Nonlinear Coupled Constitutive Relations (NCCRs) Derived from the Boltzmann Kinetic Equation Based on Balanced Closure and Mesoscopic Methods

July 25th, 2023 (2:00~2:45PM)

Rho Shin Myong

Professor, Department of Aerospace and Software Engineering
Director, Research Center for Aircraft Core Technology (ERC)
Gyeongsang National University
Jinju, South Korea
http://acml.gnu.ac.kr
myong@gnu.ac.kr

The 19th International Conference for Mesoscopic Methods in Engineering and Science

24-28 July 2023, Chengdu, China

Acknowledgements

Dr. Satyvir Singh (Graduate Student; now Postdoctoral Researcher in RWTH Aachen Univ.)

Hybrid DG code and computational simulation of rarefied & microscale gas flows

Dr. Omid Ejtehadi (Graduate Student; now Postdoctoral Research Fellow in University of Edinburgh)

Two-phase CFD codes and computational simulation of lunar landing and micro-jet two-phase gas flows; FVM-based *nccrFOAM suite*

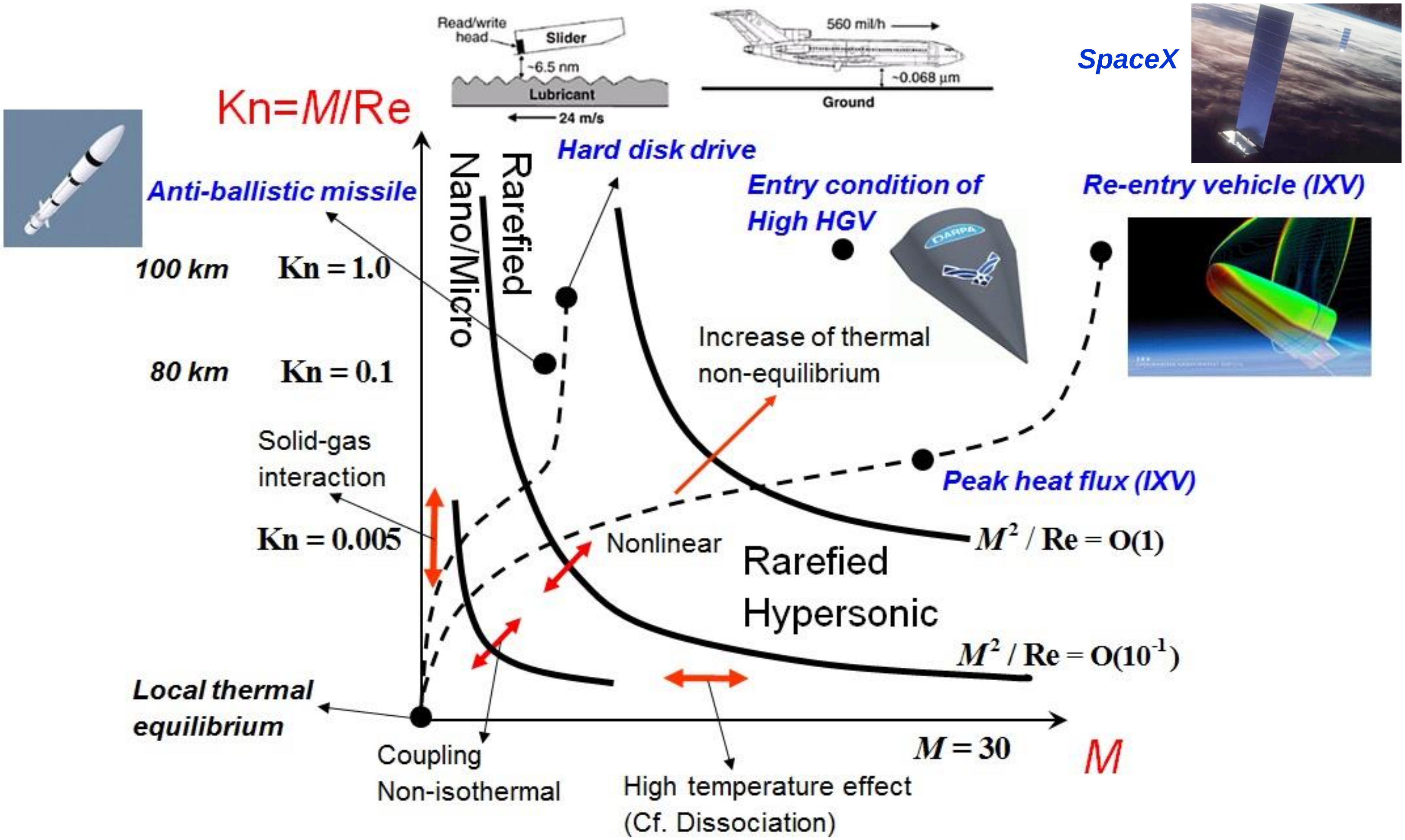
Dr. Tushar Chourushi (Graduate Student; now Assistant Professor in Amity University Mumbai)

CFD codes for viscoelastic flows with a new Boltzmann-type spring law

Dr. Tapan K. Mankodi (Postdoc; now Assistant Professor in IIT Guwahati)

Modified Boltzmann-Curtiss kinetic equation including the vibrational mode; FVM-based *nccrFOAM suite*

Classification of gas flows in non-equilibrium



$\mathbf{v}\cdot\nabla f(\mathbf{r},\mathbf{v}) = C[f, f_2]$ $\xrightarrow[\text{via statistical average}]{M\text{ appearing}}$ $\rho\mathbf{u}\cdot\nabla\mathbf{u} + \nabla\cdot p\mathbf{I} + \nabla\cdot\mathbf{\Pi} = 0$ $\Longrightarrow$ **Main parameter** $\Pi/p \sim \mathrm{Kn}\cdot M$

Two terms: Kn

Three terms: *M*, Kn

(not Kn alone)

$\frac{M^2}{\mathrm{Re}}$ or $\frac{M}{\sqrt{\mathrm{Re}}}$

Previous and ongoing studies on NCCR

PoF 1999, JCP 2001, JCP 2004: Eu's generalized hydrodynamics

PoF 2014, PoF 2016: Balanced closure & validation via MD

JCP 2014: 2D hybrid DG code for NCCR

PoF 2018: Polyatomic gases (shock-vortex interaction)

PoF 2020: Topology of NCCR

PoF 2020: Extension to the vibrational mode of energy

JCP 2020: Extension to dusty and granular flows

JCP 2022: 3D hybrid DG code for NCCR

CPC 2023 (in Revision): FVM-based *nccrFOAM suite*

Preprint: 2nd-order Boltzmann-type kinetic spring model

Conceptual revision

New closure theory

Physical insight

More validation

Discontinuous Galerkin

Topology

Two-phase flow

Vibrational mode

Viscoelastic flow

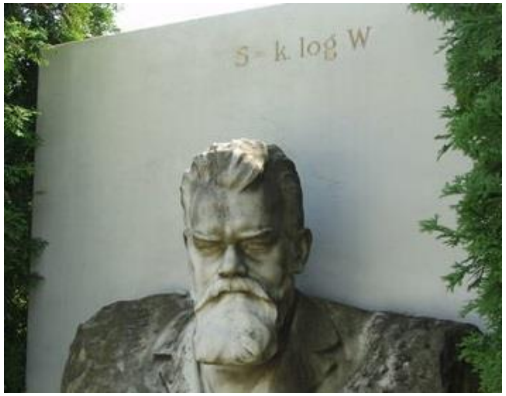
Combining with DSMC

Other independent NCCR works: Multi-species extension by Ahn & Kim (SNU, Korea, JCP09)

Implicit-FVM NCCR by Jiang, Zhao, Yuan, Chen (Zhejiang Univ., China, 2017-Present)

Boltzmann kinetic equations

- A first-order partial differential equation of **the probability density of finding a particle in phase space** with an integral collision term



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

Movement — Collision (or Interaction)

Kinematic — Dissipation

$$C[f,f_2]\sim\int|\mathbf{v}-\mathbf{v}_2|(f^* f_2^* - ff_2)d\mathbf{v}_2$$

$=$ Gain (scattered into) - Loss (scattered out) $= \left(\frac{\delta f}{\delta t}\right)^+ - \left(\frac{\delta f}{\delta t}\right)^-$

- **Maxwell's equation of transfer** for molecular expression $h^{(n)}$

$$\frac{\partial}{\partial t}\left\langle h^{(n)}f\right\rangle+\nabla\cdot\left(\mathbf{u}\left\langle h^{(n)}f\right\rangle+\left\langle \mathbf{c}h^{(n)}f\right\rangle\right)-\left\langle f\frac{d}{dt}h^{(n)}\right\rangle-\left\langle f\mathbf{c}\cdot\nabla h^{(n)}\right\rangle=\left\langle h^{(n)}C[f,f_2]\right\rangle$$

Moment method and closure theories

$$\phi^{(h)} = \left\langle h^{(k)} f \right\rangle$$

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

where

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

$$\phi^{(1)} = \rho,\ \phi^{(2)} = \rho\mathbf{u},\ \phi^{(3)} = \rho E,$$

$$\phi^{(4)} = \mathbf{\Pi} = [\mathbf{P}]^{(2)},\ \phi^{(5)} = \Delta = \frac{1}{3}\mathrm{Trace}\,\mathbf{P} - p,\ \phi^{(6)} = \mathbf{Q},$$

$$h^{(1)} = m,\ h^{(2)} = m\mathbf{v},\ h^{(3)} = \frac{1}{2}mC^2 + H_{rot},$$

$$h^{(4)} = [m\mathbf{CC}]^{(2)},\ h^{(5)} = \frac{1}{3}mC^2 - p/n,\ h^{(6)} = \left(\frac{1}{2}mC^2 + H_{rot} - m\hat{h}\right)\mathbf{C},$$

Breakdown of moment method: 1) when the statistical average is meaningless due to too few particles; 2) when thermodynamics is not definable.

Closure-first approach: Grad’s 13 moment method (1949) based on **polynomial** expansion

Levermore method (1996) based on **Gaussian** (exponential) expansion

Regularized-13 moment method (2003)

Closure-last balanced approach: Myong’s balanced closure (On the High Mach Number Shock Structure Singularity Caused by Overreach of Maxwellian Molecules, PoF 2014)

Relationship with conservation laws (moments)

Boltzmann transport equation (BTE): 10^{23}

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

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

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 BKE ($t,\mathbf{r},\mathbf{v}$ 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

$\mathbf{P}\equiv\langle m\mathbf{c}\mathbf{c}f\rangle=p\mathbf{I}+\mathbf{\Pi}$ 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

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

Conservation laws: 13

Closing-last balanced closure on open terms

$$\mathbf{\Pi} \equiv \left\langle m[\mathbf{cc}]^{(2)}\, f \right\rangle$$

Closure theory: how, where (open terms), when (last)

New balanced closure with closure-last approach (PoF 2014)

2nd-order for kinematic LH = 2nd-order for collsion RH

$$\frac{D}{Dt}\left(\mathbf{\Pi}/\rho\right) + \underbrace{\boxed{\nabla\cdot\Psi^{(\Pi)}}}_{\text{2nd-order closure}} + 2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2p[\nabla\mathbf{u}]^{(2)} = \underbrace{\boxed{\left\langle m[\mathbf{cc}]^{(2)} C[f, f_2]\right\rangle \left(\equiv \mathbf{\Lambda}^{(\Pi)}\right)}}_{\text{2nd-order closure}}$$

$$\underset{2nd}{=} -\frac{p}{\mu_{NS}}\mathbf{\Pi} q_{2nd}(\kappa_1) \text{ where } \Psi^{(\Pi)} = \left\langle m\mathbf{ccc}f\right\rangle - \left\langle m\mathrm{Tr}(\mathbf{ccc})\, f\right\rangle \mathbf{I}/3$$

$$\frac{D}{Dt}\left(\Psi^{(\Pi)}/\rho\right) + \nabla\cdot\Xi + \cdots = \left\langle h^{(\Psi^{(\Pi)})} C[f, f_2]\right\rangle$$

Other collision operator

Collision operator	$C(f_i, f_j)$
Boltzmann	$\int d\mathbf{u}_j \int_0^{\pi} d\phi \int_0^{\infty} db\, b g_{ij}(f_i^* f_j^* - f_i f_j)$
Vlasov–Landau	$2\pi e_i^2 e_j^2 \ln \Lambda \int d\mathbf{u}'\, \partial_{ij} \cdot \mathbf{U}'(\mathbf{g}) \cdot \partial_{ij} f_i(\mathbf{u}')f_j(\mathbf{u}')$
Balescu–Lenard	$\sum_{\mathbf{k}} \frac{\pi \omega_i^2 \omega_j^2}{n_i^2 m_i} (\mathbf{k}/k^2) \cdot \partial_u \int d\mathbf{u}'(\mathbf{k}/k^2) \cdot (m_j \partial_u - m_i \partial_{u'})f_i(\mathbf{u})f_j(\mathbf{u}') \frac{\delta(\mathbf{k}\cdot\mathbf{u} - \mathbf{k}\cdot\mathbf{u}')}{\lvert\epsilon(k, \mathbf{k}\cdot\mathbf{u})\rvert^2}$
Fokker–Planck	$-2\pi e_i^2 e_j^2 m_i^{-1} \ln \Lambda\, \partial_{u\alpha} \int d\mathbf{u}'[f_i(\mathbf{u})\partial_{u'\beta} f_j(\mathbf{u}')/m_j - f_j(\mathbf{u}')\partial_{u\beta} f_i(\mathbf{u})]\, U_{\alpha\beta}(\mathbf{u} - \mathbf{u}')$

$U'_{\alpha\beta}(x) = x^{-3}(x^2\delta_{\alpha\beta} - x_\alpha x_\beta)$; $\partial_{ij} = m_i^{-1}\partial_u - m_j^{-1}\partial_{u'}$; $\mathbf{g} = \mathbf{u} - \mathbf{u}'$;

$\omega_i^2 = 4\pi n_i e_i^2/m_i$; $\ln \Lambda$ = Coulomb logarithm;

$$\epsilon(\mathbf{k}, \omega) = 1 + \sum_i (\omega_i^2/k^2) \int d\mathbf{u}(\omega - \mathbf{k}\cdot\mathbf{u})\mathbf{k} \cdot \partial_u f_i(\mathbf{u}).$$

Boltzmann

(1872)

If there are no external forces, and conditions are uniform throughout the gas, this equation takes the form (equation (16)):

$$\frac{\partial f(x,t)}{\partial t} = \int_0^{\infty} \int_0^{x+x'} \left[\boxed{\frac{f(\xi,t)}{\sqrt{\xi}} \frac{f(x+x'-\xi,t)}{\sqrt{(x+x'-\xi)}}} - \boxed{\frac{\boxed{f(x,t)}}{\sqrt{x}} \frac{\boxed{f(x't)}}{\sqrt{x'}}} \right] \sqrt{(xx')}\, \psi(x, x', \xi)\, dx'\, d\xi$$

where the variables x and x' denote the energies of two molecules before a collision, and ξ and $(x+x'-\xi)$ denote their energies after the collision; $\psi(x, x', \xi)$ is a function which depends on the nature of the forces between the molecules.

Closure of dissipation terms via 2nd-law

Key ideas; exponential canonical form, consideration of entropy production σ, and non-polynomial expansion called as cumulant expansion (B. C. Eu in 80-90s)

By writing the distribution function f in the exponential form

$$f = \exp\left[-\beta\left(\frac{1}{2}mc^2 + \sum_{n=1}^{\boxed{\infty}} X^{(n)}h^{(n)} - N\right)\right],\ \beta \equiv \frac{1}{k_B T},$$

Nonequilibrium entropy Ψ: $\Psi(\mathbf{r},t) = -k_B\left\langle\left[\ln f(\mathbf{v},\mathbf{r},t) - 1\right] f(\mathbf{v},\mathbf{r},t)\right\rangle,$

Nonequilibrium entropy production: $\sigma_c \equiv -k_B\left\langle \ln f\ C[f, f_2]\right\rangle$

When f is truncated, it is truncated in such as way that the divergence problem related to the heat flux contribution containing the 3rd order term for the integrand would not arise (Al-Ghoul, M., and Eu, B. C., Nonequilibrium Partition Function in the Presence of Heat Flow, J. Chem. Phys., Vol. 115, No. 18, 2001).

$$\sigma_c = \frac{1}{4}k_B\int d\mathbf{v}\int d\mathbf{v}_2\int_0^{2\pi} d\phi\int_0^{\infty} db\ bg_{12}\ln(f^{c*}f_2^{c*}/f^c f_2^c)(f^{c*}f_2^{c*} - f^c f_2^c) \geq 0\ \text{(satisfying 2nd-law)}$$

$$\sigma_c \equiv -k_B\left\langle \ln f\ C[f, f_2]\right\rangle = \frac{1}{T}\left\langle\left(\frac{1}{2}mc^2 + \sum_{n=1}^{\infty} X^{(n)} : h^{(n)} - N\right) C[f^{(0)}\exp(-x), f_2^{(0)}\exp(-x_2)\right\rangle$$

$$= \frac{1}{4}k_B\int d\mathbf{v}\int d\mathbf{v}_2\int_0^{2\pi} d\phi\int_0^{\infty} db\ bg_{12} f^{(0)} f_2^{(0)}(x_{12} - y_{12})\left[\exp(-y_{12}) - \exp(-x_{12})\right]$$

$$= \frac{1}{4T}\int d\Gamma_{12} f^{(0)} f_2^{(0)}(x_{12} - y_{12})\left[\exp(-y_{12}) - \exp(-x_{12})\right],\quad \left(\begin{array}{l} x \equiv \beta\left(\sum_{n=1}^{\infty} X^{(n)}h^{(n)} - N\right), \\ y \text{ the post-collision value of } x \end{array}\right)$$

$$\sigma_c = \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots)\ \text{via cumulant expansion}\ \left(\kappa_1 \equiv \frac{1}{2}\left\{\left\langle(x_{12} - y_{12})^2\right\rangle_c\right\}^{1/2}\right)$$

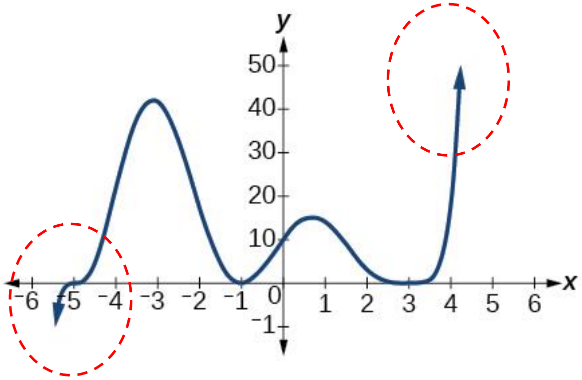
$$\text{where } q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots) \equiv \frac{1}{2\kappa_1}\left\{\exp\left[\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\kappa_l^{(+)}\right] - \exp\left[\sum_{l=1}^{\infty}\frac{(-1)^l}{l!}\kappa_l^{(-)}\right]\right\}$$

Cumulant expansion method

$$\left\langle x^l \right\rangle = \int x^l f(x)dx, \ \left\langle e^{\lambda x} \right\rangle = \int e^{\lambda x} f(x)dx$$

Then we have

$$\left\langle e^{\lambda x} \right\rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \left\langle x^l \right\rangle \boxed{= \exp\left[\sum_{l=1}^{\infty} \frac{\lambda^l}{l!} \kappa_l \right]} \text{ where}$$



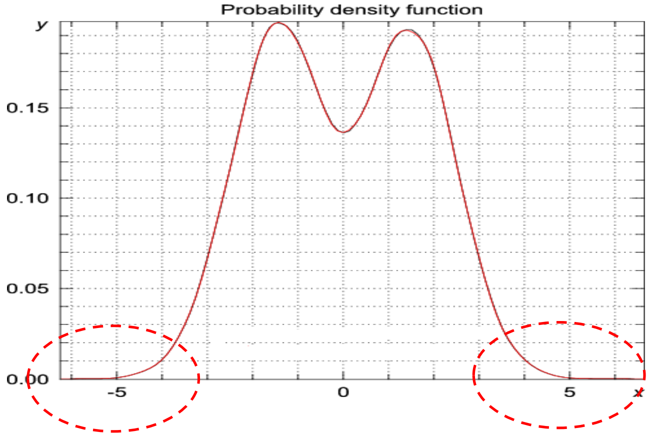
$$\kappa_l = \left[\frac{d^l}{d\lambda^l} \ln \left\langle e^{\lambda x} \right\rangle \right]_{\lambda=0} ; \ \kappa_1 = \langle x \rangle, \ \kappa_2 = \left\langle x^2 \right\rangle - \langle x \rangle^2, \cdots \text{ (mean, variance)}$$

$$\left\langle e^x \right\rangle_{\text{polynomical}} = 1 + \langle x \rangle + \frac{1}{2!} \left\langle x^2 \right\rangle + \frac{1}{3!} \left\langle x^3 \right\rangle + \cdots,$$

$$\left\langle e^x \right\rangle_{\text{cumulant}} = \exp^{\left[\langle x \rangle + \frac{1}{2!} \left(\left\langle x^2 \right\rangle - \langle x \rangle^2 \right) + \cdots \right]}$$

$$\left(\left\langle e^x \right\rangle - \left\langle e^{-x} \right\rangle \right) / 2 \Big]_{\text{polynomial}} = \langle x \rangle + \frac{1}{3} \left\langle x^3 \right\rangle + \cdots \approx \langle x \rangle$$

$$\left(\left\langle e^x \right\rangle - \left\langle e^{-x} \right\rangle \right) / 2 \Big]_{\text{cumulant}} = \exp^{\left(\frac{1}{2!} \left(\left\langle x^2 \right\rangle - \langle x \rangle^2 \right) + \cdots \right)} \left[\exp^{\left(\langle x \rangle + \cdots \right)} - \exp^{\left(-\langle x \rangle + \cdots \right)} \right] / 2 \underset{2nd}{\approx} \sinh \langle x \rangle$$



Closure of dissipation terms-continued

$$\sigma_c \equiv -k_B \left\langle \ln f\ C[f,f_2] \right\rangle = \frac{1}{T}\sum_{n=1}^{\infty} X^{(n)} \left\langle h^{(n)} C[f,f_2] \right\rangle = \frac{1}{T}\sum_{l=1}^{\infty} X^{(n)} \Lambda^{(n)} = \kappa_1^2 q(\kappa_1^{(\pm)},\kappa_2^{(\pm)},\cdots)\ ,$$

Calculating the first reduced collision integral κ_1 in terms of $X^{(n)}$,

$\kappa_1^2 = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)}$, where $R_{12}^{(nl)}$ are coefficients made up of collision bracket integrals,

$$\boldsymbol{\Lambda}^{(n)} = \frac{1}{\beta g}\sum_{l=1}^{\infty} R_{12}^{(nl)} X_2^{(l)} q(\kappa_1^{(\pm)},\kappa_2^{(\pm)},\cdots)$$

After generalizing the equilibrium Gibbs ensemble theory to nonequilibrium processes,

one can obtain the leading order terms for $X^{(n)}$, $X^{(1)} = -\dfrac{\boldsymbol{\Pi}}{2p}$, $X^{(2)} = -\dfrac{\mathbf{Q}}{pC_pT}$.

Finally, a thermodynamically-consistent constitutive equation, still exact to BKE, can be derived;

$$\rho\frac{D(\boldsymbol{\Pi}/\rho)}{Dt} + \boxed{\nabla\cdot\boldsymbol{\Psi}^{(\Pi)}} + 2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} + 2p\left[\nabla\mathbf{u}\right]^{(2)} = \boxed{\frac{1}{\beta g}\sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)},\kappa_2^{(\pm)},\cdots)}$$

$$\rho\frac{D(\mathbf{Q}/\rho)}{Dt} + \boxed{\nabla\cdot\boldsymbol{\Psi}^{(Q)} + \boldsymbol{\Psi}^{(P)}\cdot\nabla\mathbf{u}} + \frac{D\mathbf{u}}{Dt}\cdot\boldsymbol{\Pi} + \mathbf{Q}\cdot\nabla\mathbf{u} + \boldsymbol{\Pi}\cdot C_p\nabla T + pC_p\nabla T$$

$$= \boxed{\frac{1}{\beta g}\sum_{l=1}^{\infty} R_{12}^{(3l)} X_2^{(l)} q(\kappa_1^{(\pm)},\kappa_2^{(\pm)},\cdots)}$$

2^{nd}-order NCCR model

Conservation laws (exact consequence of BKE)

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

in conjunction with the 2nd-order constitutive relations (CR)

Zero in 2nd-order approximation

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

Non-local term

2nd-order coupling

Navier 1st law

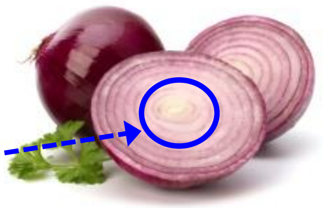
$$\Psi^{(\Pi)}\equiv\left\langle m\mathbf{ccc}f\right\rangle-\left\langle m\mathrm{Tr}(\mathbf{ccc})f\right\rangle\mathbf{I}/3$$

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

Onsager-Rayleigh dissipation function

Sinh{1st-order theory}

Navier-Fourier laws inclusive like onion!

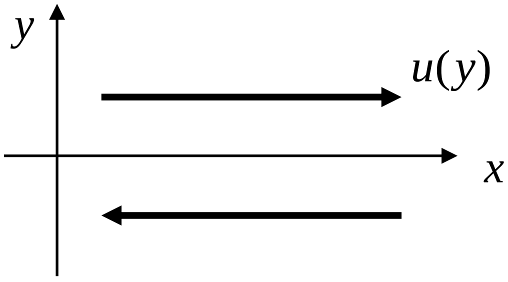


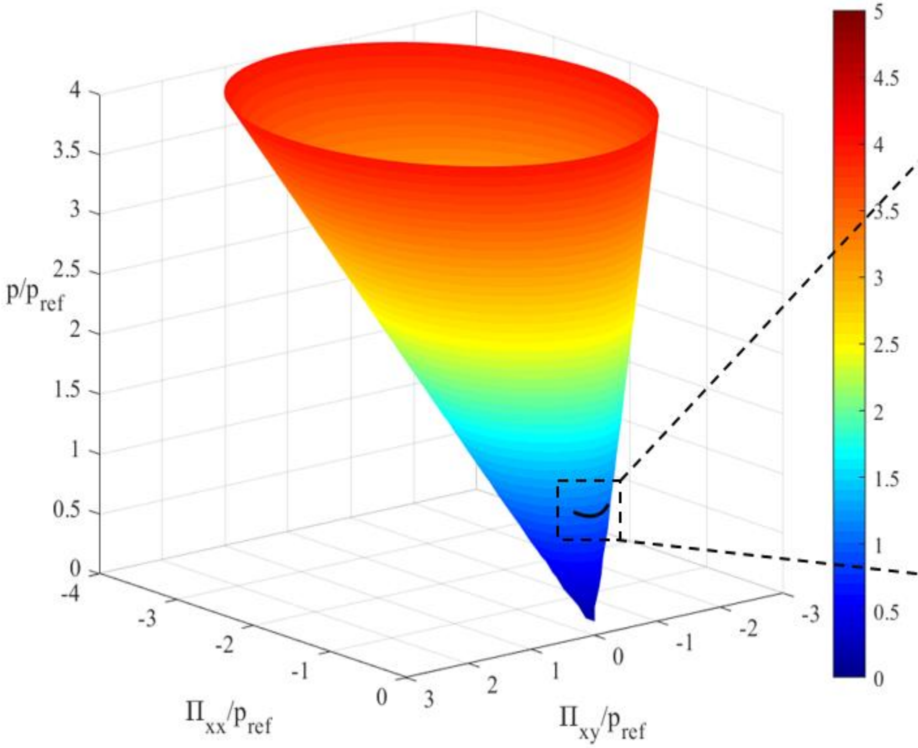
Topology of 2nd-order NCCR (velocity shear)

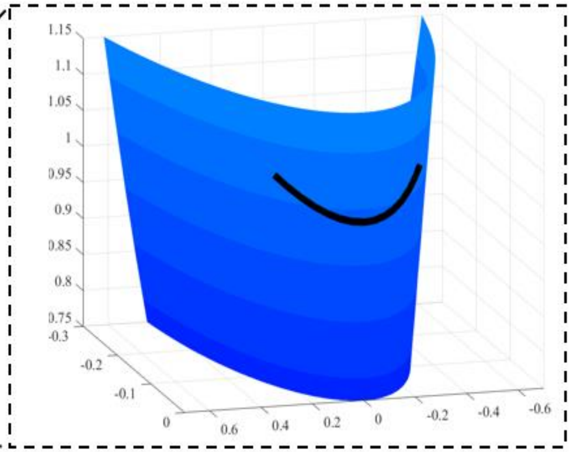
$$\mathbf{u}\cdot\nabla\mathbf{\Pi}++2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}+2p\left[\nabla\mathbf{u}\right]^{(2)}=-\frac{p}{\mu_{NS}}\mathbf{\Pi}q_{2nd}(\kappa_1)$$

Zero in velocity shear

$$\boxed{\left(\frac{\Pi_{xy}}{p}\right)^2=-\frac{3}{2}\left(1+\frac{\Pi_{yy}}{p}\right)\frac{\Pi_{yy}}{p}}$$





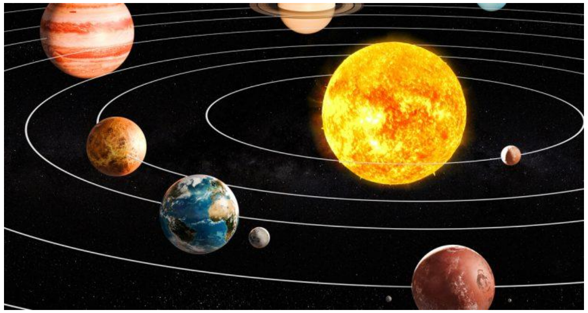


Topology of 2nd-order NCCR (velocity shear)

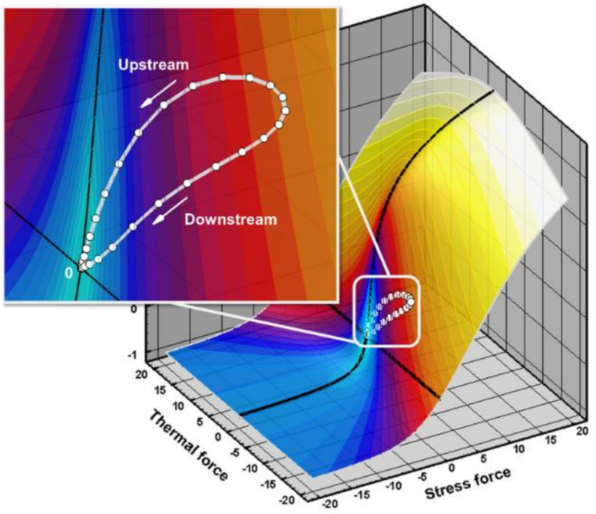
Carbon dioxide

Analogy among the second-order constitutive model, orbits of planets and comets, and Dirac cones.

	Second-order constitutive model in diatomic and polyatomic gases	Motion of the planets and comets in the two-body Kepler problem
Form of conic sections	$\left(1-\frac{9}{2}f_b^2\right)x^2+x+\frac{2}{3}y^2=0$ $f_b=\frac{\text{bulk viscosity}}{\text{shear viscosity}}$	$\left(1-e^2\right)x^2+2epx+y^2-p=0$ $p=\frac{L^2}{Gm_1^2m_2^2/(m_1+m_2)}$ L: angular momentum G: gravitational constant $m_{1,2}$: mass $E_{\min}=-\frac{G^2m_1^3m_2^3/(m_1+m_2)}{2L}$
Definition of x and y	$x=\frac{\Pi_{xx}}{p},\quad y=\frac{\Pi_{xy}}{p}$	$x=r\cos\theta,\ y=r\sin\theta$
Eccentricity	$e=\sqrt{\frac{27}{4}f_b^2-\frac{1}{2}},$ for $f_b\geq\sqrt{6}/9$	$e=\sqrt{1-\frac{E}{E_{\min}}},$ for $E\geq E_{\min}(<0)$
Topological properties	$f_b=\sqrt{6}/9;\ e=0$ (circle), $\sqrt{6}/9<f_b<\sqrt{2}/3;\ 0<e<1$ (ellipse), $f_b=\sqrt{2}/3;\ e=1$ (parabola), $f_b>\sqrt{2}/3;\ e>1$ (hyperbola)	$E=E_{\min};\ e=0$ (circle), $E_{\min}<E<0;\ 0<e<1$ (ellipse), $E=0;\ e=1$ (parabola), $E>0;\ e>1$ (hyperbola)
Direct analogy	$f_b\Leftrightarrow\frac{2\sqrt{3}}{9}\sqrt{\frac{1}{2}+e}=\frac{\sqrt{6}}{9}\sqrt{3-\frac{2E}{E_{\min}}}$ $f_b=0.2722\Leftrightarrow e_{\text{Earth}}=0.0167,$ $f_b=0.2834\Leftrightarrow e_{\text{Mercury}}=0.2056,$ $f_b=0.4611\Leftrightarrow e_{\text{Halley}}=0.967$	

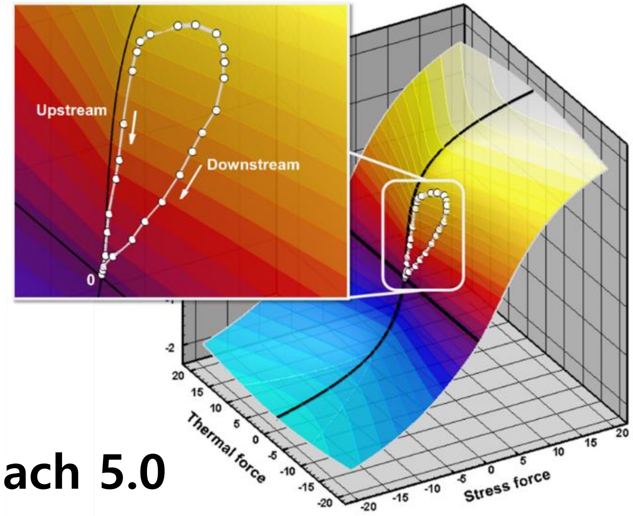


Topology of 2^{nd}-order NCCR (shock structure)

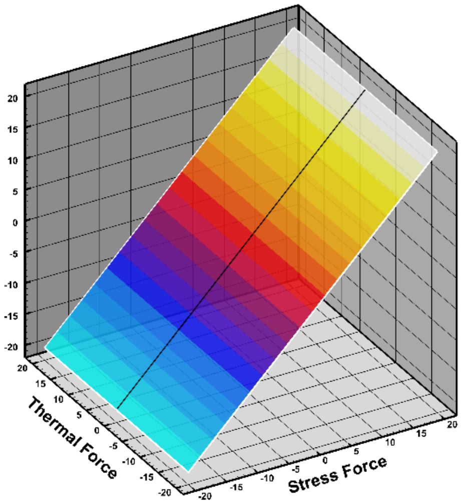


f_b=0.0

Mach 5.0



f_b=0.8



1st-order

$$\left[\hat{\mathbf{\Pi}}\cdot\nabla\hat{\mathbf{u}}\right]^{(2)}+\left(1+f_b\hat{\Delta}\right)\hat{\mathbf{\Pi}}_0=\hat{\mathbf{\Pi}}q_{2nd}(c\hat{R}),$$ (shear stress)

$$\frac{3}{2}\left(\hat{\mathbf{\Pi}}+f_b\hat{\Delta}\mathbf{I}\right):\nabla\hat{\mathbf{u}}+\hat{\Delta}_0=\hat{\Delta}q_{2nd}(c\hat{R}),$$ (excess normal stress)

$$\hat{\mathbf{\Pi}}\cdot\hat{\mathbf{Q}}_0+\left(1+f_b\hat{\Delta}\right)\hat{\mathbf{Q}}_0=\hat{\mathbf{Q}}q_{2nd}(c\hat{R}),$$ (heat flux)

$$\hat{\mathbf{\Pi}}_0=-2\mu\left[\nabla\mathbf{u}\right]^{(2)}$$
$$\hat{\Delta}_0=-\mu_b\nabla\cdot\mathbf{u}$$
$$\hat{\mathbf{Q}}_0=-k\nabla T$$

where $\hat{R}^2\equiv\hat{\mathbf{\Pi}}:\hat{\mathbf{\Pi}}+(5-3\gamma)f_b\hat{\Delta}^2+\hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}}$ (Onsager-Rayleigh dissipation function)

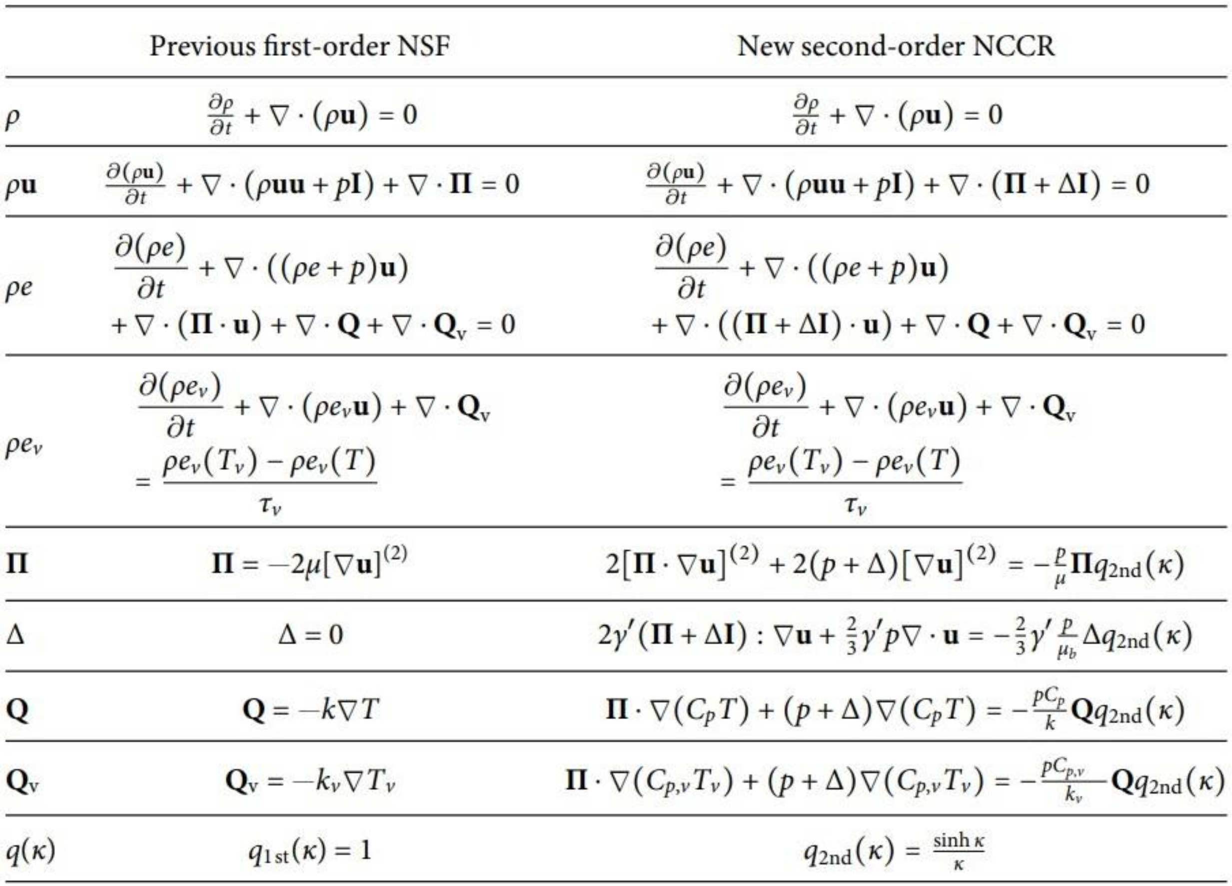
$$\Delta=\left\langle m\mathrm{Tr}(\mathbf{cc})f/3-m\mathrm{Tr}(\mathbf{cc})f^{(0)}/3\right\rangle,\ p=\left\langle m\mathrm{Tr}(\mathbf{cc})f^{(0)}/3\right\rangle$$

Vibrational mode: Modified Boltzmann-Curtiss

$$\frac{\partial f_i}{\partial t} + \mathbf{v}\cdot\nabla f_i + \mathbf{L}\cdot\nabla_r f_i = \sum_j\sum_k\sum_l \int dv_j \int d\Omega W(i, j,| k^*, l^*;\Omega)(f_k^* f_l^* - f_i f_j)$$

$$= \sum_j C[f_i\ , f_j\ ].$$

$$a(i) + a(j) \rightarrow a(k) + a(l)$$



	Previous first-order NSF	New second-order NCCR
ρ	$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$	$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$
$\rho\mathbf{u}$	$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{uu} + p\mathbf{I}) + \nabla\cdot\mathbf{\Pi} = 0$	$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot(\rho\mathbf{uu} + p\mathbf{I}) + \nabla\cdot(\mathbf{\Pi} + \Delta\mathbf{I}) = 0$
ρe	$\frac{\partial(\rho e)}{\partial t} + \nabla\cdot((\rho e + p)\mathbf{u})$ $+ \nabla\cdot(\mathbf{\Pi}\cdot\mathbf{u}) + \nabla\cdot\mathbf{Q} + \nabla\cdot\mathbf{Q}_v = 0$	$\frac{\partial(\rho e)}{\partial t} + \nabla\cdot((\rho e + p)\mathbf{u})$ $+ \nabla\cdot((\mathbf{\Pi} + \Delta\mathbf{I})\cdot\mathbf{u}) + \nabla\cdot\mathbf{Q} + \nabla\cdot\mathbf{Q}_v = 0$
ρe_v	$\frac{\partial(\rho e_v)}{\partial t} + \nabla\cdot(\rho e_v\mathbf{u}) + \nabla\cdot\mathbf{Q}_v$ $= \frac{\rho e_v(T_v) - \rho e_v(T)}{\tau_v}$	$\frac{\partial(\rho e_v)}{\partial t} + \nabla\cdot(\rho e_v\mathbf{u}) + \nabla\cdot\mathbf{Q}_v$ $= \frac{\rho e_v(T_v) - \rho e_v(T)}{\tau_v}$
$\mathbf{\Pi}$	$\mathbf{\Pi} = -2\mu[\nabla\mathbf{u}]^{(2)}$	$2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2(p + \Delta)[\nabla\mathbf{u}]^{(2)} = -\frac{p}{\mu}\mathbf{\Pi}q_{2\text{nd}}(\kappa)$
Δ	$\Delta = 0$	$2\gamma'(\mathbf{\Pi} + \Delta\mathbf{I}) : \nabla\mathbf{u} + \frac{2}{3}\gamma' p\nabla\cdot\mathbf{u} = -\frac{2}{3}\gamma'\frac{p}{\mu_b}\Delta q_{2\text{nd}}(\kappa)$
$\mathbf{Q}$	$\mathbf{Q} = -k\nabla T$	$\mathbf{\Pi}\cdot\nabla(C_p T) + (p + \Delta)\nabla(C_p T) = -\frac{pC_p}{k}\mathbf{Q}q_{2\text{nd}}(\kappa)$
$\mathbf{Q}_v$	$\mathbf{Q}_v = -k_v\nabla T_v$	$\mathbf{\Pi}\cdot\nabla(C_{p,v}T_v) + (p + \Delta)\nabla(C_{p,v}T_v) = -\frac{pC_{p,v}}{k_v}\mathbf{Q}q_{2\text{nd}}(\kappa)$
$q(\kappa)$	$q_{1\text{st}}(\kappa) = 1$	$q_{2\text{nd}}(\kappa) = \frac{\sinh\kappa}{\kappa}$

$$\hat{R}^2 \equiv \hat{\mathbf{\Pi}} : \hat{\mathbf{\Pi}} + (5 - 3\gamma) f_b \hat{\Delta}^2 + \hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}} + \boxed{\hat{\mathbf{Q}}_v\cdot\hat{\mathbf{Q}}_v}$$

3D mixed modal DG method for the 2nd-order model

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

Discretization in mixed form

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

JCP 2022

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

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

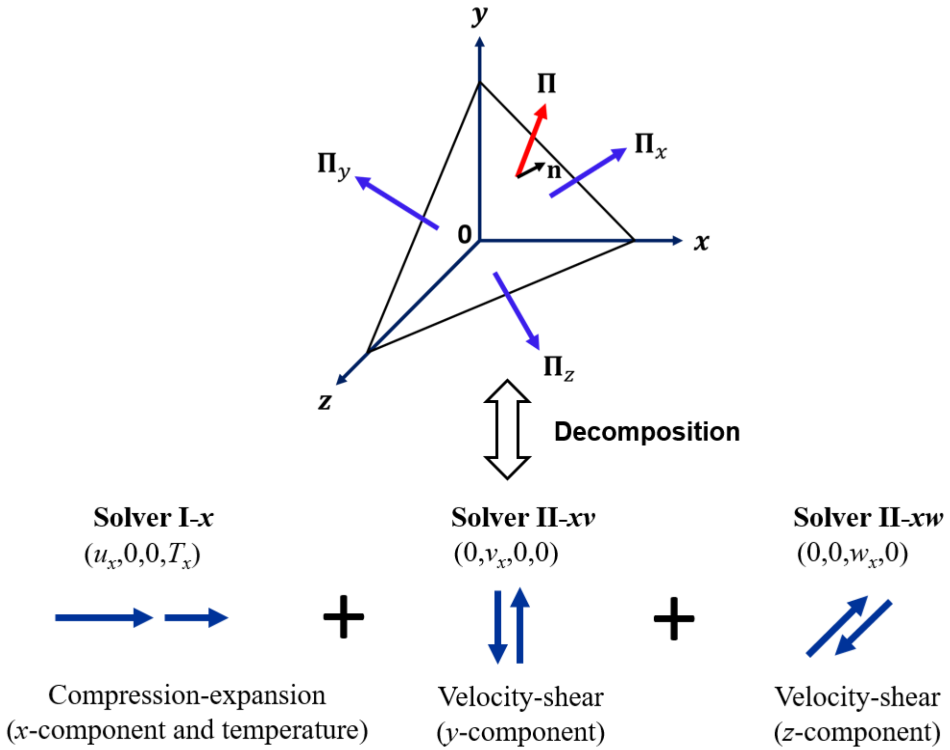
NCCR: Nonlinear Coupled Constitutive Relation

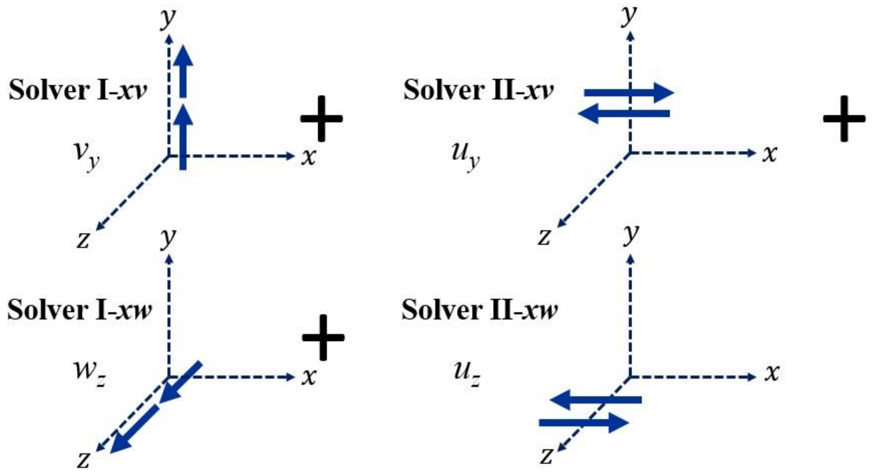
$$\mathbf{U}_h(\mathbf{x}, t) = \sum_{i=0}^{k} U_j^i(t)\varphi^i(\mathbf{x}), \quad \mathbf{S}_h(\mathbf{x}, t) = \sum_{i=0}^{k} S_j^i(t)\varphi^i(\mathbf{x})$$

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

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

Decomposition of NCCR for multi-dimensional flow

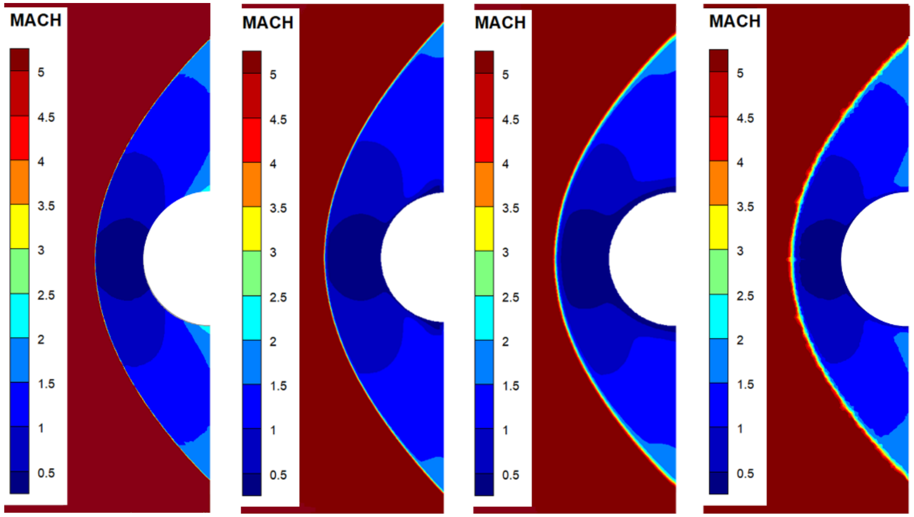




Primary surface integral

Secondary volume integral

2-D hypersonic rarefied flow past a cylinder

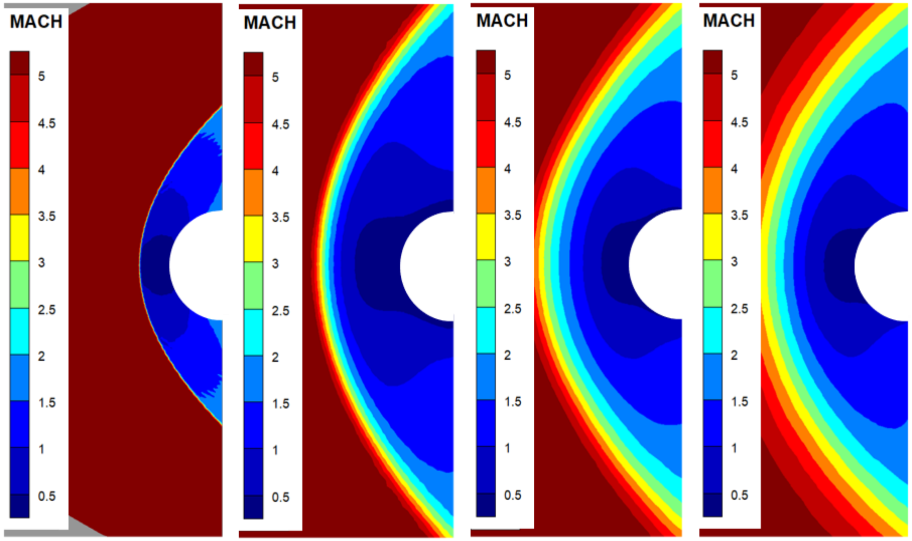


0th-order model 1st-order model 2nd-order model DSMC

Argon gas

Mach 5.48

Knudsen 0.02



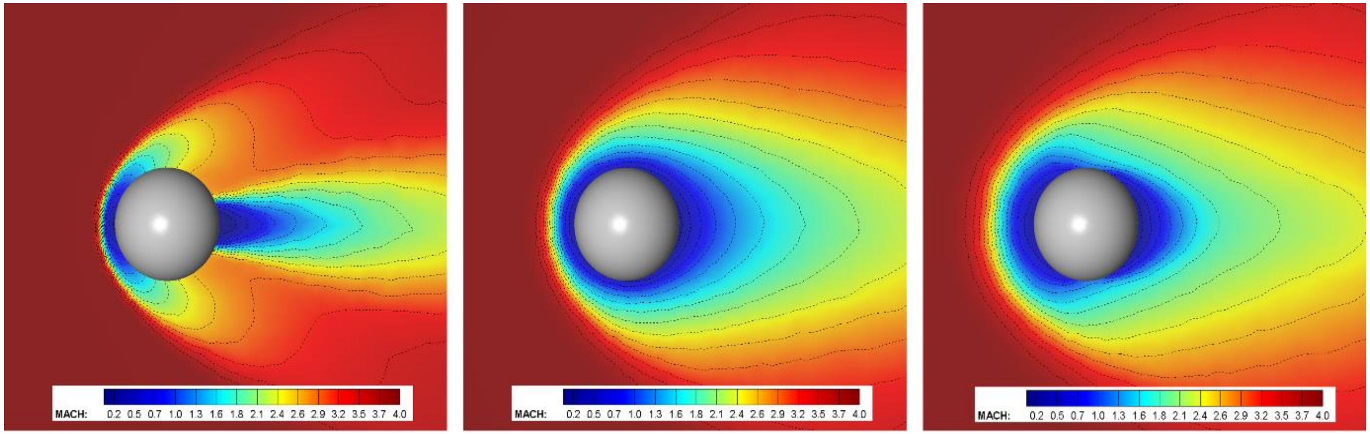
0th-order model 1st-order model 2nd-order model DSMC

Argon gas

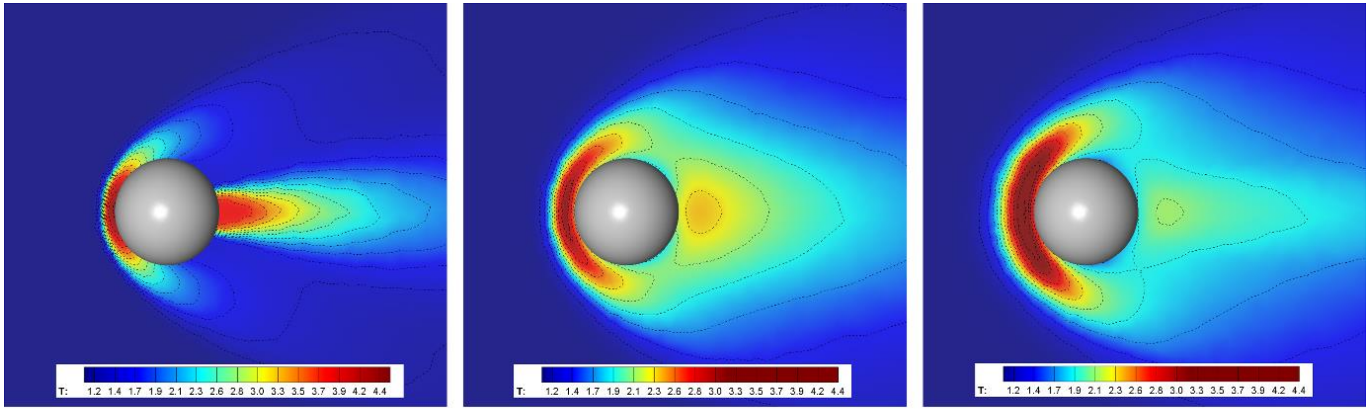
Mach 5.48

Knudsen 0.2

3-D hypersonic rarefied flow past a sphere



0th-order model 1st-order model 2nd-order model



0th-order model 1st-order model 2nd-order model

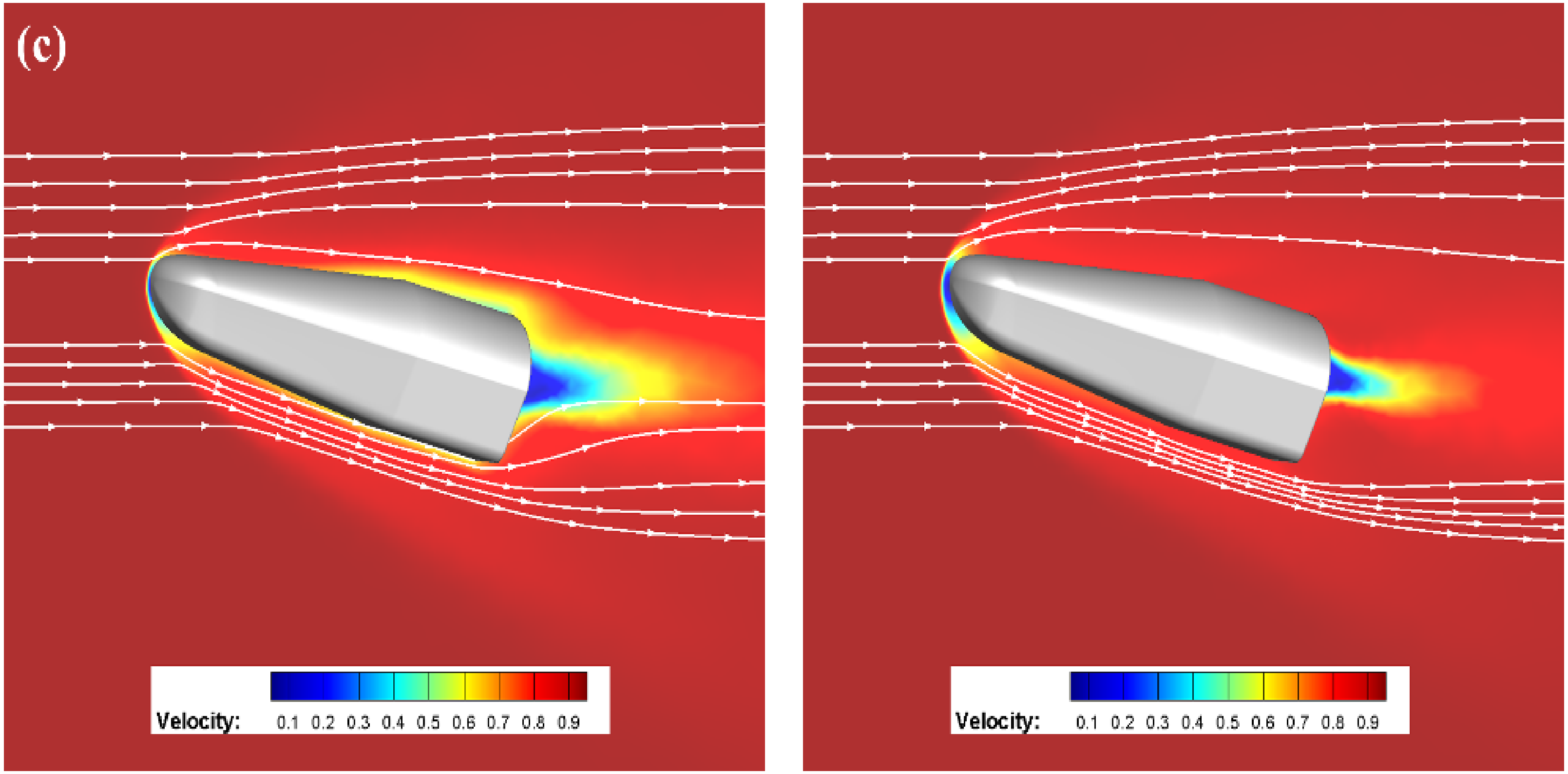
Nitrogen gas

Mach 4.0

Knudsen 0.01

3-D hypersonic rarefied flows around a vehicle

A suborbital re-entry vehicle

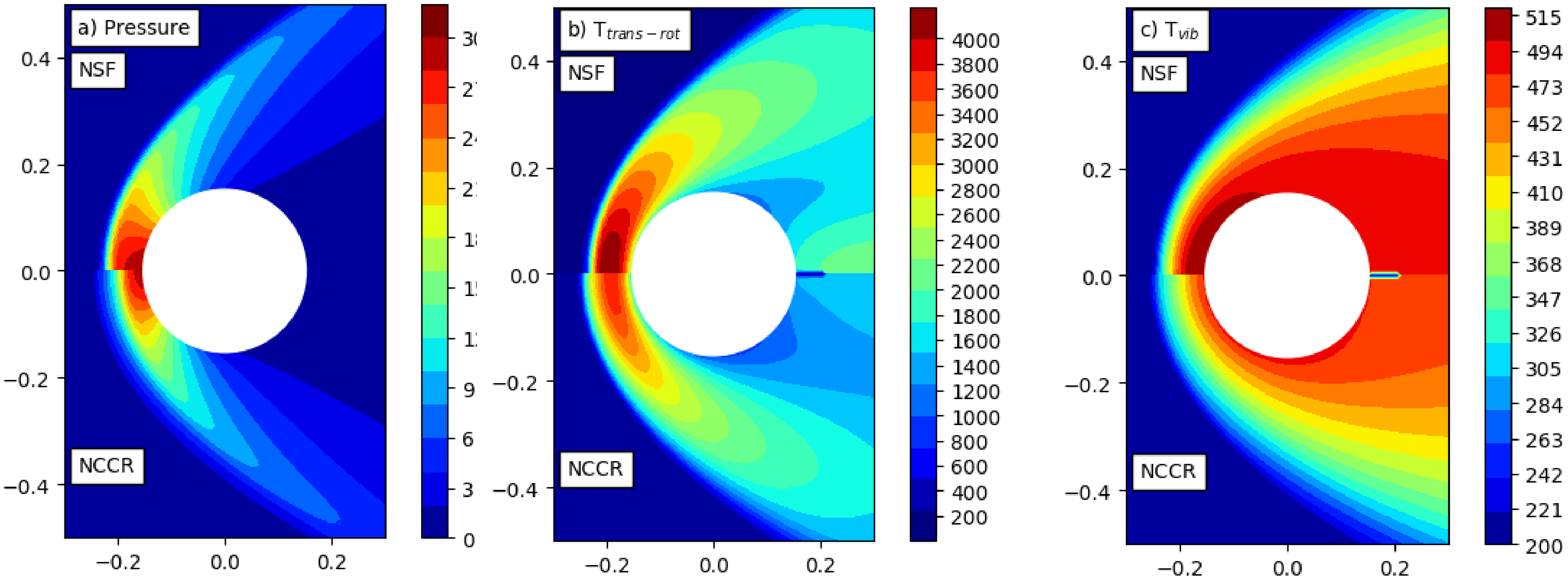


1st-order model 2nd-order model

Velocity contours of nitrogen gas flows; Mach 5.0, Knudsen 0.02

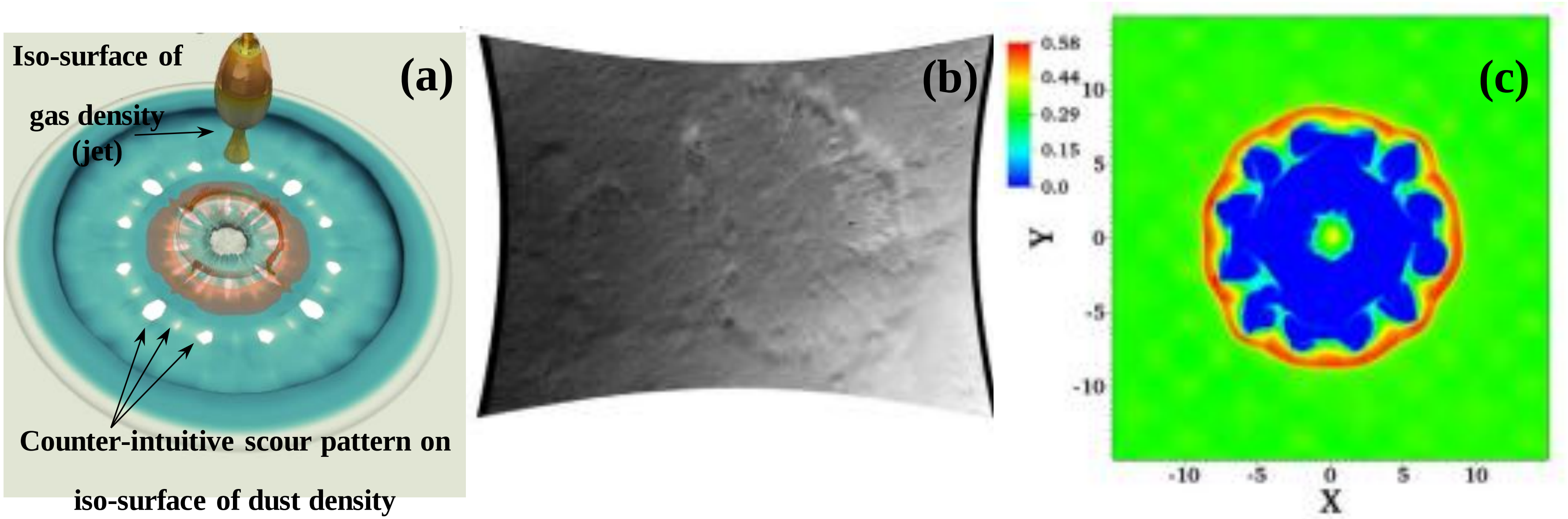
nccrVibFOAM solver for rarefied & microscale flows

Developed as an extension to the *dbnsTurbFoam* solver by implementing additional algebraic constitutive relations for the stress tensor and heat flux vector (CPC 2023 in Revision)



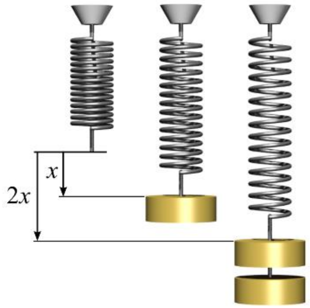
Mach 10 nitrogen gas (Kn=0.05)

nccrVibFOAM solver for rarefied & microscale flows

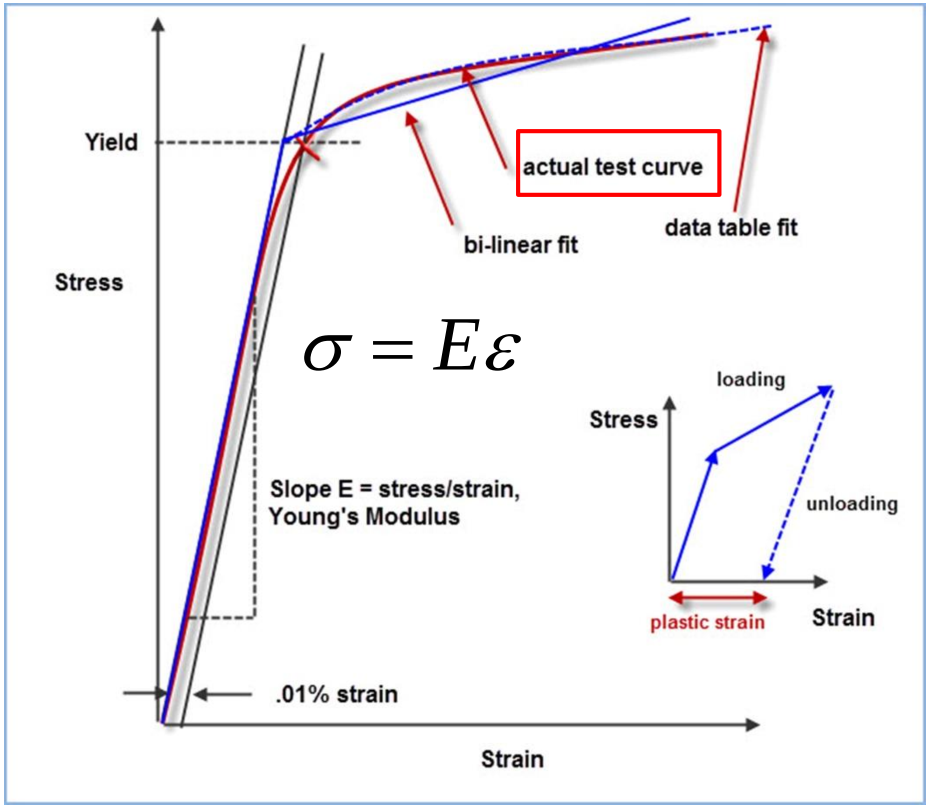


Counter-intuitive non-axisymmetric scour formation during planetary landing: (a) *nccrFOAM*; (b) NASA Mars Science Laboratory (MSL) landing image; (c) Simulation conducted in Jet Propulsion Laboratory (JPL) (PoF 2023)

Hooke's law in elasticity (1676)



$$F = -kx$$



$$\sigma = E\varepsilon$$

In the physics and mechanics of elastic solids, Hooke's law is an empirical law that states that the force needed to extend or compress a spring is proportional linearly to the distance.

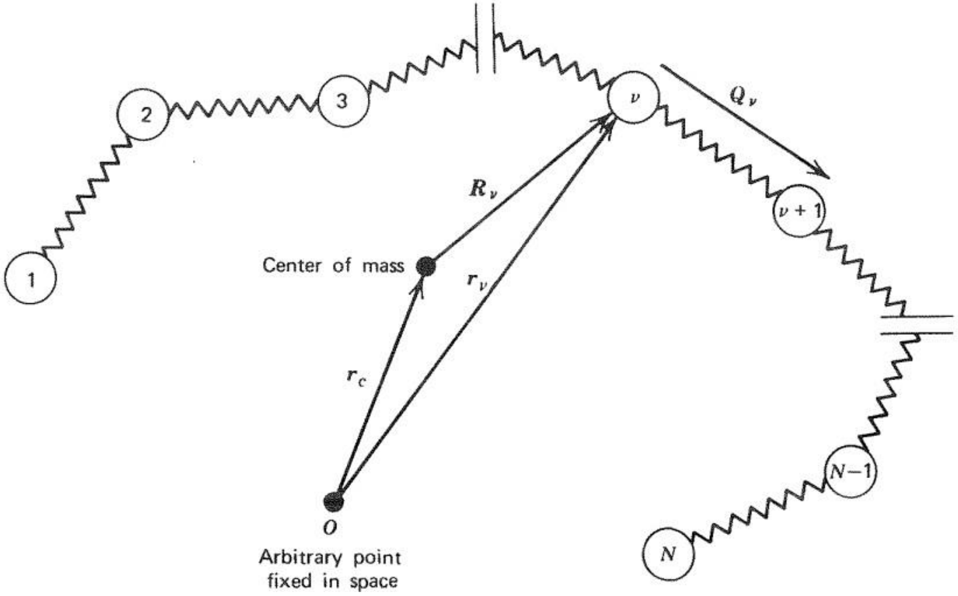
The law is named after 17th-century British physicist Robert Hooke who first stated the law in 1676.

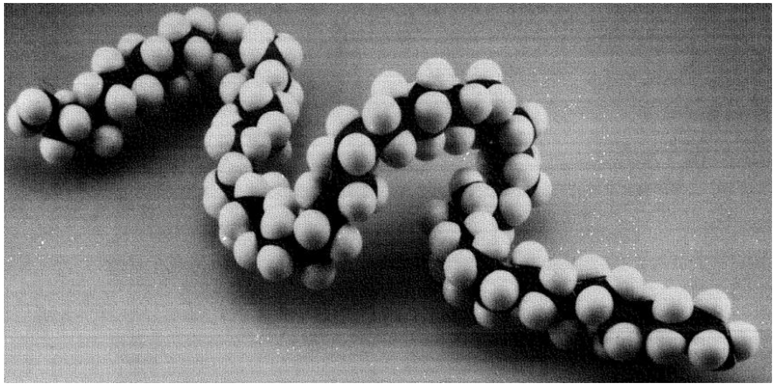
Hooke's law is only a first-order approximation to the real response of springs and other elastic bodies to applied forces.

Elastic dumbbell models: kinetic theory of polymers

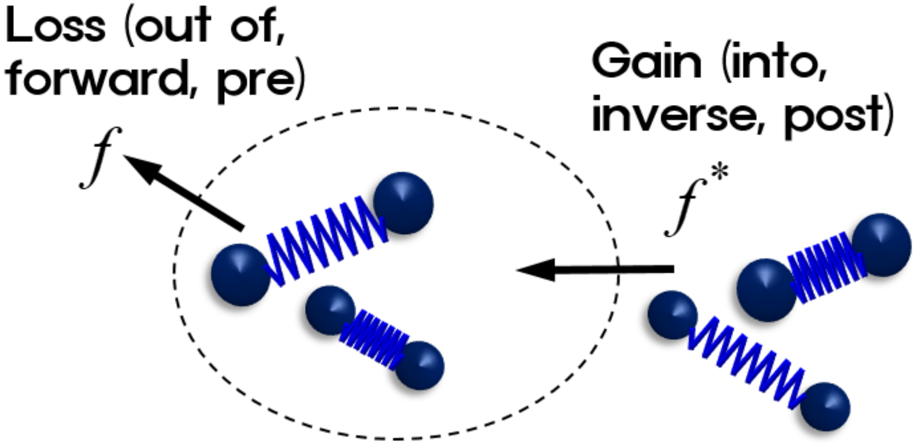
Hyper-elastic materials such as rubber (amorphous solid)

Mostly phenomenological models such as Mooney (1940)–Rivlin (1948) solid model





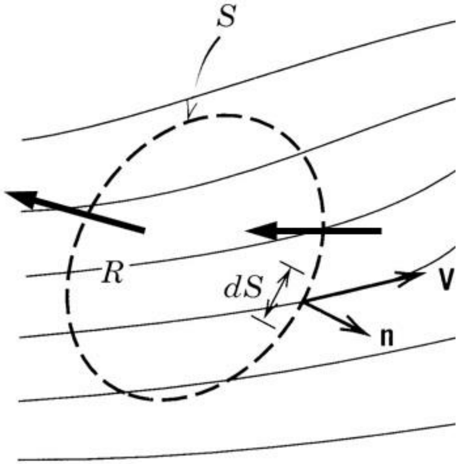
New nonlinear intramolecular interaction model



$$\frac{\delta f}{\delta t} = C[f] = \text{Gain - Loss} = \frac{1}{2\lambda}\left(f^* - f\right)$$

New nonlinear intramolecular interaction model for the “spring” in the dumbbell

When linearized, it reduces to $(f^{\mathrm{eq}} - f)/\lambda$ (BGK model, 1954)



$$\frac{\partial}{\partial t}\int_R \boldsymbol{U}dV = \text{In - Out} = \oint_S \boldsymbol{F}\cdot(-\boldsymbol{n})dS$$

Conservation in control volume

Preprint (2023): Kinetic spring model based on Boltzmann’s gain-loss-concept and application of non-Hookean models to viscoelastic fluids

Boltzmann-type intramolecular interaction model

A molecular-level equation of the marginal probability density function of finding a dumbbell in the configuration vector space $\mathbf{r}$ connecting two beads for a given time, $f\left(\mathbf{r},t\right)$($\varsigma$ friction coefficient, $\mathbf{s}$ spring force, $\lambda \equiv \varsigma / 4S_0$ relaxation)

$$\frac{\partial f}{\partial t}+\nabla\cdot\left((\nabla\mathbf{u})^T\mathbf{r}-\frac{2k_BT}{\varsigma}\nabla\right)f=\nabla\cdot\left(\frac{2\mathbf{s}}{\varsigma}f\right)$$

Fokker-Planck

$\mathbf{s}=S_0\mathbf{r}:$ Linear Hookean

$$\frac{\partial f}{\partial t}+\nabla\cdot\left((\nabla\mathbf{u})^T\mathbf{r}-\frac{2k_BT}{\varsigma}\nabla\right)f=\frac{1}{2\lambda}\left(f^*-f\right)$$

New Boltzmann-type

Note that the interaction occurs through the "spring" in the dumbbell.

For the dumbbell models the forces on the two beads are equal and opposite, leading to a connector force.

Corresponding second-order constitutive model

Nonequilibrium entropy Ψ : $\Psi(\mathbf{r},t) = -k_B \left\langle \left[\ln f(\mathbf{v},\mathbf{r},t) - 1\right] f(\mathbf{v},\mathbf{r},t) \right\rangle$,

Nonequilibrium entropy production:

$$\sigma_c \equiv -k_B \left\langle \ln f \;\, C[f] \right\rangle = \frac{1}{4\lambda} k_B \left\langle \ln\left(f^*/f\right)\left(f^* - f\right) \right\rangle \geq 0 \text{ (satisfying 2nd-law)}$$

since $\ln\left(x/y\right)\left(x-y\right) \geq 0.$

$$\sigma_c = \frac{1}{4\lambda} k_B \left\langle f^{(0)}\left(x-y\right)\left[\exp(-y) - \exp(-x)\right] \right\rangle = \kappa_1 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots) \text{ via cumulant expansion}$$

$$\sigma_c \equiv -k_B \left\langle \ln f \;\, C[f] \right\rangle = \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \left\langle h^{(n)} C[f] \right\rangle = \frac{1}{T} \sum_{l=1}^{\infty} X^{(n)} \Lambda^{(n)},$$

a thermodynamically-consistent constitutive equation can be derived;

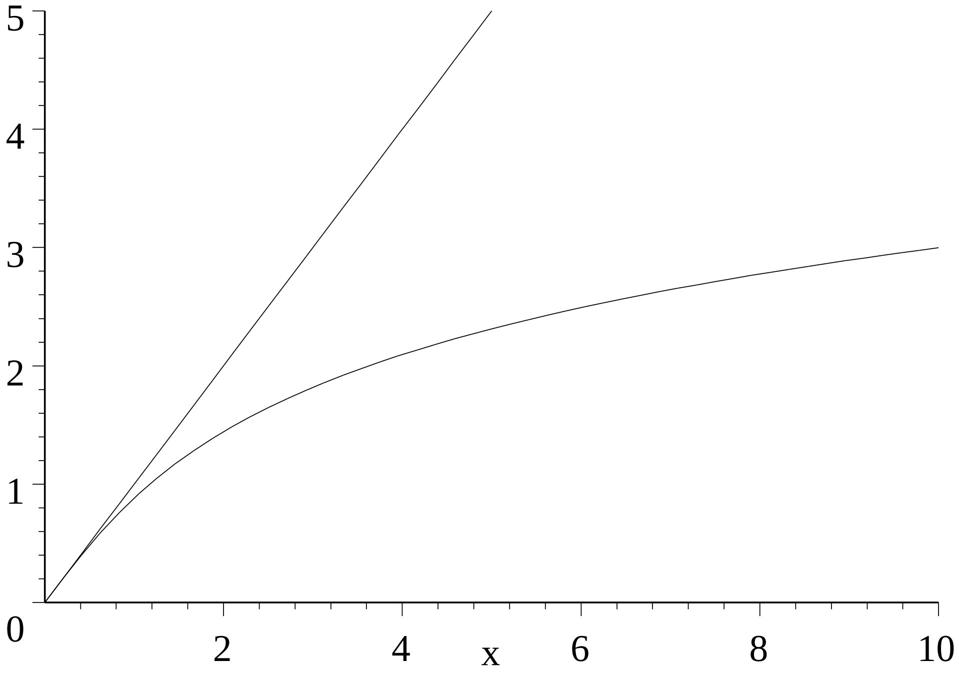
$$\frac{D\boldsymbol{\tau}}{Dt} - \left[(\nabla\mathbf{u})^T \boldsymbol{\tau} + \boldsymbol{\tau}\nabla\mathbf{u}\right] - \frac{\mu}{\lambda}(\nabla\mathbf{u}^T + \nabla\mathbf{u}) = -\frac{1}{\lambda}\boldsymbol{\tau} q_{2\text{nd}}(\kappa_1),$$

$$q_{2\text{nd}}(\kappa_1) = \frac{\sinh \kappa_1}{\kappa_1}, \;\; \kappa_1 = \alpha \frac{\sqrt{\boldsymbol{\tau} : \boldsymbol{\tau}}}{\mu/\lambda} \;\; (\boldsymbol{\tau} \equiv nS_0 \left\langle \mathbf{rr}f \right\rangle - nk_B T\mathbf{I})$$

2nd-order extension of Hooke's Law in elasticity

$$-\frac{\mu}{\lambda}(\nabla\mathbf{u}^T+\nabla\mathbf{u})=-\frac{1}{\lambda}\boldsymbol{\tau}\frac{\sinh\kappa_1}{\kappa_1},\ \ \kappa_1=\alpha\frac{\sqrt{\boldsymbol{\tau}:\boldsymbol{\tau}}}{\mu/\lambda}$$

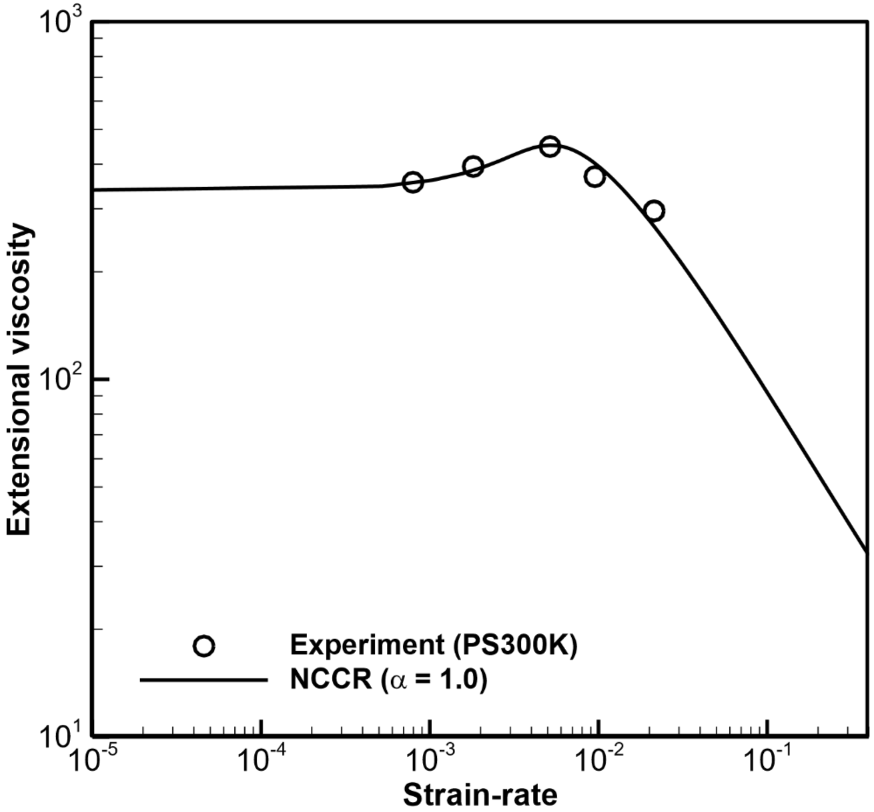
$$\Rightarrow\ \ \hat{\tau}=\frac{\sinh^{-1}(\alpha\hat{\tau}_0)}{\alpha}$$



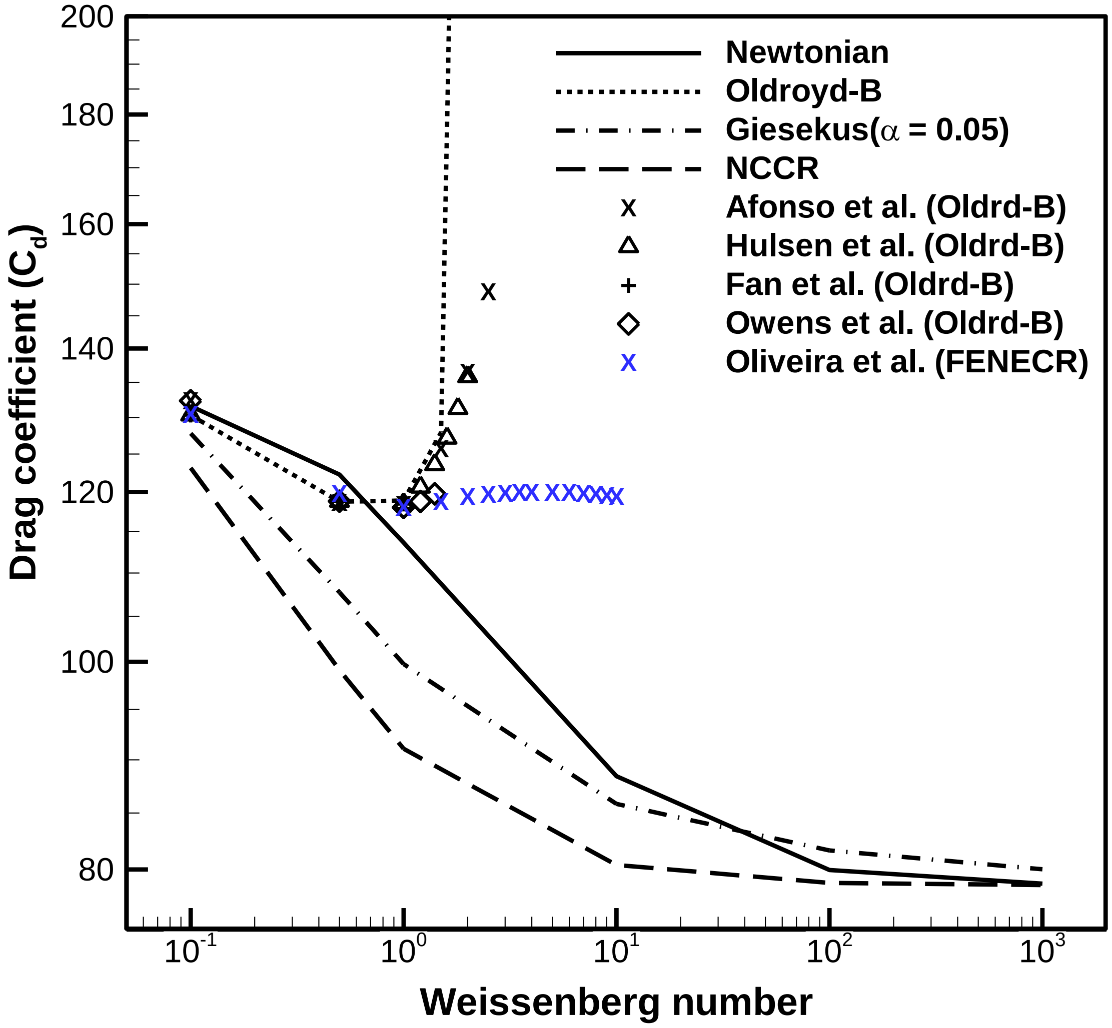
Application to viscoelastic fluids

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla p + \mu_s \nabla^2 \mathbf{u} - \nabla \cdot \boldsymbol{\tau} = 0$$

$$\frac{D\boldsymbol{\tau}}{Dt} - \left[(\nabla \mathbf{u})^T \boldsymbol{\tau} + \boldsymbol{\tau} \nabla \mathbf{u} \right] - \frac{\mu}{\lambda} (\nabla \mathbf{u}^T + \nabla \mathbf{u}) = -\frac{1}{\lambda} \boldsymbol{\tau} \frac{\sinh \kappa_1}{\kappa_1}, \ \kappa_1 = \alpha \frac{\sqrt{\boldsymbol{\tau} : \boldsymbol{\tau}}}{\mu / \lambda}$$

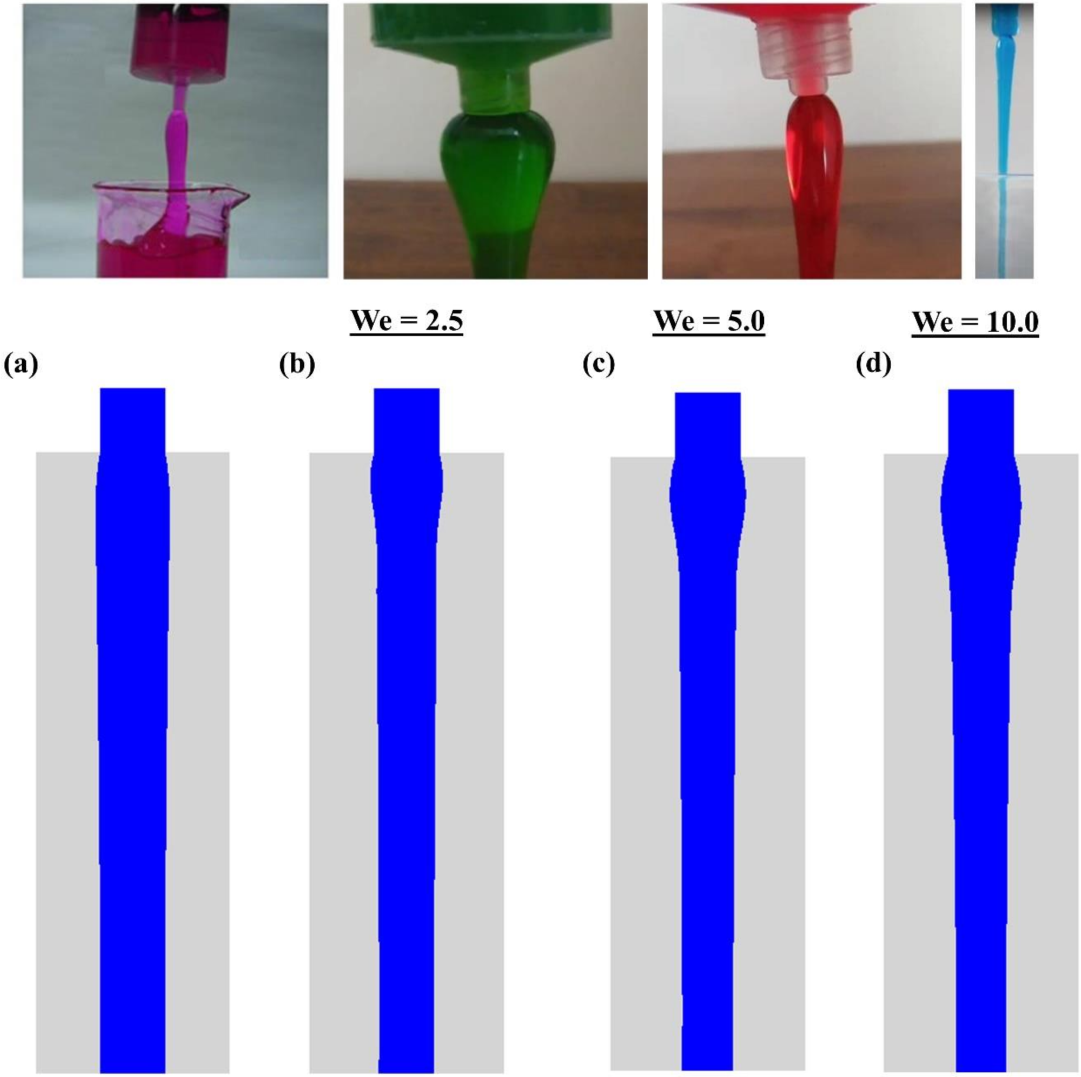


Computational simulation of viscoelastic fluids



Implementation of the new model to viscoelastic OpenFOAM (cylinder flow)

Viscoelastic fluids: Barus effect in die swell



Newtonian New New New

Future topics

- **Non-classical flow physics including mixture, chemical reaction, and radiation modeling**
- **Aerothermodynamic data for design and control**
- **More accessible (via OpenFOAM of NCCR-FVM) and efficient computational algorithms**
- **Combination with machine learning and quantum computing**
- **Investigation of viscoelastic flows based on a new Boltzmann-type kinetic spring model**

$$\frac{1}{2\lambda}\left(f^{*}-f\right) \qquad \text{Cf. } \frac{1}{\lambda}\left(f^{(0)}-f\right)$$

BGK (1954)

Yamamoto (1956), Lodge (1964), Modified network model