Second-order Extension of Hooke's Law in Elasticity Based on a New Boltzmann-type Collision Model

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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

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Development of hybrid DG code and computational simulation of rarefied & microscale gas flows

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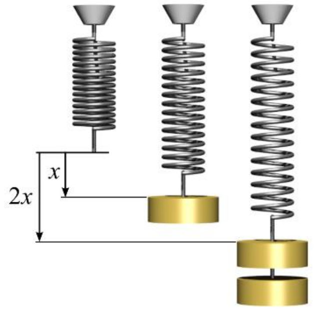
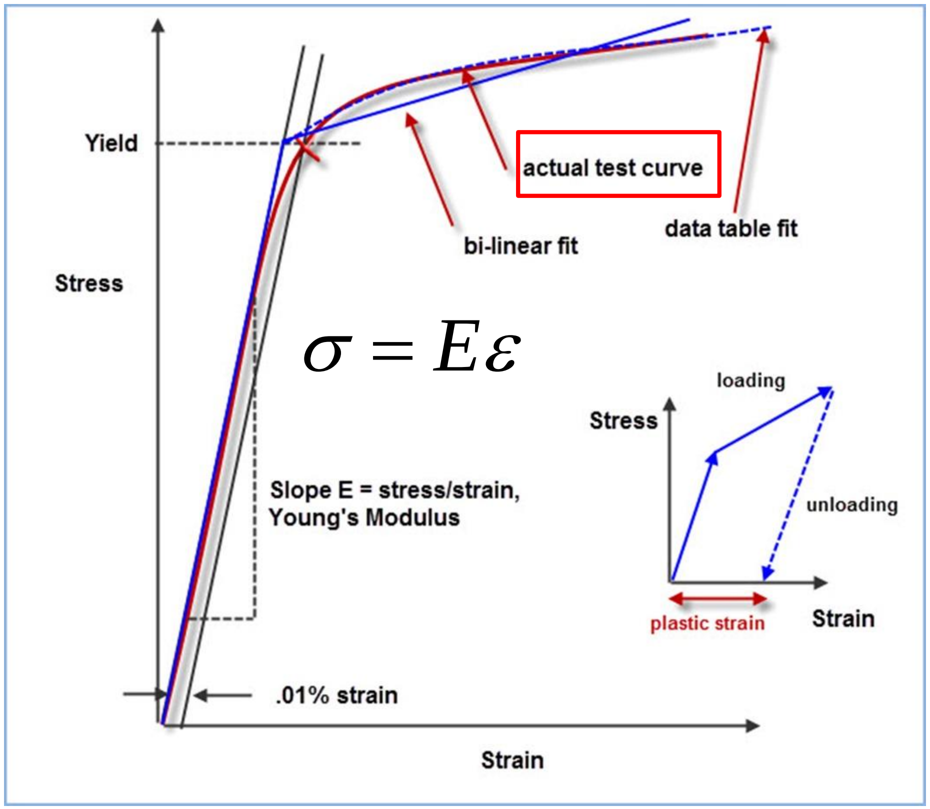
Hooke's law in elasticity (1676)



$$F = -kx$$



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.

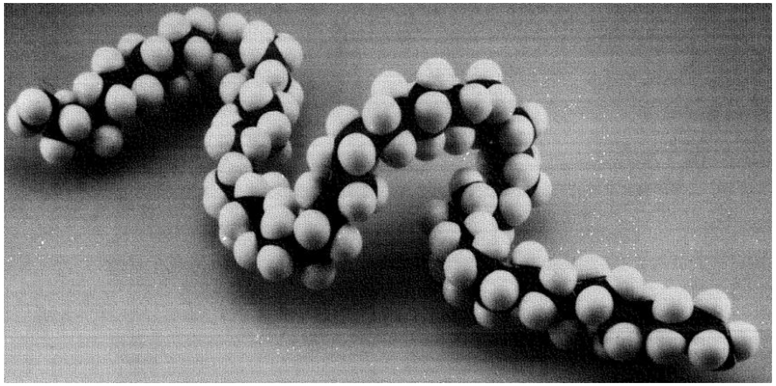
The law is named after 17th-century British physicist Robert Hooke who first stated the law in 1676.

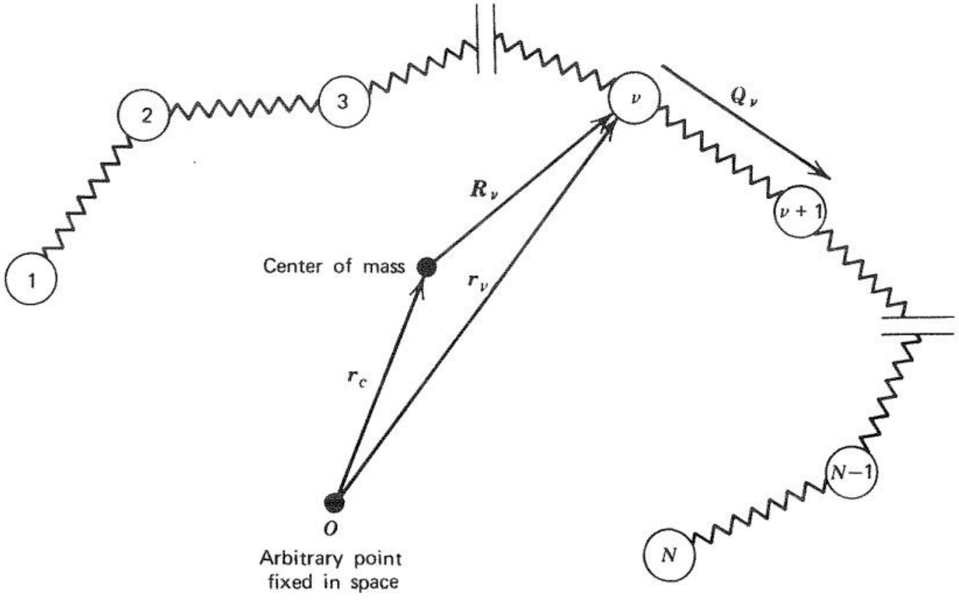
Hooke's law is only a first-order approximation to the real response of springs and other elastic bodies to applied forces.

Elastic dumbbell models: kinetic theory of polymers

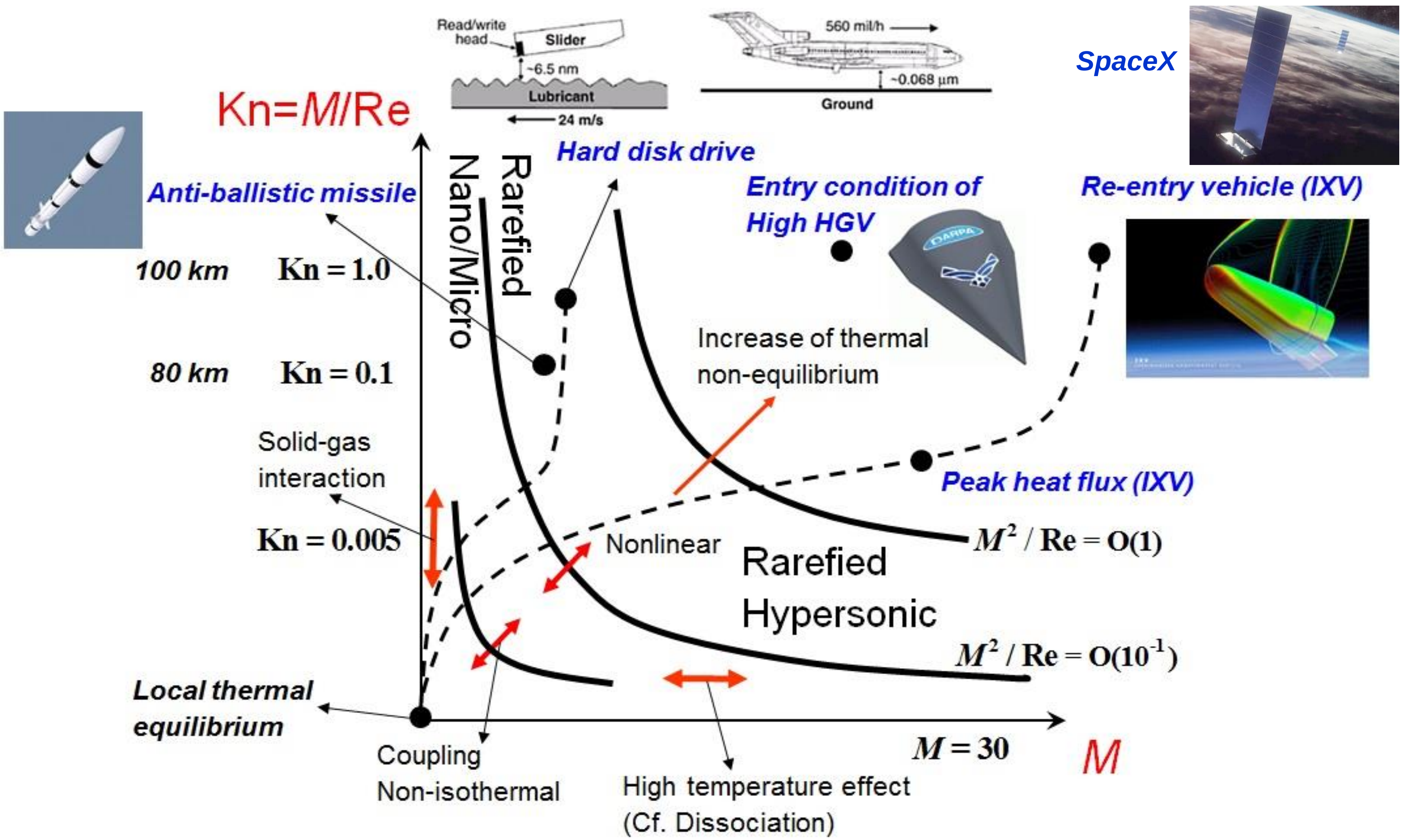
Hyper-elastic materials such as rubber (amorphous solid)

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





Classification of gas flows in non-equilibrium



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

Two terms: Kn **Three terms: *M*, Kn** **(not Kn alone)** $\dfrac{M^2}{\mathrm{Re}}$ or $\dfrac{M}{\sqrt{\mathrm{Re}}}$

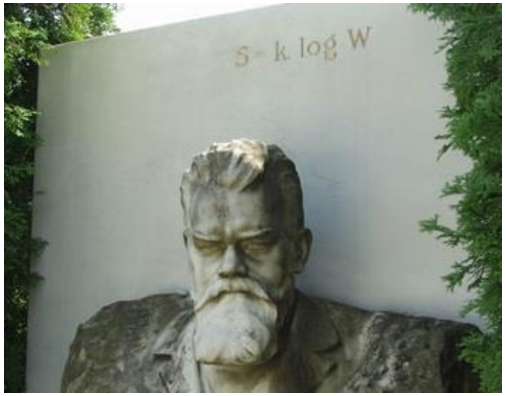
Boltzmann kinetic equations

- 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



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

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

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

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

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

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

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

$$\frac{D}{Dt}(\mathbf{\Pi}/\rho) + \boxed{\nabla\cdot\Psi^{(\Pi)}} + 2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2p[\nabla\mathbf{u}]^{(2)} = \boxed{\left\langle m[\mathbf{cc}]^{(2)} C[f, f_2] \right\rangle}$$

2nd-order closure

2nd-order closure

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

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

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	$-2\pi e_i^2 e_j^2 m_i^{-1} \ln \Lambda\, \partial_{u\alpha} \int d\mathbf{u}' [f_i(\mathbf{u}) \partial_{u'\beta} f_j(\mathbf{u}')/m_j - f_j(\mathbf{u}') \partial_{u\beta} f_i(\mathbf{u})] U_{\alpha\beta}(\mathbf{u} - \mathbf{u}')$

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

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

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

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

Boltzmann

(1872)

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

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

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

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: $\sigma_c \equiv -k_B \left\langle \ln f\ C[f, f_2]\right\rangle \geq 0$ (satisfying 2nd-law)

$\sigma_c = \kappa_1 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots)$ via cumulant expansion

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

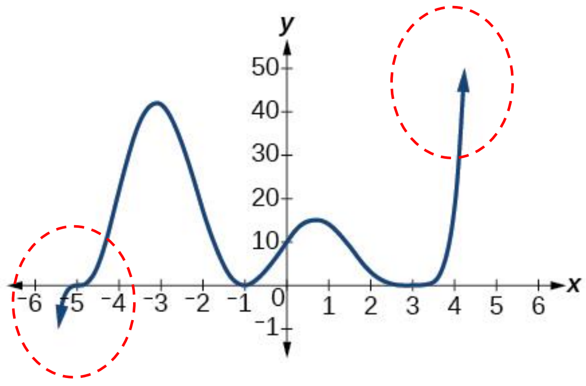
a thermodynamically-consistent constitutive equation, still exact to BKE, can be derived;

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

Note: When f is truncated to a finite number of terms, the set is truncated in such a way that the divergence problem would not arise.

Cumulant expansion method

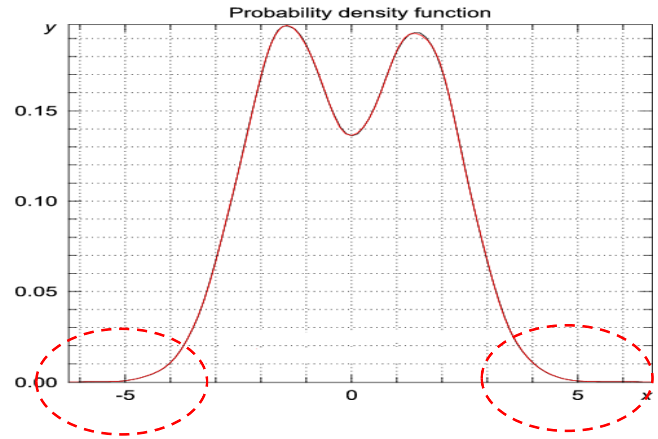
$$\left\langle x^l \right\rangle = \int x^l f(x)dx, \ \left\langle e^{\lambda x} \right\rangle = \int e^{\lambda x} f(x)dx$$



Then we have

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

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



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

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

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

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

2^{nd}-order NCCR model

NCCR: Nonlinear Coupled Constitutive Relation

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 2^{nd}-order constitutive relations (CR)

Zero in 2^{nd}-order approximation

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

Non-local term | **2^{nd}-order coupling** | **Navier 1^{st} law**

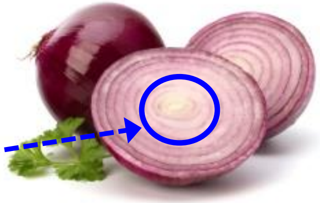
$$\Psi^{(\Pi)}\equiv\langle m\mathbf{ccc}f\rangle-\langle m\mathrm{Tr}(\mathbf{ccc})f\rangle\mathbf{I}/3$$

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

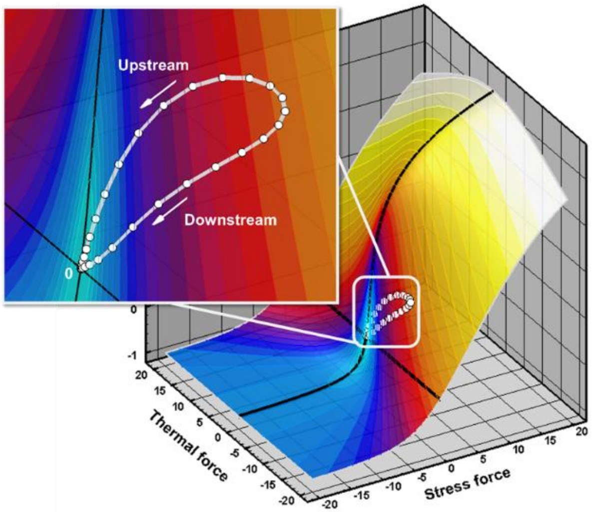
Onsager-Rayleigh dissipation function

Sinh{1^{st}-order theory}

Navier-Fourier laws inclusive like onion!

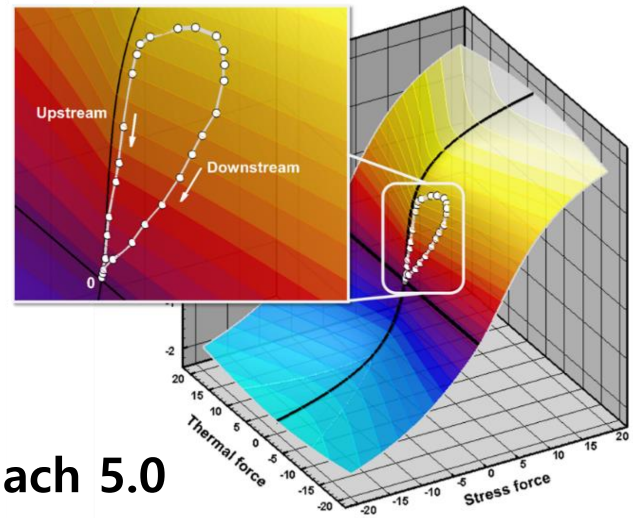


Topology of 2^{nd}-order NCCR (shock structure) (PoF 2020)

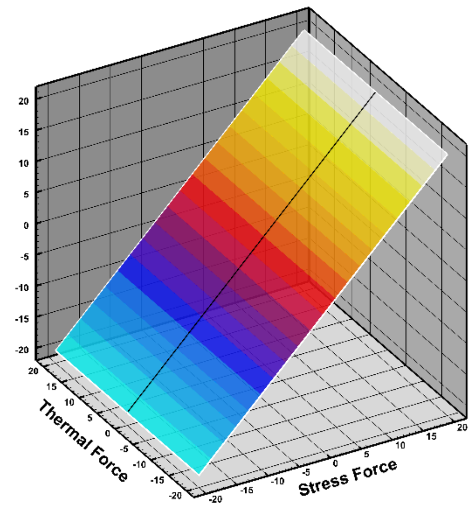


f_b=0.0

Mach 5.0



f_b=0.8



1st-order

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

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

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

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

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)

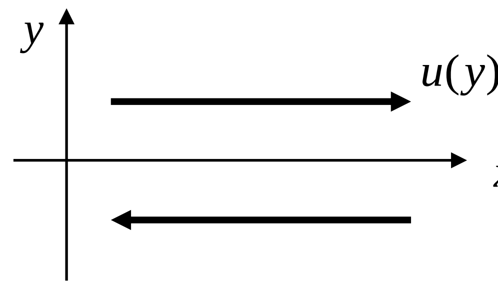
$$\Delta = \left\langle m\mathrm{Tr}(\mathbf{cc})f/3 - m\mathrm{Tr}(\mathbf{cc})f^{(0)}/3\right\rangle,\ p = \left\langle m\mathrm{Tr}(\mathbf{cc})f^{(0)}/3\right\rangle$$

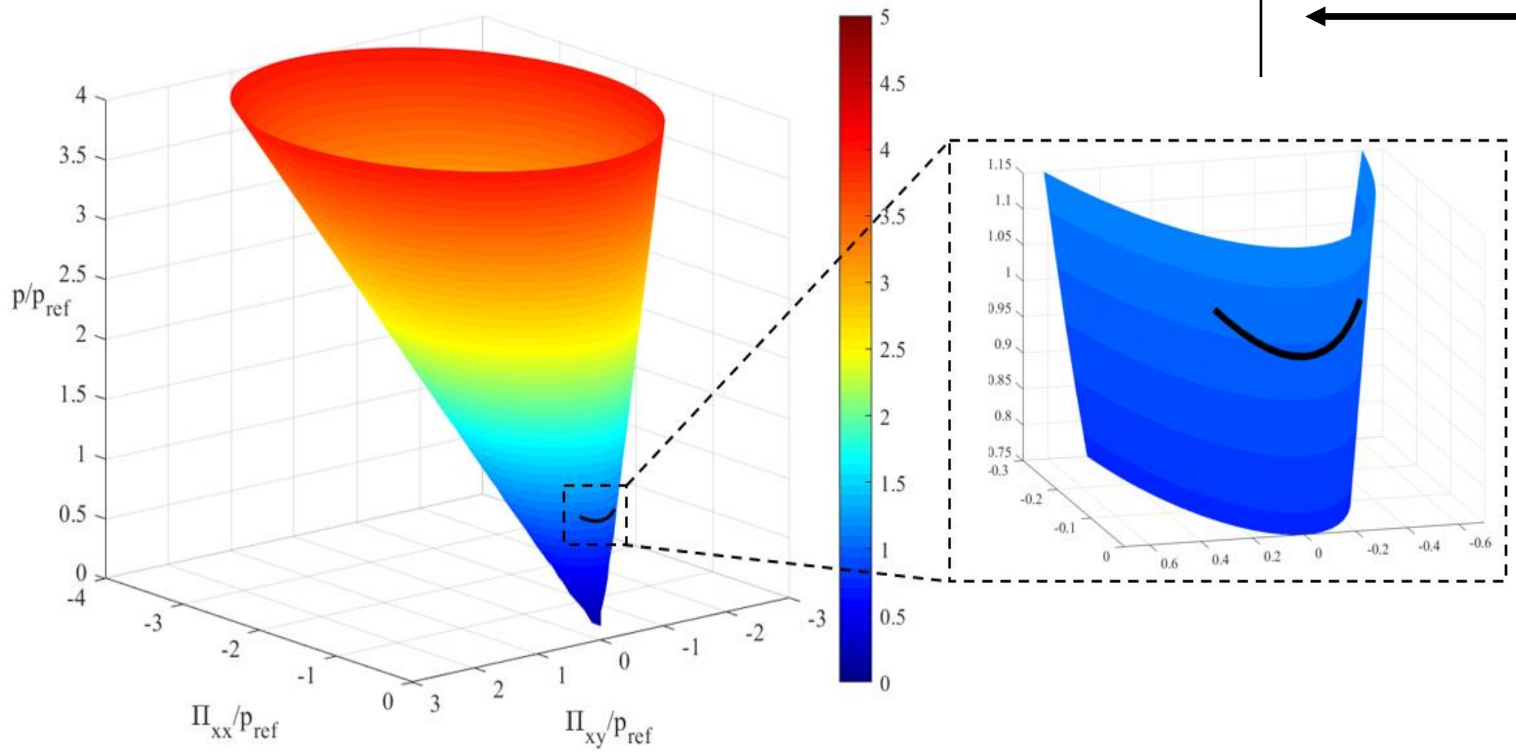
Topology of 2nd-order NCCR (velocity shear) (PoF 2016)

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

Zero in velocity shear

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





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

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

JCP 2022

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

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

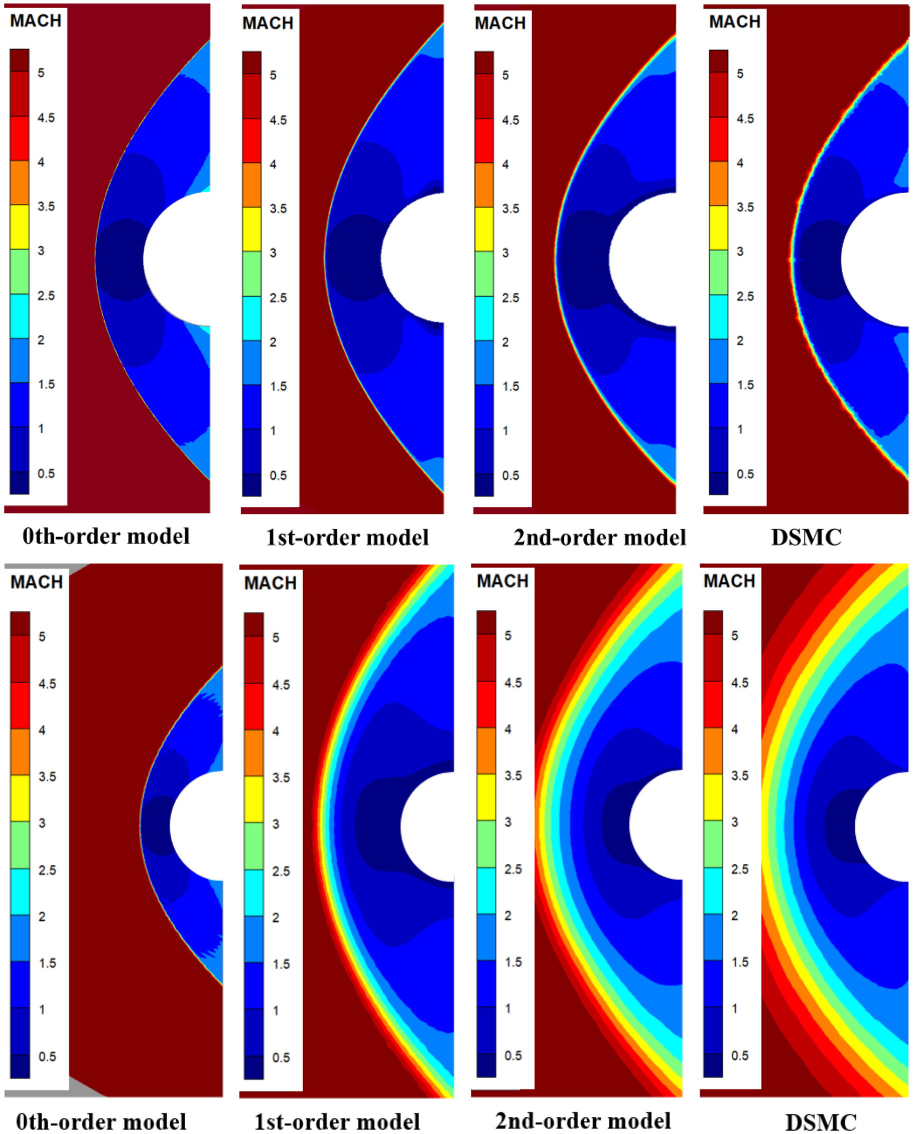
NCCR: Nonlinear Coupled Constitutive Relation

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

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

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

2-D hypersonic rarefied flow past a cylinder



Argon gas

Mach 5.48

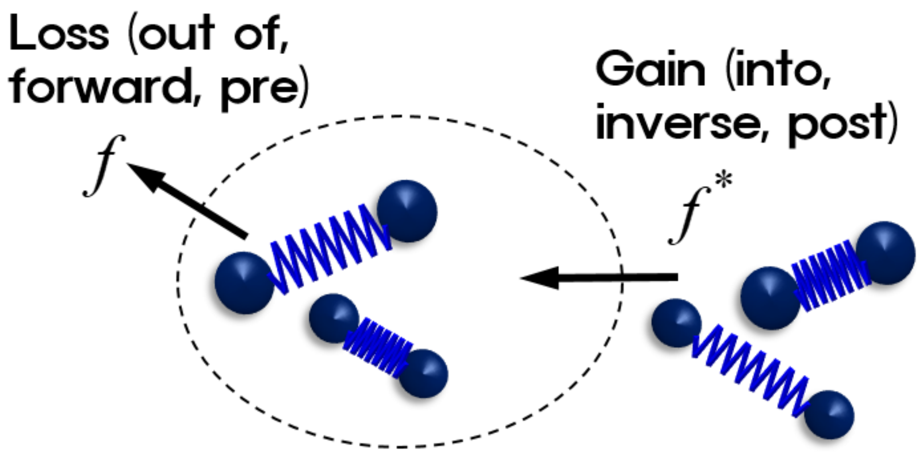
Knudsen 0.02

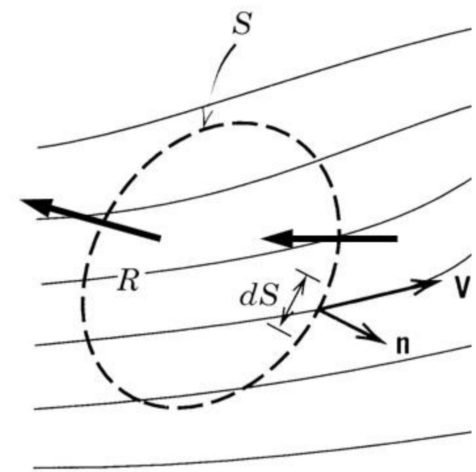
Argon gas

Mach 5.48

Knudsen 0.2

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 $(f^{\text{eq}} - f)/\lambda$ (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): A Boltzmann-type kinetic intramolecular model and its application 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)

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

Fokker-Planck

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

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

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;

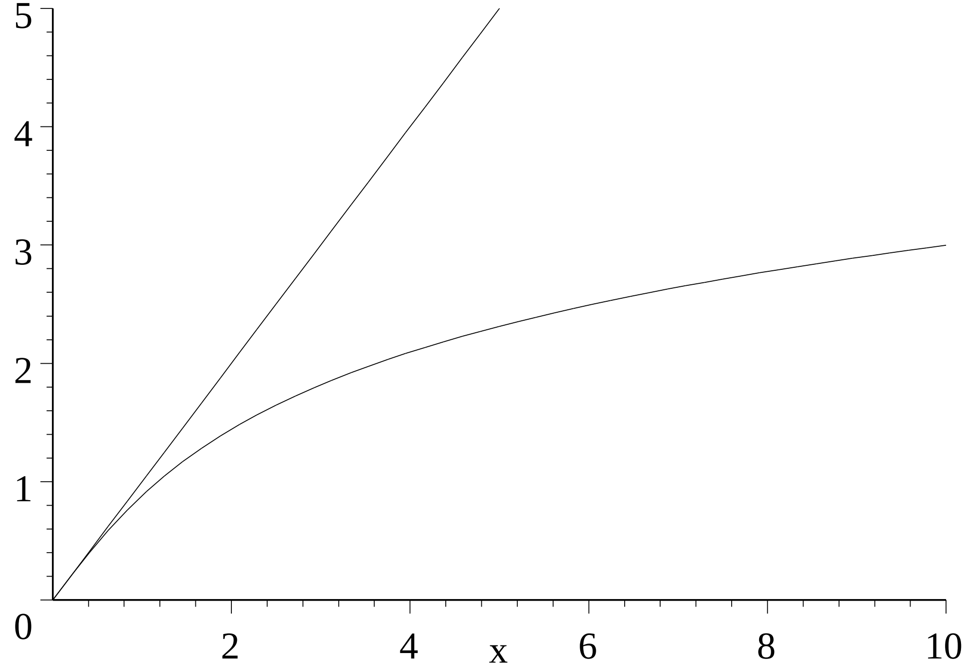
$$\frac{D\boldsymbol{\tau}}{Dt} - \left[(\nabla\mathbf{u})^T \boldsymbol{\tau} + \boldsymbol{\tau}\nabla\mathbf{u}\right] - \frac{\mu}{\lambda}(\nabla\mathbf{u}^T + \nabla\mathbf{u}) = -\frac{1}{\lambda}\boldsymbol{\tau} q_{2\text{nd}}(\kappa_1),$$

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

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

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

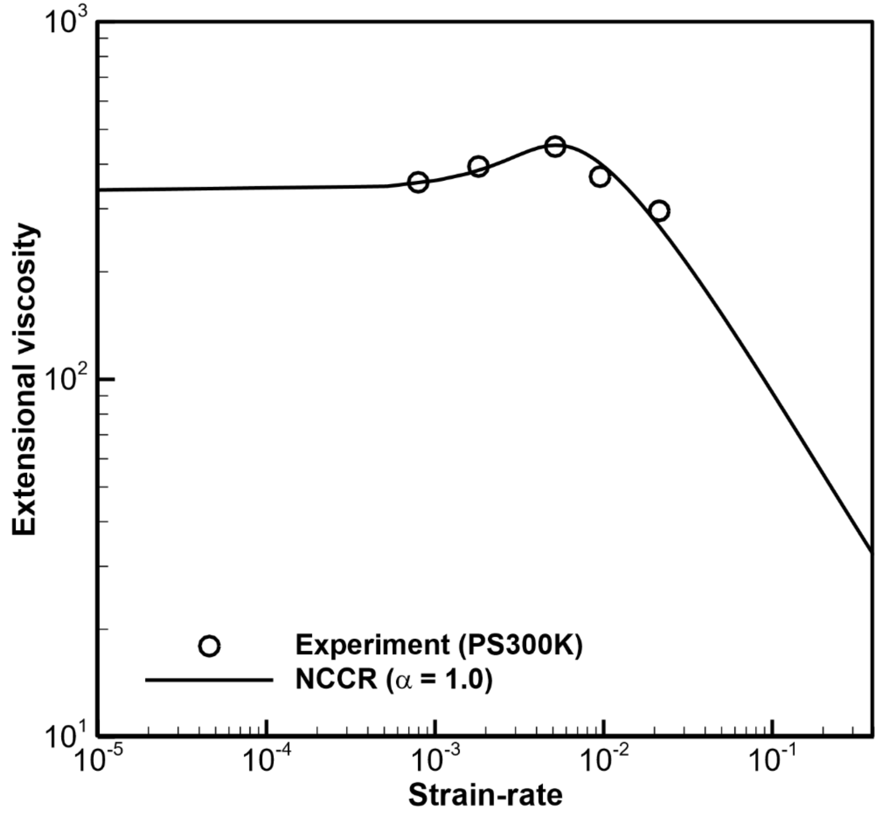
$$\Rightarrow\ \ \hat{\tau} = \frac{\sinh^{-1}(\alpha \hat{\tau}_0)}{\alpha}$$



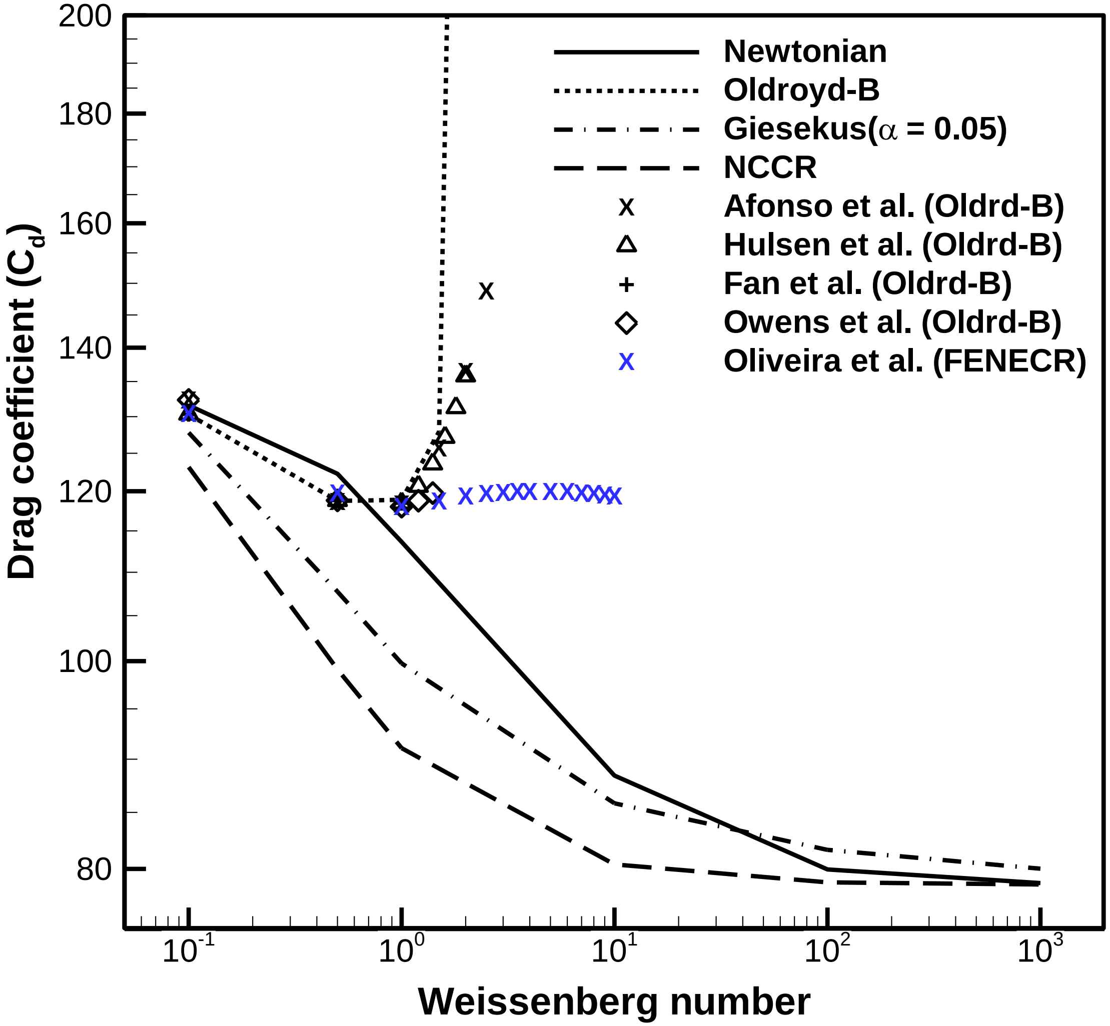
Application to viscoelastic fluids

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

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

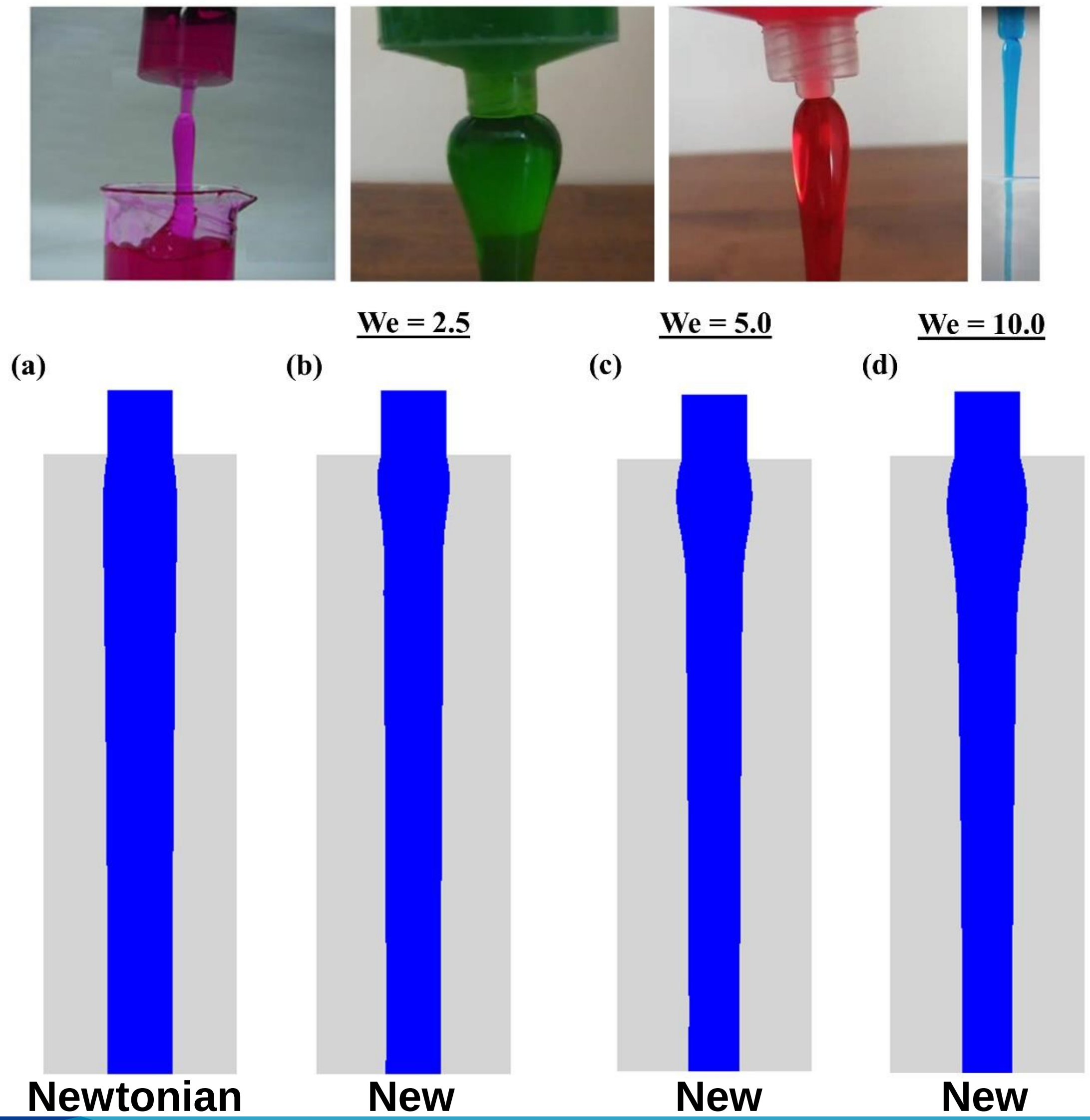


Computational simulation of viscoelastic fluids



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

Viscoelastic fluids: Barus effect in die swell



Concluding remarks

Proposal of 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

Second-order extension of Hooke's law in elasticity

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

Application to viscoelastic fluids

Similarities between rarefied gases and viscoelastic fluids