A Review of Boltzmann-Based CFD Schemes

March 18, 2015 (10:50-11:30)

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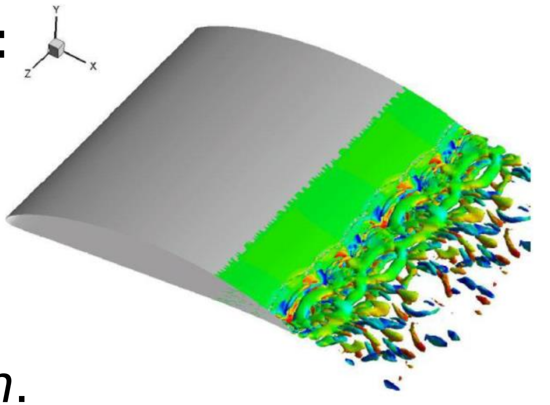
Presented at the 18th International Conference on
Finite Elements in Flow Problems
(FEF2015; Kinetic Methods in Fluid Flow)
16-18 March 2015, Taipei, Taiwan

Special thanks to
organizers of this conference
(Profs. Chao-An Lin, Jong-Shinn Wu)
for making this opportunity possible.

Background: why kinetic methods in fluids?

(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, “On the high Mach number shock structure singularity caused by overreach of Maxwellian molecules,” *Physics of Fluids*, May 2014)

Rarefied, micro- & nano- gases, viscoelastic fluids, elastic solids

Part I.

Introduction to Boltzmann-based computational schemes

Continuum vs molecular

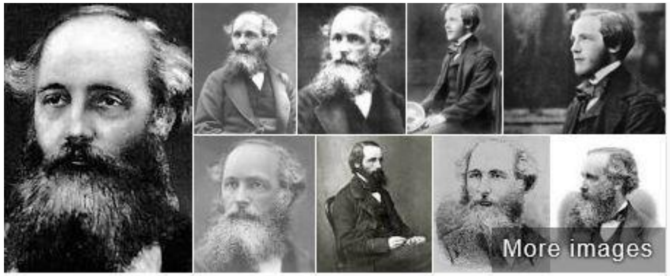
Claude-Louis Navier

Bust of Claude Louis Marie Henri Navier at the École Nationale des Ponts et Chaussées

Born	10 February 1785 Dijon, France
Died	21 August 1836 (aged 51) Paris, France
Nationality	French
Fields	Mathematical physics
Institutions	École Nationale des Ponts et Chaussées École polytechnique French Academy of Science
Alma mater	École Nationale des Ponts et Chaussées
Doctoral advisor	Joseph Fourier
Known for	Navier–Stokes equations

Navier & Fourier conservation laws and constitutive laws (1822)

Maxwell (1867), Boltzmann (1872) kinetic



James Clerk Maxwell

Physicist

James Clerk Maxwell FRS FRSE was a Scottish mathematical physicist. His most notable achievement was to formulate the classical theory of electromagnetic radiation, bringing together for the first time ... Wikipedia

Born: June 13, 1831, Edinburgh, United Kingdom

Died: November 5, 1879, Cambridge, United Kingdom

Education: University of Edinburgh, Trinity College, Cambridge, More

Awards: Rumford Medal

Ludwig Boltzmann

Ludwig Boltzmann

Born	Ludwig Eduard Boltzmann February 20, 1844 Vienna, Austrian Empire (present-day Austria)
Died	September 5, 1906 (aged 62) Tybein near Trieste, Austria-Hungary (present-day Duino, Italy) Suicide
Residence	Austria, Germany
Nationality	Austrian
Fields	Physics

$$\rho\frac{d\mathbf{u}}{dt}+\nabla p=\nabla\cdot\left(2\mu[\nabla\mathbf{u}]^{(2)}\right)$$

Equivalently, $\rho\frac{d\mathbf{u}}{dt}+\nabla\cdot\left(p\mathbf{I}+\mathbf{\Pi}\right)=\mathbf{0}$

and viscous stress $\boxed{\mathbf{\Pi}=-2\mu[\nabla\mathbf{u}]^{(2)}}$

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

How BTE is connected with continuum

Boltzmann transport equation (BTE): 10^23^ $f(t, \mathbf{r}, \mathbf{v})$

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

Nonlinear collision integral

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

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

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

Enormous reduction of information

$$\boxed{\rho \frac{d\mathbf{u}}{dt} + \nabla \cdot (p\mathbf{I} + \mathbf{\Pi})} = \boxed{0}$$

Still exact to BTE

Conservation laws & constitutive equations: 13 $(\rho, \mathbf{u}, T, \mathbf{\Pi}, \mathbf{Q}, \cdots)(t, \mathbf{r})$

Boltzmann-based CFD schemes (partial list)

Basically a game of reducing the degree of freedom of BTE from 10^{23} to 10^3-10^{10}, the level modern computers can handle

DSMC

A representative particle to cover real particles in order of 10^{13}

Then describing the motion of the particles via deterministic movement and stochastic collision

No PDE

LBM

Solving BTE on discrete lattice

Introducing finite numbers of discrete velocity

Finally replace by 1st-order accurate BGK

Gas-kinetic

Solving a discretized version of conservation laws

and discretized BGK-BTE in an iterative way

Only discretized PDE

Chapman-Enskog

Assuming

$$f(t,\mathbf{r},\mathbf{v}) \simeq f\left[\mathbf{W}(t,\mathbf{r}),\nabla\mathbf{W}(t,\mathbf{r}),\mathbf{v},\varepsilon\right]$$

and inserting into BGK-BTE and deriving 1st, 2nd, 3rd approximations

PDE of high order

Need of extra BC due to $\nabla\mathbf{W}(t,\mathbf{r})$

Moment method

Differentiating the statistical definition

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

with time

and combining with BTE

PDE of high order

Molecular ⟵ ⟶ Continuum

Boltzmann CFD schemes-continued

DSMC

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f(t,\mathbf{r},\mathbf{v}) = 0$$

Kinematic: the collision-less movement of molecules

$$\frac{\partial f}{\partial t} = \int \left|\mathbf{v}-\mathbf{v}_2\right| (f^* f_2^* - f f_2)\, d\mathbf{v}_2$$

Molecular collisions

$$\rho = \iiint m f(t,\mathbf{r},\mathbf{v})\, dv_x\, dv_y\, dv_z$$

Sampling

Constraints:

Δt < mean collision time

Δx < mean free path

Particles cross less than
 1 cell/timestep

Gas-kinetic scheme

(micro-scale)

$$f_{j,k}^{n+1} = f_{j,k}^{n} + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}} [u f_{j-1/2,k}(t) - u f_{j+1/2,k}(t)]\, dt + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int_{x_{j-1/2}}^{x_{j+1/2}} \frac{g-f}{\tau}\, dx\, dt$$

Scale up

taking conservative moments:

$$\psi = (1, u_k, \frac{1}{2}(u_k^2 + \xi^2))^T$$

Scale down

$$g^{n+1}$$

mass, momentum and energy

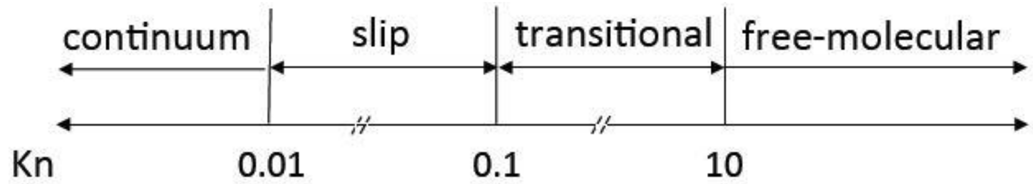
(macro-scale)

$$W_j^{n+1} = W_j^n + \frac{1}{\Delta x}\int_{t^n}^{t^{n+1}}\int u_k \psi (f_{j-1/2,k} - f_{j+1/2,k})\, du_k\, d\xi\, dt$$

K. Xu (2014)

Some points for Boltzmann-based schemes

I. Kn vs (Kn, M)



should be replaced by

FLOW REGIMES FOR DIFFERENT MACH NUMBER AND REYNOLDS NUMBER COMBINATIONS

	R		
M	$\mathcal{O}(\epsilon)$	$\mathcal{O}(1)$	$\mathcal{O}(1/\epsilon)$
$\mathcal{O}(\epsilon)$	$K=\mathcal{O}(1)$. Creeping micro-flow	$K=\mathcal{O}(\epsilon)$. Moderate micro-flow	$K=\mathcal{O}(\epsilon^2)$. Low M Fanno Flow
$\mathcal{O}(1)$	$K=\mathcal{O}(1/\epsilon)$. Transonic Free-molecular flow	$K=\mathcal{O}(1)$. Transonic micro-flow	$K=\mathcal{O}(\epsilon)$. Transonic Fanno Flow
$\mathcal{O}(1/\epsilon)$	$K=\mathcal{O}(1/\epsilon^2)$. Hypersonic Free-molecular flow	$K=\mathcal{O}(1/\epsilon)$. Hypersonic Free-molecular flow	$K=\mathcal{O}(1)$. Hypersonic "Fanno" (Transitional) Flow

Arkilic et al. (1997)

II. The equation below is an exact consequence of BTE, meaning its validity regardless of the degree of non-equilibrium.

$$\rho\frac{d\mathbf{u}}{dt}+\nabla\cdot\left(\frac{1}{\gamma M^2}p\mathbf{I}+\frac{1}{\mathrm{Re}}\mathbf{\Pi}\right)=0$$

Some points for Boltzmann-based schemes-continued

III. Conservation laws and boundary treatments

- A verification is possible based on the following property

$$\nabla \cdot \left(\rho \mathbf{u}\mathbf{u} + \frac{1}{\gamma M^2} p\mathbf{I} + \frac{1}{\mathrm{Re}} \mathbf{\Pi} \right) = 0 \ \text{ or } \ \oiint_S \mathbf{F} \cdot \mathbf{n} dS = 0 \ \text{ at steady-state}$$

- A challenge is the statement of C. Villani (2010 Field Medalist):

"The conservation laws should hold true when there are no boundaries. In presence of boundaries, however, conservation laws may be violated: momentum is not preserved by specular reflection."

In conservative PDE-based schemes, the nearest cell to the wall always satisfies the conservation laws via $\mathbf{U}_{i,j}^{n+1} = \mathbf{U}_{i,j}^{n} - \frac{\Delta t}{A_{i,j}} \sum_{k=1}^{4} \mathbf{F}_k \Delta L_k$

but it may not be true in the case of non-PDE schemes.

Part II.

CFD schemes based on the continuum version of BTE: the moment method (PDE)

Continuum version of BTE (Maxwell 1867)

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

Boltzmann collision integral

$$\boxed{\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right) f(t,\mathbf{r},\mathbf{v})} = \boxed{C[f, f_2]} \qquad \sim \int |\mathbf{v}-\mathbf{v}_2| (f^* f_2^* - f f_2) d\mathbf{v}_2$$

Differentiating the statistical definition of moments $\langle h^{(n)} f(t,\mathbf{r},\mathbf{v})\rangle$ *with time* and *then combining* with BTE

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

Non-hyperbolic
Not necessarily explicit

Two places (not one) to closure

Still exact to BTE

Conservation laws & constitutive equations: finite $(\rho, \mathbf{u}, T, \mathbf{\Pi}, \mathbf{Q}, \cdots)(t,\mathbf{r})$

Moment methods: Grad (1949)

Harold Grad (born January 23, 1923 in New York City, died November 17, 1986) was an American applied mathematician. His work specialized in the application of statistical mechanics to plasma physics and magnetohydrodynamics.

Contents [hide]

Dr. Harold Grad

Work [edit]

In statistical mechanics he had developed in his thesis new methods for the solution of the Boltzmann equation. Harold Grad was the founder of the Magneto-fluid Dynamics Division of the Courant Institute and served as its head until shortly before his death[1] From 1964 to 1967 and 1974 to 1977 he was a member of the Advisory Committee for Fusion Energy at Oak Ridge National Laboratory.[2]

Polynomial expansion with 3 terms

$$f = f^{(0)}\left[1+\frac{1}{2}\hat{\mathbf{\Pi}}:[\hat{\mathbf{c}}\hat{\mathbf{c}}]^{(2)} - \hat{\mathbf{Q}}\cdot\hat{\mathbf{c}}\left(1-\frac{1}{5}\hat{c}^2\right)\right]$$

was inserted into the Maxwell's continuum version of BTE.

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

Communications on
PURE AND APPLIED MATHEMATICS

On the Kinetic Theory of Rarefied Gases

By HAROLD GRAD

Then we have (when viscous stress $\mathbf{\Pi}=\left\langle h^{(2)} f\right\rangle$, $h^{(2)}=m[\mathbf{cc}]^{(2)}$)

$$\boxed{\rho\frac{d(\mathbf{\Pi}/\rho)}{dt}+\boxed{\frac{2}{5}[\nabla\mathbf{Q}]^{(2)}}+2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}+2p[\nabla\mathbf{u}]^{(2)}}=\boxed{-\frac{p}{\mu_{NS}}\mathbf{\Pi}F_{3rd-Approx}},$$

where $F_{3rd-Approx}=1-\dfrac{1}{6B_1^{(\Pi)}\rho\mathbf{\Pi}/m}\left[\dfrac{\rho}{m}(B_1^{(Q)}-B_1^{(\Pi)})(\text{quadratic terms of }\mathbf{\Pi}:\mathbf{\Pi})\right]$

and high order term $\nabla\cdot\left\langle \mathbf{c}h^{(2)} f\right\rangle=\nabla\cdot\left\langle m\mathbf{c}[\mathbf{cc}]^{(2)}\, f\right\rangle_{3rd-Approx}\approx\dfrac{2}{5}[\nabla\mathbf{Q}]^{(2)}$.

Genesis of the high Mach number problem (HMNP): Grad 1952

COMMUNICATIONS ON PURE AND APPLIED MATHEMATICS, VOL. V, 257–300 (1952)

The Profile of a Steady Plane Shock Wave

By HAROLD GRAD

By arguing that $\left|(B_1^{(Q)} - B_1^{(\Pi)}) / B_1^{(\Pi)}\right| < 1/7,$

Grad ignored the quadratic terms in the dissipative collision term

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \boxed{\frac{2}{5}[\nabla \mathbf{Q}]^{(2)}} + 2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2p[\nabla\mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}}\mathbf{\Pi}F_{1st-Approx}, \text{ where } \boxed{F_{1st-Approx} = 1}$$

Grad solved this equation (quadratic for left-hand side due to presence of $2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)}$, while linear for right-hand side) in 1952, but found a shock structure singularity at M=1.65 and could not figure out why.

The ultimate origin of Grad's failure was found to be the unbalanced closure; ignoring the quadratic term in the dissipation term by Myong in 2014.

While $\left|(B_1^{(Q)} - B_1^{(\Pi)}) / B_1^{(\Pi)}\right|$ can be small near the equilibrium, it will increase as the problem becomes away from equilibrium! So we cannot ignore it.

Moment methods: Truesdell (1956,1980)

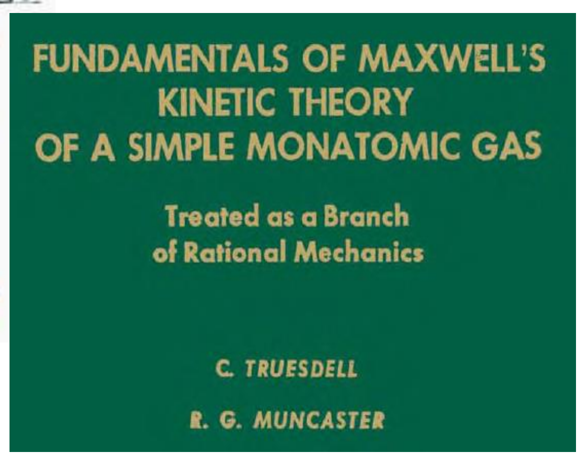
Re-enforcement of Grad's unbalanced approach

Clifford Ambrose Truesdell III

Born	February 18, 1919 Los Angeles
Died	January 14, 2000 (aged 80) Baltimore
Nationality	American
Fields	Mathematics Natural Philosophy History of Science

It was rigorously proven in the Maxwellian molecule that the linear relation in the collisional term is an exact consequence of the original Boltzmann collision integral by Truesdell ("On the pressures and the flux of energy in a gas according to Maxwell's kinetic theory," II, *J. Rational Mech. Anal*. 5 (1956), 55–128.)

$$\left\langle h^{(n)} C[f, f_2] \right\rangle \underset{\boxed{Exact}}{=} \left\langle h^{(n)} f \right\rangle$$



This misuse, the linear relation of the Maxwellian molecule, was never questioned by practitioners in the field until recently.

Summary of the origin of high Mach number shock singularity: Procrustean bed

Procrustean bed

Enforcing conformity without regard to natural variation or individuality, just as Procrustes violently adjusted his guests to fit their bed.

In order to force the constitutive equations—not necessarily hyperbolic—into a hyperbolic system (with distinct eigenvalues), over-simplify the Boltzmann collision integral by assuming the Maxwellian molecule (which is exceptional, rather than general)

$$\left\langle h^{(n)} C[f, f_2] \right\rangle = \left\langle h^{(n)} f \right\rangle$$

And this is the precious reason why the shock singularity (originally accidental) remained unsolved for several decades! (R. S. Myong, *Phys. Fluids*, 2014)

削趾適屨 **yuè zhǐ shì jù: Cut the tiptoe in order to fit the foot into a shoe** (rather than modifying the shoe)

The constitutive theory: new balanced closure

Then the solution to remove the HMNP is to abandon the 1st-order accurate linear relation in dissipative collision term.

$$\rho \frac{d}{dt}\left(\left\langle h^{(n)} f \right\rangle / \rho\right) + \nabla \cdot \left\langle \mathbf{c} h^{(n)} f \right\rangle - \left\langle f \frac{dh^{(n)}}{dt} \right\rangle - \left\langle f \mathbf{c} \cdot \nabla h^{(n)} \right\rangle = \left\langle h^{(n)} C[f, f_2] \right\rangle, \text{ where}$$

the RH terms represent the change due to the molecular collision.

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \boxed{\nabla \cdot \mathbf{\Psi}} + 2\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)} + 2p\left[\nabla \mathbf{u}\right]^{(2)} = -\frac{p}{\mu_{NS}} \mathbf{\Pi} \boxed{F_{exact}}$$

(No approximations so far!: Approximations was deferred to the last stage in order to minimize accumulated errors.)

Then, when 2nd-order balanced closure is applied; we have

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \boxed{0} + 2\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)} + 2p\left[\nabla \mathbf{u}\right]^{(2)} = -\frac{p}{\mu_{NS}} \mathbf{\Pi} \boxed{F_{2nd-order}}$$

Only remaining task is to determine $F_{2nd\text{-}order}$; nothing else!

The constitutive theory: Exponential form and 2nd law of thermodynamics

Any 2nd-order expression can basically be used for the nonlinear factor, but the hyperbolic sinh form, originally derived by B. C. Eu in 80-90s, was found adequate.

Key ideas are; exponential canonical form, consideration of entropy production σ, and non-polynomial expansion called as cumulant expansion.

By writing the distribution function f in the exponential form

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

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

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

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

The 2nd-order constitutive theory: sinh nonlinear form

The simplest closure of LH term in next level to the linear Navier-Fourier theory is $\nabla\cdot\boldsymbol{\Psi}^{(\Pi)}=0,$

while the 2nd-order closure of RH term is $R_{12}^{(21)}X_2^{(1)}q(\kappa_1^{(\pm)}).$ Then

$$\rho\frac{d(\boldsymbol{\Pi}/\rho)}{dt}+2[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}]^{(2)}+2p[\nabla\mathbf{u}]^{(2)}=-\frac{p}{\mu_{NS}}\boldsymbol{\Pi}\boxed{q(\kappa_1),}$$

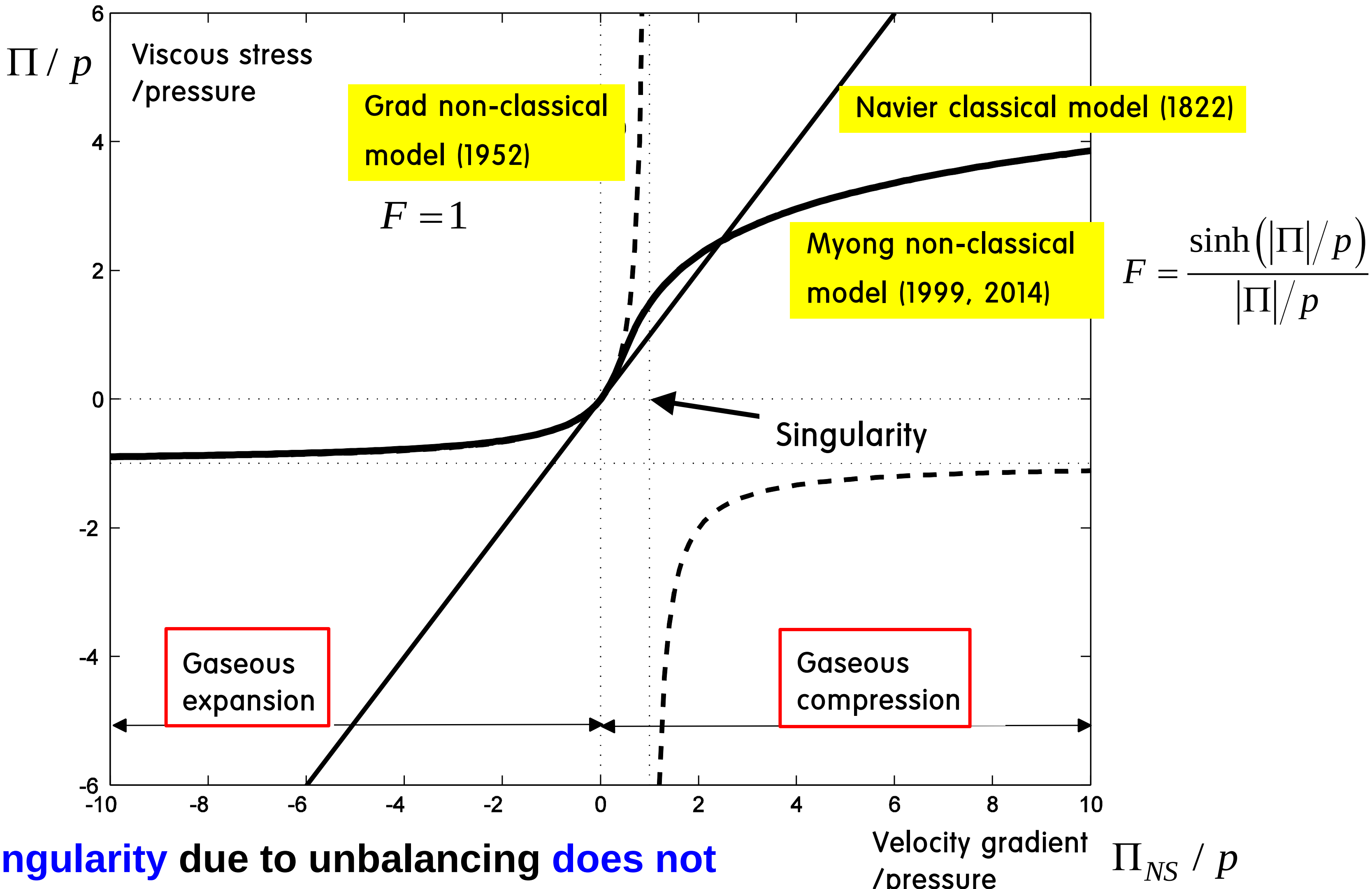
$$q(\kappa_1)\equiv\boxed{\frac{\sinh\kappa_1}{\kappa_1}},\ \kappa_1\equiv\frac{(mk_B)^{1/4}}{\sqrt{2}d}\frac{T^{1/4}}{p}\left(\frac{\boldsymbol{\Pi}:\boldsymbol{\Pi}}{\mu_{NS}}+\frac{\mathbf{Q}\cdot\mathbf{Q}/T}{k_{NS}}\right)^{1/2}.$$ **Implicit!**

This new 2nd-order constitutive equation beyond the two-century old Navier-Stokes equation, of course, recovers NS

$2p[\nabla\mathbf{u}]^{(2)}=-\frac{p}{\mu_{NS}}\boldsymbol{\Pi},$ and reduces to an algebraic equation in steady-state (also assuming 1-D)

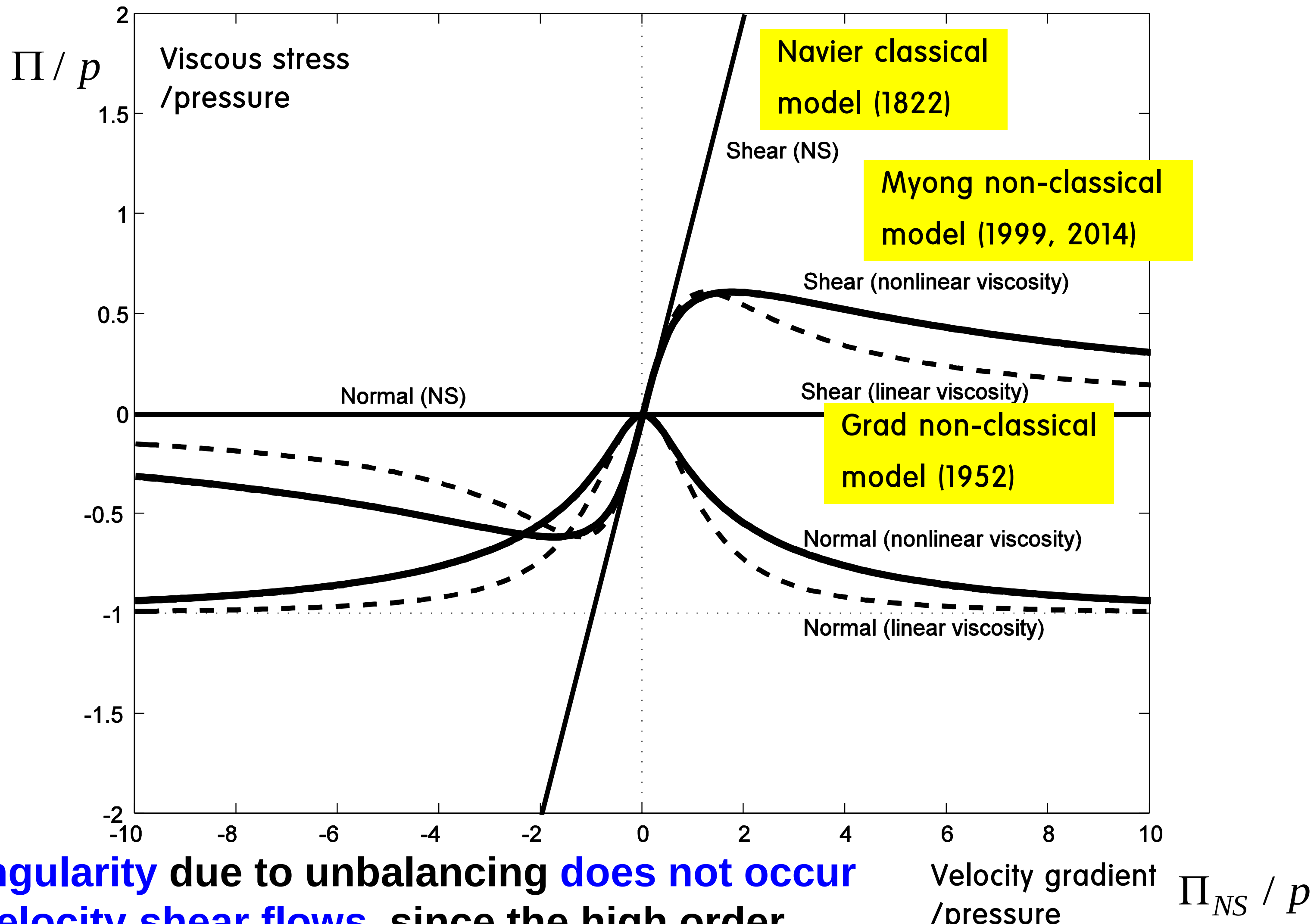
$$-\hat{\Pi}\hat{\Pi}_{NS}-\hat{\Pi}_{NS}=-\hat{\Pi}q(c|\hat{\Pi}|)\left(=-\hat{\Pi}-\frac{1}{3!}\hat{\Pi}(c\hat{\Pi})^2-\frac{1}{5!}\hat{\Pi}(c\hat{\Pi})^4-\cdots\right).$$

NCCR: Nonlinear Coupled Constitutive Relation



The singularity due to unbalancing does not occur in expansion flow, since the sign of quadratic term is opposite.

NCCR: shear-dominated flow



The **singularity** due to unbalancing **does not occur in velocity shear flows**, since the high order nonlinear effects are **cancelled under the constraint of the asymptotic behavior**.

The DG-NCCR CFD scheme

Hyperbolic (inviscid)

Conservation laws (exact consequence of BTE)

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

in conjunction with the 2nd-order constitutive equations

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

$$\rho\frac{d(\mathbf{Q}/\rho)}{dt}+\frac{d\mathbf{u}}{dt}\cdot\mathbf{\Pi}+\mathbf{Q}\cdot\nabla\mathbf{u}+\mathbf{\Pi}\cdot C_p\nabla T+C_p p\nabla T=-\frac{pC_p}{k_{NS}}\mathbf{Q}q(\kappa_1).$$

Non-hyperbolic Implicit

Thermodynamic driving force

$-2\eta\left[\nabla\mathbf{u}\right]^{(2)}$

$-k\nabla T$

$$\xrightarrow[\div p\sqrt{\frac{C_pT}{2\,\mathrm{Pr}}}]{\div p}\ \boxed{\begin{array}{c}\textbf{Nonlinear Coupled}\\ \textbf{Constitutive Relation}\\ f_\Pi, f_Q\end{array}}\ \xrightarrow[\times p\sqrt{\frac{C_pT}{2\,\mathrm{Pr}}}]{\times p}$$

Shear stress Heat flux

$\mathbf{\Pi}$

$\mathbf{Q}$

$i \qquad i+1/2 \qquad i+1$

$$\mathbf{\Pi}_{i+1/2_{NSF}}=-2\eta_{i+1/2}\left[\nabla\mathbf{u}\right]^{(2)}_{i+1/2} \qquad \mathbf{\Pi}_{i+1/2_{NCCR}}=f_\Pi\left(\mathbf{\Pi}_{i+1/2_{NSF}},\mathbf{Q}_{i+1/2_{NSF}},p_{i+1/2},T_{i+1/2}\right)$$

$$\mathbf{Q}_{i+1/2_{NSF}}=-k_{i+1/2}(\nabla T)_{i+1/2} \qquad \mathbf{Q}_{i+1/2_{NCCR}}=f_Q\left(\mathbf{\Pi}_{i+1/2_{NSF}},\mathbf{Q}_{i+1/2_{NSF}},p_{i+1/2},T_{i+1/2}\right)$$

The DG-NCCR CFD scheme

Conservation laws

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

Discretization in mixed (hybrid) form (include T^s)

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

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

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

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

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

The DG-NCCR CFD scheme

Modal basis function proposed by Dubiner for triangular element

Boundary (∂I) integrals replaced by fluxes

The Lax-Friedrichs (LxF) flux for inviscid terms

$$\mathbf{F}_{\text{inv1}} \cdot \mathbf{nx} \approx \mathbf{h}_{\text{inv1}}\left(\mathbf{U}^{-},\mathbf{U}^{+},\mathbf{nx}\right) = \frac{1}{2}\left[\mathbf{F}_{\text{inv1}}\left(\mathbf{U}^{-}\right) + \mathbf{F}_{\text{inv1}}\left(\mathbf{U}^{+}\right) - C\left(\mathbf{U}^{+} - \mathbf{U}^{-}\right)_{\text{inv1}}\right],$$

$$\text{where } C = \max\left(\left|\mathbf{u}^{-}\right| + \frac{a_s^{-}}{M},\ \left|\mathbf{u}^{+}\right| + \frac{a_s^{+}}{M}\right)$$

Central flux for viscous terms (Bassi and Rebay 1997)

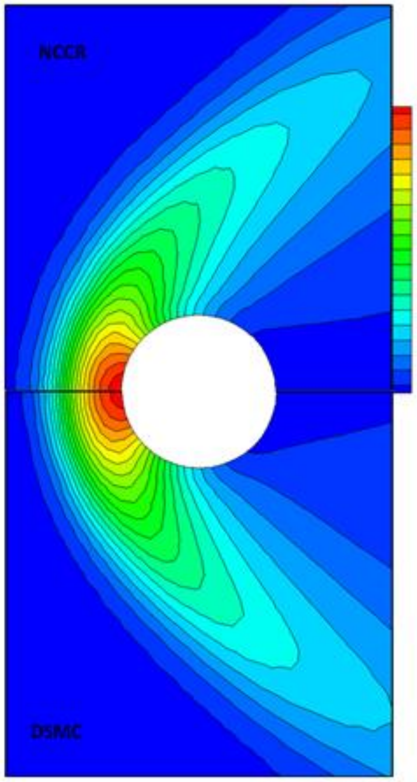
Limiter proposed by K. Kontzialis et al. in 2013

Semi-discrete form resolved by explicit Runge-Kutta time integration

$$\mathbf{L}\frac{\partial \mathbf{U}}{\partial \mathrm{t}} = \mathbf{R}(\mathbf{U})$$

Results: hypersonic case; M=5.48, Kn=0.5

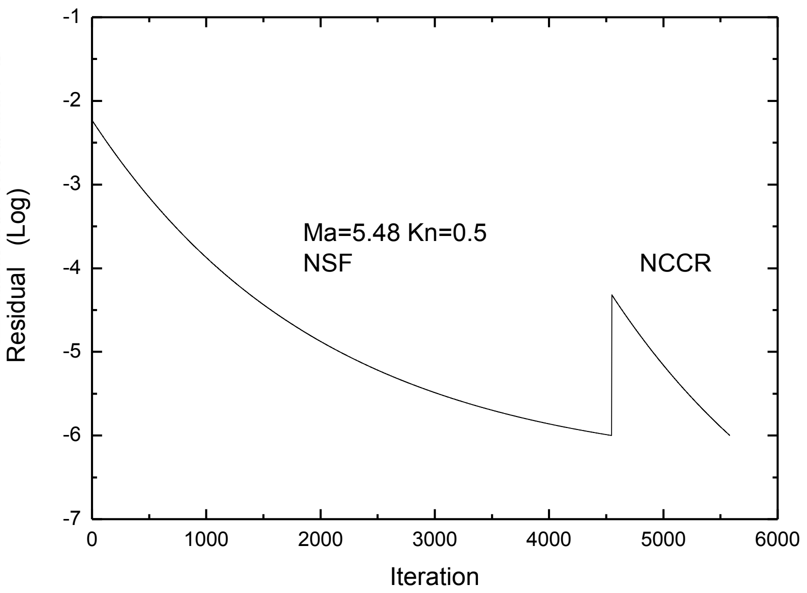
NCCR *NSF*



DSMC *DSMC*

Pressure

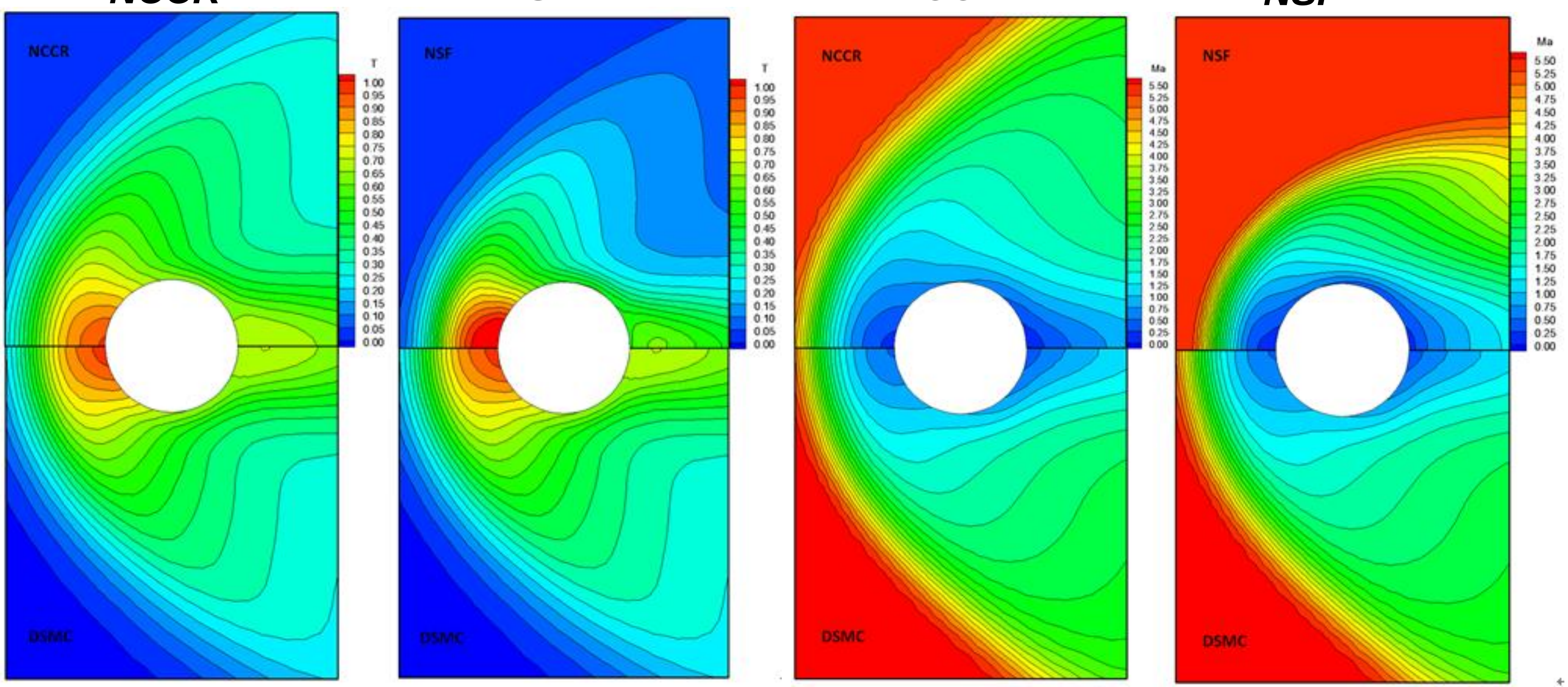
Computing time



Le, N. T. P., Xiao, H., Myong, R. S., A triangular discontinuous Galerkin method for non-Newtonian implicit constitutive models of rarefied and microscale gases, *Journal of Computational Physics*, Vol. 273, pp. 160-184, 2014.

Results: hypersonic case; M=5.48, Kn=0.5

NCCR ***NSF*** ***NCCR*** ***NSF***



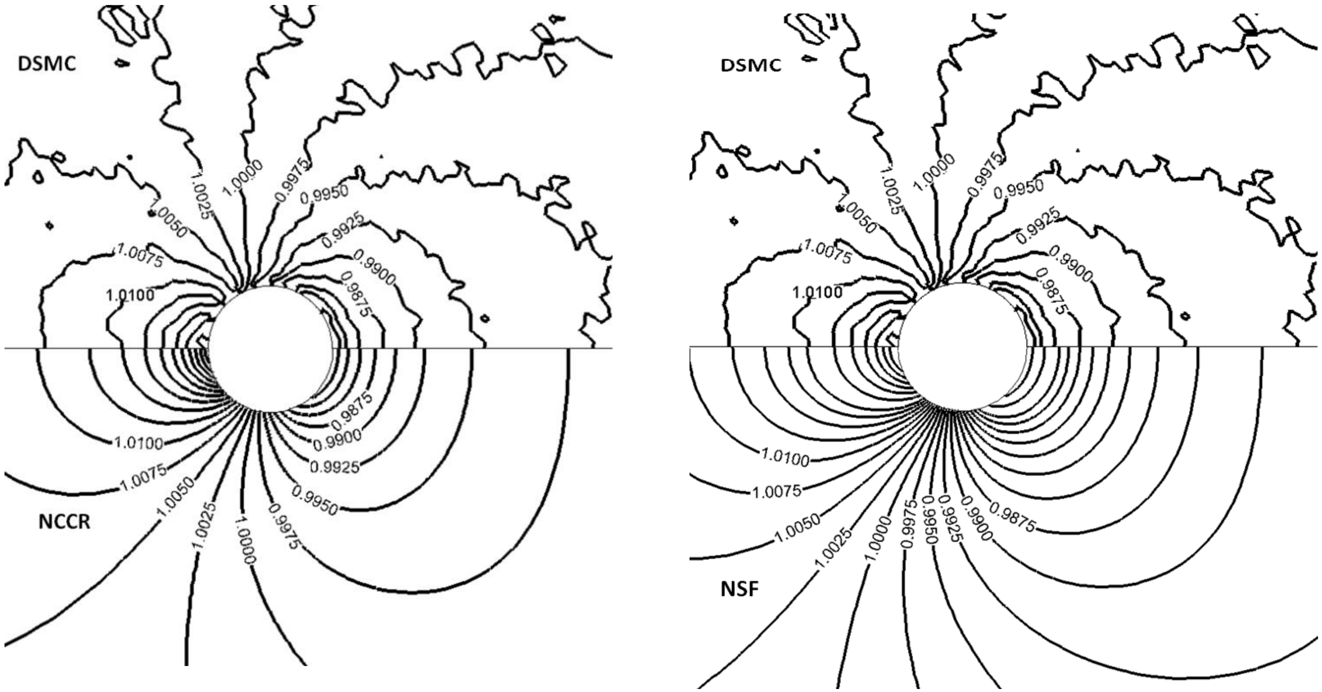
DSMC ***DSMC*** ***DSMC*** ***DSMC***

Temperature ***Mach number***

Results: low Mach no. case; M=0.1, Kn=0.1

DSMC

DSMC



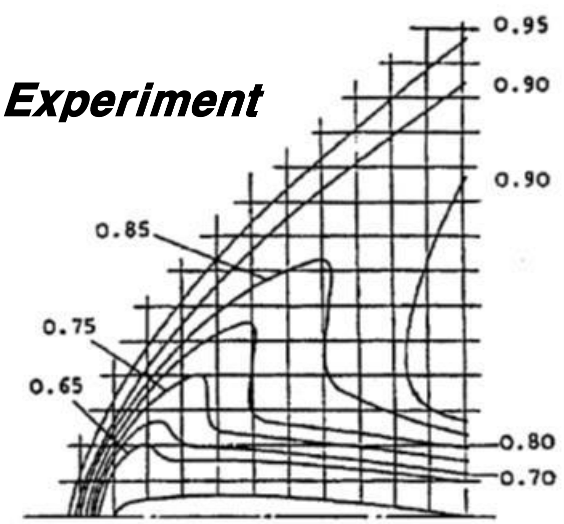
NCCR

NSF

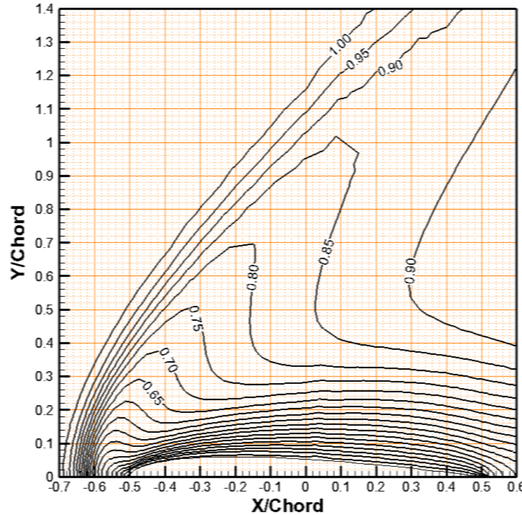
Density

Results: airfoil case; M=2.0, Re=106

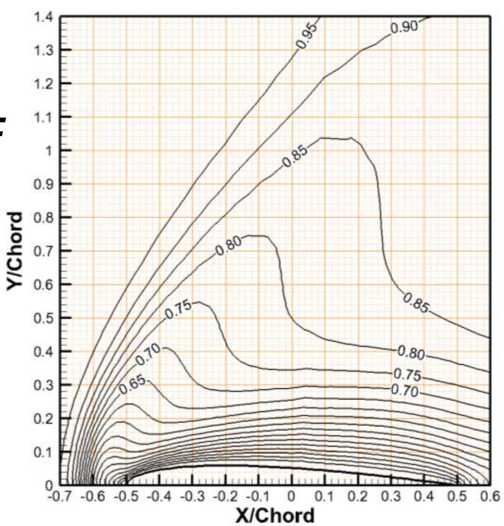
Experiment



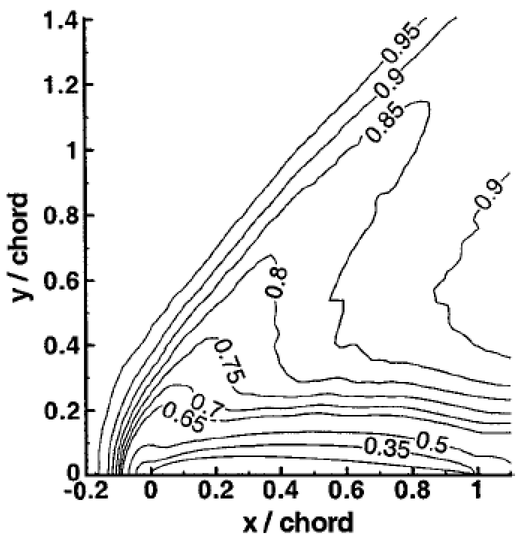
NCCR



NSF



DSMC



Velocity

Part III. Ongoing topic

Secret of Boltzmann’s success and pushing its boundary (gas to elastic solid): A unified theory for continuum media

R. S. Myong, *In Review,* 2015
“On the high Weissenberg number singularity in the Maxwell-Oldroyd model of viscoelastic fluids”

Cumulant expansion method-I

l-th moment of the distribution function and the moment-generated function (x being the non-equilibrium variables) are

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

Then we have

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

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

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

$$\left\langle e^x \right\rangle_{\text{cumulant}} = e^{\left[\kappa_1 + \frac{1}{2!}\kappa_2 + \frac{1}{3!}\kappa_3 + \cdots\right]} = e^{\left[\langle x \rangle + \frac{1}{2!}\left(\left\langle x^2 \right\rangle - \langle x \rangle^2\right) + \cdots\right]}$$

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

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

Cumulant expansion method-II

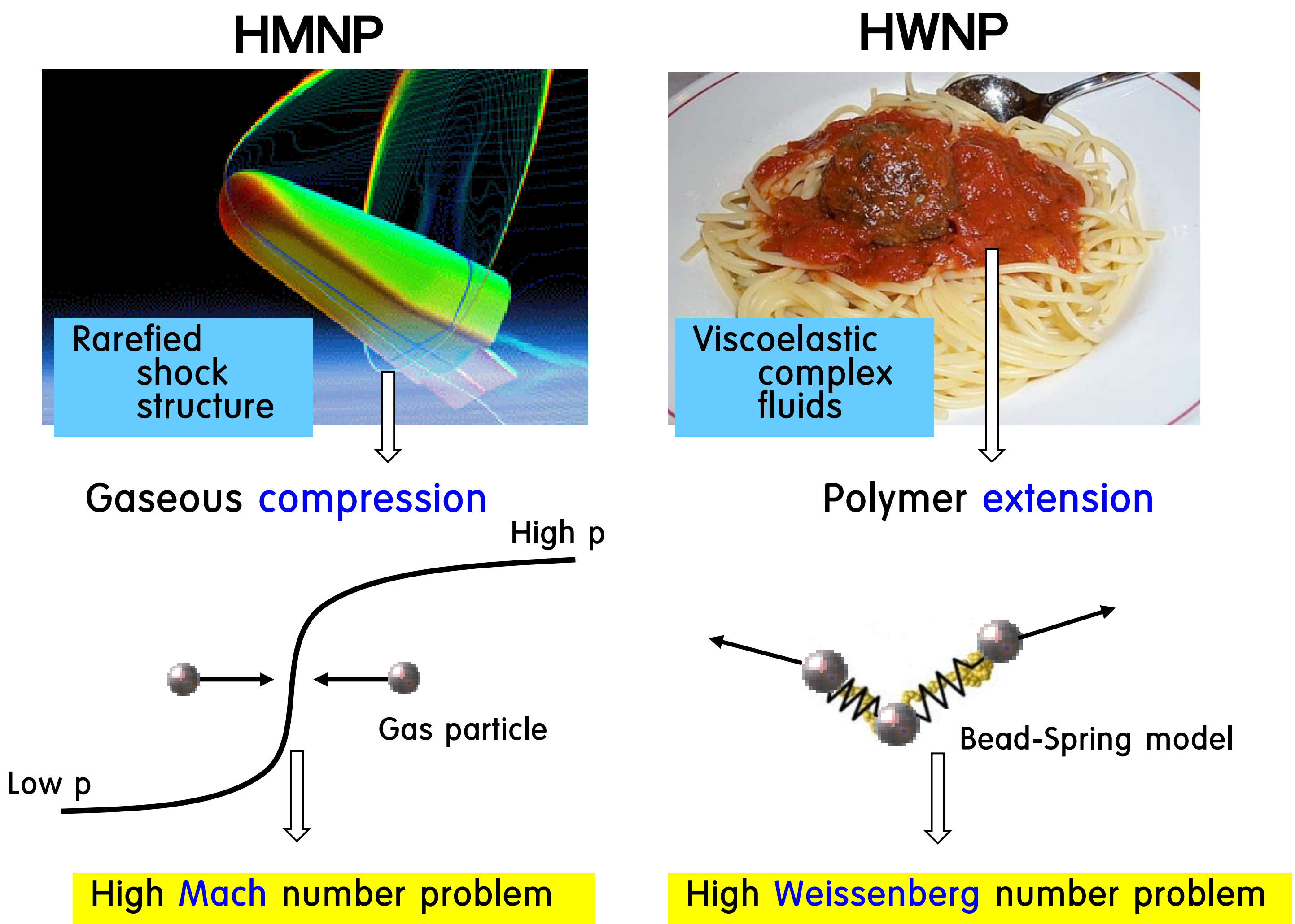
Therefore, the ratio of the cumulant expansion to the polynomial expansion becomes

$$\frac{\left.\left(\left\langle e^{x}\right\rangle-\left\langle e^{-x}\right\rangle\right)/2\right]_{\text{cumulant}}}{\left.\left(\left\langle e^{x}\right\rangle-\left\langle e^{-x}\right\rangle\right)/2\right]_{\text{polynomial}}} \approx \frac{\sinh\langle x\rangle}{\langle x\rangle} = 1+\frac{1}{3!}\langle x\rangle^{2}+\frac{1}{5!}\langle x\rangle^{4}+\cdots$$

The factor, $\sinh\langle x\rangle/\langle x\rangle$, is responsible for removing the shock singularity of the moment method and can handle transitional (and even free-molecular in cavity flow as high as Kn=6.71) flow.

Cumulant expansion: E. Meeron, *J. Chem. Phys*. 27, p. 1238, 1957.
It explicitly considers terms of all orders in the perturbation expansions.

Gain – Loss = $\left\langle e^{x}\right\rangle-\left\langle e^{-x}\right\rangle$ = sinh $\rightarrow$ **Secret of Boltzmann's success**


HMNP
HWNP
Rarefied shock structure
Viscoelastic complex fluids
Gaseous compression
Polymer extension
High p
Low p
Gas particle
Bead-Spring model
High Mach number problem
High Weissenberg number problem

The head and tail of a coin: exact analogy

Fluids category	Viscoelastic fluids (HWNP) Viscoelastic stress $\boldsymbol{\tau}$	Gases in non-equilibrium (HMNP) $\boldsymbol{\Pi}(=-\boldsymbol{\tau})$
Conserva-tion laws	$\rho\frac{D\mathbf{u}}{Dt}+\nabla\cdot\left(p\mathbf{I}-\boldsymbol{\tau}\right)=0$	$\rho\frac{D\mathbf{u}}{Dt}+\nabla\cdot\left(p\mathbf{I}+\boldsymbol{\Pi}\right)=0$
Constitutive equations	$\frac{D\boldsymbol{\tau}}{Dt}-\left[(\nabla\mathbf{u})^T\boldsymbol{\tau}+\boldsymbol{\tau}\nabla\mathbf{u}\right]-\frac{\mu}{\lambda}(\nabla\mathbf{u}^T+\nabla\mathbf{u})$ $=-\frac{1}{\lambda}\boldsymbol{\tau}$ for the Maxwell-Oldroyd model	$p\frac{D(\boldsymbol{\Pi}/p)}{Dt}+2\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}+p\left(\nabla\mathbf{u}^T+\nabla\mathbf{u}\right)$ $=-\frac{1}{\mu/p}\boldsymbol{\Pi}$ for Maxwellian molecule
Parameters	λ Wissenberg	μ/p M^2/Re

Resolving the HMNP automatically solves the HWNP.

Why analogy? Because all media follow two simple actions at a molecular level: movement and interaction among particles!

Thank you for your attention.