비평형 공기열역학: 극초음속 및 희박 공기역학 모델링
Non-equilibrium Aerothermodynamics: Modeling Hypersonic and Rarefied Aerodynamics

November 17th Thursday, 2022 (09:45~10:15AM)

명노신 (Rho-Shin Myong)

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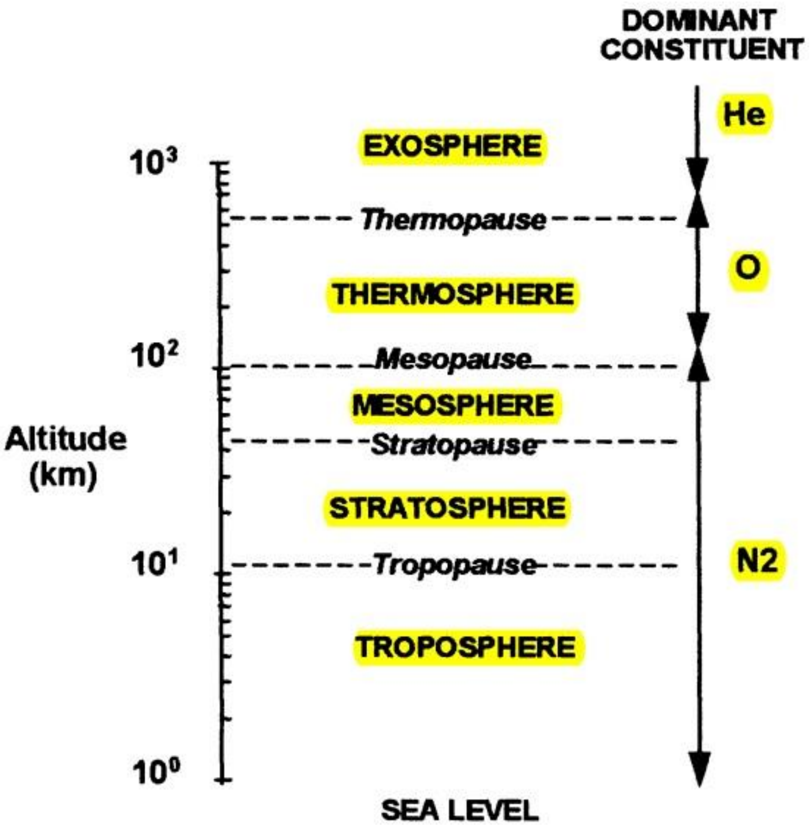
The 2022 Park Chul Aerodynamics Lecture at the Annual KSAS Fall Conference (Jeju)

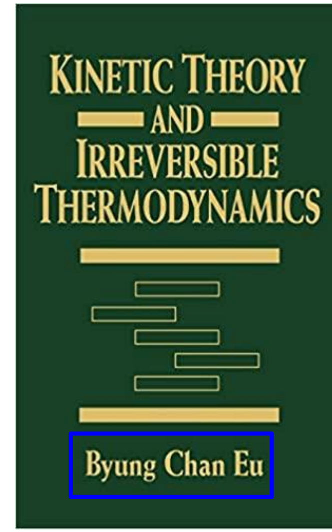
경상국립대학교
Gyeongsang National University

Aerospace Systems Research Center
항공우주시스템연구소

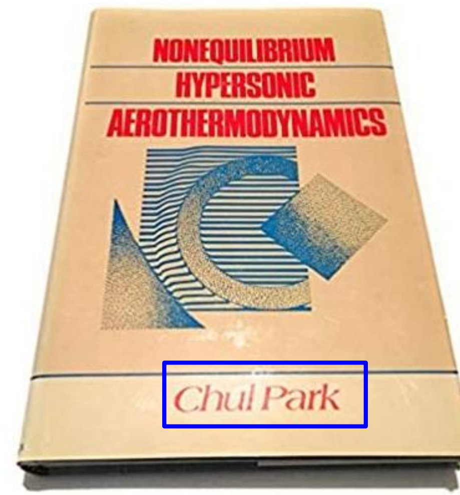
Aerodynamics? Aerothermodynamics?

Definition of air (aero): the mixture of gases that surrounds the earth



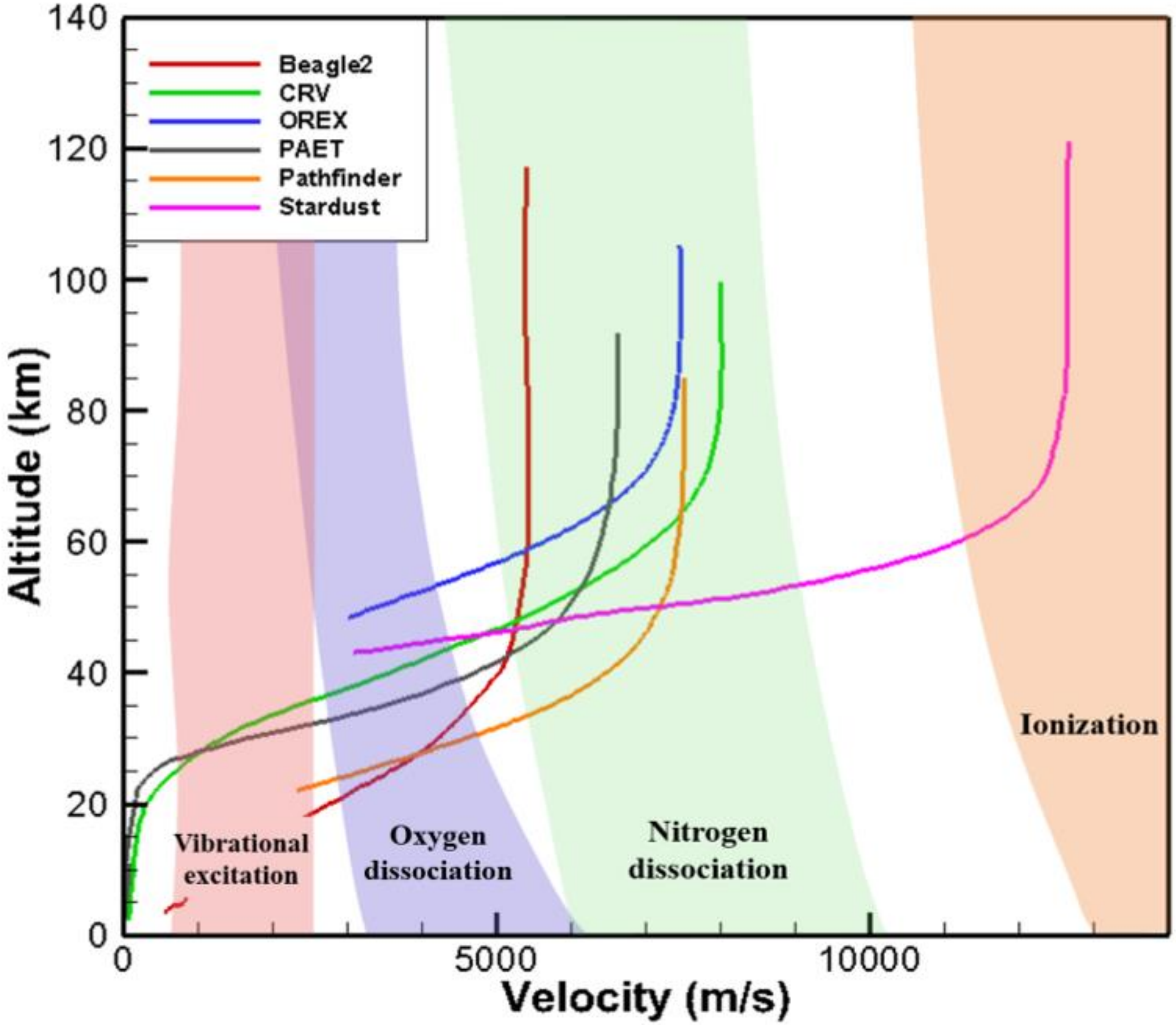


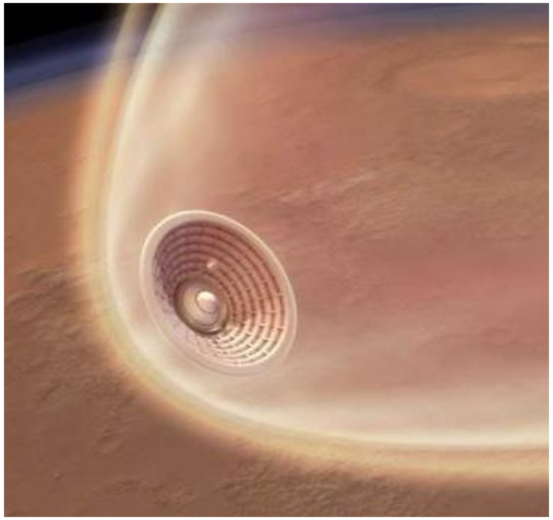
(1992, Chemistry, McGill)



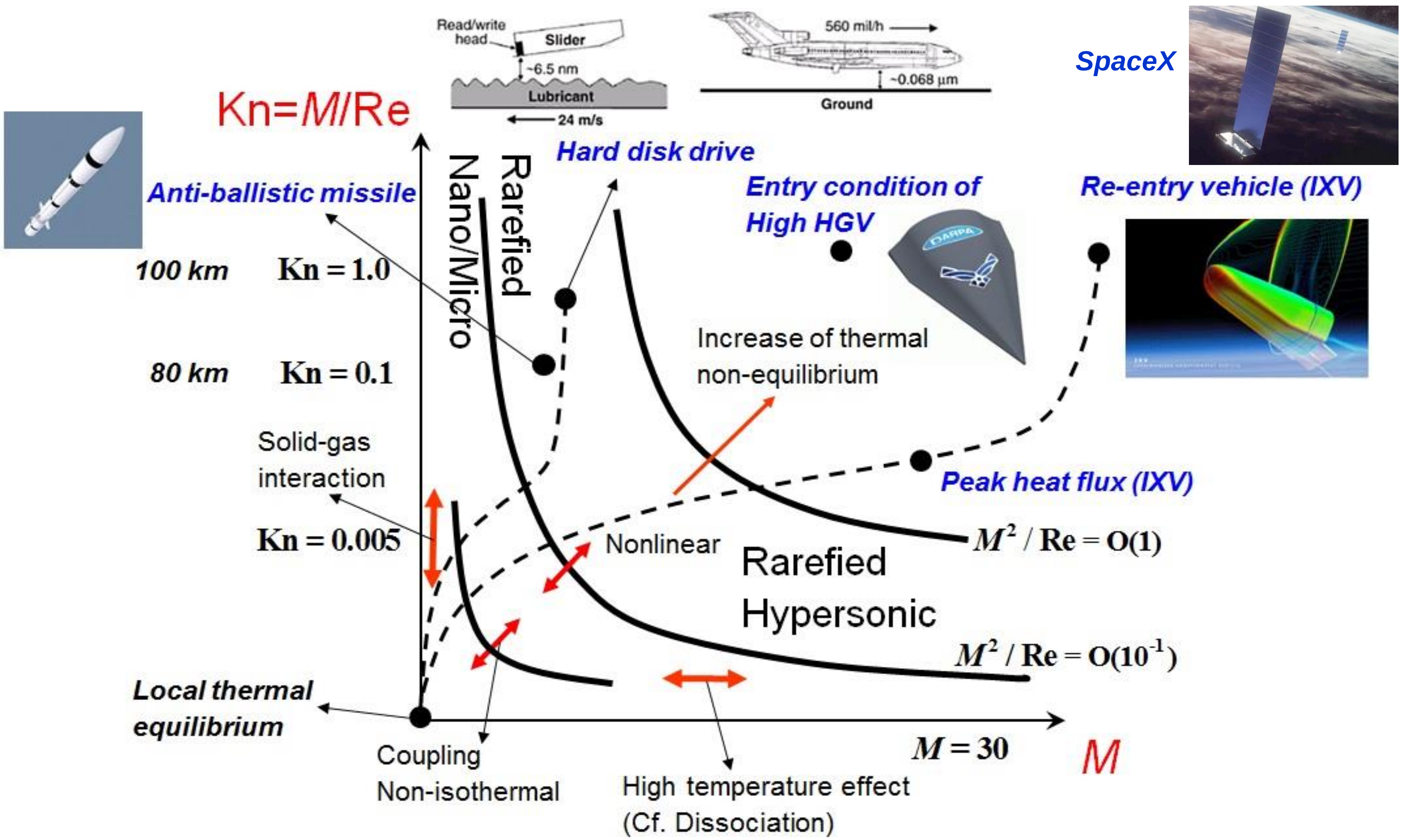
(1990, NASA Ames)

Background & motivation: Re-entry





Background & motivation: Lifting body and control



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

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

A brief history: Superaerodynamics

Albert F. Zahm (US)

"Superaerodynamics," Journal of the Franklin Institute, Vol. 217, pp. 153-166, 1934.

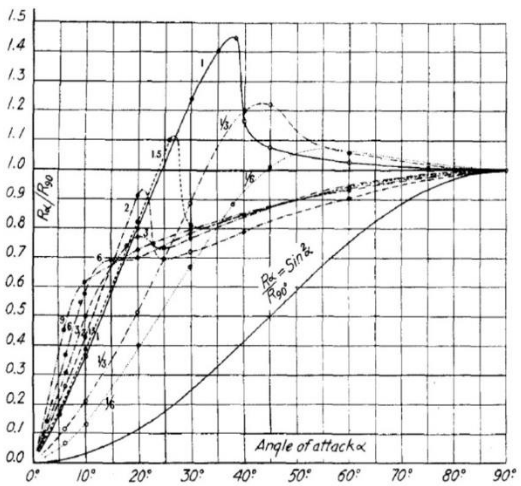
Eugene Sänger (Austria)

Silbervogel ("Silverbird") (1944)

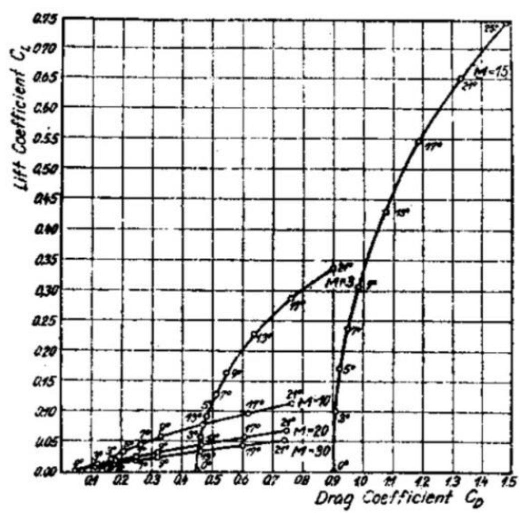
Ludwig Prandtl (Germany)

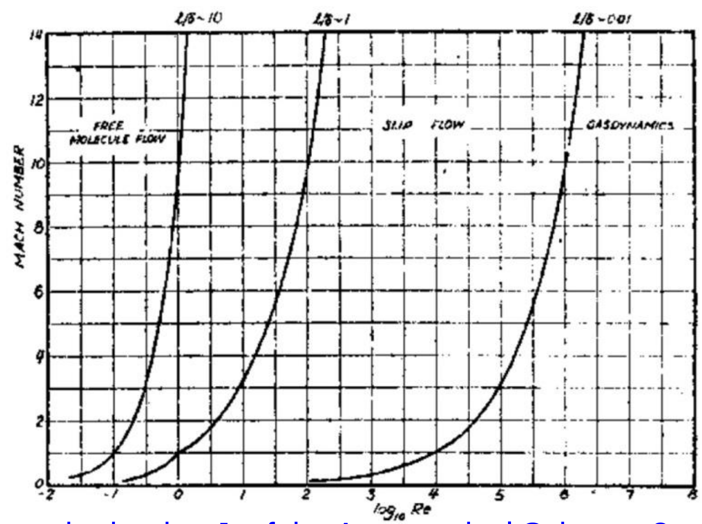
Theodore von Kármán (US, 1946)

Hsue-shen Tsien (錢學森, US)



Values of ratio R_α/R_{90} for inclined rectangles of different aspect ratios, as found by Eiffel and by discrete-fluid formula $R_\alpha/R_{90} = \sin^2\alpha$.





Munk (developer of the thin-airfoil theory) at NACA disliked Zahm's manuscript submitted to J. of the Aeronautical Sciences?

Recent: RGD32 & hypersonic shock tunnel

THIRTY-SECOND INTERNATIONAL SYMPOSIUM ON RAREFIED GAS DYNAMICS

http://www.rgd32.org/
(Seoul, July 4-8, 2022)

CAS JF12 (2012; Mach 5-9, Altitude 25-50km, 130 msec)

With Chul Park (2016, 1st HTGD, Beijing)

HGV (Hypersonic Glider Vehicle)

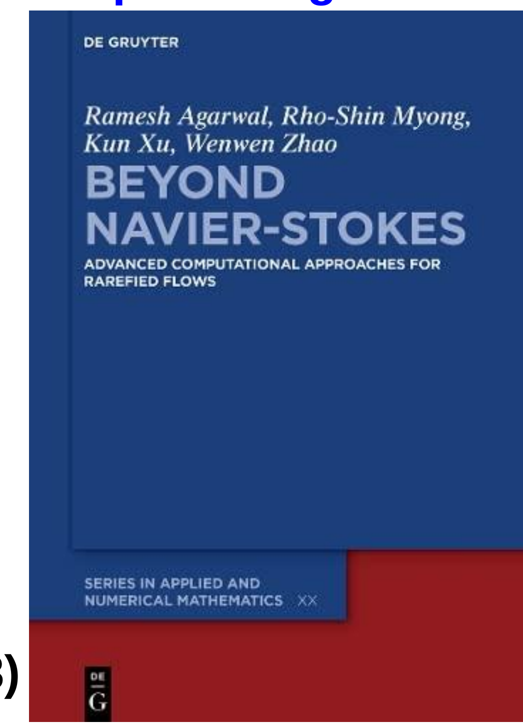
Related journal papers, article, and book

- Myong, R. S., Thermodynamically Consistent Hydrodynamic Computational Models for High-Knudsen-Number Gas Flows, ***Physics of Fluids***, Vol. 11, No. 9, pp. 2788-2802, **1999**.
- Myong, R. S., On the High Mach Number Shock Structure Singularity Caused by Overreach of Maxwellian Molecules, ***Physics of Fluids***, Vol. 26, No. 5, 056102, **2014**.
- Mankodi, T. K., Myong, R. S., Quasi-classical Trajectory-based Non-equilibrium Chemical Reaction Models for Hypersonic Air Flows, ***Physics of Fluids***, Vol. 31, 106102, **2019.**
- Singh, S., Karchani, A., Sharma, K., Myong, R. S., Topology of the Second-Order Constitutive Model Based on the Boltzmann-Curtiss Kinetic Equation for Diatomic and Polyatomic Gases, ***Physics of Fluids***, Vol. 32, 026104, **2020**.
- Mankodi, T. K., Myong, R. S., Boltzmann-based Second-order Constitutive Models of Diatomic and Polyatomic Gases including the Vibrational Mode, **Physics of Fluids**, Vol. 32, 126109, **2020**.
- Singh, S., Karchani, A., Chourushi, T., Myong, R. S., A Three-Dimensional Modal Discontinuous Galerkin Method for the Second-Order Boltzmann-Curtiss-Based Constitutive Model of Rarefied and Microscale Gas Flows, ***Journal of Computational Physics***, Vol. 457, 111052, **2022**.

http://acml.gnu.ac.kr

(2020)

(2023)



Acknowledgements: Funding, Collaborators, Students

1997-99 US National Research Council Research Associate Program (NASA Goddard Space Flight Center)

1999-03 한국과학재단 특정기초 **“**희박기체 및 **MEMS** 유동장 해석에 관한 기초연구**”**

2012-15 한국연구재단 중견연구 **“Non-classical** 열유동 물리법칙에 기초한 마이크로**-**희박 기체 연구의 새 패러다임**”**

2015-16 ADD 용역과제 **“NCCR-CFD** 기법을 이용한 연속체**-**희박 유동 통합해석 연구**” (**인하대 이승수 교수**)**

2015-18 한국연구재단 우주핵심 **“**달착륙선의 로켓플룸**-**월면 상호작용 및 표토입자 분산 연구**”**

2017-20 한국연구재단 중견연구 **“**희박**·**마이크로 다원자 기체와 점탄성 복잡유체에 관한 볼츠만 기반의 메조스케일 모델링 및 시스템 설계기법**”**

2022-25 US Air Force Research Laboratory (AFOSR Grant)

Byung-Chan Eu (Emeritus Prof., McGill University), Postdocs (Tapan K. Mankodi, IIT Guwahati) and Ph.D. Students (Satyvir Singh, Omid Ojtehadi, etc.)

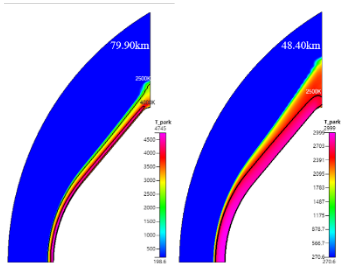
Park's two temperature model (1988)

From now on, no consideration on air-solid molecular interaction, ablation, and radiation

Average Temperature Model

In this model, the rate coefficient is assumed to be dictated by the (geometric) average temperature

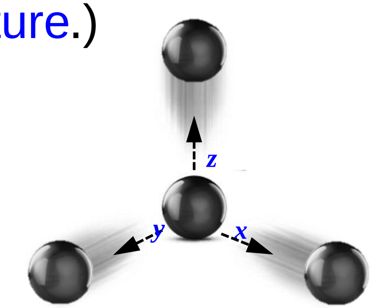
$$T_a = \sqrt{T \times T_v} \qquad (10)$$



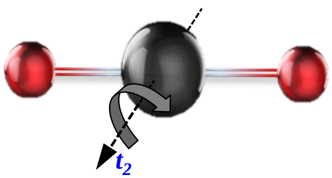
("Assessment of Two-Temperature Kinetic Model for Dissociating and Weakly-Ionizing Nitrogen," *J. of Thermophysics and Heat Transfer*, Vol. 2, pp. 8-16, 1988)

("The Limits of Two-Temperature Model," *AIAA 2010-911*: It describes what the two-temperature model is, and why it was developed. It then explains why the model is the way it is, and **what it cannot do**. It suggests a three-temperature model recognizing the rotational temperature or a radiation temperature different from heavy particle translational temperature.)

Argon **Nitrogen** **Carbon dioxide**



Translational degree of freedom



Rotational degree of freedom

NETT (Non-equilibrium Total Temperature) Model

- With the recent development of high-fidelity *ab initio* based computational chemistry algorithms, **Potential Energy Surface** information of various gas particles can be acquired using Complete Active Space Self-consistent Field (CASSCF) and Second-order Perturbation Theory (CASPT2) techniques.
- By combining this information with the **Molecular Dynamics** simulation based on the Quasi-classical Trajectory technique, the cross sections and rate coefficients of a chemical reaction can be calculated. (Luo, H., Kulakhmetov, M., and Alexeenko, A., "Ab Initio State-specific N2 + O Dissociation and Exchange Modeling for Molecular Simulations," *Journal of Chemical Physics*, Vol. 146, 074303, 2017.)
- It is crucial to realize that, although Park's two-temperature model over-predicts dissociation rates at lower vibrational temperatures, it is widely used today because of its clear and simple implementation.
- A physically-motivated model for non-equilibrium reaction rate coefficients suitable for the NSF equations is proposed. (Mankodi, T. K., Myong, R. S., Quasi-classical Trajectory-based Non-equilibrium Chemical Reaction Models for Hypersonic Air Flows, ***Physics of Fluids***, Vol. 31, 106102, **2019.)**

NETT (Non-equilibrium Total Temperature): results

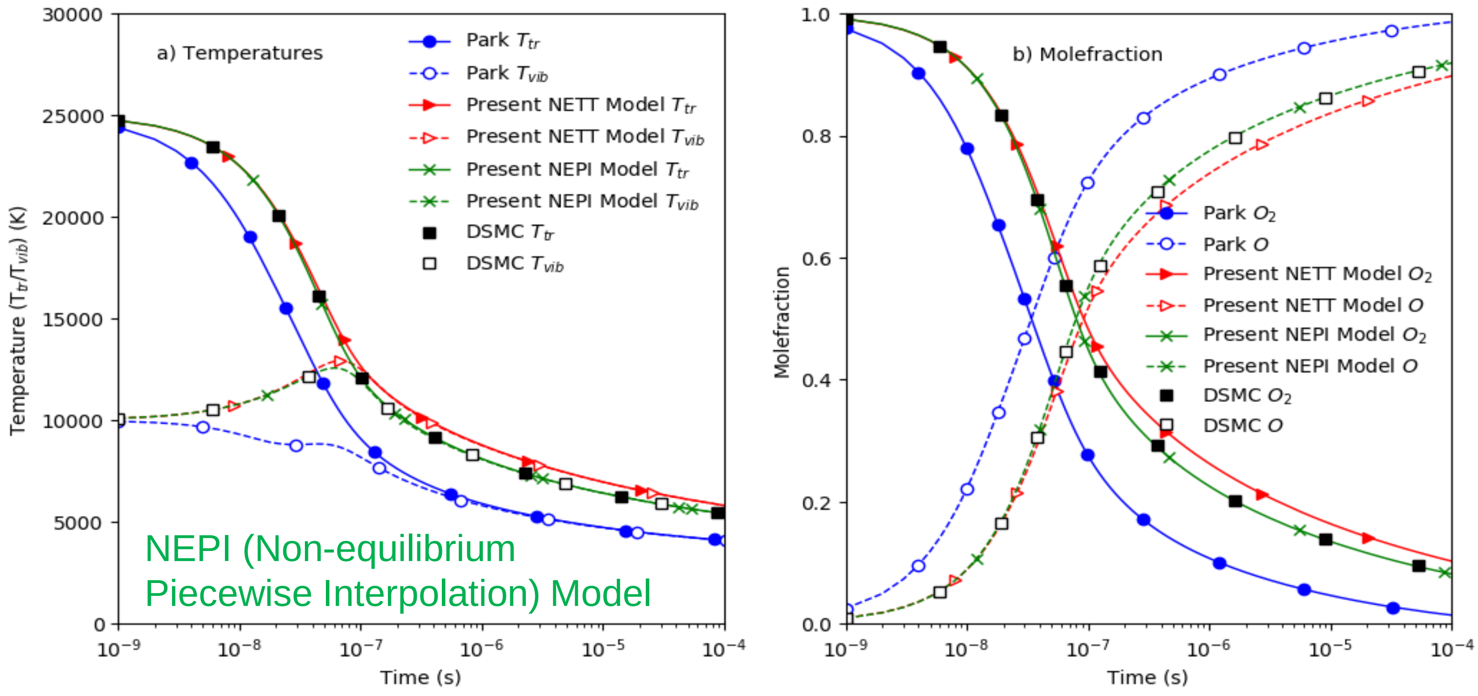
$$k(T_{tr},T_v) = A\left(\frac{T_v}{T_{tr}}\right)^{\chi} T_t^{\eta} \exp\left(-\frac{D}{T_t}\right),$$

Park's model with $\alpha = 0.5$

$$\ln T_a = \alpha \ln T_{tr} + (1-\alpha)\ln T_v$$

$$T_t = \alpha T_{tr} + (1-\alpha)T_v, \quad \alpha = \frac{\delta_{tr}}{\delta_{tr}+\delta_{vib}}, \quad \delta_{tr}(=3+2)=5, \quad \delta_{vib} = \frac{2e_{vib}}{R_S T_V}, \quad e_{vib} = \frac{R_S\theta_{vib}}{\exp(\theta_{vib}/T_v)-1}$$

NETT Model



Evolution of O and O_2 for simulation starting with vibrationally cold conditions

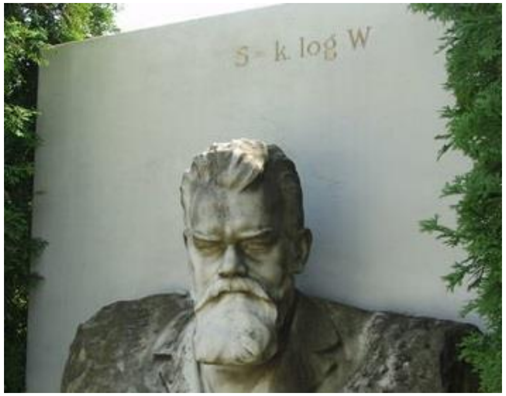
Boltzmann kinetic equations

- 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

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 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

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

PHYSICAL REVIEW E VOLUME 56, NUMBER 3 SEPTEMBER 1997

Generalized hydrodynamics and shock waves

Mazen Al-Ghoul and Byung Chan Eu*
Department of Chemistry, McGill University, 801 Sherbrooke Street West, Montreal, Quebec, Canada H3A 2K6

(Received 6 December 1996; revised manuscript received 3 March 1997)

Constitutive equations and balanced closure

Conceptual inconsistency of Eu's closure (B. C. Eu 1992)

$$\left\langle m\mathbf{cccf}\right\rangle - \left\langle m\mathrm{Tr}(\mathbf{ccc})f\right\rangle \mathbf{I}/3 = 0 \;\Rightarrow\; \text{Vanishing heat flux}$$

$$\left\langle m\mathbf{cccf}\right\rangle = 0 \;\Rightarrow\; \text{Cannot be zero in general}$$

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

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

2nd-order closure

$$\rho\frac{D}{Dt}\begin{bmatrix}\mathbf{\Pi}\left(\equiv\left\langle m[\mathbf{cc}]^{(2)}f\right\rangle\right)/\rho \\ \mathbf{Q}\left(\equiv\left\langle mc^2\mathbf{c}/2f\right\rangle\right)/\rho\end{bmatrix} + \nabla\cdot\begin{bmatrix}\left\langle m\mathbf{cccf}\right\rangle - \left\langle m\mathrm{Tr}(\mathbf{ccc})f\right\rangle\mathbf{I}/3 \\ \left\langle mc^2\mathbf{ccf}/2\right\rangle - C_pT(p\mathbf{I}+\mathbf{\Pi})\end{bmatrix} + \begin{bmatrix}0 \\ \left\langle m\mathbf{cccf}\right\rangle : \nabla\mathbf{u}\end{bmatrix}$$

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

2nd-order closure

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)

(2007)

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;

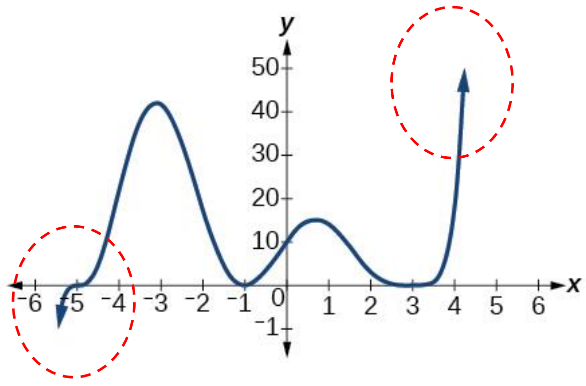
$$\rho \frac{D(\mathbf{\Pi}/\rho)}{Dt} + \nabla\cdot\mathbf{\Psi}^{(\Pi)} + 2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2p[\nabla\mathbf{u}]^{(2)} = \frac{1}{\beta g}\sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \cdots)$$

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

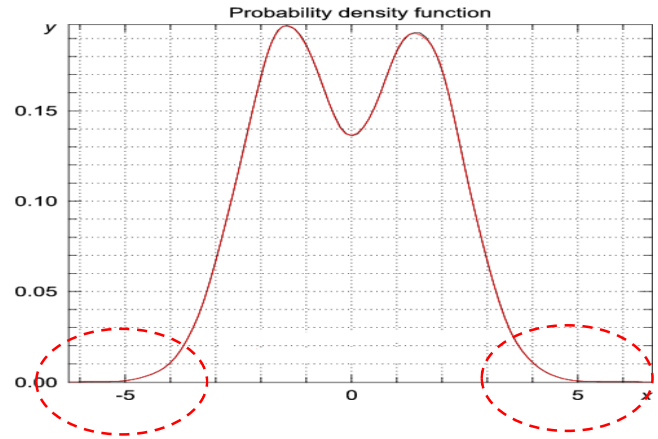
$$\left\langle e^{\lambda x} \right\rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \left\langle x^l \right\rangle = \exp\left[\sum_{l=1}^{\infty} \frac{\lambda^l}{l!} \kappa_l \right] \text{ where}$$



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

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

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



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

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

2nd-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 2nd-order constitutive relations (CR)

Zero in 2nd-order approximation

$$\frac{\partial\mathbf{\Pi}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{\Pi}+\nabla\cdot\left(\langle m\mathbf{ccc}f\rangle-\langle m\mathrm{Tr}(\mathbf{ccc})f\rangle\mathbf{I}/3\right)$$

Non-local term

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

2nd-order coupling — Navier 1st law

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

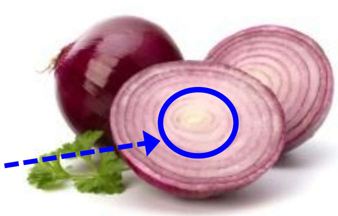
Onsager-Rayleigh dissipation function

2nd-order theory

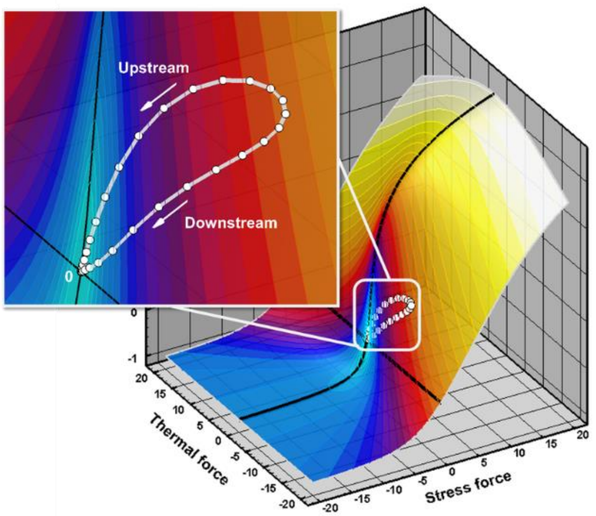
1st-order theory

Sinh{1st-order theory}

Navier-Fourier laws inclusive like onion!

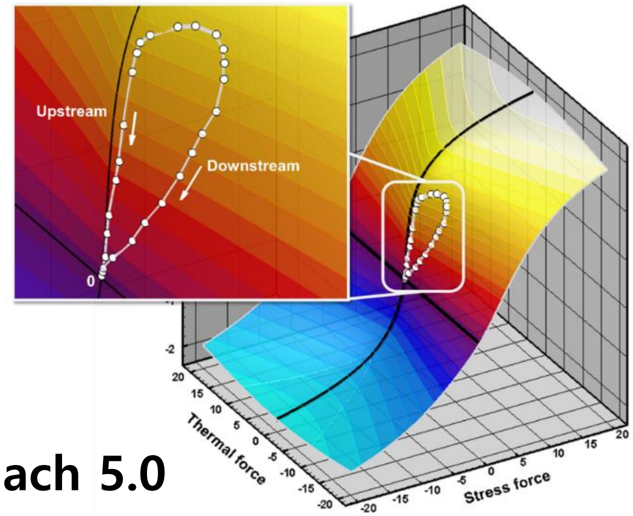


Topology of 2nd-order NCCR (shock structure) (PoF 2020a)



f_b=0.0

Mach 5.0



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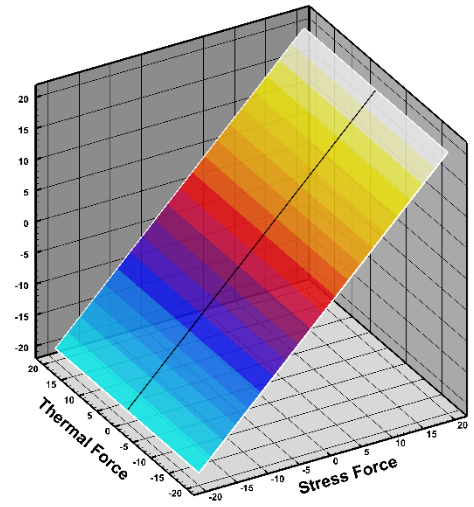


1st-order

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

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

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

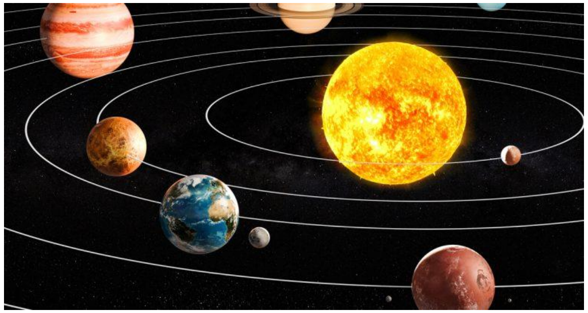
$$\hat{\mathbf{\Pi}}_0=-2\mu\left[\nabla\mathbf{u}\right]^{(2)}$$
$$\hat{\Delta}_0=-\mu_b\nabla\cdot\mathbf{u}$$
$$\hat{\mathbf{Q}}_0=-k\nabla T$$

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 2020a)

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	$\left(1-\frac{9}{2}f_b^2\right)x^2+x+\frac{2}{3}y^2=0$ $f_b=\frac{\text{bulk viscosity}}{\text{shear viscosity}}$	$(1-e^2)x^2+2epx+y^2-p=0$ $p=\frac{L^2}{Gm_1^2m_2^2/(m_1+m_2)}$ 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	$f_b\Leftrightarrow\frac{2\sqrt{3}}{9}\sqrt{\frac{1}{2}+e}=\frac{\sqrt{6}}{9}\sqrt{3-\frac{2E}{E_{\min}}}$ $f_b=0.2722\Leftrightarrow e_{\text{Earth}}=0.0167,$ $f_b=0.2834\Leftrightarrow e_{\text{Mercury}}=0.2056,$ $f_b=0.4611\Leftrightarrow e_{\text{Halley}}=0.967$	

Role of the 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	$\frac{\partial(\rho e_v)}{\partial t} + \nabla\cdot(\rho e_v\mathbf{u}) + \nabla\cdot\mathbf{Q}_v = \frac{\rho e_v(T_v) - \rho e_v(T)}{\tau_v}$	$\frac{\partial(\rho e_v)}{\partial t} + \nabla\cdot(\rho e_v\mathbf{u}) + \nabla\cdot\mathbf{Q}_v = \frac{\rho e_v(T_v) - \rho e_v(T)}{\tau_v}$
$\mathbf{\Pi}$	$\mathbf{\Pi} = -2\mu[\nabla\mathbf{u}]^{(2)}$	$2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} + 2(p+\Delta)[\nabla\mathbf{u}]^{(2)} = -\frac{p}{\mu}\mathbf{\Pi}q_{2nd}(\kappa)$
Δ	$\Delta = 0$	$2\gamma'(\mathbf{\Pi} + \Delta\mathbf{I}) : \nabla\mathbf{u} + \frac{2}{3}\gamma' p\nabla\cdot\mathbf{u} = -\frac{2}{3}\gamma'\frac{p}{\mu_b}\Delta q_{2nd}(\kappa)$
$\mathbf{Q}$	$\mathbf{Q} = -k\nabla T$	$\mathbf{\Pi}\cdot\nabla(C_pT) + (p+\Delta)\nabla(C_pT) = -\frac{pC_p}{k}\mathbf{Q}q_{2nd}(\kappa)$
$\mathbf{Q}_v$	$\mathbf{Q}_v = -k_v\nabla T_v$	$\mathbf{\Pi}\cdot\nabla(C_{p,v}T_v) + (p+\Delta)\nabla(C_{p,v}T_v) = -\frac{pC_{p,v}}{k_v}\mathbf{Q}q_{2nd}(\kappa)$
$q(\kappa)$	$q_{1st}(\kappa) = 1$	$q_{2nd}(\kappa) = \frac{\sinh\kappa}{\kappa}$

PoF 2020b

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

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

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

JCP 2022

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

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

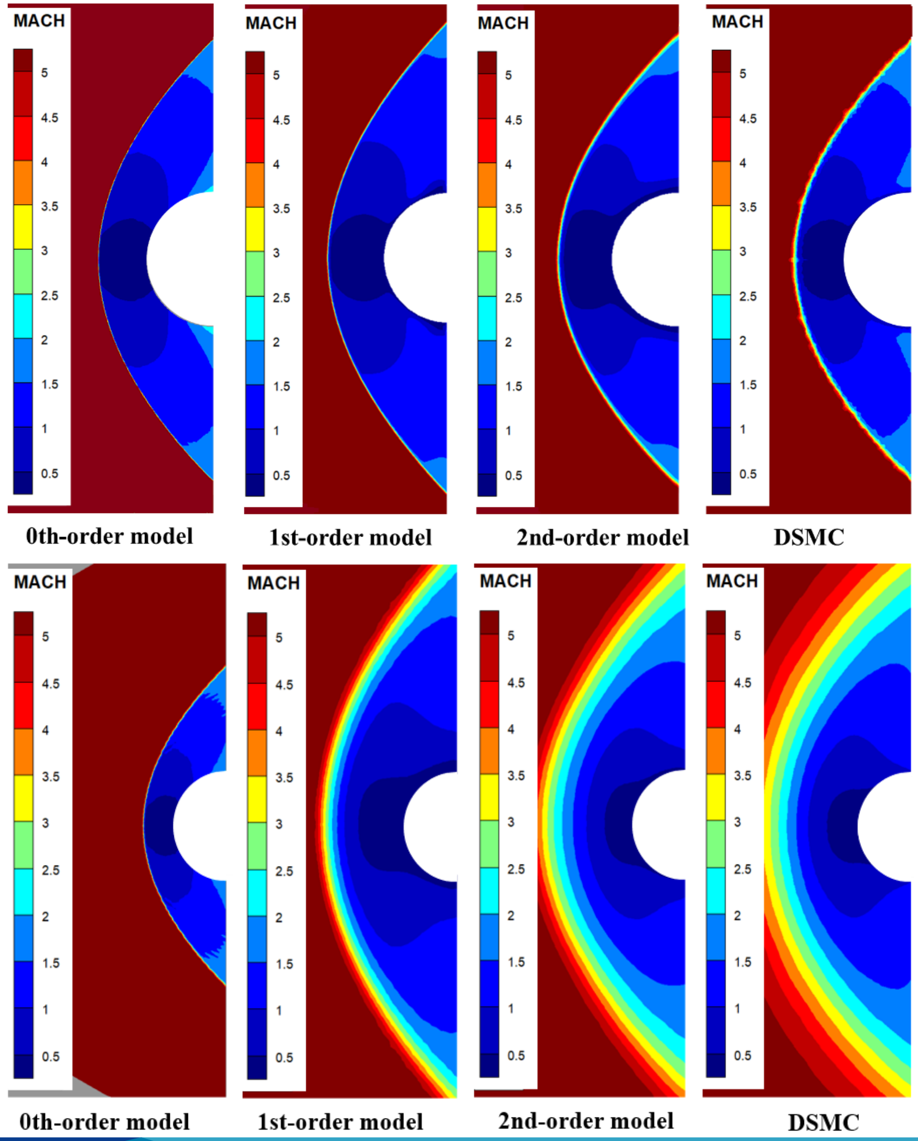
NCCR: Nonlinear Coupled Constitutive Relation

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

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

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

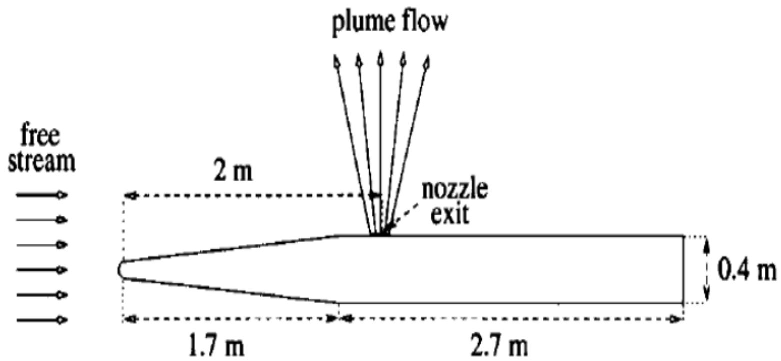
Knudsen 0.02

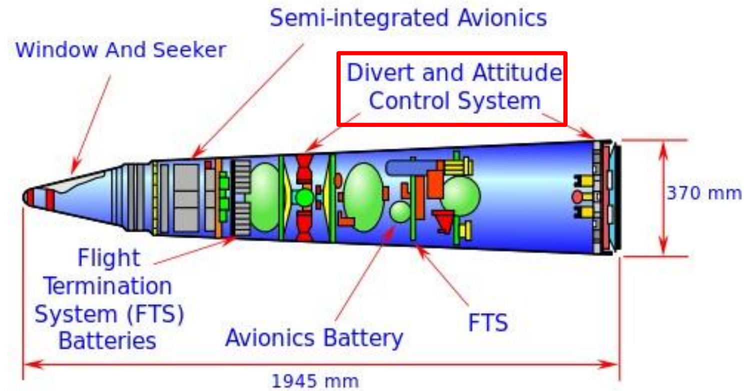
Argon gas

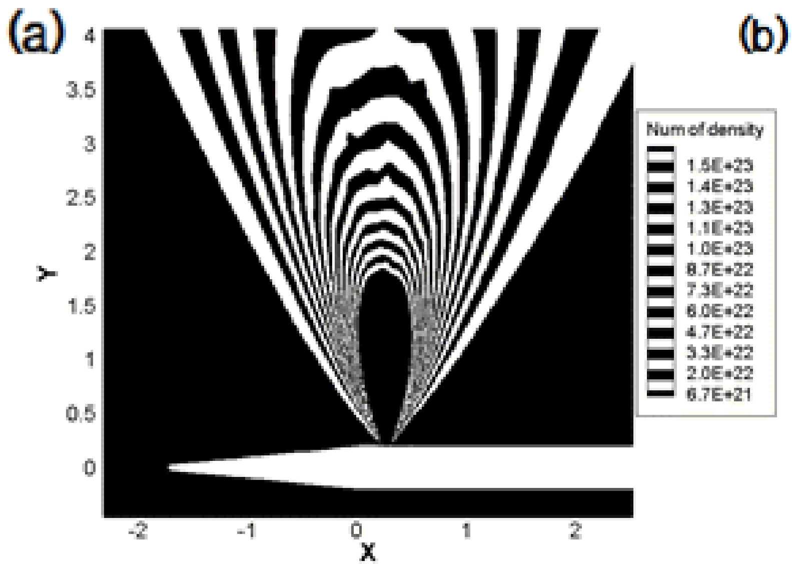
Mach 5.48

Knudsen 0.2

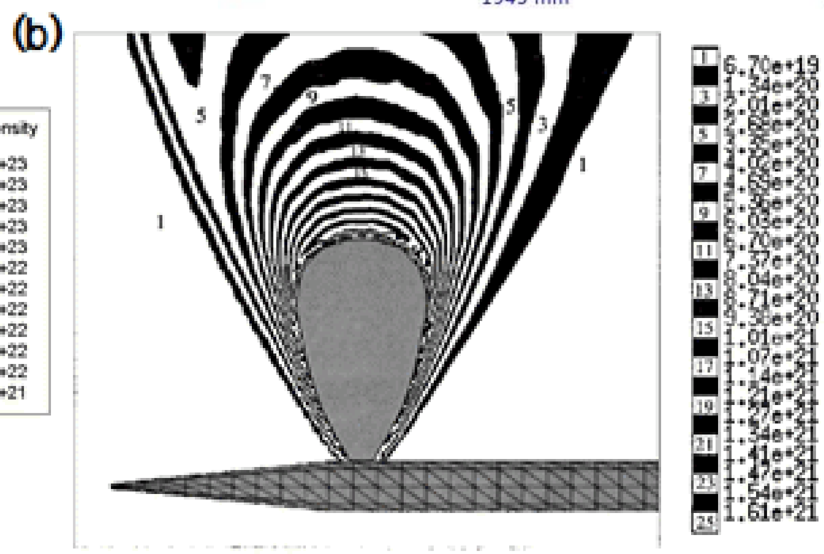
A body with side-jet: DACS (Divert Attitude Control System)







NCCR-DG

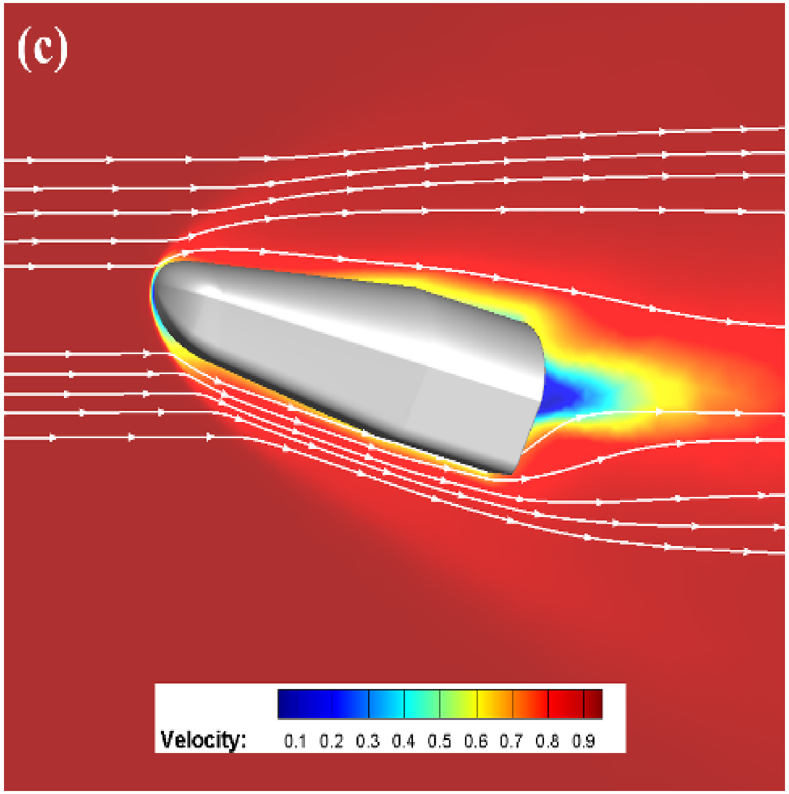


DSMC

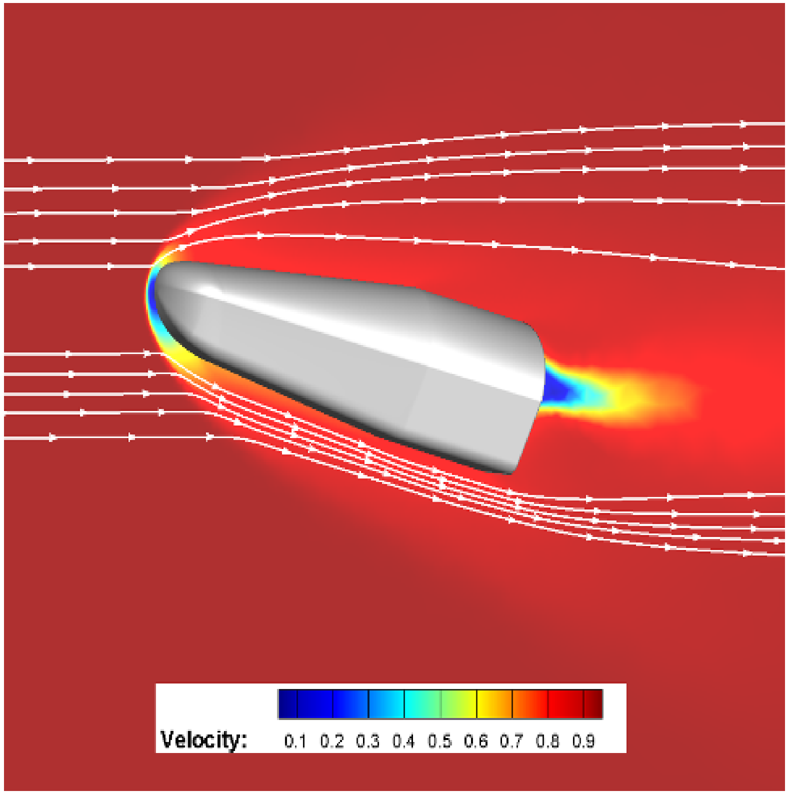
Number of density contour (nitrogen gas, velocity=2km/s, Knudsen=0.1)

Full 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

Concluding remarks and thanks

Non-classical flow physics including mixture, chemical reaction and radiation modeling
Extension to multi-phase flow problems
Aerothermodynamic data for design and control
More accessible (via OpenFOAM of NCCR-FVM) and efficient computational algorithms
Combination with machine learning and quantum computing

Pushing the Limits of Traditional Aerodynamics and Going Beyond the Navier-Stokes-Fourier!