High-order unstructured discretisations for Scale-Resolving Simulations

VKI Lecture Series on Turbomachinery Flow Simulation and Modeling 2025

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Koen Hillewaert (koen.hillewaert@uliege.be)
ULiège, Aerospace & Mechanics, DoTP[1]; Cenaero[2]; TU Department VKI [3]

A. Bilocq[1], M. Borbouse[1], M. Boxho[2], N. Deneffe[1],
M. Rasquin[2], M. Thys[1], T. Toulorge[2]

Outline

Context

Notation and nature of the Navier-Stokes equations

Mathematical entropy

Transonic CFD - challenges and physical principles

Finite Volume Method (FVM)

Discontinuous Galerkin Method (DGM)

DG shock capturing for DNS and LES

Context

High-resolution CFD for turbomachinery

Turbulence and transition paramount

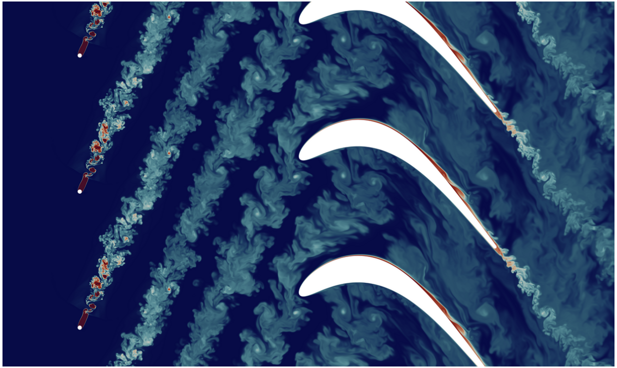
- large range of scales, smallest <<< geometry
- high loaded machinery often transonic
- conditions often between laminar and turbulent
- important source of losses/entropy
- beneficial for operational range

RANS far from comfort zone → reference data ?

- very complex (secondary) flows
- often transition ∼ low Re, high acceleration
- interaction with shocks
- vortical **and** acoustic perturbations

Challenges for DNS / LES

- high accuracy on complex geometry/flow
- (shock) stabilisation ↔ capturing turbulence
- importance of acoustic waves / effects



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

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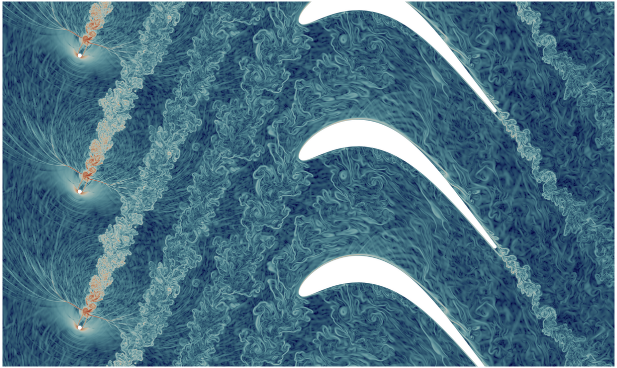

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Density gradient troughout the cascade

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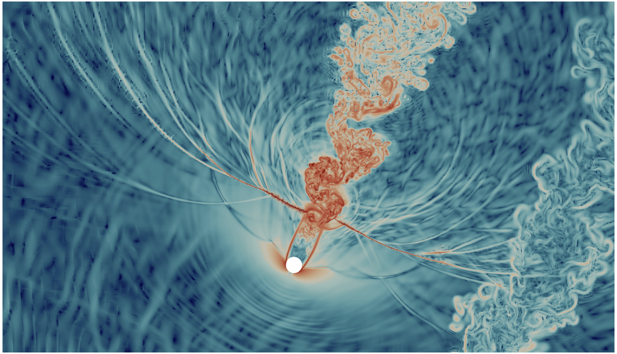

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Density gradient near the wake generator

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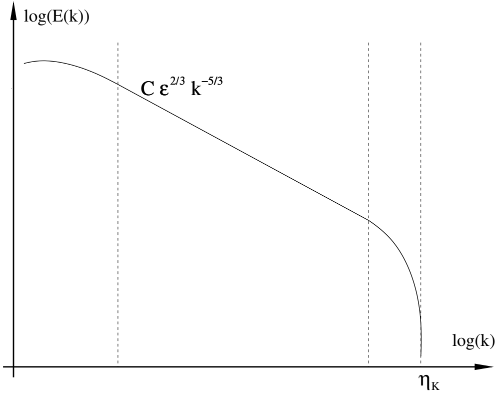
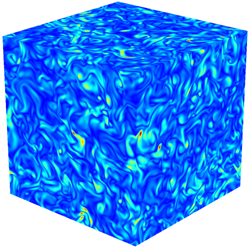
Need for high order in Scale-Resolving Simulations





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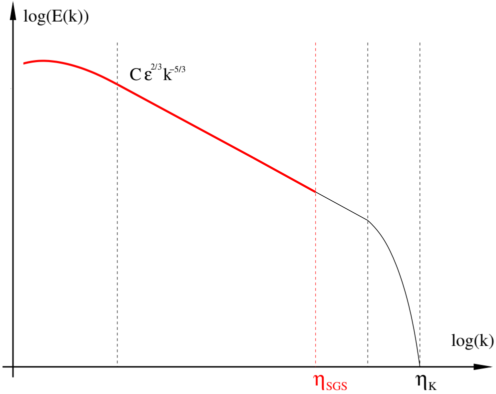

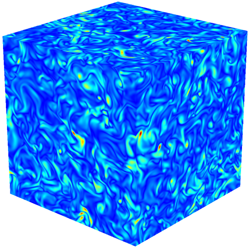

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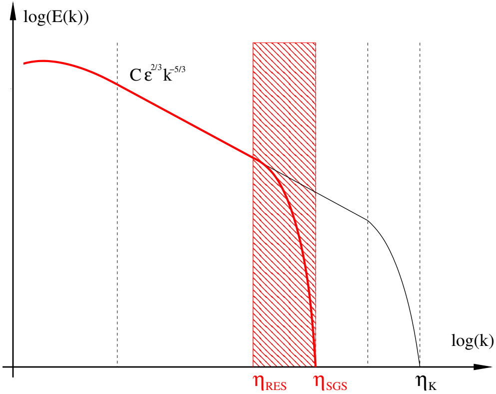

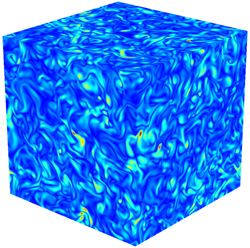

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- near cut-off, numerical error is high → sacrificial range
- sacrificial range can be made smaller by using high order

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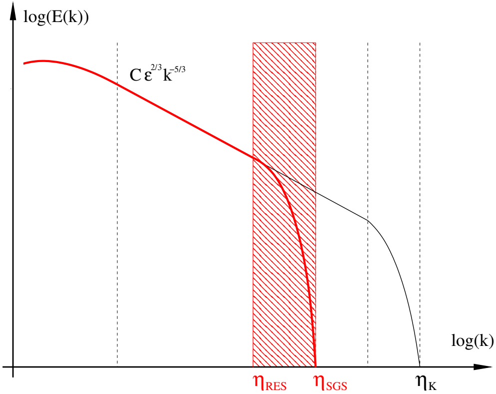

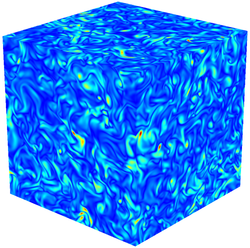

- classical LES supposes sharp cut off
- near cut-off, numerical error is high → sacrificial range
- sacrificial range can be made smaller by using high order
- global dissipation is correct if no significant error on larger scales in inertial range

Notation and nature of the Navier-Stokes equations

Conservative equations - integral form

Navier-Stokes equations

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

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

$$\int_V \frac{\partial \rho E}{\partial t}\, dV + \oint_{\partial V} \left(\left(\rho \mathbf{v} \cdot \mathbf{n} \right) H - \mathbf{v} \cdot \boldsymbol{\tau} \cdot \mathbf{n} - \mathbf{q} \cdot \mathbf{n} \right) dS = 0$$

Generalisation to set of N convection-diffusion equations in $\mathcal{U}^N$

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

with

- $\mathbf{q} \in \mathcal{U}^N$ the state vector of *conserved variables*
- $\mathbf{f} \in \mathcal{U}^{N \times D}$ the *convective flux* vector
- $\mathbf{d} \in \mathcal{U}^{N \times D}$ the *diffusive flux* vector

Notation and nature of the Navier-Stokes equations

Conservative equations - differential form

Navier-Stokes equations

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{v} \cdot \mathbf{n} &= 0 \\
\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left(\left(\rho \mathbf{v} \cdot \mathbf{n} \right) \mathbf{v} + p \mathbf{n} - \boldsymbol{\tau} \cdot \mathbf{n} \right) &= 0 \\
\frac{\partial \rho E}{\partial t} + \nabla \cdot \left(\left(\rho \mathbf{v} \cdot \mathbf{n} \right) H - \mathbf{v} \cdot \boldsymbol{\tau} \cdot \mathbf{n} - \mathbf{q} \cdot \mathbf{n} \right) &= 0
\end{aligned}
$$

Generalisation to set of N convection-diffusion equations in $\mathcal{U}^N$

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Notation and nature of the Navier-Stokes equations

Conservative equations - Convective and diffusive fluxes

- Convective fluxes correspond to *hyperbolic subsystem*: Jacobian of projected flux on any direction $\mathbf{d}$

  $$\mathcal{A}^d \in \mathbb{R}^{N \times N} : \mathcal{A}^d_{mn} = \frac{\partial \mathbf{f}_m}{\partial q_n} \cdot \mathbf{d}$$

  has N real eigenvalues λ^d_j (see [Leveque, 1992])
- Diffusive fluxes correspond to *elliptic subsystem*: Jacobian of flux wrt gradients

  $$\mathcal{D} \in \mathbb{R}^{N \times D \times D \times N} : \mathcal{D}^{kl}_{mn} = \frac{\partial d^k_m}{\partial \frac{\partial q_n}{\partial x^l}}$$

  is a positive semi-definite fourth order tensor (see *e.g.* [Chipot, 2009])

  $$A_{mk} \; \mathcal{D}^{kl}_{mn} \; A_{nl} \geq 0 \; , \; \forall A \in \mathbb{R}^{D \times N}$$

Notation and nature of the Navier-Stokes equations

Conservative equations - Change of variables

working variables u may be different from conservative variables q

- express q, $\mathbf{f}$, $\mathbf{d}$ in function of u and ∇u
- solve conservation equations for change in q

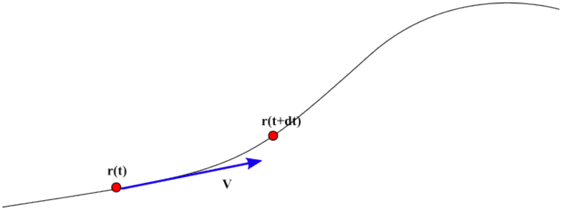
$$\frac{\partial}{\partial t} q(u) + \nabla \cdot \mathbf{f}(u) - \nabla \cdot \mathbf{d}(u, \nabla u) = 0$$

- find u corresponding to the new values of q

Notation and nature of the Navier-Stokes equations

Entropy - mechanical energy

Mechanical work along a on streamline



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

$$\Downarrow \cdot \mathbf{v}$$

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

$$\Downarrow$$

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

$$\Downarrow$$

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

Notation and nature of the Navier-Stokes equations

Entropy - entropy

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

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

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

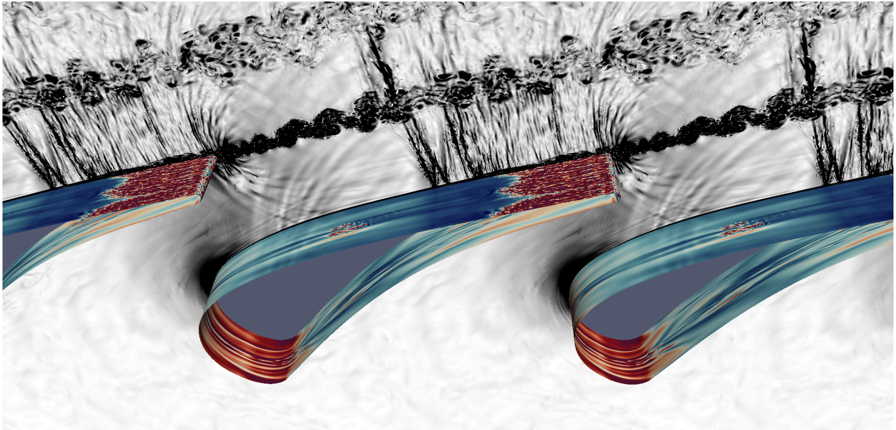
$$\frac{\partial \rho e}{\partial t} + \nabla \cdot \rho \mathbf{v} e = -p \nabla \cdot \mathbf{v} + \boldsymbol{\tau} : \nabla \mathbf{v} + \nabla \cdot \mathbf{q}$$

Conservation equation for entropy *density*

$$\frac{\partial \rho s}{\partial t} + \nabla \cdot \rho \mathbf{v} s - \nabla \cdot \frac{q}{T} = \frac{\boldsymbol{\tau} : \nabla \mathbf{v}}{T} - \frac{\nabla T \cdot \mathbf{q}}{T^2} \geq 0$$

Notation and nature of the Navier-Stokes equations

Shocks



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

Notation and nature of the Navier-Stokes equations

Shocks - linear effects - characteristics

Linearise

$$\frac{\partial q_m}{\partial t} + \nabla \cdot \mathbf{f}_m = 0$$

around mean solution $q_m = \overline{q_m} + \delta q_m$

$$\frac{\partial \delta q_m}{\partial t} + \mathcal{A}_n \cdot \nabla \delta q_n = 0$$

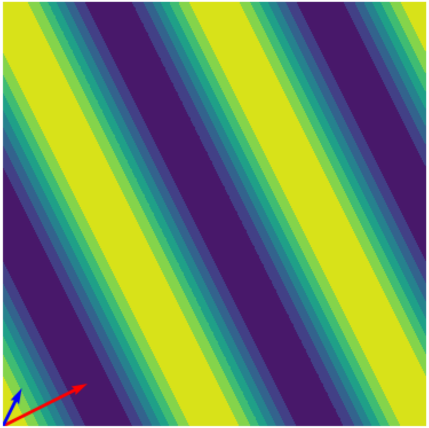
δq consists of plane waves moving along $\mathbf{d}$ with wave number k

$$\delta q_m = \sum \widehat{\delta c}_j r_{jm} e^{ik(\mathbf{d}\cdot\mathbf{r} - \lambda_j t)}$$

since all eigenvalues λ_j

$$(\mathcal{A} \cdot \mathbf{d}) \;\; r_j^d = \lambda_j^d r_j^d$$

are real



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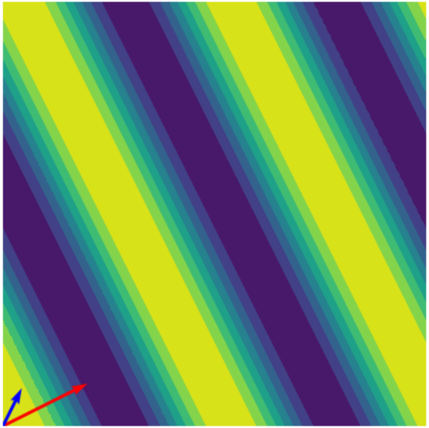
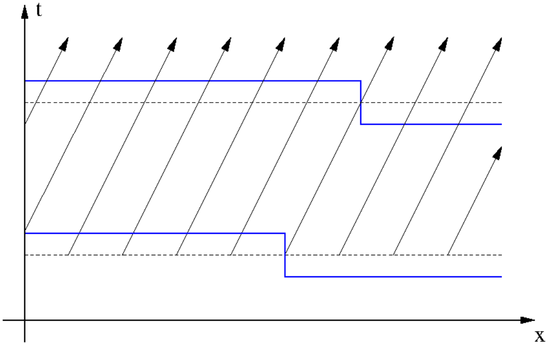


Notation and nature of the Navier-Stokes equations

Shocks - non-linear propagation in 1D - scalar equation



δq no impact on $\lambda \rightarrow$ contact

Notation and nature of the Navier-Stokes equations

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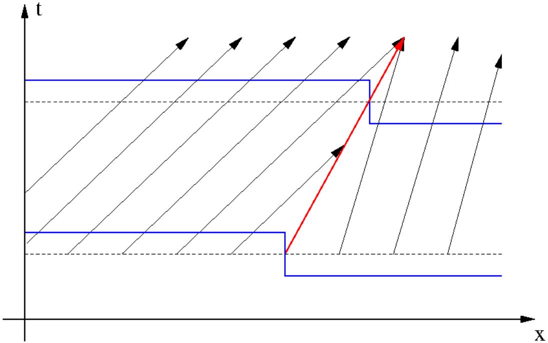

δq increases $\lambda \rightarrow$ compression shock

Notation and nature of the Navier-Stokes equations

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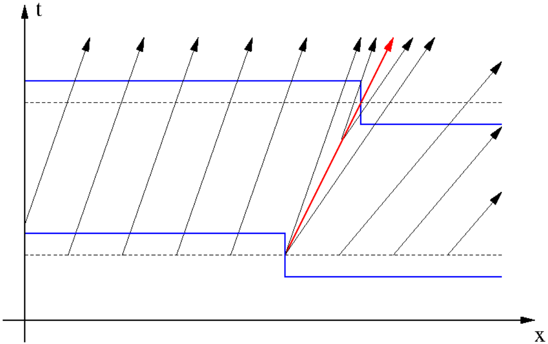

δq decreases $\lambda \rightarrow$ expansion shock

Notation and nature of the Navier-Stokes equations

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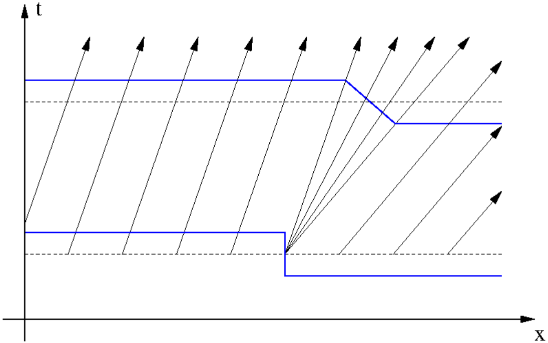
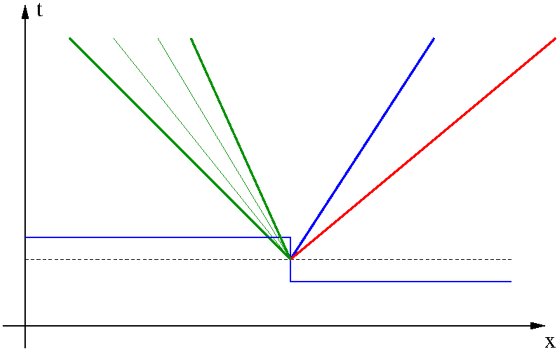


δq decreases λ + vanishing viscosity / entropy consistency → expansion fan

Notation and nature of the Navier-Stokes equations

Shocks - non-linear propagation in 1D - Riemann problem



N characteristics containing contacts, shocks and fans

Notation and nature of the Navier-Stokes equations

Shocks - weak solutions

Strong differential form of the convection system not usable for discontinous solutions

$$\frac{\partial q_m}{\partial t} + \nabla \cdot \mathbf{f}_m = 0$$

Regularity requirements lifted in *weak solution* which satisfies

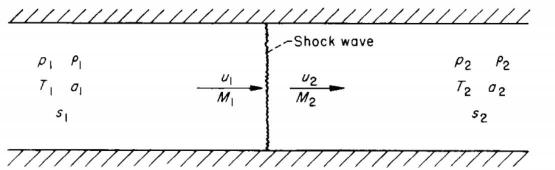
$$\int_\Omega v \frac{\partial q}{\partial t} dV - \int_\Omega \nabla v \cdot \mathbf{f}(q) \; dV = 0 \; , \; \forall v \in \mathcal{V}^N$$

However

- weak solutions not necessarily unique (*e.g.* expansion fan and shock both possible)
- complement with entropy consistency

Notation and nature of the Navier-Stokes equations

Shocks

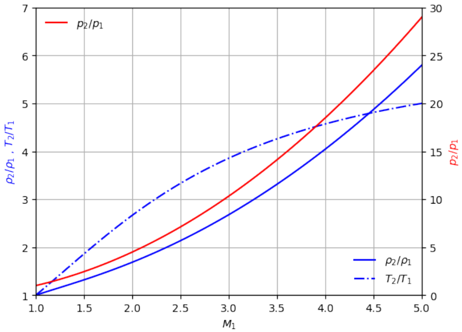


- conservation of mass, momentum and energy

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

- second law $s_2 > s_1$

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



Notation and nature of the Navier-Stokes equations

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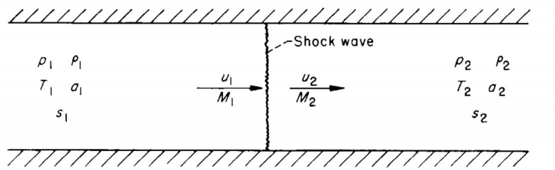

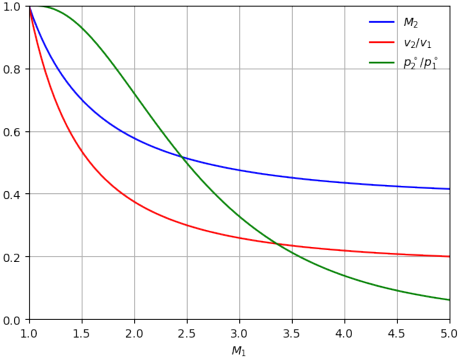

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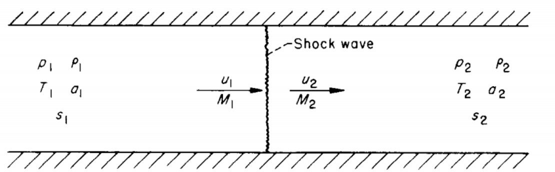

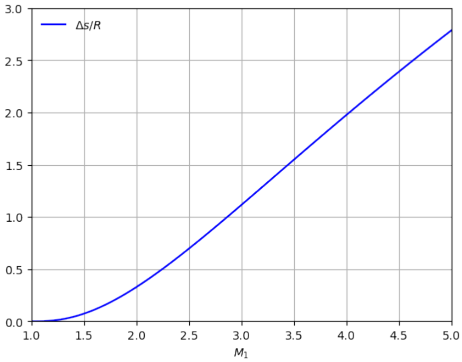

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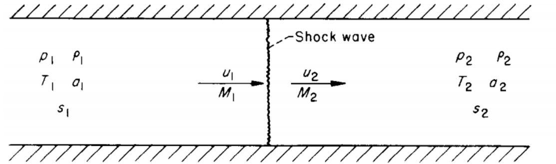

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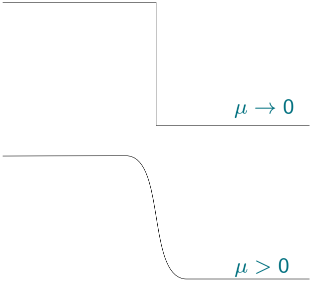

Generation of entropy by viscous effects $\boldsymbol{\tau} : \nabla \mathbf{v}$, $-\nabla T \cdot \mathbf{q}$

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

Notation and nature of the Navier-Stokes equations

Take-away messages

Entropy embedded equation within the Navier-Stokes equations

- ensures stability of the system
- ensures a unique weak solution

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 $\mu \rightarrow 0$

Mathematical entropy

definition

Generalisation of physical entropy to mathematical entropy $\mathcal{S}$ and flux $\mathcal{F}$ to study generic non-linear hyperbolic and combined hyperbolic-elliptic systems [Harten, 1983, Harten et al., 1998, Tadmor, 1987]

- conservation equation is constructed by combining N conservation equations
- can only decrease ($\leftrightarrow$ increase) monotonically

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

- **entropy variables** w

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

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

$$\frac{\partial \boldsymbol{\mathcal{F}}}{\partial q_m} = \frac{\partial \mathcal{S}}{\partial q_n} \frac{\partial \mathbf{f}_n}{\partial q_m}$$

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

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Dual: potential flux $\mathcal{Q}$ and potential flux $\mathcal{G}$

- **conservative variables** q

$$q_m = \frac{\partial \mathcal{Q}}{\partial w_m}$$

- existence of (scalar) **potential flux** $\mathcal{G}$

$$\frac{\partial \mathcal{G}}{\partial w_m} = \mathbf{f}_m$$

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- **entropy variables** w

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

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

$$\frac{\partial \mathcal{F}}{\partial q_m} = \frac{\partial \mathcal{S}}{\partial q_n}\frac{\partial \mathbf{f}_n}{\partial q_m}$$

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

Dual: potential flux $\mathcal{Q}$ and potential flux $\mathcal{G}$

- **conservative variables** q

$$q_m = \frac{\partial \mathcal{Q}}{\partial w_m}$$

- existence of (scalar) **potential flux** $\mathcal{G}$

$$\frac{\partial \mathcal{G}}{\partial w_m} = \mathbf{f}_m$$

Navier-Stokes equations : $\mathcal{S} = -\rho s$ [Hughes et al., 1986]

Mathematical entropy

conditions - conservation

Since

$$\frac{\partial \mathcal{S}}{\partial q_m}\frac{\partial \mathbf{f}_m}{\partial q_n} = \frac{\partial \boldsymbol{\mathcal{F}}}{\partial q_n}$$

we find

$$\frac{\partial \mathcal{S}}{\partial q_m}\nabla \cdot \mathbf{f}_m = \frac{\partial \mathcal{S}}{\partial q_m}\frac{\partial f_m^k}{\partial x^k} = \frac{\partial \mathcal{S}}{\partial q_m}\frac{\partial f_m^k}{\partial q_n}\frac{\partial q_n}{\partial x^k} = \frac{\partial \mathcal{F}^k}{\partial q_n}\frac{\partial q_n}{\partial x^k} = \frac{\partial \mathcal{F}^k}{\partial x^k} = \nabla \cdot \boldsymbol{\mathcal{F}}$$

and hence

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

Mathematical entropy
conditions - convexity

Integral form of entropy conservation

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

Developing the volume production term

$$-\nabla w_m \cdot \mathbf{d}_m dV = -\frac{\partial w_m}{\partial \boldsymbol{q}_n} \mathcal{D}^{kl}_{mo} \frac{\partial \boldsymbol{q}_o}{\partial x^l} = -\frac{\partial \boldsymbol{q}_n}{\partial x^k} \frac{\partial^2 \mathcal{S}}{\partial \boldsymbol{q}_n \boldsymbol{q}_m} \mathcal{D}^{kl}_{mo} \frac{\partial \boldsymbol{q}_o}{\partial x^l}$$

we see it is negative if $\mathcal{S}$ is a convex function of the state vector q

Mathematical entropy

Take-away messages

Existence of mathematical entropy : stability of convection/hyperbolic 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, providing stability
- ensures unicity of the weak solution

Consequences for numerical approximations

- entropy equation is derived from conservation equations and therefore not necessarily satisfied
- embedding *entropy-consistency* in the discretisation is desirable

Transonic CFD - challenges and physical principles

Shock position, strength and speed

- discrete exact conservation mass, momentum, energy
- generation of small yet positive amount of entropy

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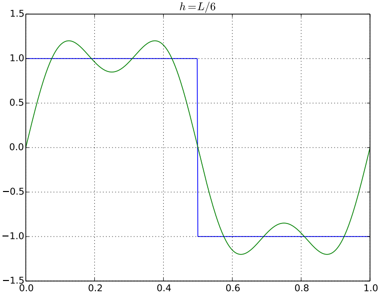
Shock capturing / representation with high order methods

- 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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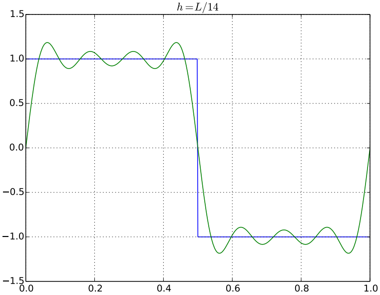

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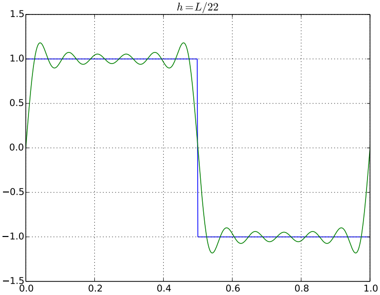

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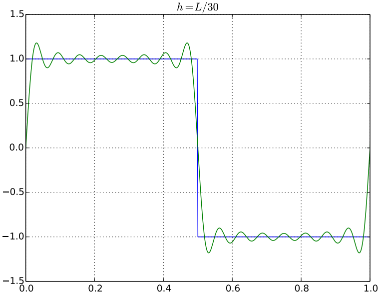

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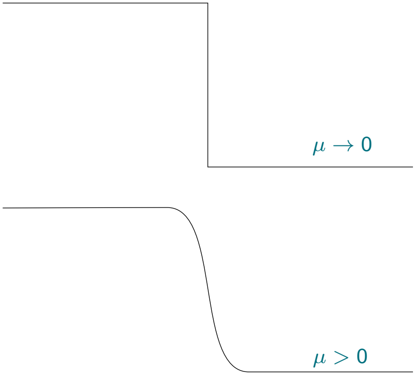

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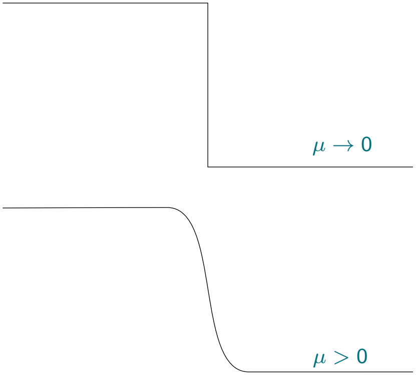
Non-linear stability required near shocks

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



Finite Volume Method (FVM)

Principle

Vanishing diffusion conservation equation

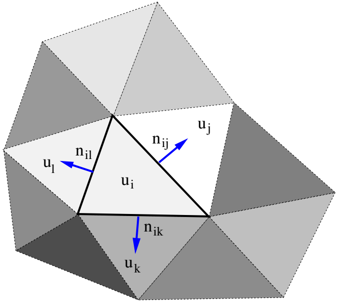
$$\int_V \frac{\partial q_m}{\partial t} dV + \oint_{\partial V} \mathbf{f}_m \cdot \mathbf{n} dS = 0$$

Solving for average q^i on control volume V_i

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

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

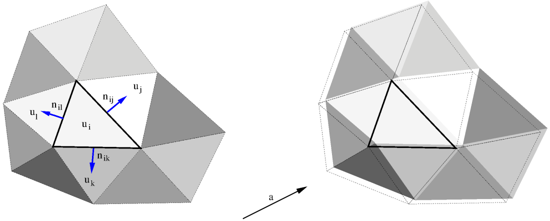
- conservativity $\mathcal{H}\left(q^j, q^i; -\mathbf{n}^{ij}\right) = -\mathcal{H}\left(q^i, q^j; \mathbf{n}^{ij}\right)$
- consistency $\mathcal{H}_m\left(q, q; \mathbf{n}\right) = \mathbf{f}_m \cdot \mathbf{n}$
- stability ?

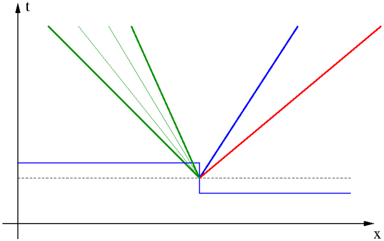


Finite Volume Method (FVM)

Upwind fluxes

Main idea: $\mathcal{H}\left(q^-, q^+; \mathbf{n}\right) = \lim_{dt \to 0} \mathbf{f}(\tilde{q}(t+dt)) \cdot \mathbf{n}$





- Godunov scheme: $\tilde{q}(t+dt)$ is solution of the Riemann problem between q^+ and q^-
- Riemann problem is expensive to solve → *approximate Riemann solvers* (see [Toro, 2009] for review)
- using upwind flux $\mathcal{H}\left(q^+, q^*; \mathbf{n}\right)$ on boundary ensures well-posed Dirichlet boundary conditions since coherent with characteristic propagation (see [Giles, 1988])

Finite Volume Method (FVM)

Entropy consistent FVM

FVM for cell V_i

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

Finite Volume Method (FVM)
Entropy consistent FVM

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

Evolution of cell entropy,

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

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Evolution of cell entropy, considering $\sum_j \mathbf{n}^{ij}$

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

Finite Volume Method (FVM)

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Evolution of entropy over the whole domain Ω

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

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$$= -\sum_{i,j} \left(w^i_m - w^j_m\right)\left(\mathcal{H}_m\left(q^i, q^j; \mathbf{n}^{ij}\right) - \frac{\partial \boldsymbol{\mathcal{G}}}{\partial w_m}(\tilde{q}) \cdot \mathbf{n}^{ij}\right) \ , \ \exists \tilde{q} \in [q^i, q^j]$$

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$$\begin{aligned}
\sum_i V_i \frac{\mathrm{d}\mathcal{S}^i}{\mathrm{dt}} &= -\sum_{i,j} \left(w_m^i - w_m^j\right) \mathcal{H}_m\left(q^i, q^j; \mathbf{n}^{ij}\right) - \left(\boldsymbol{\mathcal{G}}(q^i) - \boldsymbol{\mathcal{G}}(q^j)\right) \cdot \mathbf{n}^{ij} \\
&= -\sum_{i,j} \left(w_m^i - w_m^j\right) \left(\mathcal{H}_m\left(q^i, q^j; \mathbf{n}^{ij}\right) - \frac{\partial \boldsymbol{\mathcal{G}}}{\partial w_m}(\tilde{q}) \cdot \mathbf{n}^{ij}\right) \ , \ \exists \tilde{q} \in [q^i, q^j] \\
&= -\sum_{i,j} \underbrace{\left(w_m^i - w_m^j\right) \left(\mathcal{H}_m\left(q^i, q^j; \mathbf{n}^{ij}\right) - \mathbf{f}_m(\tilde{q}) \cdot \mathbf{n}^{ij}\right)}_{>0?} \ , \ \exists \tilde{q} \in [q^i, q^j]
\end{aligned}$$

Finite Volume Method (FVM)

Take-away messages

- discontinuity → interface fluxes $\mathcal{H}\left(u^{+}, u^{-}; \mathbf{n}\right)$
    - conservativity: $\mathcal{H}\left(u^{+}, u^{-}; \mathbf{n}\right) = -\mathcal{H}\left(u^{-}, u^{+}; -\mathbf{n}\right)$
    - consistency: $\mathcal{H}\left(u, u; \mathbf{n}\right) = \mathbf{f}(u) \cdot \mathbf{n}$
    - stability ?
- rigourous non-linear stability: *Entropy Consistent Fluxes* "E-flux" [Oleinik]

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

- *Approximate Riemann Solvers* usually are E-fluxes
- E-fluxes positive dissipation → correct shock representation
- Entropy consistent FVM
    - use of E-fluxes
    - *maximum criteria on high order reconstruction*

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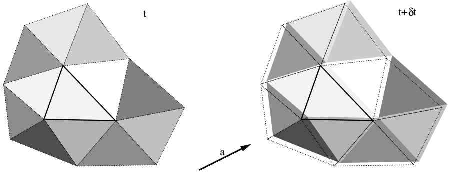


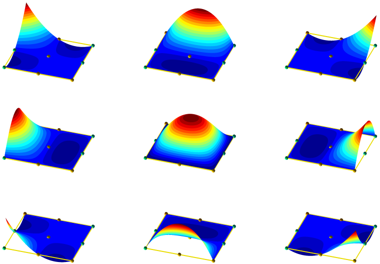
Discontinuous Galerkin Method (DGM)

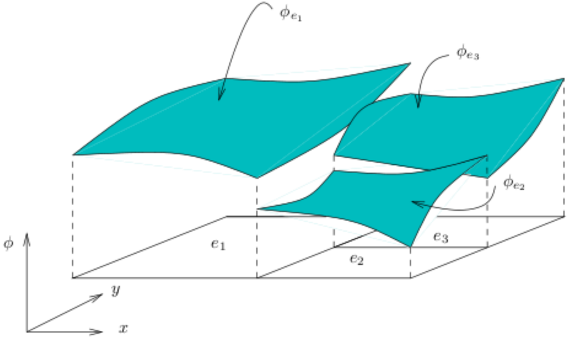
Interpolation

Elementwise polynomial interpolation of working variables u of arbitrary order p

$$u \in \mathcal{V}^N : (u_m)_e = \sum_i \mathbf{u}_{im} \phi_i^e$$

ϕ_i^e shape functions of order $p = 2$ for element e





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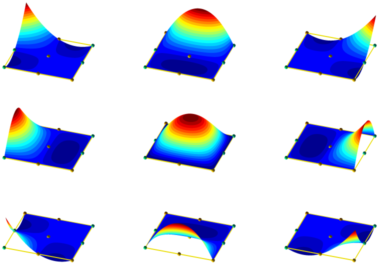

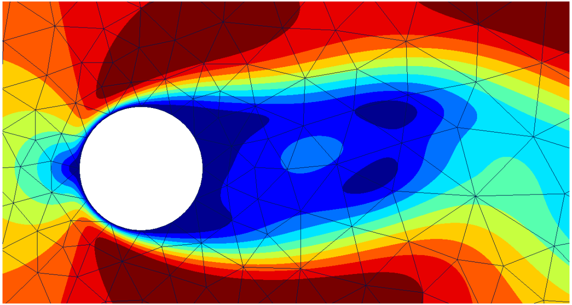

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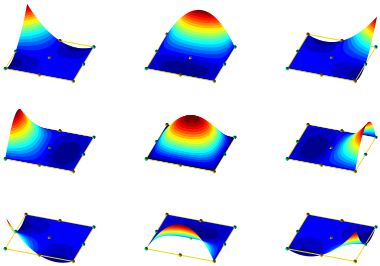
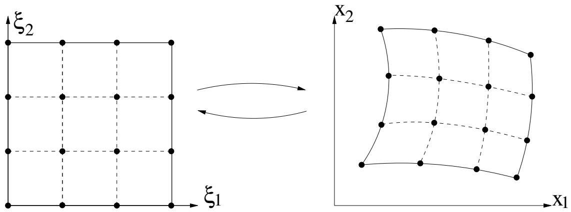


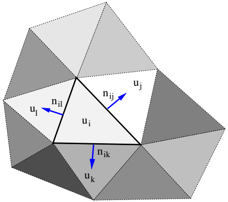


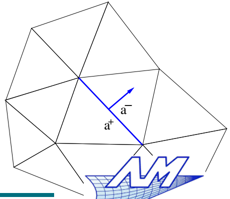
Discontinuous Galerkin Method (DGM)

Variational formulation

Galerkin

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





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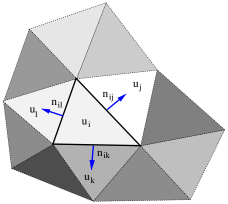

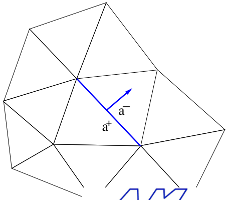

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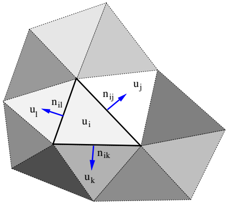
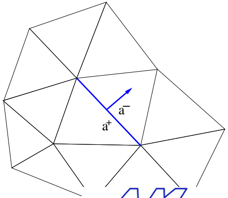
$$\sum_e \left(\int_e \left(v_m \frac{\partial q}{\partial t} - \nabla v_m \cdot \mathbf{f}_m \right) dV + \sum_{f \in e} \int_f v \mathbf{f}_m \cdot \mathbf{n} dS \right) = 0$$





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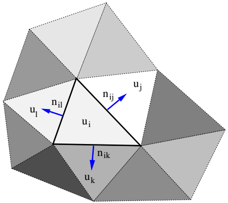
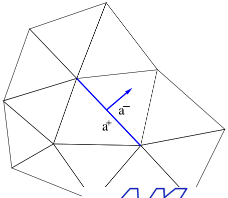
$$\sum_e \int_e v_m \frac{\partial q_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \mathbf{f}_m dV + \sum_f \int_f \left(v_m^+ \mathbf{f}_m(u^+) - v_m^- \mathbf{f}_m(u^-) \right) \cdot \mathbf{n} dS = 0$$





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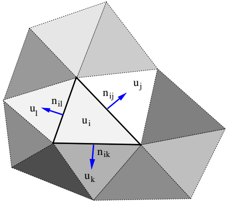
Galerkin

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

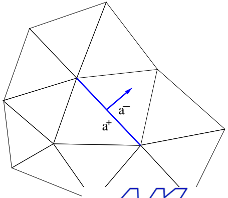
$$\sum_e \left(\int_e \left(v_m \frac{\partial q}{\partial t} - \nabla v_m \cdot \mathbf{f}_m \right) dV + \sum_{f \in e} \int_f v \mathbf{f}_m \cdot \mathbf{n} dS \right) = 0$$

$$\sum_e \int_e v_m \frac{\partial q_m}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \mathbf{f}_m dV + \sum_f \int_f \left(v_m^+ \mathbf{f}_m(u^+) - v_m^- \mathbf{f}_m(u^-) \right) \cdot \mathbf{n} dS = 0$$



Discretisation: choice for interface flux

$$\sum_e \int_e v \frac{\partial q}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \mathbf{f}_m dV + \sum_f \int_f \gamma(u^+, v^+, u^-, v^-, \mathbf{n}) dS = 0$$



Consistency ?

$$\gamma(u, v^+, u, v^-, \mathbf{n}) = \left(v^+ - v^- \right) \mathbf{f}(u) \cdot \mathbf{n}$$

Discontinuous Galerkin Method (DGM)

Variational formulation - interface flux

DGM(p=0), $v = 1$ on e and zero elsewhere

$$\int_e \frac{\partial q}{\partial t} dV + \int_f \gamma(u^+, 1, u^-, 0, \mathbf{n}) dS = 0$$

first order FVM

$$\int_e \frac{\partial q}{\partial t} dV + \int_f \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

Both coincide if

$$\gamma(u^+, v^+, u^-, v^-, \mathbf{n}) = \left(v^+ - v^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right)$$

so we find a high order extension of the FVM

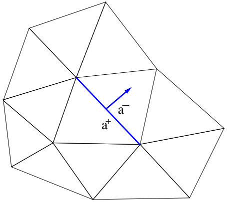
$$\sum_e \int_e v \frac{\partial q}{\partial t} dV - \sum_e \int_e \nabla v_m \cdot \mathbf{f}_m dV + \sum_f \int_f \left(v^+ - v^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

Discontinuous Galerkin Method (DGM)

Entropy consistency

Use entropy variables $u = w \rightarrow$ choose $w \in \mathcal{V}^N$

$$\sum_e \int_e w_m \frac{\partial q_m}{\partial t} dV - \int_e \nabla w_m \cdot \mathbf{f} dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$



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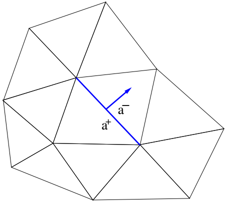
$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV - \sum_e \int_e \nabla w_m \cdot \frac{\partial \mathcal{G}}{\partial w_m} dV + \sum_f \int_f \left(w_m^+ - w_m^- \right) \mathcal{H} \left(u^+, u^- ; \mathbf{n} \right) dS = 0$$



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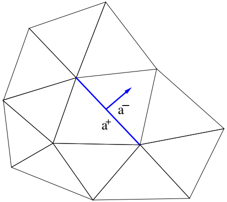
$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV - \sum_e \int_e \nabla \cdot \mathcal{G} dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$



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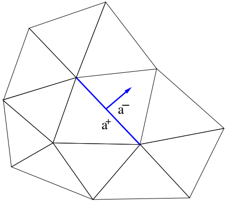
$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV - \sum_e \int_e \nabla \cdot \mathcal{G} \, dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV + \sum_f \int_f \left(\left(w_m^+ - w_m^-\right) \mathcal{H}_m\left(u^+, u^-; \mathbf{n}\right) - \left(\mathcal{G}^+ - \mathcal{G}^-\right) \cdot \mathbf{n}\right) dS = 0$$



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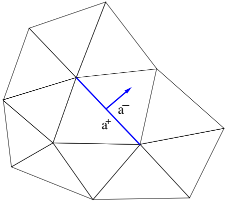

$$\sum_e \int_e w_m \frac{\partial q_m}{\partial t} dV - \int_e \nabla w_m \cdot \mathbf{f} \, dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

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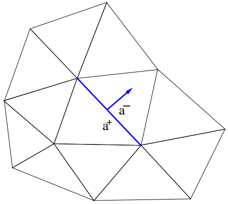
$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV = -\sum_f \int_f \left(w_m^+ - w_m^-\right) \left(\mathcal{H}_m\left(u^+, u^-; \mathbf{n}\right) - \frac{\partial \mathcal{G}}{\partial w_m}(\tilde{w})\right) dS \ , \ \exists \tilde{w} \in \left[w^+, w^-\right]$$

Discontinuous Galerkin Method (DGM)

Entropy consistency

Use entropy variables $u = w \rightarrow$ choose $w \in \mathcal{V}^N$



$$\sum_e \int_e w_m \frac{\partial q_m}{\partial t} dV - \int_e \nabla w_m \cdot \mathbf{f} dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV - \sum_e \int_e \nabla w_m \cdot \frac{\partial \mathcal{G}}{\partial w_m} dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV - \sum_e \int_e \nabla \cdot \mathcal{G} dV + \sum_f \int_f \left(w_m^+ - w_m^-\right) \mathcal{H}\left(u^+, u^-; \mathbf{n}\right) dS = 0$$

$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV + \sum_f \int_f \left(\left(w_m^+ - w_m^-\right) \mathcal{H}_m\left(u^+, u^-; \mathbf{n}\right) - \left(\mathcal{G}^+ - \mathcal{G}^-\right) \cdot \mathbf{n}\right) dS = 0$$

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$$\sum_e \int_e \frac{\partial \mathcal{S}}{\partial t} dV = -\underbrace{\sum_f \int_f \left(w_m^+ - w_m^-\right) \left(\mathcal{H}_m\left(u^+, u^-; \mathbf{n}\right) - \mathbf{f}(\tilde{w})\right) dS}_{>0}$$

Discontinuous Galerkin Method (DGM)

Take-away messages

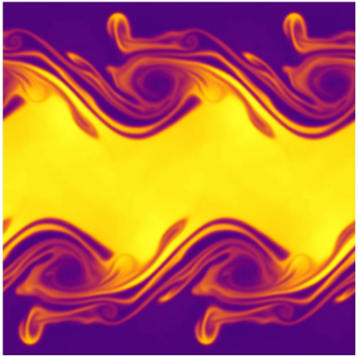
- DGM natural high order extension of first order FVM
  - inherits consistency and stability
  - arbitrary order of accuracy / interpolation
  - exact accounting for curved element shape
  - compact stencil and computational efficiency
- Using upwind fluxes, DGM can be seen as combination of small elementwise defined FEM problems, coupled by Dirichlet fluxes
- Entropy stable DG (ESDG)
  - use w as working variables $\in \mathcal{V}$ instead of conservative q
  - use of E-fluxes
  - *integration by parts* should be discretely mimicked *summation by parts*
  - quadrature error since update in conservative, not in working variables !

DG shock capturing for DNS and LES

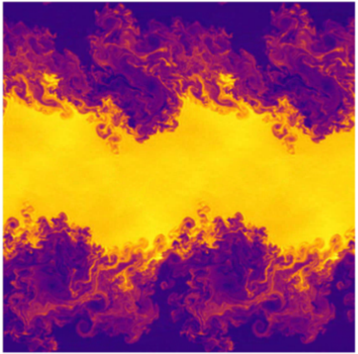
Methods

Challenges

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



Artificial viscosity



Entropy stable DG

DG shock capturing for DNS and LES

Methods

Study submitted to Journal of Computational Physics [Bilocq24*]

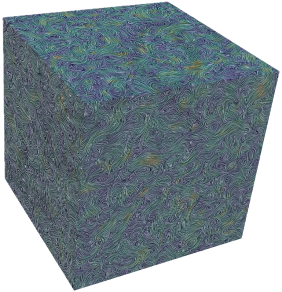
- **DG**: vanilla DG without shock capturing (DG)
  - most accurate (no quadrature error)
  - no stabilisation
- **DG-AV**: DG + sensor based artificial viscosity [Persson and Peraire, 2006, Hennemann et al., 2021]
  - additional viscosity at shocks → dissipates turbulence
  - sensors to detect underresolution
- **ESDG**: Entropy stable DG [Gassner et al., 2016, Chan et al., 2019]
  - formulation in w error in update
  - full quadrature
  - expensive
- **ESDGSEM**: Spectral Element Entropy Stable DG [Gassner et al., 2016, Chan et al., 2019]
  - 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

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - test case

Compressible homogeneous isotropic turbulence

- $M_t = 0.6,\ Re_\lambda = 100$
- starting from incompressible flow field
- high vorticity → ϵ_s
- acoustic transient → $epsilon_d$ 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 $n = (p+1)N = 66$



DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - convergence criterion

Kinetic energy budget on generic control volume

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

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - convergence criterion

Kinetic energy budget on fully periodic domain

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

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - convergence criterion

Kinetic energy budget on

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

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

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

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - convergence criterion

Kinetic energy budget on

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

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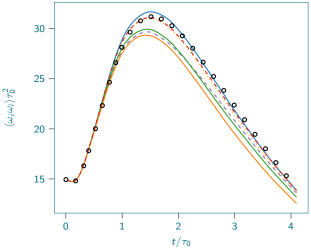
and therefore

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

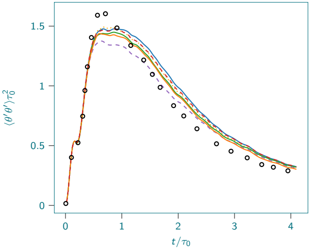
Kinetic energy budget $\Delta\epsilon = \epsilon_s + \epsilon_d + \mathcal{D}_p - \epsilon_k$ is measure for instantaneous error

DG shock capturing for DNS and LES

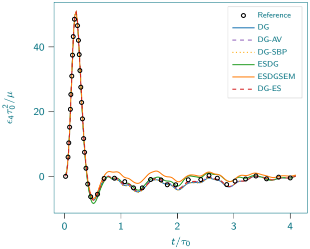
Compressible homogeneous isotropic turbulence - contributions



Solenoidal dissipation ϵ_s



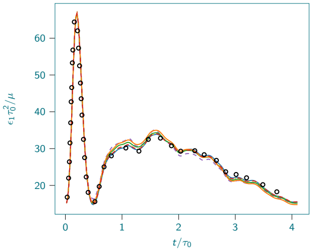
Dilatational dissipation ϵ_d



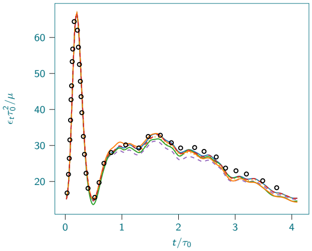
Pressure diffusion $\mathcal{D}_p$

DG shock capturing for DNS and LES

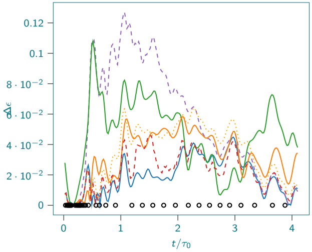
Compressible homogeneous isotropic turbulence - budgets



Measured dissipation ϵ_k



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



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

DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - stability

	$p = 3$			$p = 4$			$p = 5$		
	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	✓	✓	✓	✓	✓	✓	✓	✓	✓

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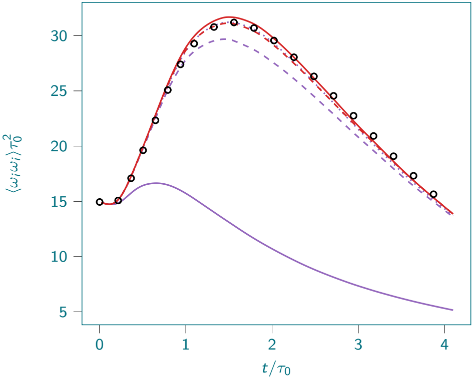
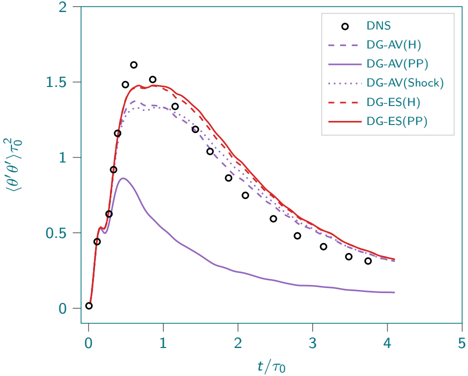
DG shock capturing for DNS and LES

Compressible homogeneous isotropic turbulence - sensor dependence



Solenoidal dissipation ϵ_s



Dilatational dissipation ϵ_d

DG shock capturing for DNS and LES

Conclusions

Conclusions

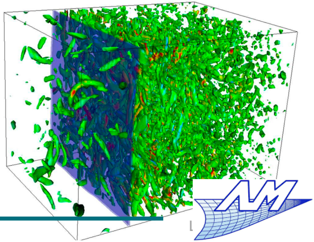
- ESDGSEM and ESDGSEM provide robustness, but not fully accurate
- DG-AV worst accuracy, high dependence on sensor
- vanilla DG, using conserved variables, most accurate
- summation by parts operator is not stabilising DG, but not jeopardizing accuracy
- best of both worlds: vanilla DG + ESDG in “troubled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



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