The pivotal role of entropy in the development of compressible Computational Fluid Dynamics algorithms

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Outline

Turbulence paramount in turbomachinery

- large range of scales, smallest <<< geometry
- high loaded machinery often transonic
- conditions often between laminar and turbulent
- important source of losses/entropy
- beneficial for operational range

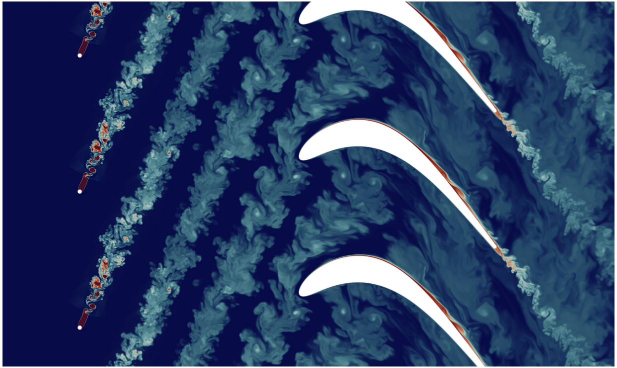
Turbulence models far from comfort zone

- very complex secondary flows
- often transition $\sim$ low Re, high acceleration
- interaction with shocks and shocklets
- transition, production, dissipation . . . $\sim$ vorticity **and** acoustics

Need for detailed turbulence budgets (DNS, LES)

Challenges:

- (shock) stabilisation $\leftrightarrow$ capturing turbulence
- importance of acoustic waves / effects



DNS of Spleen LPT cascade + wake generator experiment (Courtesy VKI and Cenaero)
Entropy generation and transport through cascade

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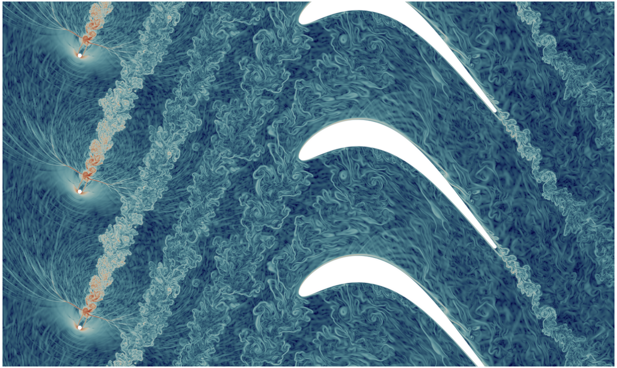

DNS of Speen LPT cascade + wake generator experiment (Courtesy VKI and Cenaero)
Density gradient troughout the cascade

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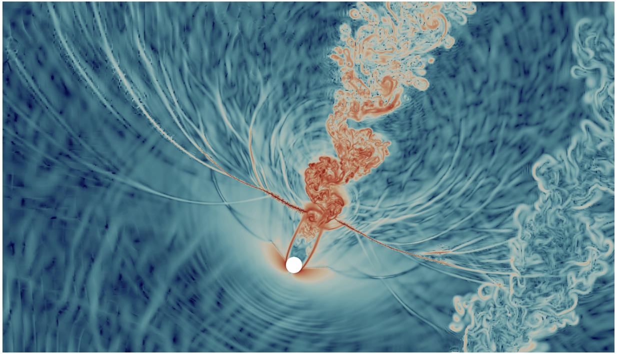
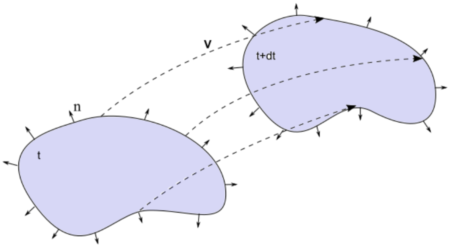


DNS of Speen LPT cascade + wake generator experiment (Courtesy VKI and Cenaero)
Density gradient near the wake generator

Conservation applied to volume moving with the flow

- mass conservation

$$\frac{\mathrm{d}}{\mathrm{dt}} \int_V \rho \, dV = 0$$



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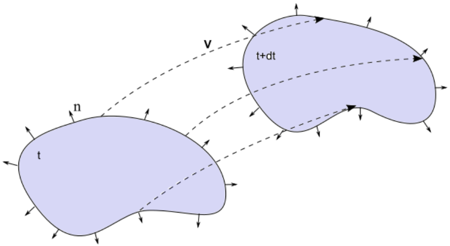
$$\int_V \frac{\partial \rho}{\partial t}\, dV + \oint_{\partial V} \rho \boldsymbol{v} \cdot \boldsymbol{n}\, dS = 0$$



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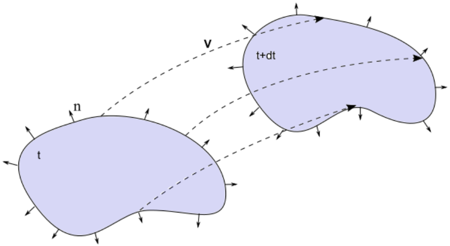

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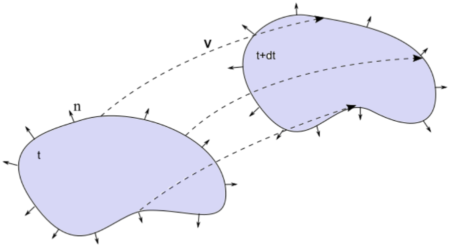

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- First law of thermodynamics: change of total energy $E = e + \mathcal{E}_k$ = work + heat exchage

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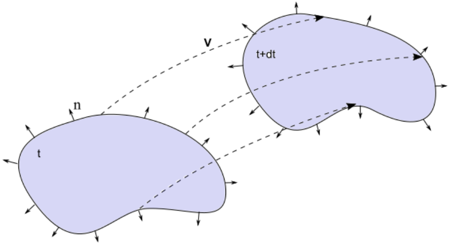

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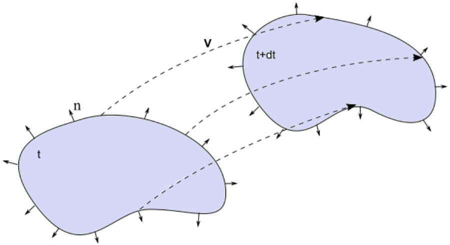

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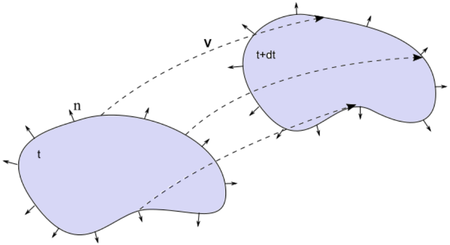

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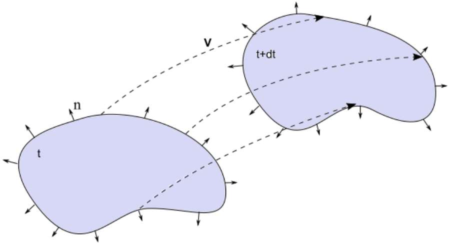

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$$\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \boldsymbol{v} = 0$$

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$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot \rho \boldsymbol{v} \boldsymbol{v} + \nabla p = \nabla \cdot \boldsymbol{\tau}$$

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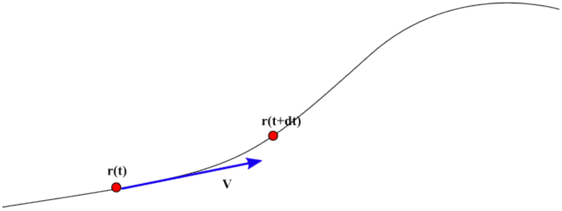
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot \rho \boldsymbol{v} H = \nabla \cdot \boldsymbol{v} \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{q}$$

Mechanical work along a on streamline



$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot \rho \boldsymbol{v} \boldsymbol{v} + \nabla p = \nabla \cdot \boldsymbol{\tau}$$

$$\Downarrow \cdot \boldsymbol{v}$$

$$\frac{\partial \rho \mathcal{E}_k}{\partial t} + \nabla \cdot \rho \boldsymbol{v} \mathcal{E}_k = \boldsymbol{v} \cdot (-\nabla p + \nabla \cdot \boldsymbol{\tau})$$

$$\Downarrow$$

$$\frac{\partial \rho \mathcal{E}_k}{\partial t} + \nabla \cdot \rho \boldsymbol{v} \mathcal{E}_k = -\nabla \cdot \boldsymbol{v} p + \nabla \cdot \boldsymbol{v} \cdot \tau + p \nabla \cdot \boldsymbol{v} - \boldsymbol{\tau} : \nabla \boldsymbol{v}$$

$$\Downarrow$$

$$\int_V \frac{\partial \mathcal{E}_k}{\partial t} \, dV + \oint_{\partial V} (\rho \boldsymbol{v} \cdot \boldsymbol{n}) \, \mathcal{E}_k \, dS = \underbrace{\oint_{\partial V} -\boldsymbol{v} \cdot p \boldsymbol{n} \, dS}_{\mathcal{W}_p} + \underbrace{\oint_{\partial V} \boldsymbol{v} \cdot \boldsymbol{\tau} \cdot \boldsymbol{n} \, dS}_{\mathcal{W}_\tau} + \underbrace{\int_V p \nabla \cdot \boldsymbol{v} \, dV}_{\mathcal{D}_p} - \underbrace{\int_V \boldsymbol{\tau} : \nabla \boldsymbol{v} \, dV}_{\epsilon > 0}$$

Subtract mechanical energy from total energy equation → conservation of internal energy

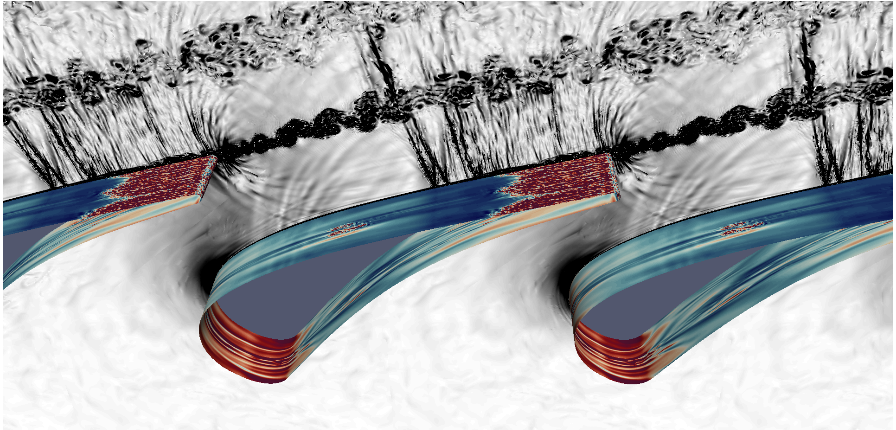
$$\frac{\partial \rho E}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} E + p\boldsymbol{v}) = \nabla \cdot \boldsymbol{v} \cdot \boldsymbol{\tau} + \nabla \cdot \boldsymbol{q}$$

$$\frac{\partial \rho \mathcal{E}_k}{\partial t} + \nabla \cdot (\rho \boldsymbol{v} \mathcal{E}_k + p\boldsymbol{v}) = \nabla \cdot \boldsymbol{v} \cdot \tau + p\nabla \cdot \boldsymbol{v} - \boldsymbol{\tau} : \nabla \boldsymbol{v}$$

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho \boldsymbol{v} e = -p\nabla \cdot \boldsymbol{v} + \boldsymbol{\tau} : \nabla \boldsymbol{v} + \nabla \cdot \boldsymbol{q}$$

Conservation equation for entropy *density*

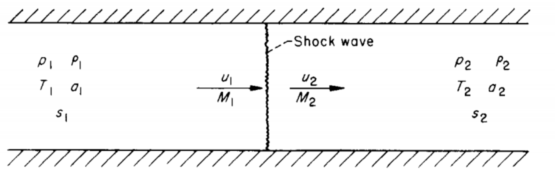
$$\frac{\partial \rho s}{\partial t} + \nabla \cdot \rho \boldsymbol{v} s = \frac{1}{T}\left(\underbrace{\boldsymbol{\tau} : \nabla \boldsymbol{v}}_{dq_{irr}} + \underbrace{\nabla \cdot \boldsymbol{q}}_{dq_{rev}}\right)$$

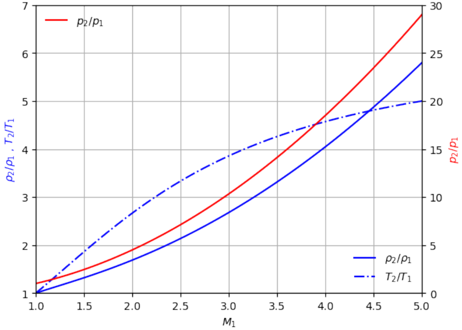


LES of the VKI LS89 high-pressure turbine inlet guide vane, condition MUR235
Numerical schlieren and wall heat flux (courtesy Cenaero and VKI)

Entropy in fluid dynamics

Shocks



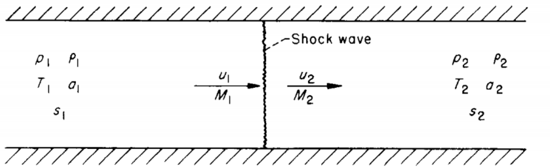


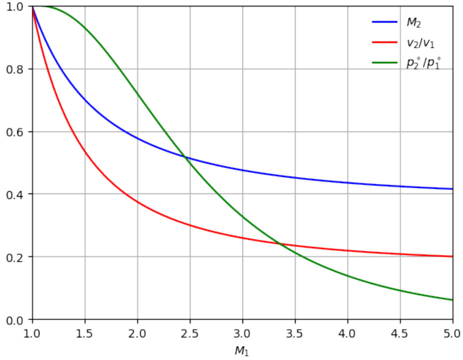
- conservation of mass, momentum and energy

  $$(p_1, T_1, v_1) \leftrightarrow (p_2, T_2, v_2)$$

- second law $s_2 > s_1$

  $$(p_1, T_1, v_1) \rightarrow (p_2, T_2, v_2)$$





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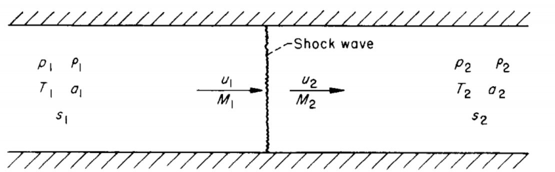

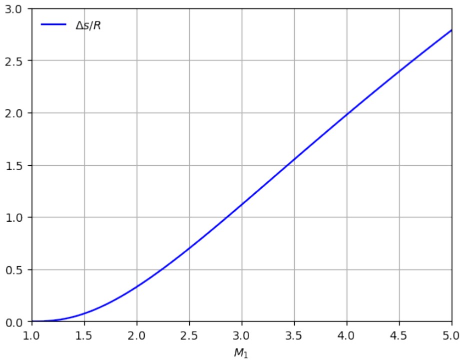

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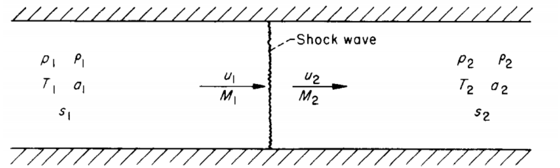

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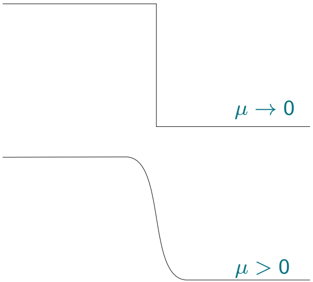

Effect of viscosity on dissipation $\boldsymbol{\tau} : \nabla \boldsymbol{v}$

- shock thickness depends on μ
- Δs independent
- Euler = vanishing viscosity solution

Thermodynamic conservation equations

- embedded in the Navier-Stokes equations
  - **total enthalpy**
  - **static enthalpy**: follows from the change from Lagrangian to Eulerian frame
  - **mechanical energy**: follows from calculating work along a stream line
  - **internal energy/entropy**: total energy - mechanical energy
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Shocks

- strength determined by conservation of mass, momentum and energy
- entropy generation - by viscous stresses - is independent of the viscosity
- **vanishing viscosity solution**: inviscid flow is limit $\mu \rightarrow 0$

Navier-Stokes equations

$$\int_V \frac{\partial \rho}{\partial t}\, dV + \oint_{\partial V} \rho \boldsymbol{v} \cdot \boldsymbol{n}\, dS = 0$$
$$\int_V \frac{\partial \rho \boldsymbol{v}}{\partial t}\, dV + \oint_{\partial V} \left((\rho \boldsymbol{v} \cdot \boldsymbol{n})\, \boldsymbol{v} + p\boldsymbol{n} - \boldsymbol{\tau} \cdot \boldsymbol{n} \right)\, dS = 0$$
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Generic set of conservation equations

$$\int_V \frac{\partial \boldsymbol{u}}{\partial t}\, dV + \oint_{\partial V} \left(\mathbf{f}(\boldsymbol{u}) \cdot \boldsymbol{n} - \mathbf{d}(\boldsymbol{u}, \nabla \boldsymbol{u}) \cdot \boldsymbol{n} \right)\, dS = 0$$

with conservative variables $\boldsymbol{u}$, convective $\mathbf{f}$ and diffusive flux vector $\mathbf{d}$

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Mathematical entropy $\mathcal{S}$ and entropy flux $\mathcal{F}$

- **entropy variables w**

$$w_m = \frac{\partial \mathcal{S}}{\partial u_m}$$

- existence of (scalar) **entropy flux** $\mathcal{F}$

$$\frac{\partial \mathcal{F}}{\partial u_m} = \frac{\partial \mathcal{S}}{\partial u_n} \frac{\partial \mathbf{f}_n}{\partial u_m}$$

- convexity of diffusive flux **d**

$$\nabla w_m \cdot \mathbf{d}_m \geq 0$$

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Navier-Stokes equations : $\mathcal{S} = -\rho s$ [Hughes1986]

Variational formulation of conservation equations

$$w_m \cdot \frac{\partial u_m}{\partial t} + w_m \nabla \cdot \mathbf{f}_m = w_m \nabla \cdot \mathbf{d}_m$$

$$\Downarrow$$

$$\frac{\partial \mathcal{S}}{\partial u_m} \frac{\partial u_m}{\partial t} + \frac{\partial \mathcal{S}}{\partial u_m} \frac{\partial \mathbf{f}_m}{\partial u_n} \cdot \nabla u_n = w_m \nabla \cdot \mathbf{d}_m$$

$$\Downarrow$$

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{\partial \boldsymbol{\mathcal{F}}}{\partial u_m} \cdot \nabla u_m = w_m \nabla \cdot \mathbf{d}_m$$

$$\Downarrow$$

$$\frac{\partial \mathcal{S}}{\partial t} + \nabla \cdot \boldsymbol{\mathcal{F}} = \mathbf{w}_m \cdot \nabla \cdot \mathbf{d}_m$$

Conservation formulation $\rightarrow$ bound for entropy [Harten1983,Tadmor2003]

$$\int_V \frac{\partial \mathcal{S}}{\partial t} \, dV + \oint_{\partial V} \boldsymbol{\mathcal{F}} \cdot \boldsymbol{n} \, dS = \oint_{\partial V} w_m \mathbf{d}_m \cdot \boldsymbol{n} \, dS - \int_V \nabla w_m \cdot \mathbf{d}_m \, dV$$

Existence of mathematical entropy : stability of physical systems

- all conservation equations can be collapsed onto a single one
- this equation describes the convection of entropy and it's destruction
- the entropy serves as a bounded energy, proving stability of the system of equations

Numerical approximations

- entropy equation is derived from conservation equations and therefore not necessarily satisfied
- embedding a discrete equivalent of the entropy equation can bound numerical solution

Shock position, strength and speed

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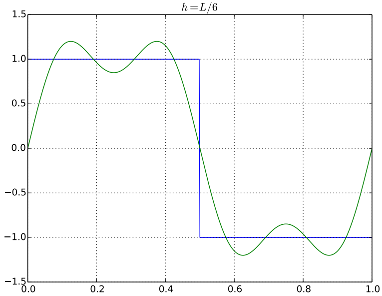
Shock capturing / representation

- numerical methods represent solutions by polynomials
- try to represent first p orders in Taylor expansion
- Gibbs oscillations due to non-convergence Taylor near shock



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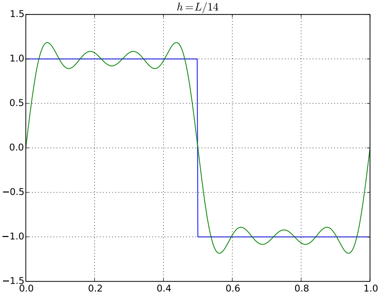
Shock capturing / representation

- numerical methods represent solutions by polynomials
- try to represent first p orders in Taylor expansion
- Gibbs oscillations due to non-convergence Taylor near shock



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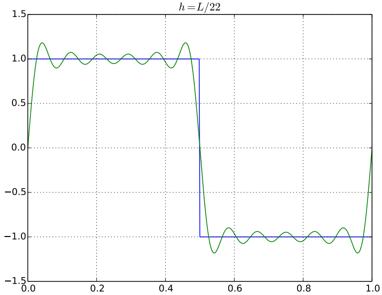

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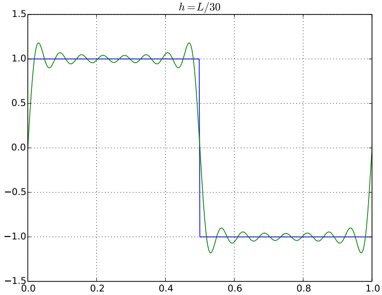

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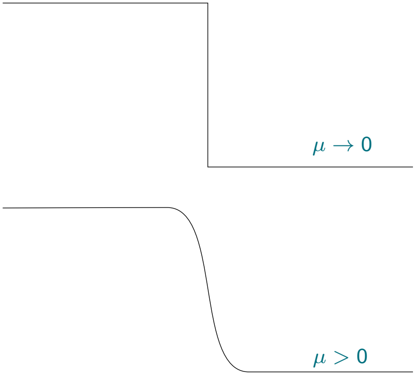

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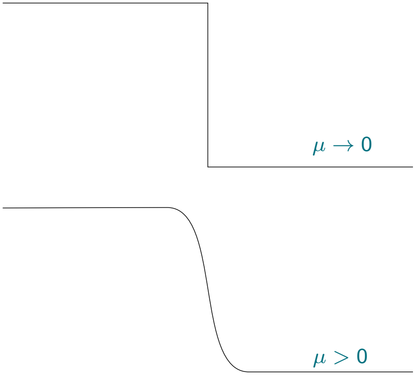
Non-linear stability required near shocks

- mimick physics: collapse all discrete equations onto entropy equation
- entropy generation mechanism ?
- discrete entropy variables

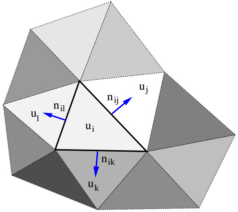


Vanishing diffusion conservation equation

$$\int_V \frac{\partial u_m}{\partial t} dV + \oint_{\partial V} \mathbf{f}_m \cdot \boldsymbol{n} dS = 0$$

Solving for average $\boldsymbol{u}^i$ on control volume V_i

$$V_i \frac{\mathrm{d}u_m^i}{\mathrm{dt}} = -\sum_j \mathcal{H}_m \left(\boldsymbol{u}^i, \boldsymbol{u}^j; \boldsymbol{n}^{ij}\right) = 0$$

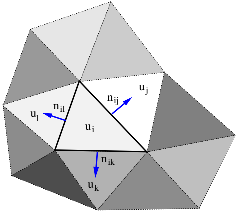


with the following requirements for the interface flux $\mathcal{H}(.,.;.)$

- conservativity $\mathcal{H}\left(\boldsymbol{u}^j, \boldsymbol{u}^i; -\boldsymbol{n}^{ij}\right) = -\mathcal{H}\left(\boldsymbol{u}^i, \boldsymbol{u}^j; \boldsymbol{n}^{ij}\right)$
- consistency $\mathcal{H}_m(\boldsymbol{u}, \boldsymbol{u}; \boldsymbol{n}) = \mathbf{f}_m \cdot \boldsymbol{n}$
- stability ?

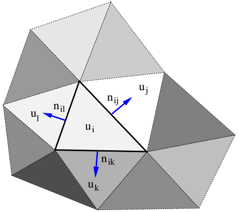
Evolution of entropy in each cell V_i

$$V_i \frac{\mathrm{d}u_m^i}{\mathrm{d}t} = -\sum_j \mathcal{H}_m\left(\boldsymbol{u}^i, \boldsymbol{u}^j; \boldsymbol{n}^{ij}\right)$$



Evolution of entropy in each cell V_i

$$V_i \, w_m^i \, \frac{\mathrm{d}u_m^i}{\mathrm{dt}} = -\sum_j w_m^i \, \mathcal{H}_m \left(\boldsymbol{u}^i, \boldsymbol{u}^j; \boldsymbol{n}^{ij} \right) - \boldsymbol{\mathcal{G}}(\boldsymbol{u}^i) \cdot \sum_j \boldsymbol{n}^{ij}$$



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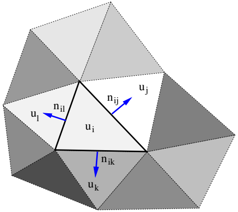
$$\sum_i V_i \frac{\mathrm{d}\mathcal{S}^i}{\mathrm{dt}} = -\sum_{i,j}\left(w_m^i - w_m^j\right)\mathcal{H}_m\left(\boldsymbol{u}^i, \boldsymbol{u}^j; \boldsymbol{n}^{ij}\right) - \left(\boldsymbol{\mathcal{G}}(\boldsymbol{u}^i) - \boldsymbol{\mathcal{G}}(\boldsymbol{u}^j)\right)\cdot \boldsymbol{n}^{ij}$$



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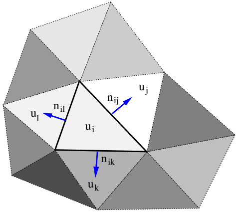

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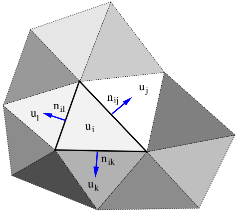
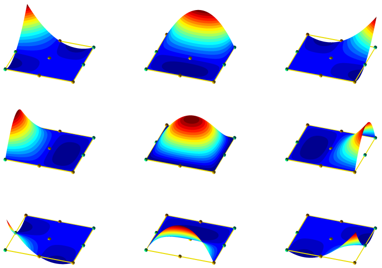
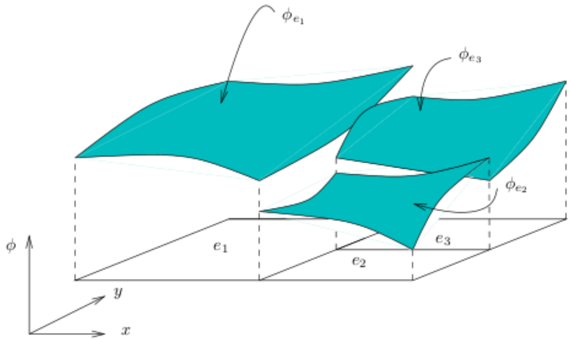


FEM interpolation of working variables $\boldsymbol{q}$

$$\boldsymbol{q} \in \mathcal{V}^N : (\boldsymbol{q}_m)_e = \sum_i \boldsymbol{q}_{im} \phi_i^e$$

ϕ_i^e shape functions for element e





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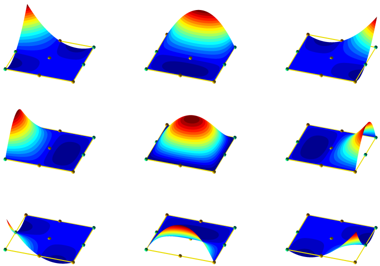
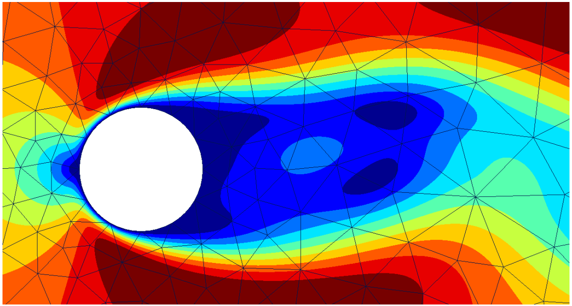
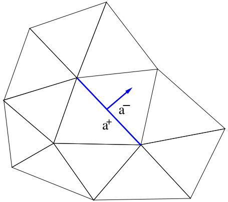




Galerkin variational formulation

$$\int_{\Omega} v_m \left(\frac{\partial u_m}{\partial t} + \nabla \cdot \mathbf{f}_m \right) dV = 0 \ , \ \forall v_m \in \mathcal{V}$$



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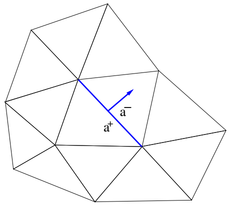

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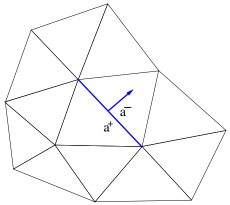

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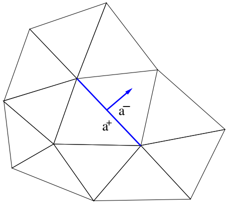

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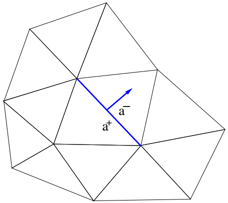

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Interface flux $\sim$ FVM

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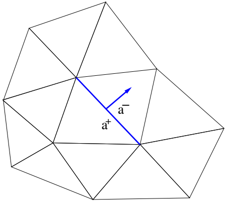

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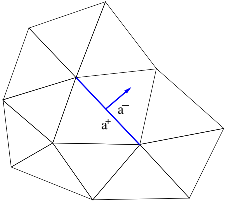

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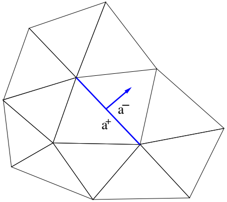

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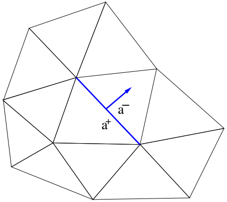

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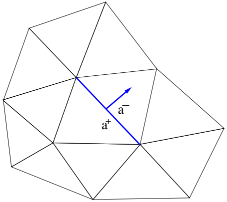

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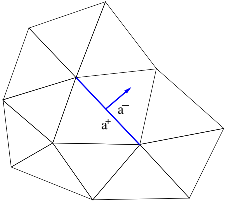

- discontinuity $\rightarrow$ interface fluxes $\mathcal{H}\left(\boldsymbol{q}^{+}, \boldsymbol{q}^{-}; \boldsymbol{n}\right)$
  - conservativity: $\mathcal{H}\left(\boldsymbol{q}^{+}, \boldsymbol{q}^{-}; \boldsymbol{n}\right) = -\mathcal{H}\left(\boldsymbol{q}^{-}, \boldsymbol{q}^{+}; -\boldsymbol{n}\right)$
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  - stability ?

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- rigourous non-linear stability: *Entropy Consistent Fluxes* "E-flux" [Oleinik]

$$\left(w_m^{+} - w_m^{-}\right)\left(\mathcal{H}_m\left(\boldsymbol{q}^{+}, \boldsymbol{q}^{-}; \boldsymbol{n}\right) - \mathbf{f}_m\left(\tilde{\boldsymbol{q}}\right) \cdot \boldsymbol{n}\right) \geq 0 \ , \ \forall \tilde{\boldsymbol{q}} \in \left[\boldsymbol{q}^{+}, \boldsymbol{q}^{-}\right]$$

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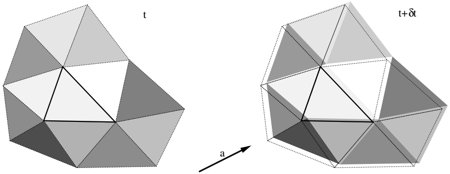
- *Approximate Riemann Solvers* usually are E-fluxes



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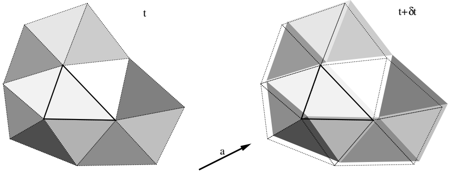
- E-fluxes positive dissipation $\rightarrow$ correct shock representation



- discontinuity → interface fluxes $\mathcal{H}\left(\boldsymbol{q}^+, \boldsymbol{q}^-; \boldsymbol{n}\right)$
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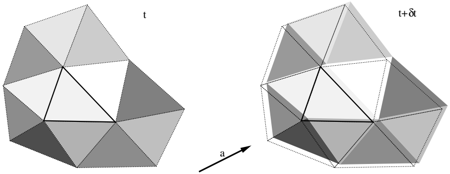
- Entropy consistent FVM
  - use of E-fluxes
  - *maximum criteria on high order reconstruction*



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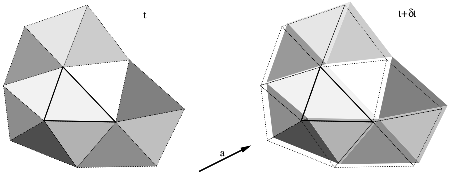
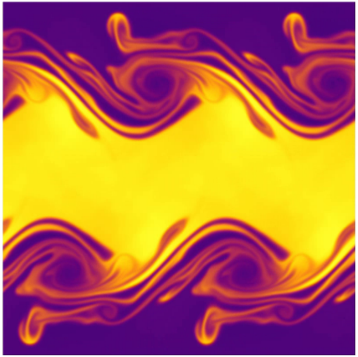
- *Approximate Riemann Solvers* usually are E-fluxes
- E-fluxes positive dissipation $\rightarrow$ correct shock representation
- Entropy consistent FVM
  - use of E-fluxes
  - *maximum criteria on high order reconstruction*
- Entropy stable DG (ESDG)
  - use $\mathbf{w}$ as working variables $\in \mathcal{V}$ instead of conservative $\boldsymbol{u}$
  - use of E-fluxes
  - *integration by parts* should be discretely mimicked *summation by parts*
  - quadrature error since update in conservative variables !

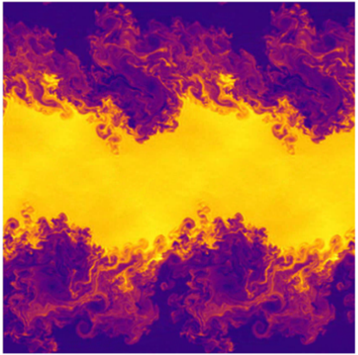


Challenges

- robustness with respect to shocks through energy stability
- minimal impact on turbulent flow features



Artificial viscosity



Entropy stable DG

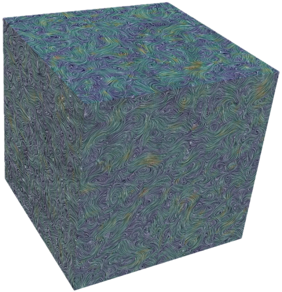
Kelvin-Helmholtz instability - impact of shock capturing strategies

Study submitted to Journal of Computational Physics [Bilocq24*]

- **DG**: vanilla DG without shock capturing (DG)
  - most accurate (no quadrature error)
  - no stabilisation
- **DG-AV**: DG + sensor based artificial viscosity [Person06][Henneman21]
  - additional viscosity at shocks $\rightarrow$ dissipates turbulence
  - sensors to detect underresolution
- **ESDG**: Entropy stable DG [Gassner16][Chan]
  - formulation in $\mathbf{w}$ error in update
  - full quadrature
  - expensive
- **ESDGSEM**: Spectral Element Entropy Stable DG [Gassner16][Chan19]
  - formulation in w
  - *summation by parts* by reduced tensor-product quadrature
- **DG-SBP**: summation by parts DG
  - DG operator expressed in conserved variables
  - summation by parts operator
- **DG-ES**: sensor based switch between DG and ESDG

Compressible homogeneous isotropic turbulence

- $M_t = 0.6,\ Re_\lambda = 100$
- starting from incompressible flow field
- high vorticity $\rightarrow \epsilon_s$
- acoustic transient $\rightarrow$ $epsilon_d$ and $\mathcal{D}_p$
- shocklets form $M \approx 2 \rightarrow \epsilon_d$ and $\mathcal{D}_p$
- N cells per direction, order p=5, equivalent resolution $n = (p+1)N = 66$



Kinetic energy budget on generic control volume

$$\int_V \frac{\partial \mathcal{E}_k}{\partial t}\, dV + \oint_{\partial V} (\rho \boldsymbol{v} \cdot \boldsymbol{n})\, \mathcal{E}_k \, dS = \oint_{\partial V} -\boldsymbol{v} \cdot p\boldsymbol{n}\, dS + \oint_{\partial V} \boldsymbol{v} \cdot \boldsymbol{\tau} \cdot \boldsymbol{n}\, dS + \int_V p \nabla \cdot \boldsymbol{v}\, dV - \int_V \boldsymbol{\tau} : \nabla \boldsymbol{v}\, dV$$

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - convergence criterion

Kinetic energy budget on fully periodic domain

$$\int_V \frac{\partial \mathcal{E}_k}{\partial t}\, dV + \cancel{\oint_{\partial V} (\rho \boldsymbol{v} \cdot \boldsymbol{n})\, \mathcal{E}_k \, dS} = \cancel{\oint_{\partial V} -\boldsymbol{v} \cdot p\boldsymbol{n}\, dS} + \cancel{\oint_{\partial V} \boldsymbol{v} \cdot \boldsymbol{\tau} \cdot \boldsymbol{n}\, dS} + \int_V p \nabla \cdot \boldsymbol{v}\, dV - \int_V \boldsymbol{\tau} : \nabla \boldsymbol{v}\, dV$$

Kinetic energy budget on

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Newtonian fluid $\boldsymbol{\tau} = \mu \left(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T - \frac{2}{3} \nabla \cdot \boldsymbol{v} \boldsymbol{I} \right)$ Split in solenoidal (vorticity) and dilatational dissipation

$$\int_V \boldsymbol{\tau} : \nabla \boldsymbol{v} dV = \underbrace{2 \int_V \mu \frac{\boldsymbol{\omega} \cdot \boldsymbol{\omega}}{2} dV}_{\epsilon_s} + \underbrace{\frac{4}{3} \int_V \mu \left(\nabla \cdot \boldsymbol{v} \right)^2 dV}_{\epsilon_d}$$

Kinetic energy budget on

$$\int_V \frac{\partial \mathcal{E}_k}{\partial t}\, dV + \cancel{\oint_{\partial V} (\rho \boldsymbol{v}\cdot\boldsymbol{n})\,\mathcal{E}_k\, dS} = \cancel{\oint_{\partial V} -\boldsymbol{v}\cdot p\boldsymbol{n}\, dS} + \cancel{\oint_{\partial V} \boldsymbol{v}\cdot\boldsymbol{\tau}\cdot\boldsymbol{n}\, dS} + \int_V p\nabla\cdot\boldsymbol{v}\, dV - \int_V \boldsymbol{\tau} : \nabla\boldsymbol{v}\, dV$$

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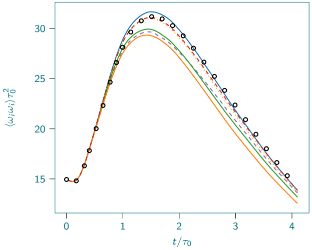
and therefore

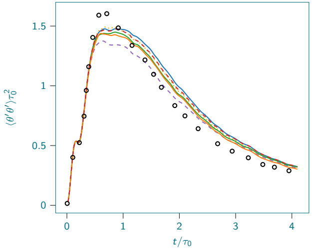
$$\underbrace{-\frac{\mathrm{d}\int_V}{\mathrm{d}t}\mathcal{E}_k dV}_{\epsilon_k} = \underbrace{2\int_V \mu\frac{\boldsymbol{\omega}\cdot\boldsymbol{\omega}}{2} dV}_{\epsilon_s} + \underbrace{\frac{4}{3}\int_V \mu\left(\nabla\cdot\boldsymbol{v}\right)^2 dV}_{\epsilon_d} - \underbrace{\int_V p\nabla\cdot\boldsymbol{v}\, dV}_{\mathcal{D}_p}$$

Kinetic energy budget $\Delta\epsilon = \epsilon_s + \epsilon_d + \mathcal{D}_p - \epsilon_k$ is measure for instantaneous error

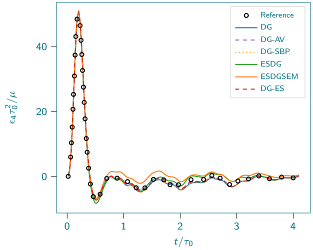
Compressible homogeneous isotropic turbulence - contributions



Solenoidal dissipation ϵ_s

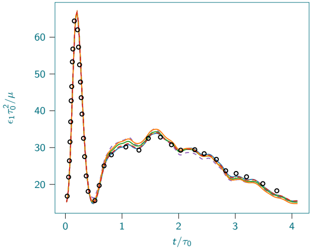


Dilatational dissipation ϵ_d

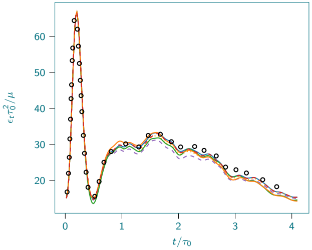


Pressure diffusion $\mathcal{D}_p$

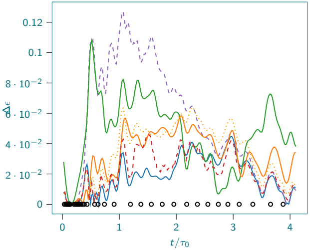
Compressible homogeneous isotropic turbulence - budgets



Measured dissipation ϵ_k

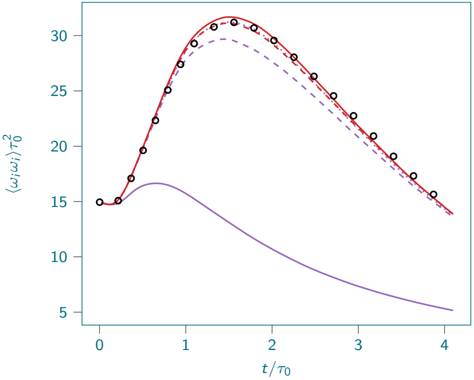


Total dissipation $\epsilon_s + \epsilon_d + \mathcal{D}_p$

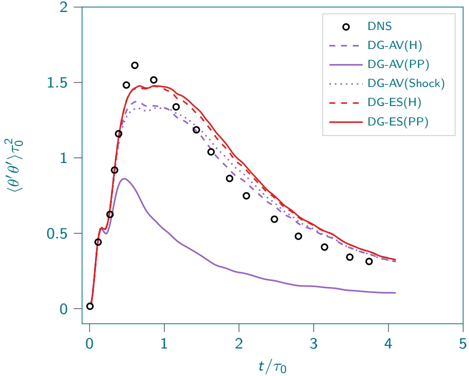


Budget error $\epsilon_s + \epsilon_d + \mathcal{D}_p - \epsilon_k$

	$p=3$			$p=4$			$p=5$		
	4^3	8^3	16^3	3^3	6^3	13^3	3^3	5^3	11^3
DG	✗	✗	✓	✗	✗	✓	✗	✗	✓
DG-AV	✓	✓	✓	✓	✓	✓	✓	✓	✓
DG-SBP	✗	✗	✓	✗	✗	✗	✗	✗	✓
ESDGSEM	✓	✓	✓	✓	✓	✓	✓	✓	✓
ESDG	✓	✓	✓	✓	✓	✓	✓	✓	✓
DG-ES	✓	✓	✓	✓	✓	✓	✓	✓	✓



Solenoidal dissipation ϵ_s



Dilatational dissipation ϵ_d

Conclusions

- ESDGSEM and ESDGSEM provide robustness, but not fully accurate
- DG-AV worst accuracy, high dependence on sensor
- vanilla DG, using conserved variables, most accurate
- summation by parts operator is not stabilising DG, but not jeopardizing accuracy
- best of both worlds: vanilla DG + ESDG in “troubled cells”
- DG-ES: low dependence on sensor

Future work

- validation on shock-turbulence interaction (shock stabilisation)
- integration methods in body-fitted solver ArgoDG w/ Cenaero

Targeted applications

- DNS and LES of high-speed turbomachinery
- hypersonic flow during atmospheric reentry