

**GIAN Course on
Rarefied & Microscale Gases and Viscoelastic Fluids:
a Unified Framework**

**Lecture 7
Method of Moment, 2nd Law of
Thermodynamics, Cumulant Expansion,
and Balanced Closure**

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Content

I. Method of moment

II. 2nd law of thermodynamics

III. Cumulant expansion

IV. Balanced closure

I. Method of moment

Boltzmann transport equation (BTE): 10²³

$f(t, \mathbf{r}, \mathbf{v})$

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

**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



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

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

Enormous reduction of information

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

Conservation laws & constitutive equations: 13

$(\rho, \mathbf{u}, T, \mathbf{\Pi}, \mathbf{Q}, \dots)(t, \mathbf{r})$

I. Method of moment

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

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 $\mathbf{v} = \mathbf{u} + \mathbf{c}$)

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

$$\text{Here } - \langle m (\mathbf{v} \cdot \nabla f) \mathbf{v} \rangle = - \nabla \cdot \langle m \mathbf{v} \mathbf{v} f \rangle = - \nabla \cdot \{ \rho \mathbf{u} \mathbf{u} + \langle m \mathbf{c} \mathbf{c} f \rangle \}$$

After the decomposition of the stress

$$\mathbf{P} \equiv \langle m \mathbf{c} \mathbf{c} f \rangle = p \mathbf{I} + \mathbf{\Pi} \text{ where } p \equiv \langle m \text{Tr}(\mathbf{c} \mathbf{c}) f / 3 \rangle, \mathbf{\Pi} \equiv \langle m [\mathbf{c} \mathbf{c}]^{(2)} f \rangle,$$

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

we have

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

I. Method of moment

The same for the heat flux, $\mathbf{Q} \equiv \langle mc^2 \mathbf{c} f / 2 \rangle$, with the derivation of the energy conservation law.

In fact, this procedure can be generalized for arbitrary molecular expressions of general moment $h^{(n)}$

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

For $h^{(1)} = [m\mathbf{c}\mathbf{c}]^{(2)}$, the constitutive equation of the viscous shear stress $\mathbf{\Pi} \equiv \langle m[\mathbf{c}\mathbf{c}]^{(2)} f \rangle$

$$\rho \frac{d(\mathbf{\Pi} / \rho)}{dt} + \nabla \cdot \mathbf{\Psi}^{(\mathbf{\Pi})} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \langle h^{(1)} C[f, f_2] \rangle,$$

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

Again exact consequence of BTE

No approximation introduced so far!

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

For $h^{(3)} = (mc^2 / 2 - mC_p T) \mathbf{c}$, the constitutive equation of the heat flux $\mathbf{Q} \equiv \langle mc^2 \mathbf{c} f / 2 \rangle$

(assuming $\mathbf{J} \equiv \langle m \mathbf{c} f \rangle = 0$ in monatomic gas)

$$\rho \frac{d(\mathbf{Q} / \rho)}{dt} + \nabla \cdot \Psi^{(Q)} + \langle m \mathbf{c} \mathbf{c} \mathbf{c} f \rangle \cdot \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T + p C_p \nabla T$$

$$= \langle h^{(3)} C[f, f_2] \rangle, \quad \Psi^{(Q)} \equiv \langle mc^2 \mathbf{c} \mathbf{c} f / 2 \rangle - C_p T (p \mathbf{I} + \mathbf{\Pi}).$$

Again no approximation!

This critical fact can not be found on codified textbooks!

This constitutive equation was not presented in Grad's 1949 work, since his 13-moment closure was already in place. In fact, to the best of my knowledge, it was never derived explicitly until B. C. Eu (1992).

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In the derivation of constitutive equation of heat flux, the following relations are used

$$\langle h^{(3)} f \rangle = \mathbf{Q} - C_p T \mathbf{J},$$

$$\langle \mathbf{c} h^{(3)} f \rangle = \langle \mathbf{c} (mc^2 / 2 - m C_p T) \mathbf{c} f \rangle = \langle mc^2 \mathbf{c} \mathbf{c} f / 2 \rangle - C_p T \mathbf{P},$$

$$\begin{aligned} \left\langle f \frac{\partial}{\partial t} h^{(3)} \right\rangle &= \left\langle f \frac{\partial}{\partial t} (mc^2 \mathbf{c} / 2) \right\rangle - \left\langle f \frac{\partial}{\partial t} (C_p T) m \mathbf{c} \right\rangle - \left\langle m f C_p T \frac{\partial \mathbf{c}}{\partial t} \right\rangle = -\frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{P} - \rho E \mathbf{I} \cdot \frac{\partial \mathbf{u}}{\partial t} \\ &\quad - \mathbf{J} \frac{\partial}{\partial t} (C_p T) + \rho C_p T \frac{\partial \mathbf{u}}{\partial t} = -\frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{\Pi} - \mathbf{J} \frac{\partial}{\partial t} (C_p T), \end{aligned}$$

$$\begin{aligned} \langle \mathbf{f} \mathbf{u} \cdot \nabla h^{(3)} \rangle &= \langle \mathbf{f} \mathbf{u} \cdot \nabla (mc^2 \mathbf{c} / 2) \rangle - \langle m \mathbf{f} \mathbf{u} \cdot \nabla (C_p T \mathbf{c}) \rangle = \langle f m c^2 \mathbf{u} \cdot \nabla \mathbf{c} / 2 \rangle + \langle f m (\mathbf{u} \cdot \nabla c^2) \mathbf{c} / 2 \rangle \\ &\quad - \langle m \mathbf{f} (\mathbf{u} \cdot \nabla C_p T) \mathbf{c} \rangle - \langle m \mathbf{f} C_p T \mathbf{u} \cdot \nabla \mathbf{c} \rangle = -\rho E \mathbf{u} \cdot \nabla \mathbf{u} - \mathbf{u} \cdot \nabla \mathbf{u} \cdot \mathbf{P} - \mathbf{J} (\mathbf{u} \cdot \nabla C_p T) + \rho C_p T \mathbf{u} \cdot \nabla \mathbf{u}, \end{aligned}$$

$$\begin{aligned} \langle \mathbf{f} \mathbf{c} \cdot \nabla h^{(3)} \rangle &= \langle \mathbf{f} \mathbf{c} \cdot \nabla (mc^2 \mathbf{c} / 2) \rangle - \langle m \mathbf{f} \mathbf{c} \cdot \nabla (C_p T \mathbf{c}) \rangle = \langle f m c^2 \mathbf{c} \cdot \nabla \mathbf{c} / 2 \rangle + \langle f m (\mathbf{c} \cdot \nabla c^2) \mathbf{c} / 2 \rangle \\ &\quad - \langle m \mathbf{f} (\mathbf{c} \cdot \nabla C_p T) \mathbf{c} \rangle - \langle m \mathbf{f} C_p T \mathbf{c} \cdot \nabla \mathbf{c} \rangle = -\mathbf{Q} \cdot \nabla \mathbf{u} - \psi^{(P)} \cdot \nabla \mathbf{u} - \mathbf{P} \cdot \nabla C_p T + C_p T \mathbf{J} \cdot \nabla \mathbf{u}, \end{aligned}$$

$$\psi^{(P)} \equiv \langle m \mathbf{c} \mathbf{c} \mathbf{c} f \rangle, \quad \rho E \equiv \langle mc^2 f / 2 \rangle, \quad C_p T = p / \rho + E, \quad \mathbf{P} = p \mathbf{I} + \mathbf{\Pi}.$$

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An alternative form of (13) is

$$\begin{aligned}
 (5.15) \quad & \frac{\partial p_{ij}}{\partial t} + \frac{\partial}{\partial x_r} (u_r p_{ij}) + \frac{\partial S_{ijr}}{\partial x_r} - \frac{1}{3} \delta_{ij} \frac{\partial S_r}{\partial x_r} \\
 & + p_{ir} \frac{\partial u_j}{\partial x_r} + p_{jr} \frac{\partial u_i}{\partial x_r} - \frac{2}{3} \delta_{ij} p_{rs} \frac{\partial u_r}{\partial x_s} \\
 & + p \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_r}{\partial x_r} \right) = \bar{J}_{ij}^{(2)}.
 \end{aligned}$$

The moment equations (13), (14), and (15) are exact; to reduce them to third order, Q_{ijk} must be replaced by its third order equivalent from $a_{ijk}^{(4)} = 0$ (cf. equation (4.11)),

$$\begin{aligned}
 (5.16) \quad Q_{ijk} &= RT(p_{ij} \delta_{kr} + p_{ik} \delta_{jr} + p_{ir} \delta_{jk} + p_{jk} \delta_{ir} + p_{jr} \delta_{ik} + p_{kr} \delta_{ij}) \\
 &+ pRT(\delta_{ij} \delta_{kr} + \delta_{ik} \delta_{jr} + \delta_{ir} \delta_{jk});
 \end{aligned}$$

also, $\bar{J}_{ij}^{(2)}$ and $\bar{J}_{ijk}^{(3)}$ are replaced by their values from equation (4.32) and the approximation (11). Adding the conservation equations for completeness, we have the system

$$\left\{ \begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_r} (\rho u_r) &= 0 \\
 \frac{\partial u_i}{\partial t} + u_r \frac{\partial u_i}{\partial x_r} + \frac{1}{\rho} \frac{\partial P_{ir}}{\partial x_r} &= 0 \\
 \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_r} (u_r p) + \frac{2}{3} P_{ir} \frac{\partial u_i}{\partial x_r} + \frac{1}{3} \frac{\partial S_r}{\partial x_r} &= 0
 \end{aligned} \right.$$

I. Method of moment

which, when averaged over velocity, yield the traceless part of the stress tensor, its excess trace part, the heat flux, the diffusion flux, and so on. We will denote them by the symbol $\Phi_i^{(\alpha)}$:

$$\Phi_i^{(\alpha)} = \langle h_i^{(\alpha)} f_i(\mathbf{v}_i, \mathbf{r}; t) \rangle, \quad (10.128)$$

where $\alpha = 1, 2, 3, 4, \dots$ and $i = 1, 2, \dots, r$. The meaning of a few leading $\Phi_i^{(\alpha)}$ is as follows:

$$\begin{aligned} \Phi_i^{(1)} &= \Pi_i = [\mathbf{P}_i]^{(2)}, & \Phi_i^{(2)} &= \Delta_i = \frac{1}{2} \text{Tr } \mathbf{P}_i - p_i, \\ \Phi_i^{(3)} &= \mathbf{Q}_i = \mathbf{Q}_i - \hat{h}_i J_i, & \Phi_i^{(4)} &= J_i, \text{ etc.} \end{aligned}$$

In the case of dilute gases $\Delta = \sum_i \Delta_i = 0$ for the reason that $p = \text{Tr } \mathbf{P}/3$ as is clear from (10.55), but we keep the term for generality's sake. Although a little repetitive, we list the set of relevant evolution equations in one place:

$$\frac{\partial}{\partial t} \rho = -\nabla \cdot \rho \mathbf{u} \text{ or } \rho \frac{d\mathbf{v}}{dt} = \nabla \cdot \mathbf{u}, \quad v = 1/\rho, \quad (10.129a)$$

$$\rho \frac{d}{dt} c_i = -\nabla \cdot \mathbf{J}_i, \quad (10.129b)$$

$$\rho \frac{d}{dt} \mathbf{u} = -\nabla \cdot \mathbf{P} + \rho \mathbf{E}, \quad (10.129c)$$

$$\rho \frac{d}{dt} \mathcal{E} = -\nabla \cdot \mathbf{Q} - \mathbf{P} : \nabla \mathbf{u} + \sum_{i=1}^r \mathbf{F}_i \cdot \mathbf{J}_i, \quad (10.129d)$$

$$\rho \frac{d}{dt} \hat{\Phi}_i^{(\alpha)} = Z_i^{(\alpha)} + \Lambda_i^{(\alpha)}, \quad (10.129e)$$

where

$$\begin{aligned} \hat{\mathbf{P}} &= (p + \Delta) \hat{\delta} + \hat{\Pi}, \\ \hat{\Phi}_i^{(\alpha)} &= \Phi_i^{(\alpha)} / \rho, \\ \Lambda_i^{(\alpha)} &= \sum_{j=1}^r \langle h_i^{(\alpha)} C(f_i, f_j) \rangle, \end{aligned} \quad \text{Compare with (10.91-93)} \quad (10.130)$$

$$Z_i^{(\alpha)} = -\nabla \cdot \langle \mathcal{E}_i h_i^{(\alpha)} f_i \rangle + \langle f_i (d_i + \mathcal{E}_i \cdot \nabla + \mathbf{F}_i \cdot \nabla_{v_i}) h_i^{(\alpha)} \rangle \quad (10.131b)$$

and other symbols are defined in the previous sections. Explicit forms for $Z_i^{(\alpha)}$ are summarized in Table 10.1.

We have seen that owing to the H theorem the equilibrium distribution function has been uniquely determined as an equilibrium solution of the Boltzmann equation, and the parameters therein are identified with the equilibrium temperature, density, and chemical potential in the spirit of the Gibbs ensemble theory. As in the Chapman-Enskog and the conventional moment method, in the modified moment method the nonequilibrium distri-

$$\begin{aligned} \Delta_\rho &= -\gamma \nabla \cdot \hat{\mathbf{u}} \\ \hat{\mathbf{u}} &= -2\eta \nabla \hat{\mathbf{u}}^{(2)}, \quad \frac{\eta}{\gamma} = 0.8 \text{ for He} \end{aligned}$$

(constant temp, Lythell 1956, Vincenti p 412)

TABLE 10.1 Kinematic Terms* $Z_i^{(\alpha)}$ in the Presence of Electromagnetic Fields

α	Kinematic Terms
1	$-\nabla \cdot \psi_i^{(1)} - 2[(d_i \mathbf{u} - \mathbf{F}_i) \cdot \mathbf{J}_i]^{(2)} + 2[\Pi_i \cdot \boldsymbol{\gamma}]^{(2)} + [\Pi_i \cdot \boldsymbol{\omega}_{\text{eff}}] + 2\Delta_i \boldsymbol{\gamma}$ $-\frac{2}{3} \Pi_i \nabla \cdot \mathbf{u} + 2\rho_i \boldsymbol{\gamma}$ $-2 \int \hat{\mathbf{u}} \cdot \nabla \hat{\mathbf{u}}^{(2)}$
2	$-\nabla \cdot \psi_i^{(2)} - \frac{2}{3}(d_i \mathbf{u} - \mathbf{F}_i) \cdot \mathbf{J}_i + \frac{2}{3} \Pi_i \cdot \boldsymbol{\gamma} - \frac{2}{3} \Delta_i \nabla \cdot \mathbf{u} - \rho_i d_i \ln(p_i v_i^{2/3}) - \nabla \cdot (\mathbf{J}_i \rho_i / \rho)$
3	$-\nabla \cdot \psi_i^{(3)} - (d_i \mathbf{u} - \mathbf{F}_i) \cdot (\mathbf{P}_i - \rho_i \mathbf{U}) + \mathbf{Q}_i \cdot (\boldsymbol{\gamma} + \boldsymbol{\omega}_{\text{eff}} - \frac{1}{2} \mathbf{U} \nabla \cdot \mathbf{u})$ $+ \phi_i^{(3)} (\boldsymbol{\gamma} - \boldsymbol{\omega}_{\text{eff}} - \frac{1}{2} \mathbf{U} \nabla \cdot \mathbf{u}) - \mathbf{J}_i \cdot d_i \hat{\mathbf{h}}_i - \mathbf{P}_i \cdot \nabla \hat{\mathbf{h}}_i$ $\nabla \hat{\mathbf{u}} = -\boldsymbol{\gamma} - \hat{\mathbf{u}} + \frac{1}{2} \nabla \hat{\mathbf{u}} \cdot \hat{\mathbf{u}}$
4	$-\nabla \cdot \mathbf{P}_i - \rho_i (d_i \mathbf{u} - \mathbf{F}_i) + \mathbf{J}_i \cdot (\boldsymbol{\gamma} - \frac{1}{2} \mathbf{U} \nabla \cdot \mathbf{u}) + \mathbf{J}_i \cdot \boldsymbol{\omega}_{\text{eff}}$ $\boldsymbol{\gamma} = -\xi [\nabla \mathbf{u}]^{(2)}$

Notation:
 $\mathbf{F}_i = z_i (\mathbf{E} + c^{-1} \mathbf{u} \times \mathbf{B})$ (Lorentz force), $z_i = e_i / m_i$
 $\boldsymbol{\omega}_{\text{eff}} = \frac{1}{2} [\nabla \mathbf{u} - (\nabla \mathbf{u})'] + c^{-1} z_i [\nabla \mathbf{A} - (\nabla \mathbf{A})']$ $\mathbf{A} = \nabla \times \mathbf{B}$
 $[\Pi_i \cdot \boldsymbol{\omega}_{\text{eff}}] = \Pi_i \cdot \boldsymbol{\omega}_{\text{eff}} - \boldsymbol{\omega}_{\text{eff}} \cdot \Pi_i$ $\psi_i^{(2)} = \langle \hat{\mathbf{C}}_i h_i \psi_i \rangle$
 $\phi_i^{(3)} = \langle m_i \mathcal{E}_i \mathcal{E}_i f_i \rangle$

*Note: For dilute monatomic gases the case of $\alpha = 2$ does not appear since $\Delta_i = 0$ identically. The kinematic terms given here are in the corotating frame, that is, the sign of the terms $[\Pi_i \cdot \boldsymbol{\omega}_{\text{eff}}]$, $\mathbf{Q}_i \cdot \boldsymbol{\omega}_{\text{eff}}$, and $\mathbf{J}_i \cdot \boldsymbol{\omega}_{\text{eff}}$ in a fixed coordinate system are changed to the opposite sign in accordance with the rules formulated in by the author; see *J. Chem. Phys.* **82**, 3773 (1985).

tribution function is built on the equilibrium distribution function. But this approach to the nonequilibrium solution of the Boltzmann equation requires an extension of the meanings of the parameters such as the temperature and so on in the equilibrium distribution function into the nonequilibrium domain. The extension is accomplished by the assumption of local equilibrium by which the equilibrium density and temperature in the equilibrium distribution function are interpreted as quantities depending on position and time. This extension is in effect an act of assigning to the equilibrium parameters the nonequilibrium quantities suitably defined as statistical mechanical averages for the nonequilibrium system in question. If this act of assignment is mathematically formalized, it may be represented by the following set of equations:

$$\rho \frac{d(\rho/\rho_e)}{dt} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\hat{\mathbf{u}} \rho) \quad \rho_{ie} = \rho_i, \quad (10.132a)$$

$$\rho_e \mathbf{u} = \rho \mathbf{u}, \quad \rho_e u = \rho u, \quad (10.132b)$$

$$T_e = T \text{ or } \rho_e \mathcal{E}_e = \rho \mathcal{E}, \quad (10.132c)$$

where the symbol $\hat{=}$, borrowed from the computer algorithm language,

I. Method of moment

Finally, the conservation laws and constitutive equations, **all of which are an exact consequence** of the Boltzmann equation

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

$$\rho \frac{d}{dt} \begin{bmatrix} \mathbf{\Pi} / \rho \\ \mathbf{Q} / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(Q)} + \psi^{(P)} : \nabla \mathbf{u} \end{bmatrix} + \begin{bmatrix} 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} \\ \frac{d\mathbf{u}}{dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T \end{bmatrix} + \begin{bmatrix} 2p[\nabla \mathbf{u}]^{(2)} \\ C_p p \nabla T \end{bmatrix} = \begin{bmatrix} \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{\Lambda}^{(Q)} \end{bmatrix}.$$

Key observations: 1) Even though we used various $\langle \dots f \rangle$, f disappeared except for

$\mathbf{\Psi}^{(\Pi)}$ (kinematic high order) and $\mathbf{\Lambda}^{(\Pi)}$ (dissipation)

2) Thus the number of places to close is two, rather one.

Lesson: **Monitor exactly where they go from micro (kinetic) to macro (average)**

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(t, \mathbf{r}, \mathbf{v}) = C[f, f_2] \Rightarrow 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)}$$

I. Method of moment

Let us tackle the dissipation term first, since we cannot get away from it.

$$\Lambda^{(\Pi)} \left(\equiv \left\langle m[\mathbf{cc}]^{(2)} C[f, f_2] \right\rangle \right)$$

But, before we move on, let us **think of what we are trying to do here first**: the seat of energy dissipation coming from the collision integral. Therefore, we might need to recall the 2nd law of thermodynamics (lecture 3)

$$\oint d\Psi = 0 \quad \text{where } \Psi \text{ is calortropy}$$

$d\Psi = T^{-1}(dE + dW) + dN$: extended **nonequilibrium** Gibbs relation

Let us start from the balance equation for the calortropy (nonequilibrium entropy)

$$\rho \hat{\Psi}(\mathbf{r}, t) = -k_B \left\langle \left[\ln f^c(\mathbf{v}, \mathbf{r}, t) - 1 \right] f(\mathbf{v}, \mathbf{r}, t) \right\rangle$$

where f^c the thermodynamic branch of the Boltzmann equation

Memo (a preparation before tackling 2nd law)

Arnold Sommerfeld (1868-1951):

“Thermodynamics is a funny subject. The first time you go through it, you don't understand it at all. The second time you go through it, you think you understand it, except for one or two small points. The third time you go through it, you know you don't understand it, but by that time you are so used to it, it doesn't bother you anymore.”

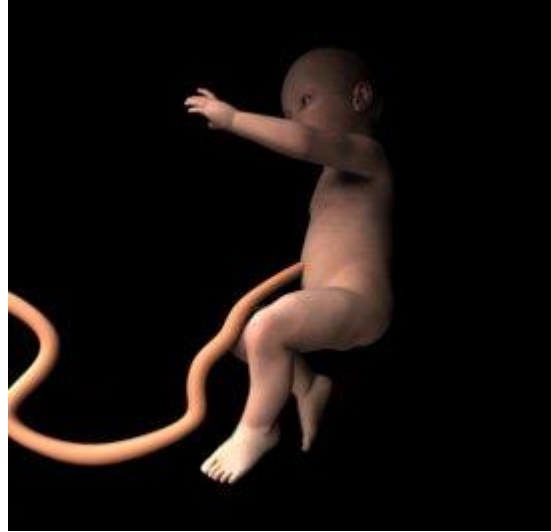
What?

2nd-law?

Why is it anything to do with here?

Is it dead animal?

Memo (a preparation before tackling 2nd law)



Recall lecture 3! Calortropy?

II. 2nd law of thermodynamics

By differentiating the local calortropy density with time and combining it with BTE

$$\rho \frac{d\hat{\Psi}}{dt} + \nabla \cdot \left(-k_B \langle \mathbf{c} (\ln f^c - 1) f \rangle \right) + k_B \left\langle f \left(\frac{d}{dt} + \mathbf{c} \cdot \nabla \right) \ln f^c \right\rangle = \sigma_c \left(\equiv -k_B \langle \ln f^c C[f, f_2] \rangle \right).$$

After assuming $f = f^c$, the positive calortropy production σ_c becomes ($g_{12} \equiv |\mathbf{v} - \mathbf{v}_2|$)

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

Then, if the calortropy production σ_c is worked out first, instead of the dissipation term $\Lambda^{(n)}$ in the conventional approach, and if there is a direct relation between them, a thermodynamically consistent form of $\Lambda^{(n)}$ can be obtained.

From the logarithmic form of the calortropy production, it will be convenient to write the distribution function in the exponential form, instead of Grad's polynomial form;

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

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

II. 2nd law of thermodynamics

In this expression N is the normalization factor, n_d is the number density, and $X^{(n)}$, unknown macroscopic quantities, are the conjugate variables to the molecular expressions for moment, $h^{(n)}$. The advantage of this exponential form is obvious; in the physical sense it is the only form that satisfies the additive property of the calortropy and calortropy production, all of which are in the logarithmic form; in the mathematical sense it assures the non-negativity of the distribution function regardless of the level of approximations. It must also be noted that no finite approximation for moments is made in (3.5); that is, the number of moments goes to infinity as shown in $\sum_{n=1}^{\infty} X^{(n)}h^{(n)}$. This is in contrast with a common practice in considering only the first 13 moments from the outset in the formulation of the theory. After the superscripts c in the distribution function f^c are dropped for simplicity and with a short notation for the exponent, the distribution function can be rewritten

$$f = f^{(0)} \exp(-x), \text{ where } x \equiv \beta \left(\sum_{n=1}^{\infty} X^{(n)}h^{(n)} - N \right). \quad (3.6)$$

With further introduction of notations and dimensionless variables (y being the post-collision value of x),

$$\begin{aligned} x_{12} &= x_1 + x_2, y_{12} = y_1 + y_2 = x_{12}^*, \\ \bar{\sigma}_c &= \frac{\sigma_c}{k_B / g}, g \equiv \frac{1}{n^2 d^2} \sqrt{\frac{m}{2k_B T}}, \\ \bar{b} &= \frac{b}{d}, \bar{g}_{12} = g_{12} \sqrt{\frac{m}{2k_B T}}, \end{aligned} \quad (3.7a)$$

II. 2nd law of thermodynamics

$$\mathbf{w} = \mathbf{c} \sqrt{\frac{m}{k_B T}}, \quad \omega(\mathbf{w}) \equiv \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{1}{2} w^2\right), \quad \omega_{12}(\mathbf{w}, \mathbf{w}_2) \equiv \frac{1}{(2\pi)^3} \exp\left(-\frac{1}{2} w^2 - \frac{1}{2} w_2^2\right),$$

$$\langle A \rangle_c \equiv \int d\hat{\Gamma}_{12} \omega_{12}(\mathbf{w}, \mathbf{w}_2) A(\mathbf{w}, \mathbf{w}_2), \quad (3.7b)$$

$$\int d\hat{\Gamma}_{12} \cdots \equiv \int d\mathbf{w} \int d\mathbf{w}_2 \int_0^{2\pi} d\phi \int_0^\infty d\bar{b} \bar{b} \bar{g}_{12} \cdots,$$

$$\int d\Gamma_{12} \cdots \equiv \int d\mathbf{v} \int d\mathbf{v}_2 \int_0^{2\pi} d\phi \int_0^\infty db b g_{12} \cdots,$$

the calortropy production can be expressed as

$$\begin{aligned} \sigma_c &\equiv -k_B \langle \ln f C[f, f_2] \rangle = \frac{1}{T} \left\langle \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} : h^{(n)} - N \right) C[f^{(0)} \exp(-x), f_2^{(0)} \exp(-x_2)] \right\rangle \\ &= \frac{1}{4} k_B \int d\mathbf{v} \int d\mathbf{v}_2 \int_0^{2\pi} d\phi \int_0^\infty db b g_{12} f^{(0)} f_2^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \quad (3.8) \\ &= \frac{1}{4T} \int d\Gamma_{12} f^{(0)} f_2^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \end{aligned}$$

or

$$\bar{\sigma}_c = \frac{1}{4} \langle (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \rangle_c. \quad (3.9)$$

II. 2nd law of thermodynamics

This form of mathematical equation is suitable for so-called cumulant expansion; from Appendix B, it can be written as

$$\bar{\sigma}_c = \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \quad \text{where } \kappa_1 \equiv \frac{1}{2} \{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2},$$

$$q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) \equiv \frac{1}{2\kappa_1} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(+)} \right] - \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(-)} \right] \right\}. \quad (3.10)$$

Note that this form guarantees the positivity of the calortropy production regardless of the level of approximations. In addition, when the distribution function (3.6) is inserted into the definition of calortropy production, the dissipation term $\Lambda^{(n)}$ is shown to be directly related to the calortropy production σ_c ,

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

$$= \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \langle h^{(n)} C[f, f_2] \rangle = \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)}. \quad (3.11)$$

II. 2nd law of thermodynamics

Now the explicit form of the dissipation term $\Lambda^{(n)}$ can be derived from (3.10) and (3.11) by calculating the first reduced collision integral κ_1 in terms of $X^{(n)}$; since x appearing in κ_1 consists of a sum of various moments, $x \equiv \beta \left(\sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right)$, with the definition $\Delta h^{(n)} = h^{(n)} - h^{(n)*}$, etc., κ_1^2 may be expressed as a quadratic form of X and X_2 ,

$$\kappa_1^2 = \frac{1}{4} \sum_{n,l=1}^{\infty} \left\langle \left(X^{(n)} \Delta h^{(n)} + X_2^{(n)} \Delta h_2^{(n)} \right) \left(X^{(l)} \Delta h^{(l)} + X_2^{(l)} \Delta h_2^{(l)} \right) \right\rangle_c. \quad (3.12)$$

On rearrangement of the terms it may become

$$\kappa_1^2 = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)}, \quad (3.13)$$

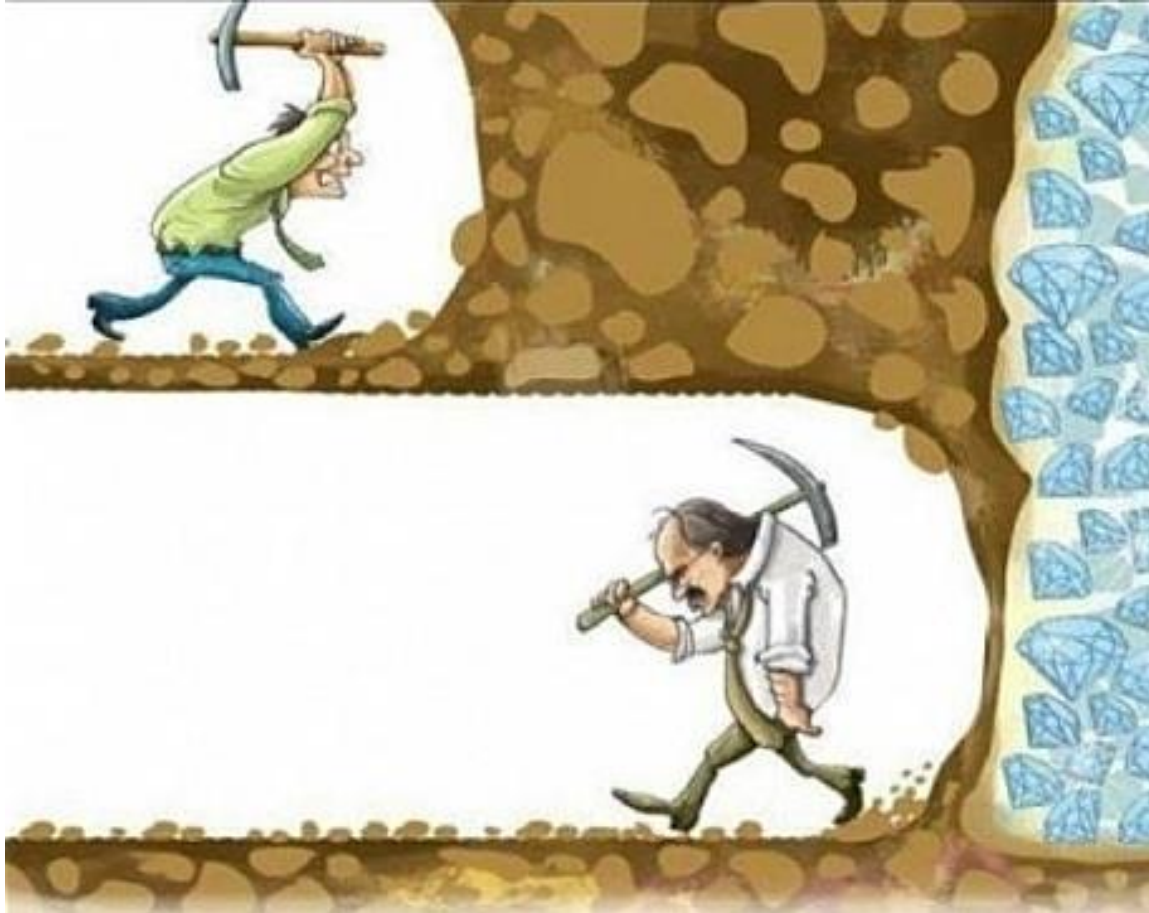
where $R_{12}^{(nl)}$ are scalar coefficients made up of collision bracket integrals of $h^{(n)}$ and $h_2^{(l)}$ for an isotropic system of dilute gases. After comparing (3.10), (3.11) and (3.13),

$$\bar{\sigma}_c = \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) = \beta g \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)} = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \quad (3.14)$$

the following dissipation term can be derived:

$$\Lambda^{(n)} = \frac{1}{\beta g} \sum_{l=1}^{\infty} R_{12}^{(nl)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots). \quad (3.15)$$

II. 2nd law of thermodynamics (???)



Just a little extra push is all it takes!

II. 2nd law of thermodynamics

In the meantime, the unknown conjugate variables $X^{(n)}$, which were first introduced in (3.5) of the distribution function, need to be determined in terms of macroscopic variables, consistent with the laws of thermodynamics. One way to achieve this is to generalize the equilibrium Gibbs ensemble theory—providing the relationship between thermodynamic variables and the partition functions—to nonequilibrium processes. Such nonequilibrium generalization was developed by Eu⁷ and the main result relevant to the present work can be summarized as

$$\langle h^{(n)} f \rangle / \rho = -k_B T \left(\frac{\partial}{\partial X^{(n)}} \ln Z \right), \text{ where } Z \equiv \frac{1}{n_d} \left\langle \exp \left[-\frac{1}{k_B T} \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} \right) \right] \right\rangle. \quad (3.16)$$

Then the $X^{(n)}$ can be determined in terms of the macroscopic flux $\langle h^{(n)} f \rangle$ by solving the differential equation (3.16). The leading order approximate solutions are known to be

$$X^{(1)} = -\frac{\Pi}{2p}, \quad X^{(2)} = -\frac{Q}{pC_p T}. \quad (3.17)$$

Finally, the moment equation for general type of molecules (2.1) can be rewritten as ($n = 2$ for shear stress); *still exact to the original Boltzmann equation*,

$$\rho \frac{d(\Pi/\rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \frac{1}{\beta g} \sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots). \quad (3.18)$$

III. Cumulant expansion

After the canonical distribution function is inserted into the calortropy balance equation, the calortropy production term can be expressed in terms of exponential function as follows:^{6,7}

$$\bar{\sigma}_c \equiv -g \langle \ln f C[f, f_2] \rangle = \frac{1}{4} \langle (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \rangle_c. \quad (\text{B1})$$

This form of mathematical equation is suitable for so-called cumulant expansion. It can further be cast into

$$\bar{\sigma}_c = \frac{1}{4} [R^{(+)}(\lambda) - R^{(-)}(\lambda)]_{\lambda=1}, \quad (\text{B2})$$

$$R^{(+)}(\lambda) \equiv \langle (x_{12} - y_{12}) [\exp(-\lambda y_{12}) - 1] \rangle_c, \quad R^{(-)}(\lambda) \equiv \langle (x_{12} - y_{12}) [\exp(-\lambda x_{12}) - 1] \rangle_c.$$

Here the parameter λ is introduced as a bookkeeping index. After expansion in series of $R^{(\pm)}(\lambda)$, it will be set $\lambda = 1$. A description of the cumulant expansion will be helpful here. Let $f(x)$ be the probability distribution of x . The l th moment of this probability distribution is defined as the expectation value of x^l :

$$\langle x^l \rangle = \int x^l f(x) dx, \quad (\text{B3})$$

and the moment-generated function as the expectation value of $e^{\lambda x}$

$$\langle e^{\lambda x} \rangle = \int f(x) e^{\lambda x} dx. \quad (\text{B4})$$

The following relations hold for the power series and derivatives:

$$\langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \int f(x) x^l dx = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \langle x^n \rangle \text{ or } \langle x^l \rangle = \left[\frac{d^l}{d\lambda^l} \langle e^{\lambda x} \rangle \right]_{\lambda=0}. \quad (\text{B5})$$

The logarithm of the characteristic function is called the cumulant-generating function and its series coefficients $\kappa_l^{(+)}$ in the Taylor expansion for λ are called cumulants of the variable x :

$$\ln \langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \kappa_l^{(+)} \text{ or } \kappa_l^{(+)} = \left[\frac{d^l}{d\lambda^l} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0}. \quad (\text{B6})$$

III. Cumulant expansion

Expressions for cumulants in terms of moments may be obtained directly from the definition and Eq. (B5), for example,

$$\begin{aligned}\kappa_1^{(+)} &= \left[\frac{d}{d\lambda} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[\frac{1}{\langle e^{\lambda x} \rangle} \frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[\frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \langle x \rangle, \\ \kappa_2^{(+)} &= \left[\frac{d^2}{d\lambda^2} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[-\frac{1}{\langle e^{\lambda x} \rangle^2} \left(\frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right)^2 + \frac{1}{\langle e^{\lambda x} \rangle} \frac{d^2}{d\lambda^2} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \langle x^2 \rangle - \langle x \rangle^2, \dots\end{aligned}\quad (\text{B7})$$

It should be noted that $\langle e^{\lambda x} \rangle = 1$ for $\lambda = 0$. Then the relationship between moments and cumulants may be summarized as follows:

$$\langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \langle x^l \rangle = \exp \left[\sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \kappa_l^{(+)} \right]. \quad (\text{B8})$$

When this is applied to $R^{(\pm)}(\lambda)$ in (B2), the following cumulant expansion can be obtained:

$$R^{(\pm)}(\lambda) = \left\{ \langle (x_{12} - y_{12})^2 \rangle_c \right\}^{1/2} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-\lambda)^l}{l!} \kappa_l^{(\pm)} \right] - 1 \right\}. \quad (\text{B9})$$

In this step, since there is a term $(x_{12} - y_{12})$ in (B2), it is convenient to introduce a pre-factor $\left\{ \langle (x_{12} - y_{12})^2 \rangle_c \right\}^{1/2}$ in the front and then define subsequent cumulants. With such a factor the cumulants are constructed systematically by expansion and the resulting leading (1st-mean, 2nd-variance, 3rd-skewness) cumulants $\kappa_{1,2,3}^{(\pm)}$ are given by the moments of reduced collision integrals $\kappa_{1,2,3}$

$$\kappa_1^{(\pm)} = \mp \kappa_1, \kappa_2^{(\pm)} = \mp \frac{\kappa_2}{\kappa_1} - \kappa_1^2, \kappa_3^{(\pm)} = \mp \frac{\kappa_3}{\kappa_1} - 3\kappa_2 \mp 2\kappa_1^3, \quad (\text{B10})$$

where

$$\kappa_1 = \frac{1}{2} \left\{ \langle (x_{12} - y_{12})^2 \rangle_c \right\}^{1/2}, \kappa_2 = \frac{1}{4} \left\{ \langle (x_{12} - y_{12})(x_{12}^2 - y_{12}^2) \rangle_c \right\}, \kappa_3 = \frac{1}{4} \left\{ \langle (x_{12} - y_{12})(x_{12}^3 - y_{12}^3) \rangle_c \right\}. \quad (\text{B11})$$

III. Cumulant expansion

The cumulant expansion may be regarded as a partial resummation of the expansion of the Boltzmann collision integral in a series of the parameter $\text{Kn} \cdot M$, and as such, it takes into account highly nonlinear irreversible processes to infinite order. Finally, the calortropy production can be written as

$$\begin{aligned}\bar{\sigma}_c &= \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \\ \kappa_1 &\equiv \frac{1}{2} \left\{ \langle (x_{12} - y_{12})^2 \rangle_c \right\}^{1/2}, \\ q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) &= \frac{1}{2\kappa_1} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(+)} \right] - \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(-)} \right] \right\}.\end{aligned}\tag{B12}$$

Using three leading cumulants given in (B11) the expanded form can be expressed as

$$\begin{aligned}\bar{\sigma}_c &= \frac{\kappa_1}{2} \left\{ \exp \left[\kappa_1 - \frac{1}{2} \left(\frac{\kappa_2}{\kappa_1} + \kappa_1^2 \right) + \frac{1}{3!} \left(\frac{\kappa_3}{\kappa_1} + 3\kappa_2 + 2\kappa_1^3 \right) + \dots \right] \right. \\ &\quad \left. - \exp \left[-\kappa_1 + \frac{1}{2} \left(\frac{\kappa_2}{\kappa_1} - \kappa_1^2 \right) - \frac{1}{3!} \left(\frac{\kappa_3}{\kappa_1} - 3\kappa_2 + 2\kappa_1^3 \right) + \dots \right] \right\}.\end{aligned}\tag{B13}$$

Notice that the source of different sign of the exponent is traced to the calortropy production, $\ln(f^* f_2^*/f f_2)(f^* f_2^* - f f_2)$, in (3.4). Finally, if the first-order cumulant approximation is applied, it reduces to

$$\bar{\sigma}_c = \kappa_1^2 q(\kappa_1) = \kappa_1 \sinh \kappa_1.\tag{B14}$$

IV. Balanced closure (Myong PoF 2014)

A thermodynamically-consistent constitutive equation, still exact to BTE,

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

The simplest closure in 2nd-order level is $\nabla \cdot \mathbf{\Psi}^{(\mathbf{\Pi})} = 0$,

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

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

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

This is the 2nd-order constitutive equation beyond the two-century old Navier-Stokes equation and recovers NS,

$$2p[\nabla \mathbf{u}]^{(2)} = -p\mathbf{\Pi} / \mu_{NS}.$$

IV. Balanced closure (Myong PoF 2014)

The lesson: Type of closure may not be important. Rather, **balanced treatment of two open terms! Remember 'balanced' does not mean anything in case of only one term.**

Though looking trivial at first glance, we will appreciate **the beauty and real power of the balanced closure**, when we tackle the high Mach number shock singularity in Lecture 11.

Q & A
