Complexity out of simplicity in Boltzmann equation and decomposed computation

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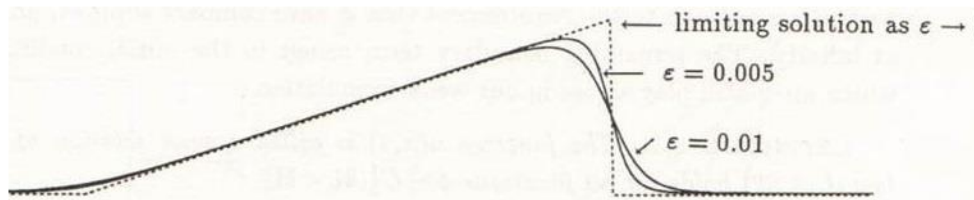
Maxwell Centre, Cambridge, UK

Research Center for Aircraft Core Technology

Models in fluid dynamics

1*1 (simple) Burgers (1948) **Navier-Stokes (1822)**

$$\frac{\partial u}{\partial t}+\boxed{\frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right)}=\frac{\partial}{\partial x}\left(\eta\frac{\partial u}{\partial x}\right) \quad \xleftarrow[p\sim u^2]{\rho\approx 1} \quad \frac{\partial(\rho u)}{\partial t}+\frac{\partial}{\partial x}\left(\rho u^2+p\right)=\frac{\partial}{\partial x}\left(\eta\frac{\partial u}{\partial x}\right)$$



- **Shock formation** ($s[u]=[u^2/2]$)
- **Dissipation in turbulence**

  (with the RHS viscous term)
- **Further extension (complexity)**

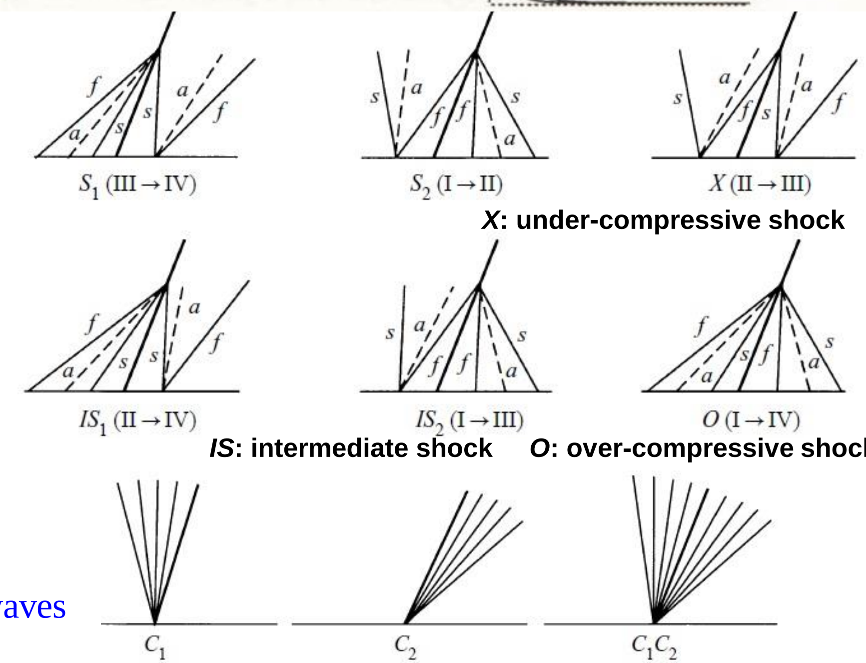
- Reynolds (turbulent) stress ($u=\bar{u}+u'$)
- Shock formation in 3*3 MHD system

  (p, B_y, B_z), instead of $u(\sim p)$

(B_y, B_z) magnetic field

s, f : slow and fast magnetoacoustic waves

a : Alfven wave



X: under-compressive shock

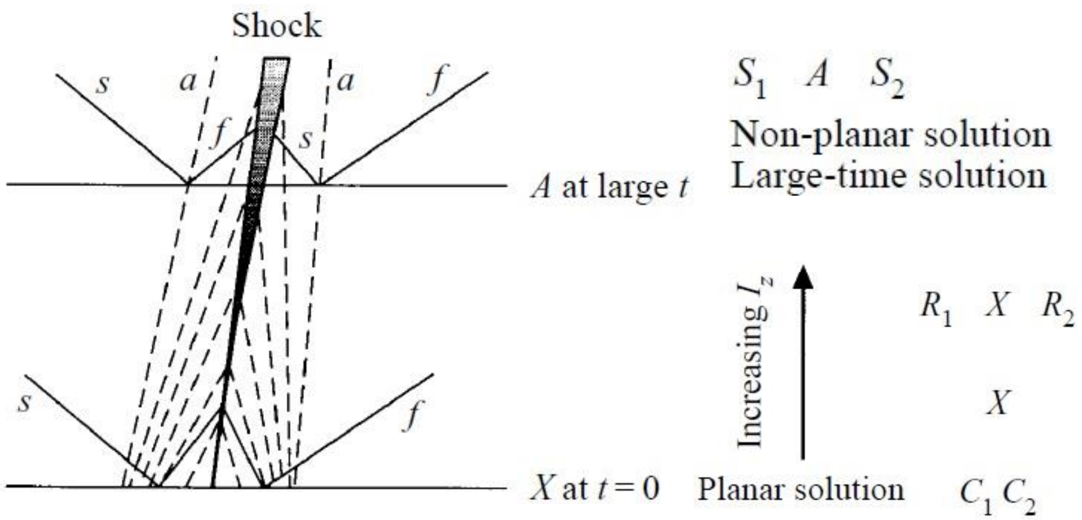
IS: intermediate shock **O**: over-compressive shock

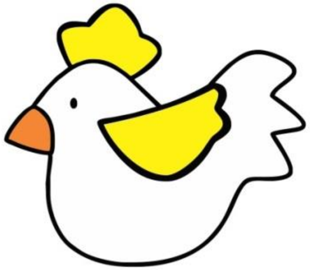
C: compound wave

Models in magneto-hydrodynamics (MHD)

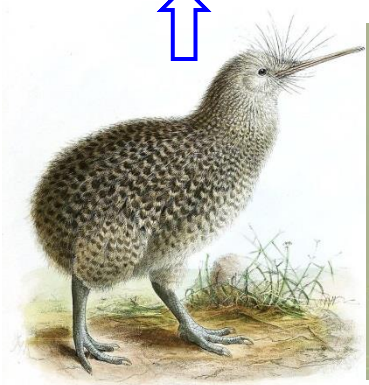
3*3 quadratic MHD model (1997; Myong & Roe)

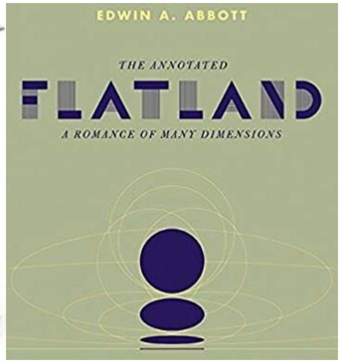
$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \\ w \end{bmatrix} + \boxed{\frac{\partial}{\partial x}\begin{bmatrix} (\gamma+1)u^2+v^2+w^2 \\ 2uv \\ 2uw \end{bmatrix}} = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \eta & -\chi \\ 0 & -\chi & \eta \end{bmatrix}\frac{\partial^2}{\partial x^2}\begin{bmatrix} u \\ v \\ w \end{bmatrix}$$





A: Alfven wave kicks in!



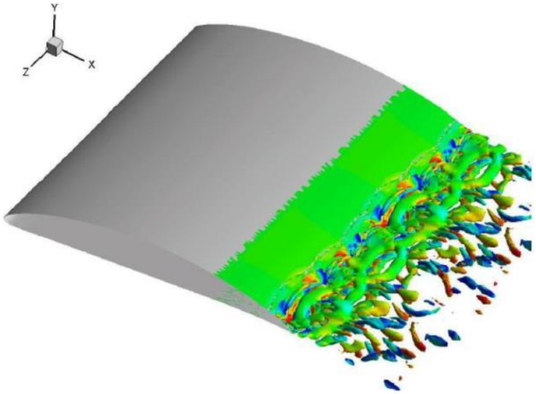


2*2 planar model for **flatland**

$$\frac{\partial}{\partial t}\begin{bmatrix} u \\ v \end{bmatrix} + \boxed{\frac{\partial}{\partial x}\begin{bmatrix} (\gamma+1)u^2+v^2+w^2 \\ 2uv \end{bmatrix}} = \begin{bmatrix} \mu & 0 \\ 0 & \eta \end{bmatrix}\frac{\partial^2}{\partial x^2}\begin{bmatrix} u \\ v \end{bmatrix}$$

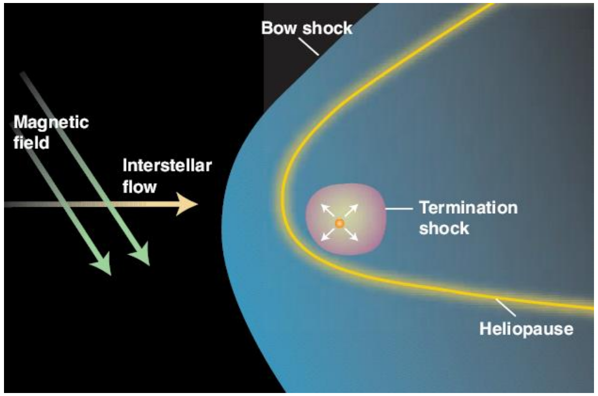
Holistic big picture of fluid dynamics; two extremes

(High Reynolds) fluid dynamics is difficult because:



*At extremely small scales, even turbulent flow is very simple. It is smooth and well behaved. At larger scales, however, a fluid is subject to very few constraints. It can develop arbitrary levels of **complexity** like the effect of turbulence on separation*. (P. L. Roe, "Future developments in CFD," ICAAT-GNU, May 2014)

(Low Reynolds mesoscopic) fluid dynamics is difficult because:



*It involves **microscopic** collisional interactions among fluid particles and their **interplay** with the kinematic motion of particles in the macroscopic framework. This challenge is vividly illustrated by the high Mach number shock singularity problem (HMNP)*. (R. S. Myong, PoF 2014)

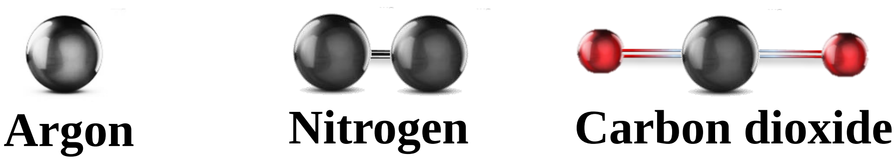
⇨ **Rarefied & microscale gases**

Shift of focus in Burgers and need of kinetic theory

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right)=\boxed{\frac{\partial}{\partial x}\left(\eta\frac{\partial u}{\partial x}\right)} \quad \Longleftarrow \quad \frac{\partial(\rho u)}{\partial t}+\frac{\partial}{\partial x}\left(\rho u^2+p\right)=\boxed{\frac{\partial}{\partial x}\left(\eta\frac{\partial u}{\partial x}\right)}$$

What does **interplay** mean? Between the **kinematic motion** of particles in the macroscopic framework and microscopic **collisional interactions** among fluid particles.

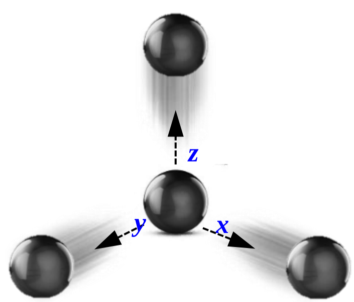
In order to answer this question, one needs to look at the molecular description of gas particles; **gas kinetic theory** or **Boltzmann-based gas dynamics**



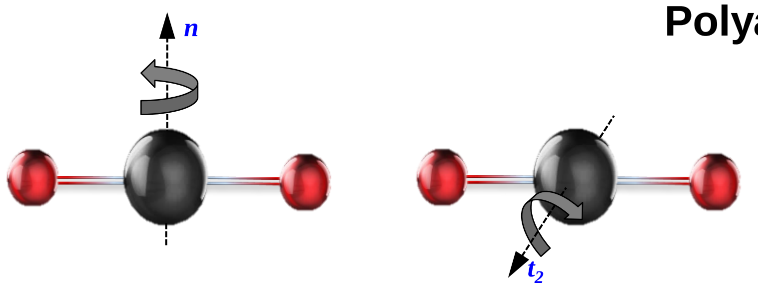
Monatomic

Diatomic

Polyatomic



Translational degree of freedom



Rotational degree of freedom

Simplicity in Boltzmann transport equation (BTE)

- **Assumptions**; 1) the mean free path >> the effective range of the intermolecular forces; 2) the velocities of the colliding particles are uncorrelated (molecular chaos and break of time reversal)
- A first-order **partial differential** equation with an **integral** collision term

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f(t,\mathbf{r},\mathbf{v})=\frac{1}{Kn}C[f,f_2]$$

Only two effects! (Simplicity)

Movement — Collision (or Interaction)

Kinematic — Dissipation

$C[f,f_2]=$ Gain (scattered into) - Loss (scattered out)

$$=\left(\frac{\delta f}{\delta t}\right)^{+}-\left(\frac{\delta f}{\delta t}\right)^{-}$$

$$\sim\int\left|\mathbf{v}-\mathbf{v}_2\right|(f^{*}f_2^{*}-ff_2)d\mathbf{v}_2$$

How complexity out of simplicity? - I

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f(t,\mathbf{r},\mathbf{v})=C[f,f_2]$$

$\rho\mathbf{u}=\langle m\mathbf{v}f(t,\mathbf{r},\mathbf{v})\rangle$

where $\langle\cdots\rangle=\iiint\cdots dv_x dv_y dv_z$

Differentiating the statistical definition $\rho\mathbf{u}\equiv\langle m\mathbf{v}f(t,\mathbf{r},\mathbf{v})\rangle$ *with time* and *then combining* with BTE ($t,\mathbf{r},\mathbf{v}$ are independent and $\mathbf{v}=\mathbf{u}+\mathbf{c}$)

$$\frac{\partial}{\partial t}\langle m\mathbf{v}f\rangle=\left\langle m\mathbf{v}\frac{\partial f}{\partial t}\right\rangle=-\langle m(\mathbf{v}\cdot\nabla f)\mathbf{v}\rangle+\langle m\mathbf{v}C[f,f_2]\rangle$$

$[\mathbf{A}]^{(2)}$: Traceless symmetric part of tensor $\mathbf{A}$

Here $-\langle m(\mathbf{v}\cdot\nabla f)\mathbf{v}\rangle=-\nabla\cdot\langle m\mathbf{v}\mathbf{v}f\rangle=-\nabla\cdot\{\rho\mathbf{u}\mathbf{u}+\langle m\mathbf{c}\mathbf{c}f\rangle\}$

After the decomposition of the stress into pressure and viscous shear stress $\mathbf{\Pi}$

$\mathbf{P}\equiv\langle m\mathbf{c}\mathbf{c}f\rangle=p\mathbf{I}+\mathbf{\Pi}$ where $p\equiv\langle m\mathrm{Tr}(\mathbf{c}\mathbf{c})f/3\rangle$, $\mathbf{\Pi}\equiv\langle m[\mathbf{c}\mathbf{c}]^{(2)}f\rangle$,

and using the collisional invariance of the momentum, $\langle m\mathbf{v}C[f,f_2]\rangle=0$,

we have

$$\frac{\partial(\rho\mathbf{u})}{\partial t}+\nabla\cdot(\rho\mathbf{u}\mathbf{u}+p\mathbf{I}+\mathbf{\Pi})=0.$$

Exact consequence of the original BTE!

How complexity out of simplicity? - II

This procedure can be generalized for arbitrary molecular expressions of general moment (**viscous shear stress** $\mathbf{\Pi}$ and **heat flux** $\mathbf{Q}$)

2nd-order closure

$$\rho \frac{D}{Dt}\begin{bmatrix} \mathbf{\Pi}\left(\equiv\left\langle m[\mathbf{cc}]^{(2)} f\right\rangle\right)/\rho \\ \mathbf{Q}\left(\equiv\left\langle mc^2\mathbf{c}/2f\right\rangle\right)/\rho \end{bmatrix} + \boxed{\nabla\cdot\begin{bmatrix} \langle m\mathbf{ccc}f\rangle - \langle m\mathrm{Tr}(\mathbf{ccc})f\rangle \mathbf{I}/3 \\ \langle mc^2\mathbf{cc}f/2\rangle - C_pT(p\mathbf{I}+\mathbf{\Pi}) + \langle m\mathbf{ccc}f\rangle : \nabla\mathbf{u}\end{bmatrix}} +$$

$$\begin{bmatrix} 2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} \\ \frac{D\mathbf{u}}{Dt}\cdot\mathbf{\Pi} + \mathbf{Q}\cdot\nabla\mathbf{u} + \mathbf{\Pi}\cdot C_p\nabla T\end{bmatrix} + \begin{bmatrix} 2p[\nabla\mathbf{u}]^{(2)} \\ pC_p\nabla T\end{bmatrix} = \boxed{\begin{bmatrix}\left\langle m[\mathbf{cc}]^{(2)} C[f,f_2]\right\rangle \\ \left\langle \left(mc^2/2 - mC_pT\right)\mathbf{c}C[f,f_2]\right\rangle\end{bmatrix}}$$

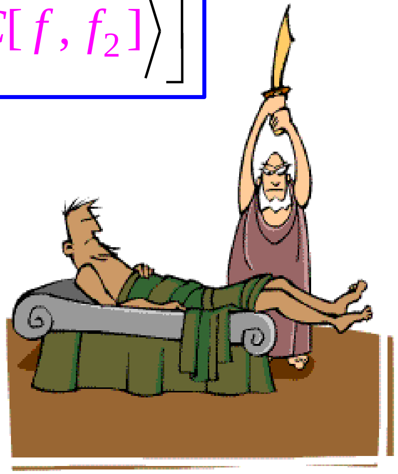
2nd-order closure

Key points: 1) No approximation: exact consequence of the original BTE

2) **Balanced closure for two open terms** (Myong, 2014)

Different from previous practice misguided by Maxwellian molecule assumption

Do not cut the tiptoe in order to fit the foot into a shoe! (削趾適履)



Procrustean bed

How complexity out of simplicity? - III

Hyperbolic (inviscid)

Conservation laws (exact consequence of BTE)

$$\boxed{\rho \frac{D}{Dt}\begin{bmatrix}1/\rho\\ \mathbf{u}\\ E_t\end{bmatrix} + \nabla\cdot\begin{bmatrix}-\mathbf{u}\\ p\mathbf{I}\\ p\mathbf{u}\end{bmatrix}} + \nabla\cdot\begin{bmatrix}0\\ \boldsymbol{\Pi}\\ \boldsymbol{\Pi}\cdot\mathbf{u}+\mathbf{Q}\end{bmatrix} = \mathbf{0}$$

in conjunction with the (complex) 2nd-order constitutive equations

$$\rho\frac{D(\boldsymbol{\Pi}/\rho)}{Dt} + \underbrace{2[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}]^{(2)}}_{\text{2nd-order coupling}} + \underbrace{2p[\nabla\mathbf{u}]^{(2)}}_{\text{Navier 1st law}} = -\frac{p}{\mu_{NS}}\boldsymbol{\Pi}\, q_{2nd}(\kappa_1),$$

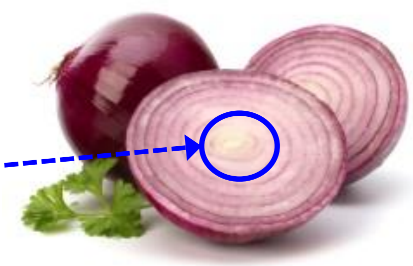
$$\rho\frac{D(\mathbf{Q}/\rho)}{Dt} + \underbrace{\frac{D\mathbf{u}}{Dt}\cdot\boldsymbol{\Pi} + \mathbf{Q}\cdot\nabla\mathbf{u} + \boldsymbol{\Pi}\cdot C_p\nabla T}_{\text{2nd-order coupling}} + \underbrace{C_p p\nabla T}_{\text{Fourier 1st law}} = -\frac{pC_p}{k_{NS}}\mathbf{Q}\, q_{2nd}(\kappa_1),$$

Non-hyperbolic

Implicit

$$q_{2nd}(\kappa_1) \equiv \frac{\sinh\kappa_1}{\kappa_1},\quad \kappa_1 \equiv \frac{T^{1/4}}{p}\left(\frac{\boldsymbol{\Pi}:\boldsymbol{\Pi}}{\mu_{NS}} + \frac{\mathbf{Q}\cdot\mathbf{Q}/T}{k_{NS}}\right)^{1/2}$$

Navier-Fourier laws inclusive like onion!



A model for 2nd-order constitutive law

$$\rho\frac{D(\mathbf{\Pi}/\rho)}{Dt}+2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}+2p[\nabla\mathbf{u}]^{(2)}=-\frac{p}{\mu_{NS}}\mathbf{\Pi}\left(\frac{\sinh\kappa_1}{\kappa_1}\right),\ \kappa_1\equiv\frac{T^{1/4}}{p}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{\mu_{NS}}+\frac{\mathbf{Q}\cdot\mathbf{Q}/T}{k_{NS}}\right)^{1/2}$$

No heat flux

$$\rho\frac{D(\mathbf{\Pi}/\rho)}{Dt}(-\mu_{NS})+[\mathbf{\Pi}\cdot(-2\mu_{NS})\nabla\mathbf{u}]^{(2)}+p(-2\mu_{NS})[\nabla\mathbf{u}]^{(2)}=p\mathbf{\Pi}\left(\frac{\sinh\kappa_1}{\kappa_1}\right),\ \kappa_1\equiv\frac{T^{1/4}}{p}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{\mu_{NS}}\right)^{1/2}$$

One-dimension

$$\mathbf{\Pi}_{NS}\equiv-2\mu_{NS}[\nabla\mathbf{u}]^{(2)}$$

$$\hat{t}\equiv\frac{t}{\mu_{NS}/p},\ \hat{\Pi}\equiv\frac{\Pi}{p},\ \Pi_{NS}\equiv-\frac{4}{3}\mu_{NS}\frac{\partial u}{\partial x}$$

$$\frac{D\hat{\Pi}}{D\hat{t}}-\hat{\Pi}\hat{\Pi}_{NS}-\hat{\Pi}_{NS}=-\hat{\Pi}\,q(|\hat{\Pi}|),\ \text{where } q(|\hat{\Pi}|)\equiv\sinh|\hat{\Pi}|/|\hat{\Pi}|$$

$$t_{stress}(10^{-8}\ \text{sec})\ll t_{flow}$$

Or steady-state

$$\boxed{\hat{\Pi}\hat{\Pi}_{NS}+\hat{\Pi}_{NS}=\hat{\Pi}\,q(|\hat{\Pi}|)}$$

2nd-order | 1st-order | 1st-order x 2nd-order

Kinematic motion | **Collision**

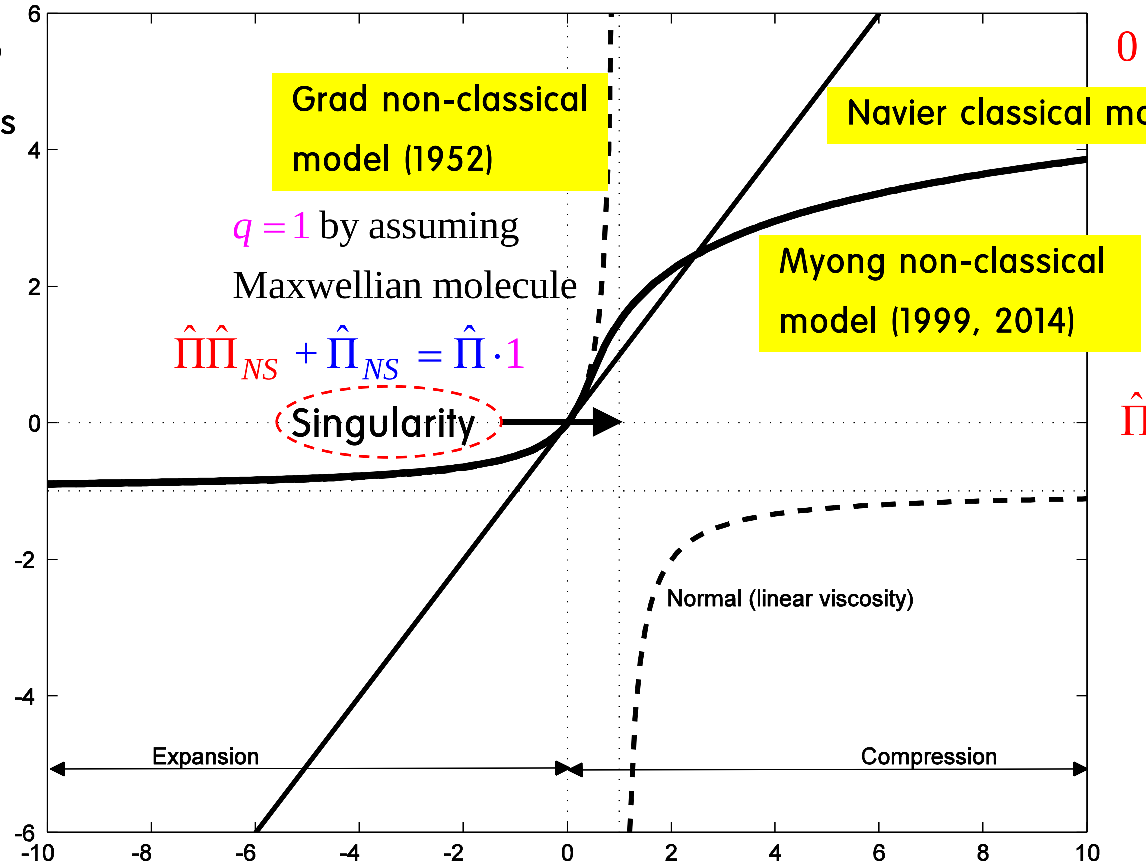
NCCR: Nonlinear Coupled Constitutive Relation

2^{nd}-order constitutive laws beyond Navier law I

1-D compression and expansion

Π / p

Viscous stress /pressure



$$0 + \hat{\Pi}_{NS} = \hat{\Pi}\cdot 1$$

$$q = \frac{\sinh\left(\Pi/p\right)}{\Pi/p}$$

$$\hat{\Pi}\hat{\Pi}_{NS} + \hat{\Pi}_{NS} = \hat{\Pi}q(\hat{\Pi})$$

Π_{NS} / p Velocity gradient /pressure

2nd-order constitutive laws beyond Navier law II

$$\rho\frac{D(\mathbf{\Pi}/\rho)}{Dt}+2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}+2p\left[\nabla\mathbf{u}\right]^{(2)}=-\frac{p}{\mu_{NS}}\mathbf{\Pi}q_{2nd}(\kappa_1),$$

$$\rho\frac{D(\mathbf{Q}/\rho)}{Dt}+\frac{D\mathbf{u}}{Dt}\cdot\mathbf{\Pi}+\mathbf{Q}\cdot\nabla\mathbf{u}+\mathbf{\Pi}\cdot C_p\nabla T+C_p p\nabla T=-\frac{pC_p}{k_{NS}}\mathbf{Q}q_{2nd}(\kappa_1)$$

1-D velocity shear → **No heat flux**

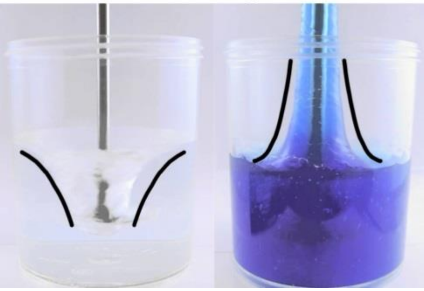
$$\frac{1}{\mu_{NS}}\begin{bmatrix}2\Pi_{xy}\Pi_{xy_{NS}}/3\\-\Pi_{yy}\Pi_{xy_{NS}}\end{bmatrix}-\frac{1}{\mu_{NS}}\begin{bmatrix}0\\p\Pi_{xy_{NS}}\end{bmatrix}=-\frac{p}{\mu_{NS}}\begin{bmatrix}\Pi_{yy}\\\Pi_{xy}\end{bmatrix}q_{2nd}(\kappa_1)$$

$$\boxed{\hat{\Pi}_{xy}^2=-\frac{3}{2}\left(1+\hat{\Pi}_{yy}\right)\hat{\Pi}_{yy}}$$

Stress constraint due to 2nd-order coupling!

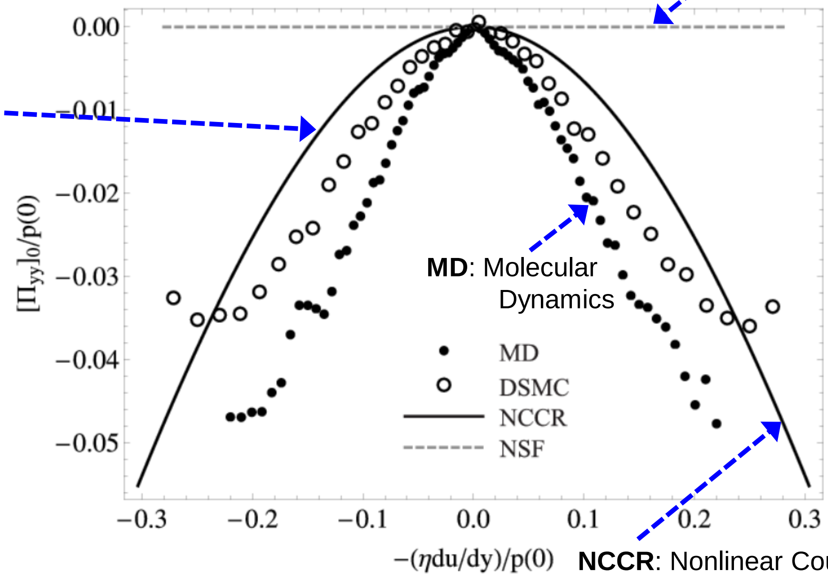
No such thing in 1st-order Navier law!

Rod Climbing Effect



Newtonian **Visco-elastic**

NSF: Navier-Stokes-Fourier



MD: Molecular Dynamics

NCCR: Nonlinear Coupled Constitutive Relation

1-D shock result: inverse shock thickness

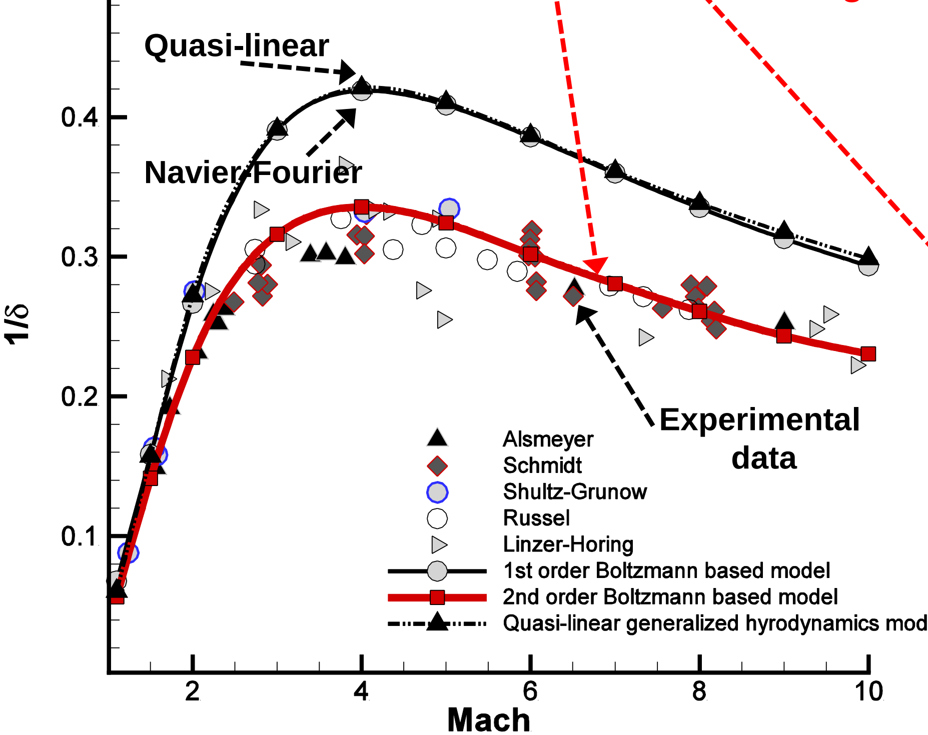
New 2nd-order & 2nd-order: **Best**

Navier 1st-order & 1st-order: Reference

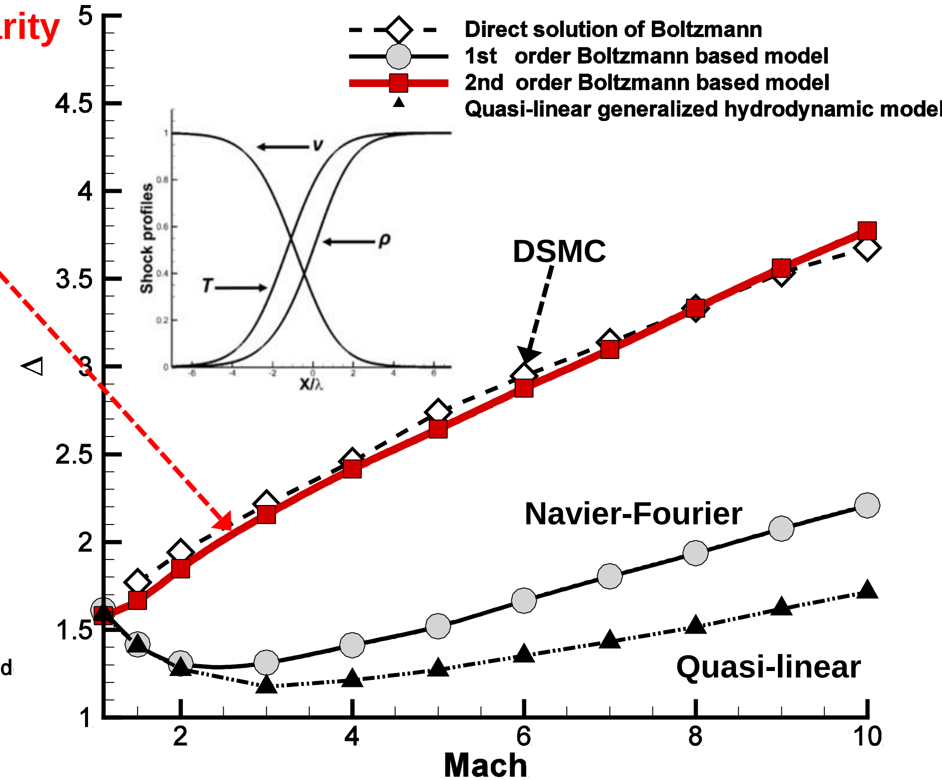
$0+\hat{\Pi}_{NS} = \hat{\Pi}q(\hat{\Pi})$ ←-- Quasi-linear 1st-order & 2nd-order: **Worse** than Navier

Grad 2nd-order & 1st-order: **Singularity**

⇨ Importance of **balanced** closure



Shock density thickness of argon gas



Shock temperature-density distance

(Karchani, *PhD Thesis*, GNU, 2017)

Multi-dimensional CFD based on decomposition

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Comparison with 1st-order simple Burger

$$\frac{\partial u}{\partial t}+\frac{\partial}{\partial x}\left(\frac{1}{2}u^2\right)+\boxed{\frac{\partial \Pi}{\partial x}}= \text{ where } \Pi_{NS}\Pi+\Pi_{NS}=\Pi q(\Pi) \text{ and } \Pi_{NS}=-\eta\frac{\partial u}{\partial x}$$

New 2nd-order model

$$\begin{cases} \dfrac{\partial u}{\partial t}+\dfrac{\partial}{\partial x}\left(\dfrac{1}{2}u^2+\Pi\right)=0, \\ \Pi=f^{-1}(-S) \text{ where } f(\Pi)=\dfrac{\sinh \Pi}{\Pi+1}, \\ S=\eta\dfrac{\partial u}{\partial x} \end{cases}$$

Original 1st-order Burger

$$\begin{cases} \dfrac{\partial u}{\partial t}+\dfrac{\partial}{\partial x}\left(\dfrac{1}{2}u^2+\Pi\right)=0, \\ \Pi=-S, \\ S=\eta\dfrac{\partial u}{\partial x} \end{cases}$$

$\Pi_{NS}\Pi+\Pi_{NS}=\Pi q(\Pi)$ can be solved for given Π_{NS} via method of iteration

$$\Pi_{n+1}=\sinh^{-1}(\Pi_{NS}(1+\Pi_n)) \text{ for positive } \Pi_{NS},$$

$$\Pi_{n+1}=\frac{\Pi_{NS}}{q(\Pi_n)-\Pi_{NS}} \qquad \text{for negative } \Pi_{NS}$$

Decomposed computation in multi-dimension I

Edge based finite volume formulation in general coordinates

$$\frac{\partial}{\partial t}\int_V \mathbf{U}dV + \int_S \mathbf{F}\cdot\mathbf{n}dS = 0$$

$$\mathbf{\Pi} = f_\Pi\left(\mathbf{\Pi}_{\mathrm{NSF}}, \mathbf{Q}_{\mathrm{NSF}}, p, T\right),$$

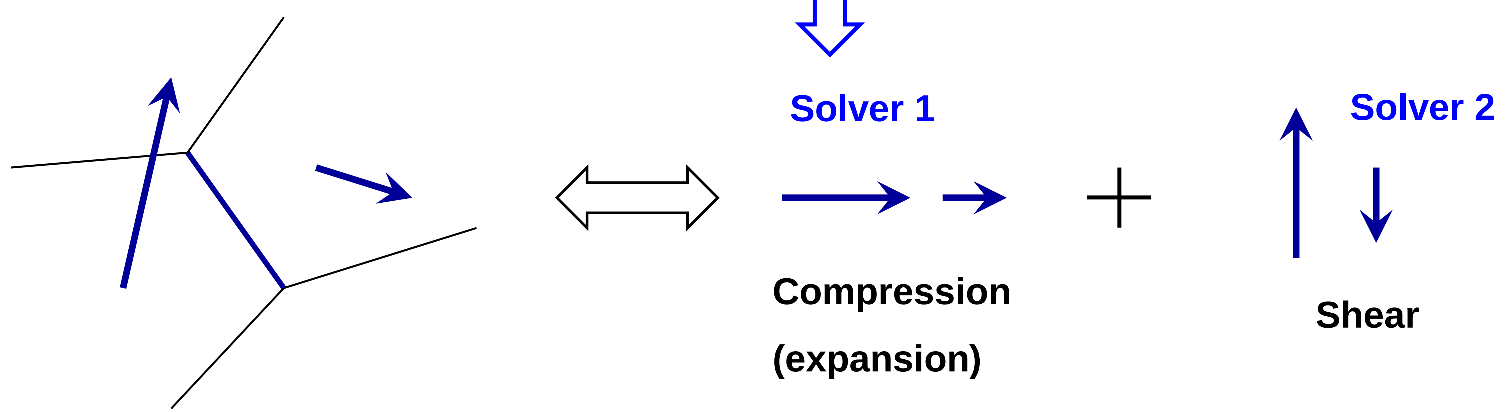
$$\mathbf{Q} = f_Q\left(\mathbf{\Pi}_{\mathrm{NSF}}, \mathbf{Q}_{\mathrm{NSF}}, p, T\right)$$

$$(-2\eta)\begin{bmatrix} 2u_x/3 & v_x/2 & w_x/2 \\ v_x/2 & -u_x/3 & 0 \\ w_x/2 & 0 & -u_x/3 \end{bmatrix} \xRightarrow{f_\Pi} \begin{bmatrix} \Pi_{xx} & \Pi_{xy} & \Pi_{xz} \\ \Pi_{yx} & \Pi_{yy} & \Pi_{yz} \\ \Pi_{zx} & \Pi_{zy} & \Pi_{zz} \end{bmatrix}$$

f_Π : complex 5-dimensional mapping

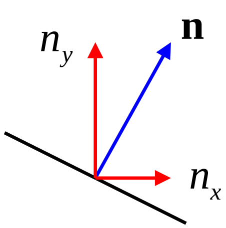
$$\because\ q_{2nd}(\kappa_1) \equiv \frac{\sinh \kappa_1}{\kappa_1},\quad \kappa_1 \equiv \frac{T^{1/4}}{p}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{\mu_{NS}} + \frac{\mathbf{Q}\cdot\mathbf{Q}/T}{k_{NS}}\right)^{1/2}$$

Decomposition



Decomposed computation in two-dimension II

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho v\\ \rho E\end{pmatrix}+\nabla\cdot\begin{pmatrix}\rho(\mathbf{u}\cdot\mathbf{n})\\ \rho u(\mathbf{u}\cdot\mathbf{n})+n_x p\\ \rho v(\mathbf{u}\cdot\mathbf{n})+n_y p\\ \rho H(\mathbf{u}\cdot\mathbf{n})\end{pmatrix}+\nabla\cdot\begin{pmatrix}0\\ n_x\Pi_{xx}+n_y\Pi_{xy}\\ n_x\Pi_{yx}+n_y\Pi_{yy}\\ n_x\Theta_x+n_y\Theta_y\end{pmatrix}=0$$



where $\Theta_x=u\Pi_{xx}+v\Pi_{xy}+Q_x,\ \Theta_y=u\Pi_{yx}+v\Pi_{yy}+Q_y$

In the case of *x*-direction, (Π_{xx},Π_{xy},Q_x) on interface for a given input (u_x,v_x,T_x) can be **decomposed** as

$$\boxed{\begin{aligned} f_x(u_x,v_x,T_x)&=f_{1x}(u_x,0,T_x)+f_{2x}(0,v_x,0).\\ f_y(u_y,v_y,T_y)&=f_{1y}(0,v_y,T_y)+f_{2y}(u_y,0,0).\end{aligned}}$$

Similarly,

Finally we have

$$\Pi_{xx}=\Pi_{xx-1x}+\Pi_{xx-2x}+\Pi_{xx-1y}+\Pi_{xx-2y},$$

$$\Pi_{xy}=\Pi_{xy-2x}+\Pi_{xy-2y},$$

$$\Pi_{yy}=\Pi_{yy-1x}+\Pi_{yy-2x}+\Pi_{yy-1y}+\Pi_{yy-2y},$$

$$Q_x=Q_{x-1x},\ Q_y=Q_{y-1y}$$

$$2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}+2p[\nabla\mathbf{u}]^{(2)}=-\frac{p}{\mu_{NS}}\mathbf{\Pi}q_{2nd}(\kappa_1),$$

$$\frac{D\mathbf{u}}{Dt}\cdot\mathbf{\Pi}+\mathbf{Q}\cdot\nabla\mathbf{u}+\mathbf{\Pi}\cdot C_p\nabla T+C_p p\nabla T=-\frac{pC_p}{k_{NS}}\mathbf{Q}q_{2nd}(\kappa_1)$$

$$q_{2nd}(\kappa_1)\equiv\frac{\sinh\kappa_1}{\kappa_1},\ \kappa_1\equiv\frac{T^{1/4}}{p}\left(\frac{\mathbf{\Pi}:\mathbf{\Pi}}{\mu_{NS}}+\frac{\mathbf{Q}\cdot\mathbf{Q}/T}{k_{NS}}\right)^{1/2}$$

Mixed modal DG method for the 2nd-order model I

$$\partial_t \mathbf{U} + \nabla \mathbf{F}_{\text{inv}}(\mathbf{U}) + \nabla \mathbf{F}_{\text{vis}}(\mathbf{U}, \nabla \mathbf{U}) = 0$$

Discretization in mixed form

$$\begin{cases} \boxed{\mathbf{S} - \nabla \mathbf{U} = 0} \\ \partial_t \mathbf{U} + \nabla \mathbf{F}_{\text{inv}}(\mathbf{U}) + \nabla \mathbf{F}_{\text{vis}}(\mathbf{U}, \mathbf{S}) = 0 \end{cases}$$

NSF model $(\mathbf{\Pi}, \mathbf{Q}) = \mathbf{f}_{\mathbf{linear}}(\mathbf{S}(\mathbf{U}))$

NCCR model $(\mathbf{\Pi}, \mathbf{Q})_{\mathbf{NCCR}} = \mathbf{f}_{\mathbf{non\text{-}linear}}(\mathbf{S}(\mathbf{U}), p, T)$

NCCR: Nonlinear Coupled Constitutive Relation

$$\mathbf{U}_h(\mathbf{x}, t) = \sum_{i=0}^{k} U_j^i(t) \varphi^i(\mathbf{x}), \quad \mathbf{S}_h(\mathbf{x}, t) = \sum_{i=0}^{k} S_j^i(t) \varphi^i(\mathbf{x})$$

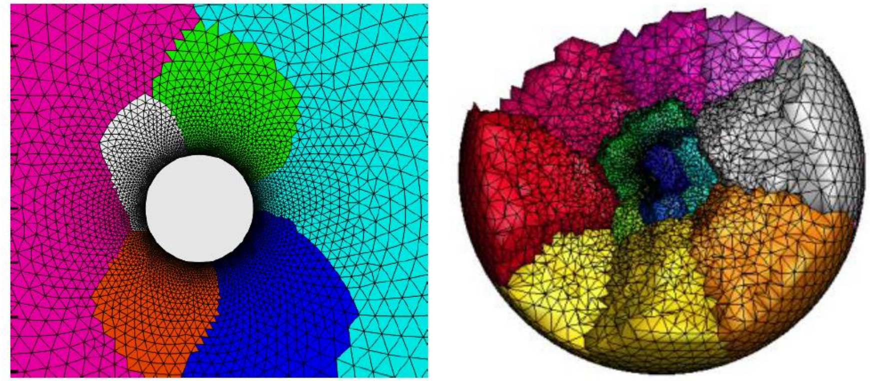
$$\begin{cases} \dfrac{\partial}{\partial t} \displaystyle\int_I \mathbf{U} \varphi dV - \int_I \nabla \varphi \mathbf{F}_{\text{inv}} dV + \int_{\partial I} \varphi \mathbf{F}_{\text{inv}} \cdot \mathbf{n} d\Gamma - \int_I \nabla \varphi \mathbf{F}_{\text{vis}} dV + \int_{\partial I} \varphi \mathbf{F}_{\text{vis}} \cdot \mathbf{n} d\Gamma = 0, \\ \displaystyle\int_I \mathbf{S} \varphi dV + \int_I T^s \nabla \varphi \mathbf{U} dV - \int_{\partial I} T^s \varphi \mathbf{U} \cdot \mathbf{n} d\Gamma = 0, \end{cases}$$

Dubiner basis function, Lax-Friedrichs inviscid flux, central flux for viscous terms

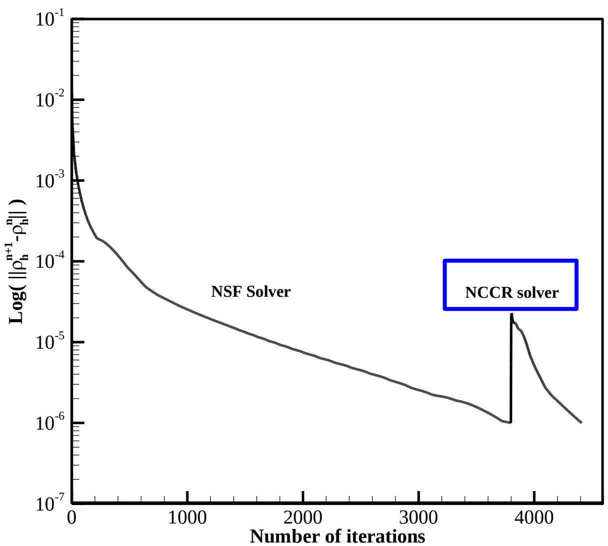
Mixed modal DG method for the 2nd-order model II

Convergence property and super-parallel performance

$$\hat{\Pi}\hat{\Pi}_{NS} + \hat{\Pi}_{NS} = \hat{\Pi} q(\hat{\Pi})$$

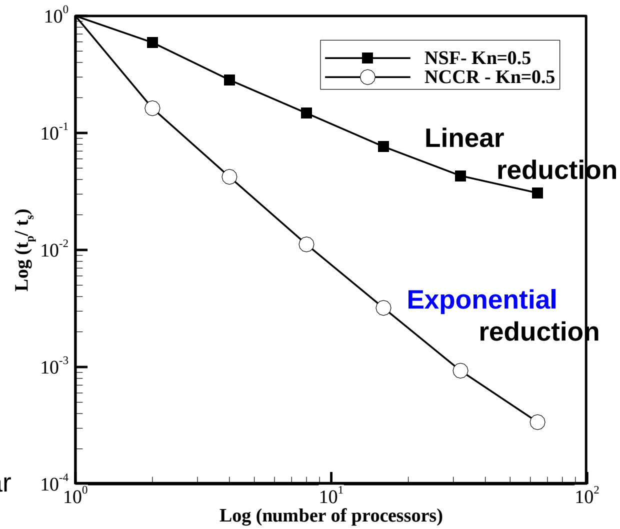


Triangular mesh partition using ParMETIS.; different colors represent sub-domains owned by different processors.



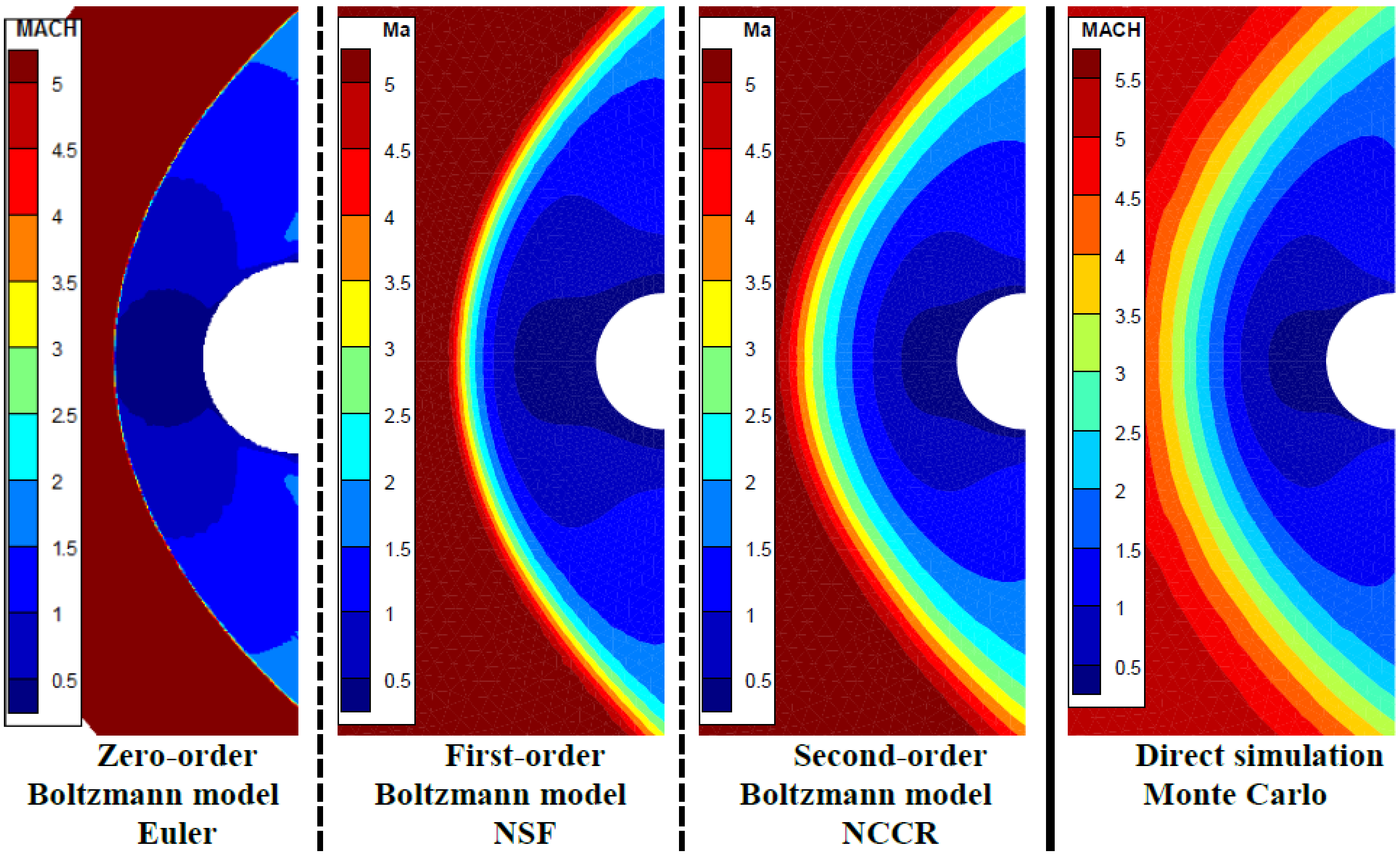
Convergence property

NCCR: Nonlinear Coupled Constitutive Relation



Super-parallel performance (via the rate of cost reduction)

Two-dimensional shock structure around cylinder



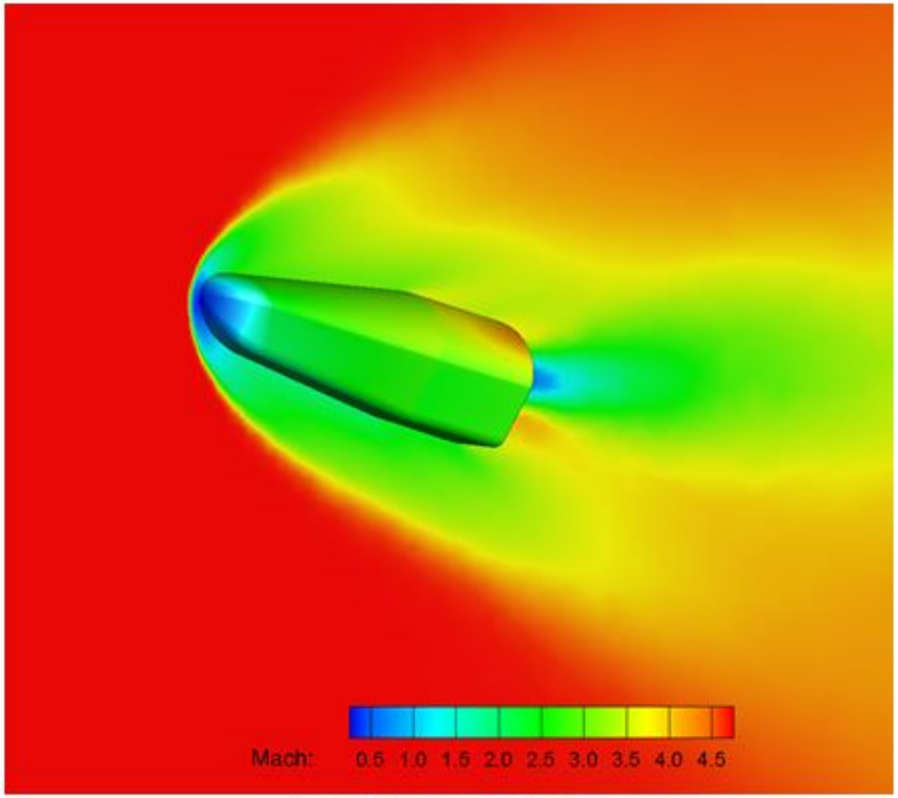
Computed Mach contours over cylinder (Mach 5.48, Kn=0.2)

NCCR: Nonlinear Coupled Constitutive Relation

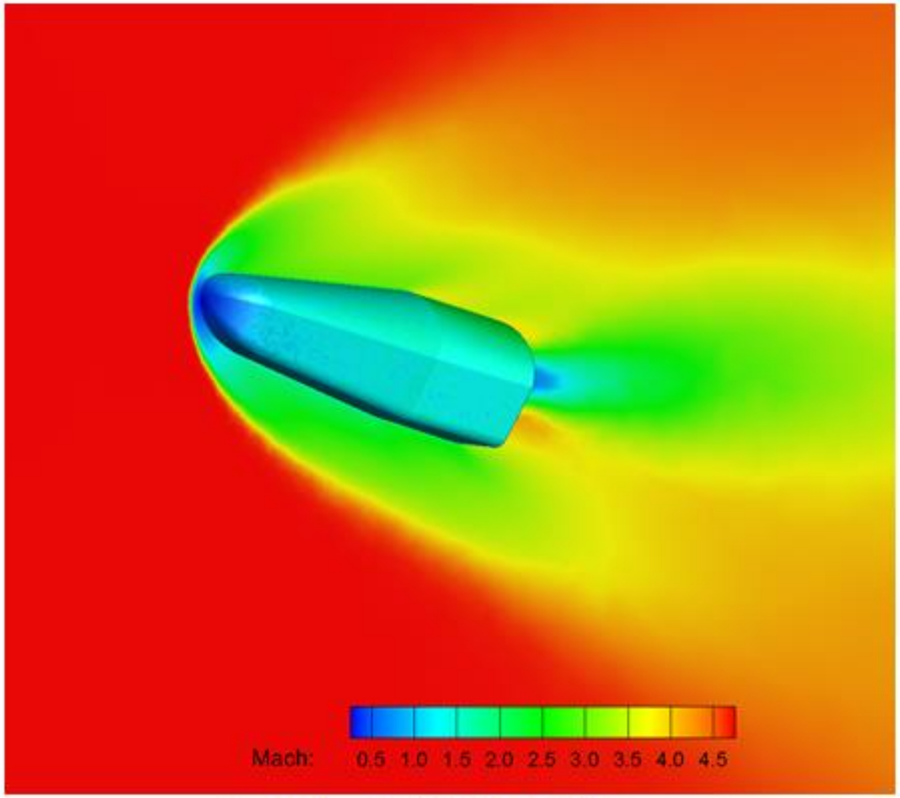
(Karchani, *PhD Thesis*, GNU, 2017)

Three-dimensional rarefied hypersonic flows

A suborbital re-entry vehicle



First-order NSF solution



Second-order NCCR solution

NCCR: Nonlinear Coupled Constitutive Relation

Mach contours of gas flows; M = 5.0, Kn = 0.02