Physics of polyatomic gases in nonequilibrium based on the second-order Boltzmann-type kinetic theory

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Rho Shin Myong

Department of Aerospace and Software Engineering Research Center for Aircraft Core Technology Gyeongsang National University South Korea

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Research Center for Aircraft Core Technology



Part I

2nd-order Boltzmann-type kinetic theory: Boltzmann-based gas dynamics (BGD):

Part II

2nd-order constitutive laws for polyatomic gases

Physics of polyatomic gases in non-equilibrium via

- Topological representation of constitutive laws
- Multi-dimensional flow fields obtained by CFD based on discontinuous Galerkin method

2nd-order Boltzmann-type kinetic theory

- PoF 1999, JCP 2001, JCP 2004: Eu's generalized hydrodynamics
- PoF 2014, PoF 2016: Balanced closure & validation via MD
- PoF 2018: Polyatomic gases (shock-vortex interaction)

Conceptual revision New closure theory Physical insight More validation Discontinuous Galerkin

- Basic information can be found in the Youtube of an Indian GIAN (Global Initiative Academic Networks) Lecture (2017; IIT Kanpur; 15 Lectures)
- Rarefied & Microscale Gases and Viscoelastic Fluids: A Unified Framework
- https://www.youtube.com/ and search "Rarefied & Microscale Gases"
- Other independent NCCR works: Multi-species extension by Ahn & Kim (SNU, Korea, JCP09) Implicit-FVM implementation by Jiang & Zhao (Zhejiang Univ., China, 2017)
- Cf. NCCR: Nonlinear Coupled Constitutive Relation

Closure-last moment method $\rho \mathbf{u} = \iiint m \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) dv_x dv_y dv_z$

Molecular		Continuum		Molecular			Continuum	
Pure (or Semi-) Simulation				PDE-based Approach				
MD	DSMC	Gas- Kinetic	LBM	Liouville Equation	Boltzmann and	Method of	Chapman- Enskog	NSF
		Scheme			Simplified	Moments	and	
					Boltzmann		Burnett	
Microscopic Mesoscopic Macroscopic				Microscopic	Mesoscopic		Macroscopic	

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 approach: Eu's generalized hydrodynamics (1980) based on

Eu's closure & equation of transfer

NCCR (2014) based on balanced closure & equation of transfer

Boltzmann transport equation (BTE)

• A first-order partial differential equation with an integral collision term

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

Movement Collision (or Interaction)

Kinematic Dissipation

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

= 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 $h^{(n)}$

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

Complexity out of simplicity: conservation laws

 $\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(t, \mathbf{r}, \mathbf{v}) = C[f, f_2] \qquad \qquad \rho \mathbf{u} = \langle m \mathbf{v} f(t, \mathbf{r}, \mathbf{v}) \rangle$ where $\langle \cdots \rangle = \iiint \cdots dv_x dv_y dv_z$

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

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

$$[\mathbf{A}]^{(2)}: \text{ Traceless symmetric}$$
Here $-\left\langle m(\mathbf{v}\cdot\nabla f)\mathbf{v} \right\rangle = -\nabla \cdot \left\langle m\mathbf{v}\mathbf{v}f \right\rangle = -\nabla \cdot \left\{ \rho\mathbf{u}\mathbf{u} + \left\langle m\mathbf{c}\mathbf{c}f \right\rangle \right\}$

$$[\mathbf{A}]^{(2)}: \text{ Traceless symmetric}$$

$$part of \text{ tensor } \mathbf{A}$$

After the decomposition of the stress into pressure and viscous shear stress $\mathbf{\Pi}$ $\mathbf{P} \equiv \langle m\mathbf{cc}f \rangle = p\mathbf{I} + \mathbf{\Pi}$ where $p \equiv \langle m\mathbf{Tr}(\mathbf{cc})f/3 \rangle$, $\mathbf{\Pi} \equiv \langle m[\mathbf{cc}]^{(2)}f \rangle$,

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

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot \left(\rho \mathbf{u} \mathbf{u} + p \mathbf{I} + \mathbf{I}\right) = \mathbf{0}.$$
 Exact consequence of the original BTE!

Further complexity: constitutive equations

For arbitrary molecular expressions of general moment (viscous shear stress Π and heat flux Q)

$$\rho \frac{D}{Dt} \begin{bmatrix} \mathbf{\Pi} \left(\equiv \left\langle m [\mathbf{cc}]^{(2)} f \right\rangle \right) / \rho \\ \mathbf{Q} \left(\equiv \left\langle mc^2 \mathbf{c} / 2f \right\rangle \right) / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \left\langle m\mathbf{ccc}f \right\rangle - \left\langle m\mathbf{Tr}(\mathbf{ccc})f \right\rangle \mathbf{I} / 3 \\ \left\langle mc^2 \mathbf{cc}f \right\rangle + \mathbf{I} \end{bmatrix} + \begin{bmatrix} 0 \\ \left\langle m\mathbf{ccc}f \right\rangle : \nabla \mathbf{u} \end{bmatrix} \\ \begin{bmatrix} 2 \left[\mathbf{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} \\ \frac{D\mathbf{u}}{Dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T \end{bmatrix} + \begin{bmatrix} 2p \left[\nabla \mathbf{u} \right]^{(2)} \\ pC_p \nabla T \end{bmatrix} = \begin{bmatrix} \left\langle m [\mathbf{cc}]^{(2)} C[f, f_2] \right\rangle \\ \left\langle (mc^2 / 2 - mC_p T) \mathbf{c} C[f, f_2] \right\rangle \end{bmatrix}$$

No approximation so far: exact consequence of the original BTE via Maxwell's equation of transfer

Balanced closure: constitutive equations

Conceptual inconsistency of Eu's closure (1992)

 $\langle m\mathbf{ccc} f \rangle - \langle m\mathrm{Tr}(\mathbf{ccc}) f \rangle \mathbf{I} / 3 = 0 \implies \text{Vanishing heat flux}$ $\langle m\mathbf{ccc} f \rangle = 0 \implies \text{Cannot be zero in general}$

New balanced closure with closure-last approach (2014)

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

$$\rho \frac{D}{Dt} \begin{bmatrix} \mathbf{\Pi} \left(\equiv \left\langle m [\mathbf{cc}]^{(2)} f \right\rangle \right) / \rho \\ \mathbf{Q} \left(\equiv \left\langle mc^{2}\mathbf{c} / 2f \right\rangle \right) / \rho \end{bmatrix} + \begin{bmatrix} \left\langle m\mathbf{ccc}f \right\rangle - \left\langle m\mathbf{Tr}(\mathbf{ccc})f \right\rangle \mathbf{I} / 3 \\ \left\langle mc^{2}\mathbf{cc}f / 2 \right\rangle - C_{p}T(p\mathbf{I} + \mathbf{\Pi}) \end{bmatrix} + \begin{bmatrix} 0 \\ \left\langle m\mathbf{ccc}f \right\rangle : \nabla \mathbf{u} \end{bmatrix} \\ \begin{bmatrix} 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} \\ \frac{D\mathbf{u}}{Dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_{p}\nabla T \end{bmatrix} + \begin{bmatrix} 2p[\nabla \mathbf{u}]^{(2)} \\ pC_{p}\nabla T \end{bmatrix} = \begin{bmatrix} \left\langle m[\mathbf{cc}]^{(2)} C[f, f_{2}] \right\rangle \\ \left\langle \left(mc^{2} / 2 - mC_{p}T\right)\mathbf{c}C[f, f_{2}] \right\rangle \end{bmatrix}$$

2nd-order closure

Conservation laws + 2nd-order constitutive relations

Conservation laws (exact consequence of BTE)

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

Hyperbolic (inviscid)

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

$$\rho \frac{D(\widehat{\Pi} \not/ \rho)}{Dt} + 2 \left[\Pi \cdot \nabla \mathbf{u} \right]^{(2)} + 2 p \left[\nabla \mathbf{u} \right]^{(2)} = -\frac{p}{\mu_{NS}} \Pi q_{2nd}(\kappa_1),$$

$$\rho \frac{D(\widehat{\mathbf{Q}} \not/ \rho)}{Dt} + \frac{D\mathbf{u}}{Dt} \cdot \Pi + \mathbf{Q} \cdot \nabla \mathbf{u} + \Pi \cdot C_p \nabla T + C_p p \nabla T = -\frac{pC_p}{k_{NS}} \mathbf{Q} q_{2nd}(\kappa_1),$$
Non-hyperbolic
mplicit
$$q_{2nd}(\kappa_1) \equiv \frac{\sinh \kappa_1}{\kappa_1}, \ \kappa_1 \equiv \frac{T^{1/4}}{p} \left(\frac{\Pi : \Pi}{\mu_{NS}} + \frac{\mathbf{Q} \cdot \mathbf{Q} / T}{k_{NS}} \right)^{1/2}$$

2nd-order theory in elementary flows



- Critical role of $q_{2nd}(\kappa_1)$ term in compression case
- Negligible role of $q_{2nd}(\kappa_1)$ term in expansion & velocity shear (simple shear thinning decreasing viscosity)

A model for 1-D compression & expansion

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2nd-order constitutive laws in compression/expansion



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1-D shock result: inverse shock thickness



Shock density thickness of argon gas

Shock temperature-density distance

(Karchani, PhD Thesis, GNU, 2017)

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2nd-order constitutive laws in velocity shear



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Multi-dimensional CFD based on DG

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Two-dimensional shock structure around cylinder



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

NCCR: Nonlinear Coupled Constitutive Relation

(Karchani, PhD Thesis, GNU, 2017)

Monatomic, diatomic, and (linear) polyatomic gases



 Once the Stokes assumption is abandoned, an additional constitutive law of the excess normal stress ∆ related to the bulk viscosity will appear

$$\Delta = \mu_b (\Delta \cdot \boldsymbol{u}).$$

- The inner structure of strong shock waves (Emanuel and Argrow 1994)
- Dilatational waves in transition in hypersonic boundary layers (Zhu et al. 2016)

Monatomic, diatomic, and (linear) polyatomic gases



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Boltzmann-Curtiss equation for polyatomic gases

$$\begin{pmatrix} \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla + \frac{j}{l} \frac{\partial}{\partial \psi} \end{pmatrix} f(\mathbf{v}, \mathbf{r}, \mathbf{j}, \psi, t) = C[f, f_2]$$

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

$$I = \text{moment of inertia}$$

$$\mathbf{j} = \text{angular momentum}$$

$$\psi = \text{azimuthal angle}$$

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

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2nd-order constitutive relations for polyatomic gases

$$\begin{aligned} \mathbf{\Pi} &= \left\langle h^{(1)} f \right\rangle \quad h^{(1)} = m \left[\mathbf{cc} \right]^{(2)} \\ \Delta &= \left\langle h^{(2)} f \right\rangle \quad h^{(2)} = mc^2 / 3 - p / n \\ \mathbf{Q} &= \left\langle h^{(3)} f \right\rangle \quad h^{(3)} = \left[mc^2 / 3 + H_{rot} - m\hat{h} \right] \mathbf{c} \\ \mathbf{2^{nd} - order} & \mathbf{1st-order} \\ \begin{bmatrix} \mathbf{\hat{\Pi}} \cdot \nabla \hat{\mathbf{u}} \end{bmatrix}^{(2)} + \left(f_b \hat{\Delta} + 1 \right) \hat{\mathbf{\Pi}}_{NF} = \hat{\mathbf{\Pi}} q_{2nd} (c\hat{R}) \\ \frac{3}{2} f_b \left(\hat{\mathbf{\Pi}} + f_b \hat{\Delta} \mathbf{I} \right) : \nabla \hat{\mathbf{u}} + \hat{\Delta}_{NF} = \hat{\Delta} q_{2nd} (c\hat{R}) \\ \hat{\mathbf{\Pi}} \cdot \hat{\mathbf{Q}}_{NS} + \left(f_b \hat{\Delta} + 1 \right) \hat{\mathbf{Q}}_{NF} = \hat{\mathbf{Q}} q_{2nd} (c\hat{R}) \\ \hat{\mathbf{\Pi}} \cdot \hat{\mathbf{Q}}_{NS} + \left(f_b \hat{\Delta} + 1 \right) \hat{\mathbf{Q}}_{NF} = \hat{\mathbf{Q}} q_{2nd} (c\hat{R}) \end{aligned}$$

Topological representation of constitutive relations is possible!

Topology of 2nd-order CR (compression/expansion)



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Topology of 2nd-order CR (compression/expansion)



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Trajectory of shock structure in topology of CR



Mach number = 5.0

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Inverse density thickness of shock wave (nitrogen)



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Multi-dimensional case: shock-vortex interaction



Talk 24/27

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Multi-dimensional case: shock-vortex interaction

Shock Mach = 2.0 Vortex Mach = 0.8 Knudsen = 0.001



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Multi-dimensional case: shock-vortex interaction



Effects of diatomic and polyatomic gases on macro SVI with $M_s = 2.0, M_v = 0.8, r_1 = 1000\lambda$ (top) and micro SVI with $M_s = 2.0, M_v = 0.8, r_1 = 10\lambda$ (bottom): sound pressure at t = 1000 ns.

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Dusty gas flows in Lunar landing



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