$\int_{\widehat{D}} \frac{\partial \eta(\boldsymbol{u}_N)}{\partial t}\, \mathrm{d}\boldsymbol{x} = \sum_{i=1}^{d} \int_{\partial \widehat{D}} (\psi_i(\Pi_N \boldsymbol{v}) - (\Pi_N \boldsymbol{v})^T \boldsymbol{f}_i^*) \boldsymbol{n}_i^k,$$

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- Test with $\boldsymbol{v}_h$. Volume contributions

$$-\mathbf{v}_h^T \mathbf{V}_h^T \left(\sum_{n=1}^{d} 2(\mathbf{Q}_{h,n} \circ \mathbf{F}_n)\mathbf{1}\right) = -\sum_{n=1}^{d} \sum_{i,j} (\mathbf{Q}_{h,n})_{ij} (\widetilde{\mathbf{v}}_i - \widetilde{\mathbf{v}}_j)^T \boldsymbol{f}_{n,S}(\widetilde{\boldsymbol{u}}_i, \widetilde{\boldsymbol{u}}_j)$$

Proof of entropy conservation

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Let $\boldsymbol{f}_{i,S}$ be an entropy conservative flux. Assuming continuity in time, if $\eta(\mathbf{u}_h)$ is convex, solutions $\mathbf{u}_h$ satisfy a semi-discrete conservation of entropy

$$\mathbf{1}^T \mathsf{W} \frac{\mathrm{d}\eta(\mathbf{u}_q)}{\mathrm{d}t} = \sum_{i=1}^{d-1} \mathbf{1}^T \mathsf{W}_f \left(\operatorname{diag}(\widehat{\mathbf{n}}_i)(\psi_i(\widetilde{\mathbf{u}}_f) - \widetilde{\mathbf{v}}_f^T \mathbf{f}_i^*)\right)$$

which are the quadrature approximations to the following

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- Test with $\boldsymbol{v}_h$. Volume contributions

$$-\mathbf{v}_h^T \mathbf{V}_h^T \left(\sum_{n=1}^{d} 2(\mathbf{Q}_{h,n} \circ \mathbf{F}_n)\mathbf{1}\right) = -\sum_{n=1}^{d} \sum_{i,j} (\mathbf{Q}_{h,n})_{ij} (\psi_n(\widetilde{\mathbf{v}}_i) - \psi_n(\widetilde{\mathbf{v}}_j))$$

Proof of entropy conservation

Theorem (Conservation of entropy)

Let $\boldsymbol{f}_{i,S}$ be an entropy conservative flux. Assuming continuity in time, if $\eta(\mathbf{u}_h)$ is convex, solutions $\mathbf{u}_h$ satisfy a semi-discrete conservation of entropy

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- Test with $\boldsymbol{v}_h$. Volume contributions

$$-\mathbf{v}_h^T \mathbf{V}_h^T (\sum_{n=1}^{d} 2(\mathbf{Q}_{h,n} \circ \mathbf{F}_n)\mathbf{1}) = -\sum_{n=1}^{d} \psi_n(\widetilde{\mathbf{v}})^T (\mathbf{Q}_{h,n} - \mathbf{Q}_{h,n}^T)\mathbf{1}$$

Proof of entropy conservation

Theorem (Conservation of entropy)

Let $\boldsymbol{f}_{i,S}$ be an entropy conservative flux. Assuming continuity in time, if $\eta(\mathbf{u}_h)$ is convex, solutions $\mathbf{u}_h$ satisfy a semi-discrete conservation of entropy

$$\mathbf{1}^T \mathbf{W} \frac{\mathrm{d}\eta(\mathbf{u}_q)}{\mathrm{d}t} = \sum_{i=1}^{d-1} \mathbf{1}^T \mathbf{W}_f (\operatorname{diag}(\widehat{\mathbf{n}}_i)(\psi_i(\widetilde{\mathbf{u}}_f) - \widetilde{\mathbf{v}}_f^T \mathbf{f}_i^*))$$

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- Test with $\boldsymbol{v}_h$. Volume contributions

$$-\mathbf{v}_h^T \mathbf{V}_h^T (\sum_{n=1}^{d} 2(\mathbf{Q}_{h,n} \circ \mathbf{F}_n)\mathbf{1}) = -\sum_{n=1}^{d-1} \psi_n(\widetilde{\mathbf{v}})^T (2\mathbf{Q}_{h,n} - \mathbf{B}_{h,n}^T)\mathbf{1} - \psi_d(\widetilde{\mathbf{v}})^T 2\mathbf{Q}_{h,d}\mathbf{1}$$

Proof of entropy conservation

Theorem (Conservation of entropy)

Let $\boldsymbol{f}_{i,S}$ be an entropy conservative flux. Assuming continuity in time, if $\eta(\mathbf{u}_h)$ is convex, solutions $\mathbf{u}_h$ satisfy a semi-discrete conservation of entropy

$$\mathbf{1}^T\mathbf{W}\frac{\mathrm{d}\eta(\mathbf{u}_q)}{\mathrm{d}t} = \sum_{i=1}^{d-1}\mathbf{1}^T\mathbf{W}_f(\operatorname{diag}(\widehat{\mathbf{n}}_i)(\psi_i(\widetilde{\mathbf{u}}_f) - \widetilde{\mathbf{v}}_f^T\mathbf{f}_i^*))$$

which are the quadrature approximations to the following

$$\int_{\widehat{D}} \frac{\partial\eta(\boldsymbol{u}_N)}{\partial t}\,\mathrm{d}\boldsymbol{x} = \sum_{i=1}^{d}\int_{\partial\widehat{D}}(\psi_i(\Pi_N\boldsymbol{v}) - (\Pi_N\boldsymbol{v})^T\boldsymbol{f}_i^*)\boldsymbol{n}_i^k,$$

- Test with $\boldsymbol{v}_h$. Volume contributions

$$-\mathbf{v}_h^T\mathbf{V}_h^T(\sum_{n=1}^{d}2(\mathbf{Q}_{h,n}\circ\mathbf{F}_n)\mathbf{1}) = \sum_{n=1}^{d-1}\psi_n(\widetilde{\mathbf{v}})^T\mathbf{B}_{h,n}^T\mathbf{1}$$

GPU implementation - Two kernel split

- Skew-symmetric formulation

$$\frac{\partial \mathsf{u}_h^k}{\partial t} = -\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_h^T\Big(\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^k - (\mathsf{Q}_{h,n}^k)^T)\circ \mathsf{F}_n^k)\mathbf{1} + 2(\mathsf{Q}_{h,3}^k \circ \mathsf{F}_3^k)\Big)$$
$$-\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_f^T\sum_{m=1}^{d-1}\mathsf{B}_m^k\mathsf{f}_m^*, \quad (\mathsf{F}_n^k)_{ij} = \boldsymbol{f}_{n,S}(\widetilde{\mathsf{u}}_i^k, \widetilde{\mathsf{u}}_j^k)$$

GPU implementation - Two kernel split

- Skew-symmetric formulation

$$\underbrace{\frac{\partial \mathsf{u}_h^k}{\partial t}}_{\text{update kernel}} = -\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_h^T\Big(\underbrace{\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^k - (\mathsf{Q}_{h,n}^k)^T)\circ \mathsf{F}_n^k)\mathbf{1}}_{\text{xy flux-differencing kernel}} + \underbrace{2(\mathsf{Q}_{h,3}^k \circ \mathsf{F}_3^k)}_{\text{z flux-differencing kernel}}\Big)$$

$$\underbrace{-\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_f^T\sum_{m=1}^{d-1}\mathsf{B}_m^k\mathsf{f}_m^*}_{\text{surface kernel}}, \quad (\mathsf{F}_n^k)_{ij} = \boldsymbol{f}_{n,S}\,\underbrace{(\widetilde{\mathsf{u}}_i^k, \widetilde{\mathsf{u}}_j^k)}_{\text{entropy projection kernel}}$$

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$$\underbrace{-\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_f^T\sum_{m=1}^{d-1}\mathsf{B}_m^k\mathbf{f}_m^*}_{\text{surface kernel}}, \quad (\mathsf{F}_n^k)_{ij} = \boldsymbol{f}_{n,S}\,(\underbrace{\widetilde{\mathbf{u}}_i^k, \widetilde{\mathbf{u}}_j^k}_{\text{entropy projection kernel}})$$

GPU implementation - Two kernel split

- Skew-symmetric formulation

$$\underbrace{\frac{\partial \mathbf{u}_h^k}{\partial t}}_{\text{update kernel}} = -\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_h^T\Big(\underbrace{\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^k - (\mathsf{Q}_{h,n}^k)^T)\circ \mathsf{F}_n^k)\mathbf{1} +}_{\text{xy flux-differencing kernel}} \underbrace{2(\mathsf{Q}_{h,3}^k \circ \mathsf{F}_3^k)}_{\text{z flux-differencing kernel}}\Big)$$

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GPU implementation - Two kernel split

- Skew-symmetric formulation

$$\underbrace{\frac{\partial \mathbf{u}_h^k}{\partial t}}_{\text{update kernel}} = -\frac{1}{J^k}\mathbf{M}^{-1}\mathbf{V}_h^T\Big(\underbrace{\sum_{n=1}^{2}\big((\mathbf{Q}_{h,n}^k - (\mathbf{Q}_{h,n}^k)^T) \circ \mathbf{F}_n^k\big)\mathbf{1}}_{\text{xy flux-differencing kernel}} + \underbrace{2(\mathbf{Q}_{h,3}^k \circ \mathbf{F}_3^k)}_{\text{z flux-differencing kernel}}\Big)$$

$$\underbrace{-\frac{1}{J^k}\mathbf{M}^{-1}\mathbf{V}_f^T\sum_{m=1}^{d-1}\mathbf{B}_m^k\mathbf{f}_m^*}_{\text{surface kernel}}, \quad (\mathbf{F}_n^k)_{ij} = f_{n,S}\underbrace{(\widetilde{\mathbf{u}}_i^k, \widetilde{\mathbf{u}}_j^k)}_{\text{entropy projection kernel}}$$

- Evalute flux matrix $\mathbf{F}$ on-the-fly

GPU implementation - Two kernel split

- Skew-symmetric formulation

$$\underbrace{\frac{\partial \mathbf{u}_h^k}{\partial t}}_{\text{update kernel}} = -\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_h^T\Big(\underbrace{\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^k - (\mathsf{Q}_{h,n}^k)^T)\circ \mathsf{F}_n^k)\mathbf{1}}_{\text{xy flux-differencing kernel}} + \underbrace{2(\mathsf{Q}_{h,3}^k \circ \mathsf{F}_3^k)}_{\text{z flux-differencing kernel}}\Big)$$

$$\underbrace{-\frac{1}{J^k}\mathsf{M}^{-1}\mathsf{V}_f^T\sum_{m=1}^{d-1}\mathsf{B}_m^k\mathbf{f}_m^*}_{\text{surface kernel}}, \quad (\mathsf{F}_n^k)_{ij} = \boldsymbol{f}_{n,S}\underbrace{(\widetilde{\mathbf{u}}_i^k, \widetilde{\mathbf{u}}_j^k)}_{\substack{\text{entropy}\\ \text{projection}\\ \text{kernel}}}$$

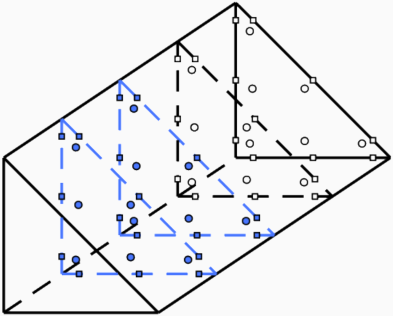
- Evalute flux matrix F on-the-fly
- Two kernel split: data locality

GPU implementation - Triangle kernel

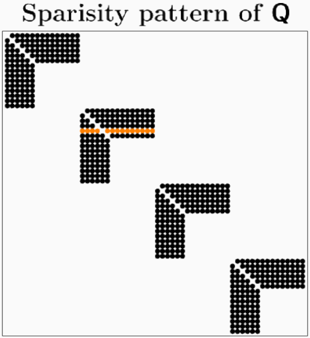
$$\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^{k} - (\mathsf{Q}_{h,n}^{k})^{T}) \circ \mathsf{F}_{n}^{k})\mathbf{1}$$

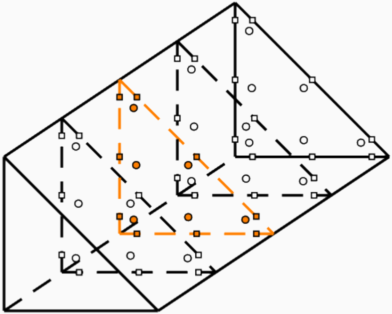
GPU implementation - Triangle kernel

$$\sum_{n=1}^{2}((\mathsf{Q}_{h,n}^{k} - (\mathsf{Q}_{h,n}^{k})^{T}) \circ \mathsf{F}_{n}^{k})\mathbf{1}$$



$$\text{At row } i: \sum_{n=1}^{2} (((\mathbf{Q}^k_{h,n} - (\mathbf{Q}^k_{h,n})^T) \circ \mathbf{F}^k_n)\mathbf{1})_i$$



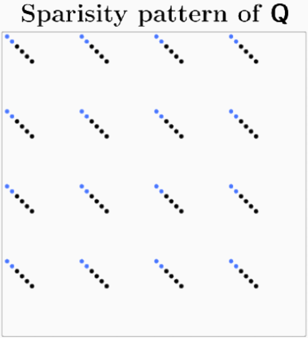


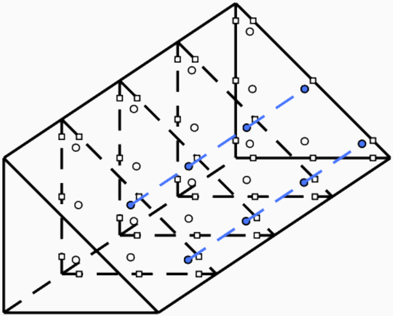
GPU implementation - Fourier mode kernel

$$(\mathsf{Q}_{h,3}^{k} \circ \mathsf{F}_3^{k})\mathbf{1}$$

GPU implementation - Fourier mode kernel

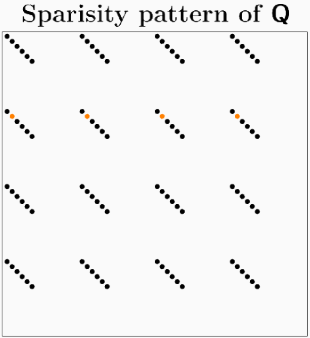
$$(\mathsf{Q}_{h,3}^{k} \circ \mathsf{F}_{3}^{k})\mathbf{1}$$

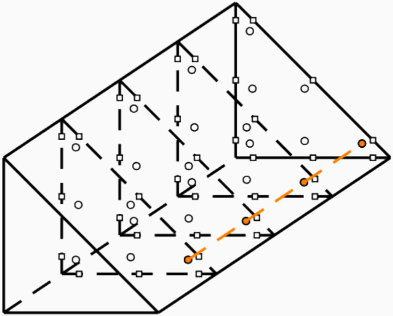




GPU implementation - Fourier mode kernel

At row i : $((\mathbf{Q}_{h,n}^{k} \circ \mathbf{F}_{n}^{k})\mathbf{1})_i$





Compressible Euler equations

- Compressible Euler equations in conservation form

$$\frac{\partial \boldsymbol{U}}{\partial t} + \sum_{i=1}^{3} \frac{\partial \boldsymbol{f}_i(\boldsymbol{U})}{\partial \boldsymbol{x}_i} = 0$$

$$\boldsymbol{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \end{bmatrix}, \quad \boldsymbol{f}_i(\boldsymbol{U}) = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ u(E+p) \end{bmatrix}, \begin{bmatrix} \rho v \\ \rho u v \\ \rho v^2 + p \\ \rho v w \\ v(E+p) \end{bmatrix}, \begin{bmatrix} \rho w \\ \rho u w \\ \rho v w \\ \rho w^2 + p \\ w(E+p) \end{bmatrix}$$

- Chandrashekar's entropy conservative flux[3], log mean $\{\!\{u\}\!\}^{\log} = \frac{u_L - u_R}{\log u_L - \log u_R}$

$$\boldsymbol{f}_{i,S}(\boldsymbol{U}_L, \boldsymbol{U}_R) = \begin{bmatrix} \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\}^2 + p_{\text{avg}} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\}\{\!\{v\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\}\{\!\{w\}\!\} \\ (E_{\text{avg}} + p_{\text{avg}})\{\!\{u\}\!\} \end{bmatrix}, \begin{bmatrix} \{\!\{\rho\}\!\}^{\log}\{\!\{v\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\}\{\!\{v\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{v\}\!\}^2 + p_{\text{avg}} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{v\}\!\}\{\!\{w\}\!\} \\ (E_{\text{avg}} + p_{\text{avg}})\{\!\{v\}\!\} \end{bmatrix}, \begin{bmatrix} \{\!\{\rho\}\!\}^{\log}\{\!\{w\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{u\}\!\}\{\!\{w\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{v\}\!\}\{\!\{w\}\!\} \\ \{\!\{\rho\}\!\}^{\log}\{\!\{w\}\!\}^2 + p_{\text{avg}} \\ (E_{\text{avg}} + p_{\text{avg}})\{\!\{w\}\!\} \end{bmatrix}$$

[3] Chandrashekar, "Kinetic energy preserving and entropy stable finite volume schemes for compressible Euler and Navier-Stokes equations".

Numerical results: doubly periodic shear layers

- Density with Mach numbers $\mathrm{Ma} = 0.3$ and $\mathrm{Ma} = 0.7$: shocks formed

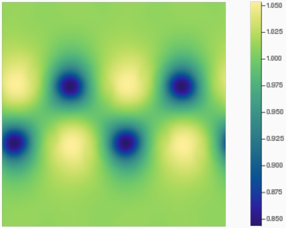


Figure 9: $\mathrm{Ma} = 0.3$, mode 4

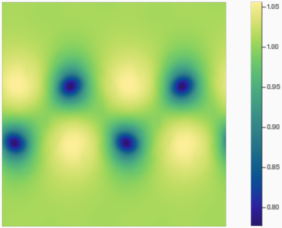


Figure 10: $\mathrm{Ma} = 0.3$, mode 8

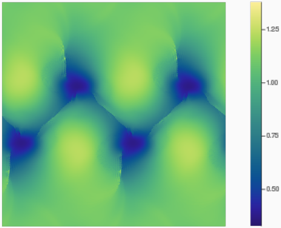


Figure 11: $\mathrm{Ma} = 0.7$, mode 4

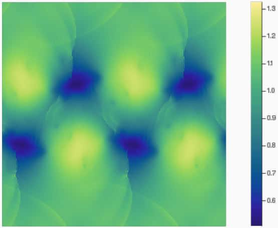


Figure 12: $\mathrm{Ma} = 0.7$, mode 8

1. Entropy Stable DG-Fourier methods

with Jesse Chan

2. Modal ESDG formulation for the compressible Navier-Stokes equation

with Jesse Chan and Tim Warburton

3. Positivity Limiting for nodal ESDG methods

with Jesse Chan, Xinhui Wu and Ignacio Tomas

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:

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

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

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

Integration by parts

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Integration by parts

$$\int_\Omega \frac{\partial \eta(\boldsymbol{u})}{\partial t} \leq \int_{\partial\Omega} \sum_{i=1}^{d} \left(\frac{1}{c_v T} \kappa \frac{\partial T}{\partial x_i} - F_i(\boldsymbol{u})\right) n_i \qquad \text{Heat entropy flow}$$

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$$\int_\Omega \frac{\partial \eta(\boldsymbol{u})}{\partial t} \leq 0 \qquad \text{Periodic}$$

Discretization of CNS

- Discretize the inviscid term by flux differencing and entropy projection

$$\frac{\partial \boldsymbol{f}_i(\boldsymbol{u})}{\partial x_i} \iff 2(\mathsf{Q} \circ \mathsf{F})\mathbf{1}$$

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

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

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- Difficult to enforce boundary condition because of $\{\{K\boldsymbol{\Theta}\}\}$

Viscous term discretization

- We write the system differently:

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

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- Viscous entropy dissipates

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

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- Easier to enforce boundary condition through $\boldsymbol{\sigma}^+$

Enforce boundary conditions

- Isothermal no-slip wall conditions

$$u_i = u_{i,\mathrm{wall}}, \quad i = 1, \ldots, d, \qquad T = T_{\mathrm{wall}}$$

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$$\begin{aligned} v_{1+i}^+ &= \frac{2u_{i,\mathrm{wall}}}{c_v T_{\mathrm{wall}}} - v_{1+i} \\ v_4^+ &= -\frac{2}{c_v T_{\mathrm{wall}}} - v_4 \\ \sigma_{2,i}^+ &= \sigma_{2,i}, \\ \sigma_{3,i}^+ &= \sigma_{3,i}, \\ \sigma_{4,i}^+ &= \sigma_{4,i}, \end{aligned}$$

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- Mimics entropy balance:

$$\sum_k (\boldsymbol{g}_{\mathrm{visc}}, \boldsymbol{v})_{D^k} = \sum_{i=1}^{d} \left\langle \frac{q_n}{c_v T_{\mathrm{wall}}}, 1 \right\rangle - \sum_k \left(\sum_{i,j=1}^{d} \left(\boldsymbol{K}_{ij} \boldsymbol{\Theta}_j, \boldsymbol{\Theta}_i \right) \right)_{D^k}$$

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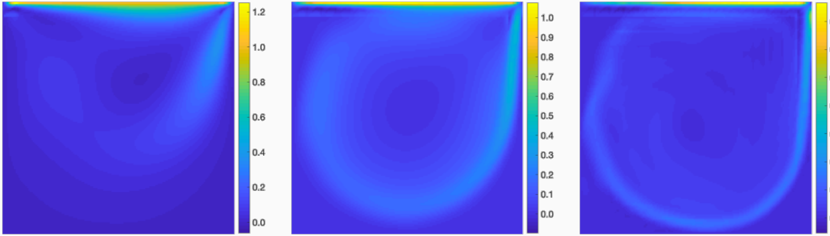
- Similarly for adiabatic no-slip and reflective wall boundary conditions.

Numerical results: Lid driven cavity

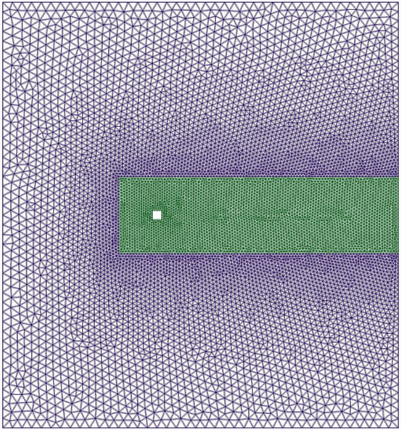
- Lid driven cavity with different *Re*



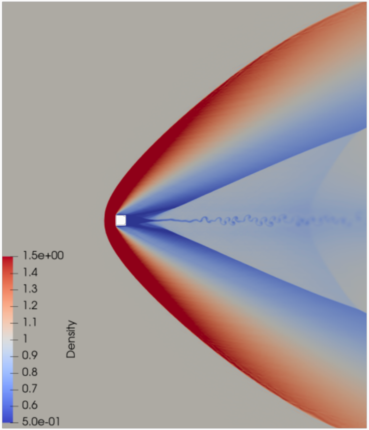
(a) Re = 100 (b) Re = 1000 (c) Re = 10000

Numerical results: Flow over cylinder

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



(a) Mesh



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

1. Entropy Stable DG-Fourier methods

with Jesse Chan

2. Modal ESDG formulation for the compressible Navier-Stokes equation

with Jesse Chan and Tim Warburton

3. Positivity Limiting for nodal ESDG methods

with Jesse Chan, Xinhui Wu and Ignacio Tomas

LeBlanc shocktube

- LeBlanc shocktube: strong shock forms

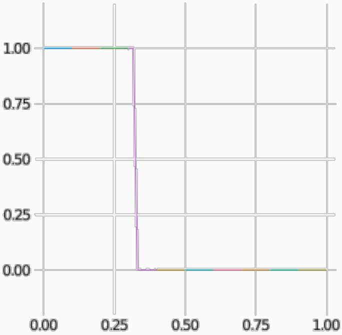


Figure 13: Initial condition

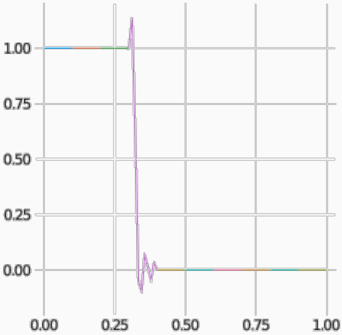
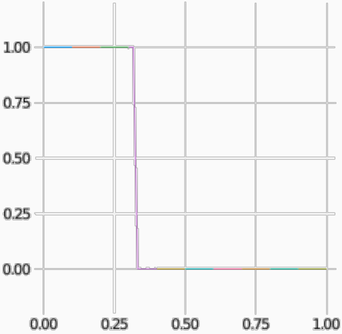


Figure 14: After a time step

LeBlanc shocktube

- LeBlanc shocktube: strong shock forms



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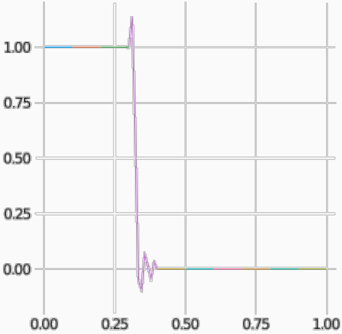

Figure 14: After a time step

- Oscillation by Gibbs phenomenon leads to negative density

Invariant sets

- A set $\mathcal{A}$ is an invariant set if the average of the solution $\boldsymbol{u}(\boldsymbol{x}, t)$ to the Riemann problem over $[-t\lambda_{\text{max}}, t\lambda_{\text{max}}]$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \frac{\partial f(\boldsymbol{u}) \cdot \boldsymbol{n}}{\partial x} = 0, \qquad \boldsymbol{u}(x, 0) = \begin{cases} \boldsymbol{u}^-, x < 0 \\ \boldsymbol{u}^+, x > 0 \end{cases}$$

remains in $\mathcal{A}$ for any $\boldsymbol{u}^+, \boldsymbol{u}^-, \boldsymbol{n}$ and $t > 0$.

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  remains in $\mathcal{A}$ for any $\boldsymbol{u}^+, \boldsymbol{u}^-, \boldsymbol{n}$ and $t > 0$.
- Compressible Euler: the set of states with positive density and internal energy is a convex invariant set.

$$\mathcal{A} = \{\boldsymbol{u} : \rho > 0, e > 0\}$$

Invariant domain discretization

- Low order IDP method could be written as

$$\underbrace{\boldsymbol{m}_i \frac{\partial \boldsymbol{u}}{\partial t} + \sum_{j \in \mathcal{N}(i)} \boldsymbol{c}_{ij} \boldsymbol{f}(\boldsymbol{u}_j)}_{\text{low order nodal DG}} - \underbrace{\sum_{j \in \mathcal{N}(i)} d_{ij}(\boldsymbol{u}_j - \boldsymbol{u}_i)}_{\text{graph viscosity}} = 0$$

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- Stiffness matrix $\boldsymbol{c}$ is a sparse low order 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:

$$d_{ij} = \max\left\{\lambda_{\max}(u_i, u_j, n_{ij})\|c_{ij}\|, \lambda_{\max}(u_j, u_i, n_{ji})\|c_{ij}\|\right\}, n_{ij} = c_{ij}/\|c_{ij}\|$$

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- (Guermond, Popov) Conservative and invariant domain preserving under certain CFL condition, so positivity preserving!

Limiting strategy

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

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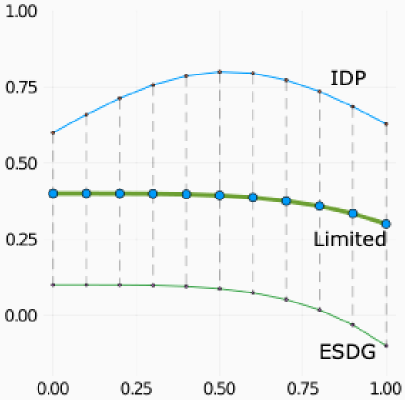
- Step 2. Compute low order IDP scheme (satisfies positivity)
- Step 3. Blend two schemes together through convex limiting



Convex Limiting

- Low order IDP and ESDG in algebraic flux form:

$$\frac{m_i}{\tau}(u_i^{L,n+1} - u_i^n) + \sum_{j \in \mathcal{N}(i)} \mathsf{F}_{ij}^{L,n} = 0$$

$$\frac{m_i}{\tau}(u_i^{H,n+1} - u_i^n) + \sum_{j \in \mathcal{N}(i)} \mathsf{F}_{ij}^{H,n} = 0$$

$$\mathsf{F}_{ij}^{L,n} = (f(u_i^n) + f(u_j^n))c_{ij} - d_{ij}(u_j - u_i), \qquad \mathsf{F}_{ij}^{H,n} = 2f_S(u_i^n, u_j^n)c_{ij}$$

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- Relation between low order IDP and ESDG solution

$$\boldsymbol{m}_i\boldsymbol{u}_i^{H,n+1} = \boldsymbol{m}_i\boldsymbol{u}_i^{L,n+1} + \sum_{j \in \mathcal{N}(i)} \tau(\mathsf{F}_{ij}^{L,n} - \mathsf{F}_{ij}^{H,n})$$

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

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

Convex Limiting

- Write limited solution as a convex combination of states

$$\boldsymbol{u}_i^{n+1} = \sum_{j \in \mathcal{N}(i)} \lambda_j (\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}), \qquad \mathsf{P}_{ij} = \frac{\tau}{\boldsymbol{m}_i \lambda_j} (\mathsf{F}_{ij}^{L,n} - \mathsf{F}_{ij}^{H,n})$$

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

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

$$\begin{aligned} l_{ij} = \max\{l \in [0,1] : \ & \rho(\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}) \geq 0, \\ & e(\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}) \geq 0\} \end{aligned}$$

Convex Limiting

- Write limited solution as a convex combination of states

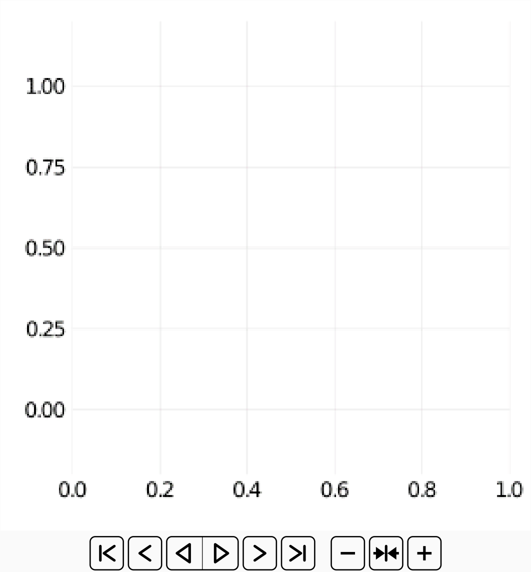
$$\boldsymbol{u}_i^{n+1} = \sum_{j \in \mathcal{N}(i)} \lambda_j (\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}), \qquad \mathsf{P}_{ij} = \frac{\tau}{\boldsymbol{m}_i \lambda_j} (\mathsf{F}_{ij}^{L,n} - \mathsf{F}_{ij}^{H,n})$$

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

$$\begin{aligned} l_{ij} = \max\{l \in [0,1] : \rho(\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}) \geq 0, \\ e(\boldsymbol{u}_i^{L,n} + l_{ij} \mathsf{P}_{ij}) \geq 0\} \end{aligned}$$

- Reduce to solving a quadratic equation

Numerical results: LeBlanc shocktube



Summary and future works

- Entropy stable high order discontinuous Galerkin-Fourier methods: semi-discrete entropy stability
- Modal ESDG formulation for the compressible Navier-Stokes equations
- Positivity limiting for nodal ESDG methods.
- Future work: curvilinear and moving meshes, positivity limiting for modal ESDG.

Thanks everyone for joining!