Finding 13-Moment System Beyond Grad [1]

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Kinetic Equations: from Modeling Computation to Analysis
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Boltzmann equation (1872)

Phase density: $f(t, \boldsymbol{x}, \boldsymbol{\xi})$, $\boldsymbol{x} = (x_1, x_2, x_3)^T$, $\boldsymbol{\xi} = (\xi_1, \xi_2, \xi_3)^T$

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{x}} f = Q(f, f).$$

Collision term:

$$Q(f, f) = \int_{\mathbb{R}^3} \int_0^{2\pi} \int_0^{\pi/2} (f'_* f' - f_* f) |\boldsymbol{\xi} - \boldsymbol{\xi}_*| \sigma \sin \Theta \, \mathrm{d}\Theta \, \mathrm{d}\varepsilon \, \mathrm{d}\boldsymbol{\xi}_*,$$

where $f' = f(t, \mathbf{x}, \boldsymbol{\xi}')$, $f_* = f(t, \mathbf{x}, \boldsymbol{\xi}_*)$, $f'_* = f(t, \mathbf{x}, \boldsymbol{\xi}'_*)$.

We only consider Maxwell molecules hereafter.

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Moment method

For h as a polynomial of $\boldsymbol{\xi}$ times by f, we denote

$$\langle h \rangle = m \int_{\mathbb{R}^3} h \, \mathrm{d}\boldsymbol{\xi},$$

m: the mass of a single particle

Density	:	$\rho = \langle f \rangle$
Velocity	:	$\boldsymbol{u} = (u_1, u_2, u_3)^T = \rho^{-1} \langle \boldsymbol{\xi} f \rangle$
Temperature	:	$T = (3\rho k_B/m)^{-1} \langle \lvert \boldsymbol{\xi} - \mathbf{u} \rvert^2 f \rangle$
Temperature tensor	:	$T_{ij} = (\rho k_B/m)^{-1} \langle (\xi_i - u_i)(\xi_j - u_j) f \rangle$
Heat flux	:	$\boldsymbol{q} = (q_1, q_2, q_3)^T = \langle \lvert \boldsymbol{\xi} - \mathbf{u} \rvert^2 (\boldsymbol{\xi} - \mathbf{u}) f/2 \rangle$

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Moment method

Rescaled temperature:

$$\theta = \frac{k_B}{m} T, \quad \theta_{ij} = \frac{k_B}{m} T_{ij}, \quad \boldsymbol{\Theta} = (\theta_{ij})_{3\times 3}.$$

Let $\boldsymbol{C} = \boldsymbol{\xi} - \boldsymbol{u}$ $(C = |\boldsymbol{C}|)$,

$$\theta = (3\rho)^{-1} \langle C^2 f \rangle, \quad \theta_{ij} = \rho^{-1} \langle C_i C_j f \rangle.$$

Closure is a problem: 1D case for example

$$\frac{\partial \langle \xi^\alpha f \rangle}{\partial t} + \frac{\partial \langle \xi^{\alpha+1} f \rangle}{\partial x} = \langle \xi^\alpha Q(f, f) \rangle$$

Specific form of the phase density.

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Specific form of the phase density.

Grad's 13-moment system

Grad [CPAM 2(4), 1949]:

$$f|_{13} = \left[1 + \frac{\theta_{ij} - \delta_{ij}\theta}{2\theta^2}\left(C_i C_j - \delta_{ij} C^2\right) + \frac{2}{5}\frac{q_k}{\rho\theta^2} C_k \left(\frac{C^2}{2\theta} - \frac{5}{2}\right)\right] f_M,$$

f_M is the Maxwellian[2], defined as

$$f_M = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(-\frac{C^2}{2\theta}\right).$$

[2] J. Maxwell, 1860.

Grad's 13-moment system

The system is obtained as

$$\left\langle \phi \frac{\partial f|_{13}}{\partial t} \right\rangle + \langle \phi (\boldsymbol{\xi} \cdot \nabla_{\mathbf{x}} f|_{13}) \rangle = \langle \phi Q(f|_{13}, f|_{13}) \rangle,$$

Ikenberry polynomial[3]:

$$\begin{aligned} \phi = (1,& \\ & C_1, C_2, C_3, \\ & C_1^2, C_2^2, C_3^2, C_1 C_2, C_1 C_3, C_2 C_3, \\ & C^2 C_1, C^2 C_2, C^2 C_3)^T. \end{aligned}$$

[3] E. Ikenberry, A system of homogeneous spherical harmonics, JMAA, 1961.

Grad's 13-moment system

Explicit form[4]:

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\frac{\partial u_k}{\partial x_k} = 0, \qquad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + u_k\frac{\partial}{\partial x_k}$$

$$\frac{\mathrm{d}u_i}{\mathrm{d}t} + \frac{\theta_{ik}}{\rho}\frac{\partial \rho}{\partial x_k} + \frac{\partial \theta_{ik}}{\partial x_k} = 0,$$

$$\frac{\mathrm{d}\theta_{ij}}{\mathrm{d}t} + 2\theta_{k(i}\frac{\partial u_{j)}}{\partial x_k} + \frac{1}{\rho}\left(\frac{4}{5}\frac{\partial q_{(i}}{\partial x_{j)}} + \frac{2}{5}\delta_{ij}\frac{\partial q_k}{\partial x_k}\right) = -\frac{\rho\theta}{\mu}(\theta_{ij} - \delta_{ij}\theta),$$

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} - (\theta_{ij}\theta_{jk} - 2\theta\theta_{ik} + \theta^2\delta_{ik})\frac{\partial \rho}{\partial x_k} + \frac{7}{5}q_i\frac{\partial u_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial u_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial u_k}{\partial x_i}$$
$$- \rho\theta_{ik}\left(\frac{\partial \theta_{jk}}{\partial x_j} - \frac{7}{6}\frac{\partial \theta_{jj}}{\partial x_k}\right) + 2\rho\theta\left(\frac{\partial \theta_{ik}}{\partial x_k} - \frac{1}{3}\frac{\partial \theta_{jj}}{\partial x_i}\right) = -\frac{2}{3}\frac{\rho\theta}{\mu}q_i.$$

[4] This system has been collected in textbooks for more than 50 years.

Local hyperbolicity of 1D Grad's moment system

1D system:

$$u_2 = u_3 = \theta_{12} = \theta_{13} = \theta_{23} = q_2 = q_3 = 0, \quad \theta_{33} = \theta_{22}$$

In quasi-linear form:

$$\frac{\partial \hat{\mathbf{w}}}{\partial t} + \hat{\mathbf{M}}(\hat{\mathbf{w}}) \frac{\partial \hat{\mathbf{w}}}{\partial x} = \hat{\boldsymbol{Q}}(\hat{\mathbf{w}}),$$

where

$$\hat{\mathbf{w}} = (\rho, u_1, \theta_{11}, \theta_{22}, q_1)^T,$$

$$\hat{\boldsymbol{Q}}(\hat{\mathbf{w}}) = \left(0, 0, \rho\theta(\theta - \theta_{11})/\mu, \rho\theta(\theta - \theta_{22})/\mu, -\frac{2}{3}\rho\theta q_1/\mu\right)^T,$$

$$\hat{\mathbf{M}}(\hat{\mathbf{w}}) = \begin{pmatrix} u_1 & \rho & 0 & 0 & 0 \\ \theta_{11}/\rho & u_1 & 1 & 0 & 0 \\ 0 & 2\theta_{11} & u_1 & 0 & 6/(5\rho) \\ 0 & 0 & 0 & u_1 & 2/(5\rho) \\ -4(\theta_{11} - \theta_{22})^2/9 & 16q_1/5 & \rho(11\theta_{11} + 16\theta_{22})/18 & \rho(17\theta_{11} - 8\theta_{22})/9 & u_1 \end{pmatrix}.$$

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Local hyperbolicity of 1D Grad's moment system [5]

The characteristic polynomial is

$$\det(\lambda \mathbf{I} - \hat{\mathbf{M}}) = (\lambda - u_1)\Big[(\lambda - u_1)^4 - \frac{2}{45}(101\theta_{11} + 16\theta_{22})(\lambda - u_1)^2 - \frac{96}{25}\frac{q_1}{\rho}(\lambda - u_1) + \frac{1}{15}(53\theta_{11}^2 - 16\theta_{11}\theta_{22} + 8\theta_{22}^2)\Big].$$

At the local equilibrium ($\theta_{11} = \theta_{22} = \theta$, $q_1 = 0$), the eigenvalues of $\hat{\mathbf{M}}$ are

$$\lambda_{1,5} = u_1 \pm \sqrt{\frac{13 + \sqrt{94}}{5}\theta}, \quad \lambda_{2,4} = u_1 \pm \sqrt{\frac{13 - \sqrt{94}}{5}\theta}, \quad \lambda_3 = u_1.$$

1D system is hyperbolic AROUND the local equilibrium.

[5] I. Müller and T. Ruggeri, Rational extented thermdynamics, Springer-Verlag, 1998.

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Lack of hyperbolicity of 3D Grad's 13-moment system

3D system in quasi-linear form:

$$\frac{\partial \boldsymbol{w}}{\partial t} + \mathbf{M}_k(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial x_k} = \boldsymbol{Q}(\boldsymbol{w}).$$

Now $\boldsymbol{w}$ is a vector with 13 entries:

$$\boldsymbol{w} = (\rho, u_1, u_2, u_3, \theta_{11}, \theta_{22}, \theta_{33}, \theta_{12}, \theta_{13}, \theta_{23}, q_1, q_2, q_3)^T.$$

It is enough to examine $\mathbf{M}_1(\boldsymbol{w})$ due to the rotational invariance.

Lack of hyperbolicity of 3D Grad's 13-moment system

$$\mathbf{M}_1(\boldsymbol{w}) =$$

$$\begin{pmatrix}
u_1 & \rho & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\theta_{11}}{\rho} & u_1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{\theta_{12}}{\rho} & 0 & u_1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
\frac{\theta_{13}}{\rho} & 0 & 0 & u_1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 2\theta_{11} & 0 & 0 & u_1 & 0 & 0 & 0 & 0 & 0 & \frac{6}{5\rho} & 0 & 0 \\
0 & 0 & 2\theta_{12} & 0 & 0 & u_1 & 0 & 0 & 0 & 0 & \frac{2}{5\rho} & 0 & 0 \\
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0 & 0 & \theta_{13} & \theta_{12} & 0 & 0 & 0 & 0 & 0 & u_1 & 0 & 0 & 0 \\
-(\theta-\theta_{11})^2-(\theta_{12}^2+\theta_{13}^2) & \frac{16q_1}{5} & \frac{2q_2}{5} & \frac{2q_3}{5} & \frac{\rho(\theta_{11}+8\theta)}{6} & \frac{\rho(7\theta_{11}-4\theta)}{6} & \frac{\rho(7\theta_{11}-4\theta)}{6} & -\rho\theta_{12} & -\rho\theta_{13} & 0 & u_1 & 0 & 0 \\
\theta_{12}\theta_{33}-\theta_{13}\theta_{23}-\theta\theta_{12} & \frac{7q_2}{5} & \frac{7q_1}{5} & 0 & \frac{\rho\theta_{12}}{6} & \frac{7\rho\theta_{12}}{6} & \frac{7\rho\theta_{12}}{6} & \rho(2\theta-\theta_{22}) & -\rho\theta_{23} & 0 & 0 & u_1 & 0 \\
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\end{pmatrix}$$

Lack of hyperbolicity of 3D Grad's 13-moment system

Local equilibrium:

$$\theta_{12} = \theta_{13} = \theta_{23} = q_1 = q_2 = q_3 = 0, \quad \theta_{11} = \theta_{22} = \theta_{33} = \theta.$$

The characteristic polynomial of $\mathbf{M}_1(\boldsymbol{w})$:

$$\det(\lambda\mathbf{I}-\mathbf{M}_1) = \frac{(\lambda-u_1)^5}{125}[5(\lambda-u_1)^2-7\theta]^2[5(\lambda-u_1)^4-26\theta(\lambda-u_1)^2+15\theta^2].$$

The eigenvalues of $\mathbf{M}_1(\boldsymbol{w})$:

$$\lambda = \quad u_1, \quad u_1 \pm \sqrt{\tfrac{7}{5}\theta}, \quad u_1 \pm \sqrt{\tfrac{13+\sqrt{94}}{5}\theta}, \quad u_1 \pm \sqrt{\tfrac{13-\sqrt{94}}{5}\theta}.$$

	u_1	$u_1 \pm \sqrt{\tfrac{7}{5}\theta}$	$u_1 \pm \sqrt{\tfrac{13+\sqrt{94}}{5}\theta}$	$u_1 \pm \sqrt{\tfrac{13-\sqrt{94}}{5}\theta}$
multiplicity	5	2	1	1

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The minimal polynomial:

$$q(\lambda) = \frac{(\lambda - u_1)}{25}[5(\lambda - u_1)^2 - 7\theta] \cdot [5(\lambda - u_1)^4 - 26\theta(\lambda - u_1)^2 + 15\theta^2].$$

$q(\mathbf{M}_1) = \mathbf{0} \Rightarrow \mathbf{M}_1(\boldsymbol{w})$ is diagonalizable AT the equilibrium.

In the neighborhood of equilibrium, we consider the case

$$\theta_{13} = \theta_{23} = q_1 = q_2 = q_3 = 0, \quad \theta_{11} = \theta_{22} = \theta_{33} = \theta.$$

f is a Gaussian distribution[6]:

$$f = \frac{\rho}{\sqrt{\det(2\pi\boldsymbol{\Theta})}} \exp\left(-\frac{1}{2}\boldsymbol{C}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C}\right), \quad \boldsymbol{\Theta} = \begin{pmatrix} \theta & \theta_{12} & 0 \\ \theta_{12} & \theta & 0 \\ 0 & 0 & \theta \end{pmatrix}. \tag{1}$$

[6] When $|\theta_{12}| < \theta$, the matrix $\boldsymbol{\Theta}$ is positive definite, and thus the distribution function (1) can be a physical configuration.

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The characteristic polynomial of $\mathbf{M}_1(\boldsymbol{w})$:

$$\det(\lambda \mathbf{I} - \mathbf{M}_1) = \frac{(\lambda - u_1)^3}{125}[5(\lambda - u_1)^2 - 7\theta] \cdot r\left(\frac{(\lambda - u_1)^2}{\theta}\right),$$

where

$$r(x) = 25x^4 - 165x^3 + \left(257 + 48\frac{\theta_{12}^2}{\theta^2}\right)x^2 + \left(8\frac{\theta_{12}^2}{\theta^2} - 105\right)x - 28\frac{\theta_{12}^2}{\theta^2}.$$

The minimal polynomial:

$$q(\lambda) = (\lambda - u_1)[5(\lambda - u_1)^2 - 7\theta] \cdot r\left(\frac{(\lambda - u_1)^2}{\theta}\right).$$

If $\mathbf{M}_1(\boldsymbol{w})$ is diagonalizable, $q(\mathbf{M}_1) = \mathbf{0}$ — But [7]

$$q(\mathbf{M}_1) = \frac{56\theta^2\theta_{12}^3}{\rho}(\rho\theta\mathbf{E}_{10,4} - \mathbf{E}_{10,13}) \neq \mathbf{0}.$$

[7] $\mathbf{E}_{i,j} = \boldsymbol{e}_i\boldsymbol{e}_j^T$, and $\boldsymbol{e}_j$ is the unit vector with the j-th entry being 1.

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$$q(\lambda) = (\lambda - u_1)[5(\lambda - u_1)^2 - 7\theta] \cdot r\left(\frac{(\lambda - u_1)^2}{\theta}\right).$$

If $\mathbf{M}_1(\boldsymbol{w})$ is diagonalizable, $q(\mathbf{M}_1) = \mathbf{0}$ — But [7]

$$q(\mathbf{M}_1) = \frac{56\theta^2\theta_{12}^3}{\rho}(\rho\theta\mathbf{E}_{10,4} - \mathbf{E}_{10,13}) \neq \mathbf{0}.$$

[7] $\mathbf{E}_{i,j} = \mathbf{e}_i\mathbf{e}_j^T$, and $\mathbf{e}_j$ is the unit vector with the j-th entry being 1.

Lack of hyperbolicity of 3D Grad's 13-moment system

$\theta_{12} \neq 0$ (can be arbitrary small)

$\Rightarrow$ Any neighborhood of equilibrium $\not\subset$ Hyperbolicity region!

$\Rightarrow$ NO local wellposedness even AROUND equilibrium! [8]

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Modified 13-moment system

Let

$$\tilde{f}|_{13} = \left[1 + \frac{2}{5\rho}\boldsymbol{s}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C}\left(\frac{1}{2}\boldsymbol{C}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C} - \frac{5}{2}\right)\right] f_G,$$

where $\boldsymbol{s} = (s_1, s_2, s_3)^T$, and f_G is a Gaussian distribution:

$$f_G = \frac{\rho}{m\sqrt{\det(2\pi\boldsymbol{\Theta})}} \exp\left(-\frac{1}{2}\boldsymbol{C}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C}\right).$$

$$\boldsymbol{s} = \frac{1}{2}\langle C_G^2 \boldsymbol{C} f\rangle,$$

where $C_G^2 = \boldsymbol{C}^T\boldsymbol{\Theta}^{-1}\boldsymbol{C}$.

Modified 13-moment system

The system obtained is as

$$\left\langle \tilde{\phi} \frac{\partial \tilde{f}|_{13}}{\partial t} \right\rangle + \left\langle \tilde{\phi} (\boldsymbol{\xi} \cdot \nabla_{\mathbf{x}} \tilde{f}|_{13}) \right\rangle = \left\langle \tilde{\phi} Q(\tilde{f}|_{13}, \tilde{f}|_{13}) \right\rangle ,$$

where

$$\begin{aligned} \tilde{\phi} = (1, & \\ & C_1, C_2, C_3, \\ & C_1^2, C_2^2, C_3^2, C_1 C_2, C_1 C_3, C_2 C_3, \\ & C_G^2 C_1, C_G^2 C_2, C_G^2 C_3)^T. \end{aligned}$$

Modified 13-moment system

Explicit form [9]:

$$
\begin{aligned}
&\frac{\mathrm{d}\rho}{\mathrm{d}t} + \rho\frac{\partial u_k}{\partial x_k} = 0,\\
&\frac{\mathrm{d}u_i}{\mathrm{d}t} + \frac{\theta_{ik}}{\rho}\frac{\partial \rho}{\partial x_k} + \frac{\partial \theta_{ik}}{\partial x_k} = 0,\\
&\frac{\mathrm{d}\theta_{ij}}{\mathrm{d}t} + 2\theta_{k(i}\frac{\partial u_{j)}}{\partial x_k} + \frac{6}{5\rho}\left(s_{(i}\frac{\partial \theta_{jk)}}{\partial x_k} + \theta_{(ij}\frac{\partial s_{k)}}{\partial x_k}\right) = -\frac{\rho\theta}{\mu}(\theta_{ij} - \delta_{ij}\theta),\\
&\frac{\mathrm{d}s_j}{\mathrm{d}t} + \frac{3}{5}\theta^{ik}s_{(j}\frac{\mathrm{d}\theta_{ik)}}{\mathrm{d}t} + \frac{1}{2}\left(\rho\theta^{ik}\theta_{jl}\frac{\partial \theta_{ik}}{\partial x_l} + 2\rho\frac{\partial \theta_{jl}}{\partial x_l}\right)\\
&\qquad + \frac{2}{5}\left(7s_{(j}\frac{\partial u_{l)}}{\partial x_l} + \theta^{ik}\theta_{jl}s_{(i}\frac{\partial u_{k)}}{\partial x_l}\right) = \tilde{Q}_j.
\end{aligned}
$$

[9] Here θ^{ij} stands for the (i,j)-entry of matrix $\boldsymbol{\Theta}^{-1}$.

Modified 13-moment system

Collision term:

$$\tilde{Q}_j = -\frac{\rho\theta}{\mu}\left(\frac{71}{30}s_j - \frac{9}{10}\theta\theta^{(ii}s_{j)} - \frac{1}{15}\theta^{ii}\theta_{jk}s_k\right).$$

The expressions of $\tilde{Q}_j$ are obtained by using the following equalities of Maxwell molecules:

$$\langle C_i C_j Q(f,f)\rangle = -\frac{\rho\theta}{\mu}\left\langle\left(C_i C_j - \frac{1}{3}C^2\delta_{ij}\right)f\right\rangle,$$

$$\langle C^2 C_j Q(f,f)\rangle = -\frac{2\rho\theta}{3\mu}\langle C^2 C_j f\rangle,$$

$$\left\langle\left(C_i C_j C_k - \frac{3C^2 C_{(i}\delta_{jk)}}{5}\right)Q(f,f)\right\rangle = -\frac{3\rho\theta}{2\mu}\left\langle\left(C_i C_j C_k - \frac{3C^2 C_{(i}\delta_{jk)}}{5}\right)f\right\rangle.$$

Modified 13-moment system

Quasi-linear form:

$$\frac{\partial \tilde{\mathbf{w}}}{\partial t} + \tilde{\mathbf{M}}_k(\tilde{\mathbf{w}}) \frac{\partial \tilde{\mathbf{w}}}{\partial x_k} = \tilde{\boldsymbol{Q}}(\tilde{\mathbf{w}}), \tag{3}$$

where

$$\tilde{\mathbf{w}} = (\rho, u_1, u_2, u_3, \theta_{11}, \theta_{22}, \theta_{33}, \theta_{12}, \theta_{13}, \theta_{23}, s_1, s_2, s_3)^T.$$

Local hyperbolicity of the modified system

Discriminant of hyperbolicity:

$$\Delta \triangleq \rho^{-2} \boldsymbol{s}^T \boldsymbol{\Theta}^{-1} \boldsymbol{s}$$

Theorem 1

$\exists \delta > 0$, *such that if* $\Delta < \delta$, $\tilde{\mathbf{M}}_k(\tilde{\mathbf{w}})$ *is real diagonalizable, thus the moment system* (3) *is hyperbolic.*

Proof.

To verify that the matrix has no multiple eigenvalues. □

Quantitative threshold[10]:

$$\delta \approx 0.095$$

[10] For Couette flow with $Kn = 0.1$, velocity should be less than 150.

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Thank You!

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Reference:

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