Non-linear Wave Propagation and Non-Equilibrium Thermodynamics - Part 6

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The study of nonequilibrium phenomena in gases is particularly important. We have two complementary approaches to rarefied gases, namely the *continuum approach* and the *kinetic approach*.

The continuum model consists in the description of the system by means of macroscopic equations (e.g., fluid-dynamic equations) obtained on the basis of conservation laws and appropriate constitutive equations. A typical example is TIP. The applicability of this classical macroscopic theory is, however, inherently restricted to a nonequilibrium state characterized by a *small* Knudsen number K_n , which is a measure to what extent the gas is rarefied:

 $K_n = \frac{\text{mean free path of molecule}}{\text{macroscopic characteristic length}}.$



The approach based on the kinetic theory postulates that the state of a gas can be described by the velocity distribution function. The evolution of the distribution function is governed by the Boltzmann equation. The kinetic theory is applicable to a nonequilibrium state characterized by a *large* K_n , and the transport coefficients naturally emerge from the theory itself. Therefore the range of the applicability of the Boltzmann equation has been limited to rarefied gases.

The RET theory, a generalization of the TIP theory, also belongs to the continuum approach but is applicable to a nonequilibrium state with larger K_n . In a sense, RET is a sort of bridge between TIP and the kinetic theory. An interesting point to be noticed is that, in the case of rarefied gases, there exists a common applicability range of the RET theory and the kinetic theory. Therefore, in such a range, the results from the two theories should be consistent with each other. Because of this, we can expect that the kinetic-theoretical considerations can motivate us to establish the mathematical structure of the RET theory.



The Extended Thermodynamics of Rarefied Monoatomic Gas

The kinetic theory describes the state of a rarefied gas through the phase density $f(\mathbf{x}, t, \mathbf{c})$, where $f(\mathbf{x}, t, \mathbf{c})d\mathbf{c}$ is the number density of atoms at point \mathbf{x} and time t that have velocities between \mathbf{c} and $\mathbf{c} + d\mathbf{c}$. The phase density obeys the Boltzmann equation

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = Q \tag{1}$$

where Q represents the collisional terms. Most macroscopic thermodynamic quantities are identified as moments of the phase density

$$F_{k_1k_2\cdots k_j} = \int_{\mathbb{R}^3} f c_{k_1} c_{k_2} \cdots c_{k_j} d\mathbf{c}, \qquad (2)$$

and due to the Boltzmann equation (1), the moments satisfy an infinity hierarchy of balance laws in which the flux in one equation becomes the density in the next one:

$$\partial_{t}F + \partial_{i}F_{i} = 0$$

$$\swarrow$$

$$\partial_{t}F_{k_{1}} + \partial_{i}F_{ik_{1}} = 0$$

$$\swarrow$$

$$\partial_{t}F_{k_{1}k_{2}} + \partial_{i}F_{ik_{1}k_{2}} = P_{\langle k_{1}k_{2} \rangle}$$

$$\swarrow$$

$$\partial_{t}F_{k_{1}k_{2}k_{3}} + \partial_{i}F_{ik_{1}k_{2}k_{3}} = P_{k_{1}k_{2}k_{3}}$$

$$\vdots$$

$$\partial_{t}F_{k_{1}k_{2}...k_{n}} + \partial_{i}F_{ik_{1}k_{2}...k_{n}} = P_{k_{1}k_{2}...k_{n}}$$

The hierarchy structure of the system

- The tensorial rank of the equations increases one by one.
- In the flux in one equation becomes the density in the next equation.

Taking into account that $P_{kk} = 0$, the first five equations are conservation laws and coincides with the mass, momentum and energy conservation respectively, while the remaining ones are balance laws.

Remark: ET with this hierarchy structure is valid only for *rarefied monatomic* gases. In fact due to the previous structure we have that the momentum flux:

$$F_{ik} = \rho v_i v_k - t_{ik}; \quad t_{ik} = -p \delta_{ik} + \sigma_{ik}, \quad \sigma_{ik} = -\Pi \delta_{ik} + \sigma_{\langle ik \rangle}$$

while the conservation of energy we have:

$$F_{II} = 2\rho\varepsilon + \rho v^2$$

then

$$3p = 2\rho\varepsilon$$
 $\Pi = 0$

that implies

$$\gamma = \frac{c_p}{c_V} = \frac{5}{3},$$

i.e. monatomic gas.

The Closure Problem

When we cut the hierarchy at the density with tensor of rank n, we have the problem of closure because the last flux end the production terms are not in the list of the densities.

The first idea of Rational Extended Thermodynamics MÜLLER and RUGGERI (Springer - Verlag 1993, 1998) was to view the truncated system as a phenomenological system of continuum mechanics and then we consider the new quantities as constitutive functions:

$$F_{k_1k_2...k_nk_{n+1}} \equiv F_{k_1k_2...k_nk_{n+1}} \left(F, F_{k_1}, F_{k_1k_2}, \dots, F_{k_1k_2...k_n} \right)$$

$$P_{k_1k_2...k_j} \equiv P_{k_1k_2...k_j} \left(F, F_{k_1}, F_{k_1k_2}, \dots F_{k_1k_2...k_n} \right) \quad 2 \le j \le n.$$

According with the continuum theory, the restrictions on the constitutive equations come only from *universal principles*, i.e.: *Entropy principle*, *Objectivity Principle* and *Causality and Stability* (convexity of the entropy).

The most interesting physical cases was the 13 fields theory in classical framework (I.S.-Liu & I. Müller - ARMA 1983) and the 14- fields in the context of relativistic fluids (I.S.-Liu, I. Müller & T. Ruggeri -ANNALS of PHYSICS 1984)



If the number of moments increase it is too difficult to adopt the pure continuum approach for a system with such a large number of field variables.

Therefore it is necessary to recall that the field variables are the moments of a distribution function truncated at some order. And then the closure of the balance equations of the moments, which is known as the *maximum entropy principle* (MEP), should be introduced. This is the procedure of the so-called *molecular extended thermodynamics* (molecular RET).

The principle of maximum entropy has its root in statistical mechanics. It is developed by Jaynes in the context of the theory of information basing on the Shannon entropy



Nowadays the importance of MEP is recognized fully due to the numerous applications in many fields, for example, in the field of computer graphics.

MEP states that the probability distribution that represents the current state of knowledge in the best way is the one with the largest entropy.

Another way of stating this is as follows: Take precisely stated prior data or testable information about a probability distribution function. Then consider the set of all trial probability distributions that would encode the prior data. Of those, one with maximal information entropy is the proper distribution, according to this principle.



Concerning the applicability of MEP in nonequilibrium thermodynamics, this was originally by the observation made by Kogan (1967) that Grad's distribution function maximizes the entropy. The MEP was proposed in RET for the first time by Dreyer (1987).

In this way the 13-moment theory can be obtained in three different ways: RET, Grad, and MEP. A remarkable point is that all closures are equivalent to each other!

The MEP procedure was then generalized by Müller and Ruggeri to the case of any number of moments in the first edition of their book (1993) and later proposed again and popularized by Levermore (1996). The complete equivalence between the entropy principle and the MEP was finally proved by Boillat and Ruggeri (1997).

Later MEP was formulated also in a quantum-mechanical context (Degond & Ringhofer -2003).



Monatomic rarefied gas with many moments

More explicit :

$$\begin{aligned} \partial_t F + \partial_i F_i &= 0, \\ \partial_t F_{k_1} + \partial_i F_{ik_1} &= 0, \\ \partial_t F_{k_1 k_2} + \partial_i F_{ik_1 k_2} &= P_{\langle ij \rangle}, \\ \partial_t F_{k_1 k_2 k_3} + \partial_i F_{ik_1 k_2 k_3} &= P_{k_1 k_2 k_3}, \end{aligned}$$

$$\vdots$$

$$\partial_t F_{k_1 \dots k_N} + \partial_i F_{ik_1 \dots k_N} &= P_{k_1 \dots k_N}, \end{aligned}$$

For simplicity, we adopt the following notation:

$$F_A = egin{cases} F & ext{ for } A = 0 \ F_{k_1 k_2 \cdots k_A} & ext{ for } 1 \leq A \leq N, \end{cases}$$

Then the system can be rewritten as simple form:

$$\partial_t F_A + \partial_i F_{iA} = P_A,$$



Maximum Entropy Principle for Monatomic gas

with

$$F_A = m \int_{\mathbb{R}^3} c_A f \, d\mathbf{c}, \quad F_{iA} = m \int_{\mathbb{R}^3} c_i c_A f \, d\mathbf{c}, \quad P_A = m \int_{\mathbb{R}^3} c_A Q \, d\mathbf{c}.$$
(4)

and

$$c_{\mathcal{A}} = egin{cases} 1 & ext{for } \mathcal{A} = 0 \ c_{k_1}c_{k_2}\cdots c_{k_A} & ext{for } 1 \leq \mathcal{A} \leq \mathcal{N}. \end{cases}$$

The variational problem from which the distribution function f_N is obtained is connected to the functional:

$$\mathcal{L}_{N}(f) = -k \int_{R^{3}} f \log f \, d\mathbf{c} + u_{A}' \left(F_{A} - m \int_{R^{3}} c_{A} f \, d\mathbf{c} \right)$$

where u'_A are the Lagrange multipliers The distribution function f_N which maximizes the functional \mathcal{L}_N is given by:

$$f_N = \exp\left(-1 - \frac{m}{k}\chi_N\right), \qquad \chi_N = u'_A c_A.$$



Then, the system may be rewritten as follows:

$$J_{AB}\partial_t u'_B + J_{iAB}\partial_i u'_B = P_A(u'_C), \qquad A = 0, \dots, N$$
(6)

where

$$J_{AB}(u'_{C}) = -\frac{m^{2}}{k_{B}} \int_{R^{3}} f_{N} c_{A} c_{B} d\mathbf{c}, \qquad J_{iAB}(u'_{C}) = -\frac{m^{2}}{k_{B}} \int_{R^{3}} f_{N} c_{i} c_{A} c_{B} d\mathbf{c}.$$
 (7)

In an equilibrium state, (5) reduces to the Maxwellian distribution function. We observe that f_N is not a solution of the Boltzmann equation. But we have the conjecture (open problem) that, for $N \to \infty$, f_N tends to a solution of the Boltzmann equation. The system (6) is symmetric hyperbolic according with the general theory of systems of balance laws with a convex entropy density (Boillat & Ruggeri Continuum Mech. Thermodyn. (1997)).



All results explained above are valid also for a case far from equilibrium provided that the integrals in (4) and (7) are convergent. The problem of the convergence of the moments is one of the main questions in a far-from-equilibrium case. In particular, as we will see, the index of truncation N must be even. This implies, in particular, that a theory with 13 moments is not allowed when far from equilibrium!

Moreover, if the conjecture that the distribution function f_N , when $N \to \infty$, tends to the distribution function f that satisfies the Boltzmann equation is true, we need another convergence requirement.

These problems were studied by Boillat and Ruggeri (1997). They first introduced a map between the components of order k of the main field $u'_{i_1i_2...i_k}$ and the corresponding variables u'_{pqr} with p + q + r = k, where p, q, r are the indices over 1,2,3. With this notation, χ is expressed as

$$\chi = \sum_{p,q,r} u'_{pqr} c_1^p c_2^q c_3^q, \quad 0 \le p + q + r \le N.$$



Since

$$\sum_{p,q,r} u'_{pqr} c_1^p c_2^q c_3^q \bigg| \le a_N c^N$$

with

$$a_N = \max_{|\mathbf{t}|=1} \nu_N(\mathbf{t}), \qquad \nu_N(\mathbf{t}) = \sum_{p,q,r} u'_{pqr} t_1^p t_2^q t_3^q,$$

when $p + q + r = N \rightarrow \infty$, the series is absolutely convergent for any **c** provided that

$$u'_{pqr} o 0, \qquad \frac{a_{N+1}}{a_N} o 0.$$

Hence the components of the main field become smaller and smaller when N increases. This justifies the truncation of the system. On the other hand, when N is finite, the integrals of moments must also be convergent. When c is large, $\chi \simeq |c|^N \nu_N$. Therefore it is easy to see, by using the spherical coordinates, that the integrals of moments converge provided that $\nu_N(\mathbf{t}) < 0$ for any unit vector \mathbf{t} . But, as $\nu(-\mathbf{t}) = (-1)^N \nu(\mathbf{t})$, we can conclude that N must be even and $\max_{|\mathbf{t}|=1} \nu(\mathbf{t}) < 0$.

Now, the distribution function obtained as the solution of the variational problem is expanded in the neighborhood of a local equilibrium state:

$$f \approx f_M \left(1 - \frac{m}{k_B} \tilde{u}'_A c_A \right), \quad \tilde{u}'_A = u'_A - u'^E_A, \tag{9}$$

where $u_A^{\prime E}$ are the main field components evaluated in the local equilibrium state and f_M is the Maxwellian equilibrium distribution function.

This is a big limitation of the theory because the theory is valid only near equilibrium and hyperbolicity exists only in some small domain of configuration space near equilibrium. Notice that f is not always positive!

The RET had success because several experiments are in agreement with the theory (sound waves in high frequencies, Light scattering, Schock waves) nevertheless have 2 weak limitations:

- The theory is valid only near equilibrium
- In the theory, as Kinetic Theory, is valid only for monatomic rarefied gas



Limit of ET and KT

ET has played crucial role for rarefied non-equilibrium gas. Nevertheless the weak point of ET and KT is that the applicable range is limited to rarefied monatomic gas.









The 14 moment phenomenological theory for dense gas and in particular polyatomic ones was recently obtained using the universal principles of ET and postulating a double hierarchy of equations by T. Arima, S. Taniguchi, T. Ruggeri and M. Sugiyama - Continuum Mech. Thermodyn., (2012). The question is if the macroscopic system have a kinetic counterpart. We will see that in the case of rarefied gas the previous structure can be explained in clear manner. We shall, therefore, briefly describe the kinetic model for polyatomic gases and point out the important consequences related to internal energy density. The idea is to consider an additional parameter in the distribution function $f(t, \mathbf{x}, \mathbf{c}, l)$ defined on extended domain $[0, \infty) \times \mathbb{R}^3 \times \mathbb{R}^3 \times [0, \infty)$. Its rate of change is determined by the Boltzmann equation which has the same form as for monatomic gas but collision integral Q(f) takes into account the influence of internal degrees of freedom through collisional cross section (Bourgat, Desvillettes, Le Tallec and Perthame, see also Borgnakke and Larsen)



Equilibrium distribution function for polyatomic gases

Collision invariants for this model form a 5-vector:

$$\psi(\mathbf{c}, \mathbf{l}) = m \left(1, c_i, \frac{1}{2}mc^2 + \mathbf{l}\right)^T, \qquad (10)$$

which lead to hydrodynamic variables in the form:

$$\begin{pmatrix} \rho \\ \rho v_i \\ \frac{1}{2}\rho v^2 + \rho \varepsilon \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^\infty \psi(\mathbf{c}, \mathbf{l}) f(t, \mathbf{x}, \mathbf{c}, \mathbf{l}) \varphi(\mathbf{l}) \, d\mathbf{l} \, d\mathbf{c}, \tag{11}$$

where ρ , **v** and ε are mass density, hydrodynamic velocity and internal energy, respectively. A non-negative measure $\varphi(I) dI$ is property of the model aimed at recovering classical caloric equation of state for polyatomic gases in equilibrium. Entropy is defined by the following relation:

$$h = -k \int_{\mathbb{R}^3} \int_0^\infty f \log f\varphi(I) \, dI \, d\mathbf{c}.$$



We shall introduce the peculiar velocity:

$$\mathbf{C} = \mathbf{c} - \mathbf{v} \tag{13}$$

and rewrite the Eq. (11) in terms of it. Then:

$$\begin{pmatrix} \rho \\ 0_i \\ 2\rho\varepsilon \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} 1 \\ C_i \\ C^2 + 2I/m \end{pmatrix} f(t, \mathbf{x}, \mathbf{C}, I)\varphi(I) \, dI \, d\mathbf{C}.$$
(14)

Note that the internal energy density can be divided into the translational part $\rho \varepsilon_T$ and part related to the internal degrees of freedom $\rho \varepsilon_I$:

$$\rho \varepsilon_{T} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} \frac{1}{2} m C^{2} f(t, \mathbf{x}, \mathbf{C}, I) \varphi(I) \, dI \, d\mathbf{C},$$

$$\rho \varepsilon_{I} = \int_{\mathbb{R}^{3}} \int_{0}^{\infty} I f(t, \mathbf{x}, \mathbf{C}, I) \varphi(I) \, dI \, d\mathbf{C}.$$
(15)

The former can be related to kinetic temperature in the following way:

$$\varepsilon_T = \frac{3}{2} \frac{k}{m} T$$



whereas the latter should determine the contribution of internal degrees of freedom to internal energy of a polyatomic gas.

In fact if D is the number of degrees of freedom of a molecule, it can be shown that $\varphi(I) = I^{\alpha}$ leads to appropriate caloric equation in equilibrium provided:

$$\alpha = \frac{D-5}{2}.$$
 (17)

In fact if the weighting function is chosen to be $\varphi(I) = I^{\alpha}$, internal energy of a polyatomic gas in equilibrium reads:

$$\varepsilon = \left(\frac{5}{2} + \alpha\right) \frac{k}{m} T, \quad \alpha > -1.$$
 (18)

The relation between α and D (17) follows directly from comparison between (18) and well-know caloric equation for polyatomic gases:

$$\varepsilon = \frac{D}{2} \frac{k}{m} T.$$

Observe that model for a monatomic gas (D = 3) cannot be recovered from the one with continuous internal energy, since the value of parameter α in monatomic case violates the overall restriction $\alpha > -1$.

Pavić, Ruggeri and Simić [5] firstly considered the Euler fluid with 5 moments and they considered the the maximum entropy principle expressed in terms of the following variational problem: determine the velocity distribution function $f(t, \mathbf{x}, \mathbf{c}, I)$ such that $h \rightarrow \max$, being subjected to the constraints (11).

Theorem

The distribution function that maximizes the entropy (12) under the constraints (14) has the form:

$$f_E = \frac{\rho}{m(k_B T)^{1+\alpha} \Gamma(1+\alpha)} \left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left\{-\frac{1}{k_B T} \left(\frac{1}{2}mC^2 + I\right)\right\}.$$
 (19)

This is the generalized Maxwell distribution function for polyatomic gases.



The following theorem was also proved:

Theorem

If (19) is the local equilibrium distribution function with $\rho \equiv \rho(t, \mathbf{x})$, $\mathbf{v} \equiv \mathbf{v}(t, \mathbf{x})$ and $T \equiv T(t, \mathbf{x})$, then the hydrodynamic variables ρ , \mathbf{v} and T satisfy the Euler system:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho v_i) = 0,$$

$$\frac{\partial}{\partial t} (\rho v_j) + \frac{\partial}{\partial x_i} (\rho v_i v_j + p \delta_{ij}) = 0,$$

$$\frac{\partial}{\partial t} \left(\rho \varepsilon + \rho \frac{v^2}{2}\right) + \frac{\partial}{\partial x_i} \left\{ \left(\rho \varepsilon + \rho \frac{v^2}{2} + p\right) v_i \right\} = 0$$
(20)

with

$$p = \frac{k_B}{m} \rho T, \qquad \varepsilon = \frac{D}{2} \frac{k_B}{m} T.$$
 (21)

This is an important result because we can obtain the Euler equations from the kinetic equation for any kind of polyatomic gases as well as monatomic gases.

Pavić, Ruggeri and Simić [5] secondly considered the case of 14 moments. This case is completely in agreement with the binary hierarchy with the moments:

$$\begin{pmatrix} F\\F_{i_1}\\F_{i_1i_2} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} 1\\c_{i_1}\\c_{i_1}c_{i_2} \end{pmatrix} f(t, \mathbf{x}, \mathbf{c}, l) \varphi(l) \, dl \, d\mathbf{c},$$

$$\begin{pmatrix} G_{pp}\\G_{ppk_1} \end{pmatrix} = \int_{\mathbb{R}^3} \int_0^\infty m \begin{pmatrix} c^2 + 2\frac{l}{m}\\(c^2 + 2\frac{l}{m})c_{k_1} \end{pmatrix} f(t, \mathbf{x}, \mathbf{c}, l) \varphi(l) \, dl \, d\mathbf{c}.$$
(22)

For the entropy defined by (12), the following variational problem, expressing the maximum entropy principle, can be formulated: determine the velocity distribution function $f(t, \mathbf{x}, \mathbf{C}, I)$ such that $h \to \max$, being subjected to the constraints (22). The solution of the problem is as follows.



Near the equilibrium state the velocity distribution function, which maximizes the entropy (12) with the constraints (22) and the weighting function $\varphi(I) = I^{\alpha}$, has the form:

$$f = f_E \left\{ 1 - \frac{\rho}{p^2} q_i C_i + \frac{\rho}{p^2} \left[-\sigma_{\langle ij \rangle} + \left(\frac{5}{2} + \alpha\right) (1 + \alpha)^{-1} \Pi \delta_{ij} \right] C_i C_j \qquad (23)$$
$$- \frac{3}{2(1 + \alpha)} \frac{\rho}{p^2} \Pi \left(\frac{1}{2} C^2 + \frac{I}{m} \right) + \left(\frac{7}{2} + \alpha \right)^{-1} \frac{\rho^2}{p^3} q_i \left(\frac{1}{2} C^2 + \frac{I}{m} \right) C_i \right\},$$

where f_E is the equilibrium distribution (19). The non-equilibrium distribution (23) reduces to the velocity distribution obtained by Mallinger for gases composed of diatomic molecules ($\alpha = 0$), and, for any $\alpha > -1$, the closure gives exactly the same equations obtained before by using the macroscopic approach and the entropy principle:

[T. Arima, S. Taniguchi, T. Ruggeri and M. Sugiyama - Continuum Mech. Thermodyn., (2012).]



The general hierarchy of moment equations for polyatomic gases

In non-equilibrium motivated by the idea of phenomenological ET, we shall generalize the moment equations for polyatomic gases by constructing two independent hierarchies. One will be much alike classical "momentum" hierarchy of monatomic gases (F-hierarchy); the other one, "energy" hierarchy, commences with the moment related to energy collision invariant and proceeds with standard increase of the order through multiplication by velocities (G-hierarchy). They read:

$$\partial_t \mathbf{F} + \partial_i \mathbf{F}_i = \mathbf{P}, \quad \partial_t \mathbf{G} + \partial_i \mathbf{G}_i = \mathbf{Q}.$$

[Pavić, Ruggeri & Simić Physica A,(2012)] [Arima, Mentrelli & Ruggeri - Annals of Physics (2014)]



Moments, fluxes and productions of F-hierarchy are defined as:

$$\begin{split} \mathbf{F}(t,\mathbf{x}) &= \int_{\mathbb{R}^3} \int_0^\infty \Psi(\mathbf{c}) f \,\varphi(l) \,dl \,d\mathbf{c}, \\ \mathbf{F}_i(t,\mathbf{x}) &= \int_{\mathbb{R}^3} \int_0^\infty c_i \Psi(\mathbf{c}) f \,\varphi(l) \,dl \,d\mathbf{c}, \\ \mathbf{P}(t,\mathbf{x}) &= \int_{\mathbb{R}^3} \int_0^\infty \Psi(\mathbf{c}) Q(f) \,\varphi(l) \,dl \,d\mathbf{c}, \end{split}$$

with:



Moments, fluxes and productions of G-hierarchy are defined as:

$$\mathbf{G}(t, \mathbf{x}) = \int_{\mathbb{R}^3} \int_0^\infty \mathbf{\Theta}(\mathbf{c}, l) f \,\varphi(l) \,dl \,d\mathbf{c},$$
$$\mathbf{G}_i(t, \mathbf{x}) = \int_{\mathbb{R}^3} \int_0^\infty c_i \mathbf{\Theta}(\mathbf{c}, l) f \,\varphi(l) \,dl \,d\mathbf{c},$$
$$\mathbf{Q}(t, \mathbf{x}) = \int_{\mathbb{R}^3} \int_0^\infty \mathbf{\Theta}(\mathbf{c}, l) Q(f) \,\varphi(l) \,dl \,d\mathbf{c},$$

with:

$$\Theta(\mathbf{c}, l) = m \begin{pmatrix} c^2 + 2\frac{l}{m} \\ (c^2 + 2\frac{l}{m})c_{k_1} \\ (c^2 + 2\frac{l}{m})c_{k_1}c_{k_2} \\ \vdots \\ (c^2 + 2\frac{l}{m})c_{k_1}\cdots c_{k_m} \\ \vdots \end{pmatrix},$$

Note that minimal order of the moment in F-hierarchy is 0, while minimal order in G-hierarchy is 2.

Polyatomic rarefied gas with many moments

More explicit :

$$\begin{split} \partial_t F &+ \partial_i F_i = 0, \\ \partial_t F_{k_1} &+ \partial_i F_{ik_1} = 0, \\ \partial_t F_{k_1 k_2} &+ \partial_i F_{ik_1 k_2} = P_{\langle ij \rangle}, \\ \partial_t F_{k_1 k_2 k_3} &+ \partial_i F_{ik_1 k_2 k_3} = P_{k_1 k_2 k_3}, \\ \vdots \\ \partial_t F_{k_1 \cdots k_N} &+ \partial_i F_{ik_1 \cdots k_N} = P_{k_1 \cdots k_N}, \end{split}$$

$$\begin{split} &\partial_t G_{LL} + \partial_i G_{iLL} = 0 \\ &\partial_t G_{LLk_1} + \partial_i G_{iLLk_1} = Q_{LLk_1}, \\ &\vdots \\ &\vdots \\ &\partial_t G_{LLk_1 \cdots k_M} + \partial_i G_{iLLk_1 \cdots k_M} = Q_{LLk_1 \cdots k_M}. \end{split}$$

For simplicity, we adopt the following notation:

$$F_{A} = \begin{cases} F & \text{for } A = 0 \\ F_{k_{1}k_{2}\cdots k_{A}} & \text{for } 1 \leq A \leq N, \end{cases} \qquad G_{LLa} = \begin{cases} G_{LL} & \text{for } a = 0 \\ G_{LLk_{1}k_{2}\cdots k_{a}} & \text{for } 1 \leq a \leq N \end{cases}$$

Then the system can be rewritten as simple form:
$$\partial_{t}F_{A} + \partial_{i}F_{iA} = P_{A}, \qquad \partial_{t}G_{LLA'} + \partial_{i}G_{iLLA'} = Q_{LLA'}. \tag{24}$$

Maximum Entropy Principle

The variational problem from which the distribution function $f_{(N,M)}$ is obtained is connected to the functional:

$$\mathcal{L}_{(N,M)}(f) = -k \int_{\mathbb{R}^3} \int_0^\infty f \log f \, I^\alpha \, dI \, d\mathbf{c} + u'_A \left(F_A - m \int_{\mathbb{R}^3} \int_0^\infty c_A f \, I^\alpha \, dI \, d\mathbf{c} \right) + v'_{A'} \left(G_{IIA'} - m \int_{\mathbb{R}^3} \int_0^\infty \left(c^2 + \frac{2I}{m} \right) c_{A'} f \, I^\alpha \, dI \, d\mathbf{c} \right),$$

where u'_A and v'_a are the Lagrange multipliers and

$$c_{A} = \begin{cases} 1 & \text{for } A = 0 \\ c_{k_{1}}c_{k_{2}}\cdots c_{k_{A}} & \text{for } 1 \leq A \leq N, \end{cases} \quad c_{A'} = \begin{cases} 1 & \text{for } A' = 0 \\ c_{k_{1}}c_{k_{2}}\cdots c_{k_{A'}} & \text{for } 1 \leq A' \leq M. \end{cases}$$

The distribution function $f_{(N,M)}$ which maximizes the functional $\mathcal{L}_{(N,M)}$ is given by:

$$f_{(N,M)} = \exp\left(-1 - \frac{m}{k}\chi_{(N,M)}\right), \qquad \chi_{(N,M)} = u'_{A}c_{A} + \left(c^{2} + \frac{2I}{m}\right)v'_{A'}c_{A}$$
(25)

Then, the system may be rewritten as follows:

$$\begin{pmatrix} J^{0}_{AB} & J^{1}_{AB'} \\ J^{1}_{A'B} & J^{2}_{A'B'} \end{pmatrix} \partial_{t} \begin{pmatrix} u'_{B} \\ v'_{B'} \end{pmatrix} + \begin{pmatrix} J^{0}_{iAB} & J^{1}_{iAB'} \\ J^{1}_{iA'B} & J^{2}_{iA'B'} \end{pmatrix} \partial_{i} \begin{pmatrix} u'_{B} \\ v'_{B'} \end{pmatrix} = \begin{pmatrix} P_{A} \\ Q_{IIA'} \end{pmatrix},$$
(26)

where

$$J_{AB}^{0} = -\frac{m}{k} \int_{R^{3}} \int_{0}^{\infty} f c_{A}c_{B}I^{\alpha} dld\mathbf{c},$$

$$J_{AB'}^{1} = -\frac{m}{k} \int_{R^{3}} \int_{0}^{\infty} f c_{A}c_{B'} \left(c^{2} + \frac{2I}{m}\right)I^{\alpha} dld\mathbf{c},$$

$$J_{A'B'}^{2} = -\frac{m}{k} \int_{R^{3}} \int_{0}^{\infty} f c_{A'}c_{B'} \left(c^{2} + \frac{2I}{m}\right)^{2}I^{\alpha} dld\mathbf{c}.$$
(27)

The system (26) is symmetric hyperbolic according with the general theory of systems of balance laws with a convex entropy density (Boillat & Ruggeri Continuum Mech. Thermodyn. (1997)).



<u>Problem</u> \Rightarrow Are N and M independent?

The following two theorems give the answer [Arima, Mentrelli and Ruggeri- Annals of Physics (2014)]:

Theorem

The differential system is Galilean invariant if and only if $M \le N - 1$.

Theorem

If M < N - 1, all characteristic velocities are independent from the internal degrees of freedom D and coincides with the one of F-hierarchy of monatomic gases with the truncation order N.

Ŷ

The relation between N and M for the physically meaningful system

The requirement that the system is Galilean invariant and the characteristic velocities are function of D require

$$M = N - 1$$

Examples:

N=1, M=0 Euler system:

$$\partial_t F + \partial_i F_i = 0,$$

$$\partial_t F_{k_1} + \partial_i F_{ik_1} = 0,$$

$$\partial_t G_{LL} + \partial_i \frac{G_{iLL}}{G_{iLL}} = 0$$

N=2, M=1 14-field system:

$$\begin{aligned} \partial_t F + \partial_i F_i &= 0, \\ \partial_t F_{k_1} + \partial_i F_{ik_1} &= 0, \\ \partial_t F_{k_1 k_2} + \partial_i \overline{F_{ik_1 k_2}} &= \overline{P_{\langle ij \rangle}} \end{aligned}$$

$$\partial_t G_{LL} + \partial_i G_{iLL} = 0$$

$$\partial_t G_{LLk_1} + \partial_i G_{iLLk_1} = Q_{LLk_1}$$

We have the same problematic in polyatomic gas concerning the convergence of the integrals. In ET of monatomic gas we need that the index of truncation N must even and M + 2 must be even in the present theory. In particular not Grad in monatomic case neither 14 moments are allowed in a theory far from equilibrium! Therefore as in the monatomic gas case, the distribution function obtained as solution of the variational problem is expanded in the neighborhood of a local equilibrium state:

$$f \approx f^{E} \left[1 - \frac{m}{k} \left(\tilde{u}'_{A} c_{A} + \left(c^{2} + \frac{2I}{m} \right) \tilde{v}'_{A'} c_{A'} \right) \right], \quad \tilde{u}'_{A} = u'_{A} - u'^{E}_{A}, \ \tilde{v}'_{A'} = v'_{A'} - v'^{E}_{A'},$$
(28)

where $u_A^{\prime E}$ and $v_{A'}^{\prime E}$ are the main field components evaluated in the local equilibrium state. The equilibrium distribution function f^E is given by the (19).



The 14 moments system for polyatomic gases

In the case of 14 moments and polyatomic gas $p = \frac{k}{m}\rho T$, $\varepsilon = \frac{D}{2}\frac{k}{m}T$, the system become:

The 6 Moments case

The most simple case of dissipative polyatomic gas is the one in which we neglect heat conductivity and shear viscosity and we suppose that only the bulk viscosity is not negligible In this case we have the most simple model after Euler in the presence of dissipation due to the role of the dynamical pressure We consider 6 independent field-variables (ρ , v_i , T, Π), and we assume the following binary hierarchy (F-series and G-series) of the balance equations proposed in the framework of ET of real gases [2]:

$$\frac{\partial F}{\partial t} + \frac{\partial F_i}{\partial x_i} = 0,$$

$$\frac{\partial F_j}{\partial t} + \frac{\partial F_{ji}}{\partial x_i} = 0,$$

$$\frac{\partial F_{ll}}{\partial t} + \frac{\partial F_{lli}}{\partial x_i} = P_{ll},$$

$$\frac{\partial G_{ll}}{\partial t} + \frac{\partial G_{lli}}{\partial x_i} = 0,$$
(29)

where $(29)_{1,2,4}$ represent the conservation laws of mass, momentum and energy provided that $F = \rho$, $F_i = \rho v_i$, $F_{ij} = \rho v_i v_j + (p + \Pi)\delta_{ij}$, $G_{II} = \rho v_I v_I + 2\rho \varepsilon$, and $G_{IIi} = (\rho v_I v_I + 2\rho \varepsilon + 2p + 2\Pi)v_i$ with p and ε being, respectively, the pressure and the specific internal energy.

with

$$\begin{pmatrix} F\\F_i\\F_{II} \end{pmatrix} = \begin{pmatrix} \rho\\\rho v_i\\\rho v^2 + 3(p+\Pi) \end{pmatrix} = \int_{R^3} \int_0^\infty m \begin{pmatrix} 1\\c_i\\c^2 \end{pmatrix} f \ I^\alpha \, dI \, d\mathbf{c} \qquad (30)$$

 and

$$G_{II} = \rho v^2 + 2\rho \varepsilon = \int_{\mathcal{R}^3} \int_0^\infty m(c^2 + 2I/m) f \ I^\alpha \, dI \, d\mathbf{c}. \tag{31}$$



Theorem

The distribution function that maximizes the entropy (12) under the constraints (30) (31) has the form:

$$f = \frac{\rho}{m(k_B T)^{1+\alpha} \Gamma(1+\alpha)} \left(\frac{m}{2\pi k_B T} \frac{1}{1+\frac{\Pi}{\rho}} \right)^{3/2} \left(\frac{1}{1-\frac{3}{2(1+\alpha)} \frac{\Pi}{\rho}} \right)^{1+\alpha} \exp\left\{ -\frac{1}{k_B T} \left(\frac{1}{2} m C^2 \left(\frac{1}{1+\frac{\Pi}{\rho}} \right) + I \left(\frac{1}{1-\frac{3}{2(1+\alpha)} \frac{\Pi}{\rho}} \right) \right) \right\}.$$
 (32)

All the moments are convergent provided that

$$-1 < \frac{\Pi}{\rho} < \frac{2}{3}(1+\alpha), \qquad \alpha > -1.$$
 (33)



Then the system (29) is written in terms of the physical variables:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{i}} (\rho v_{i}) = 0,
\frac{\partial \rho v_{j}}{\partial t} + \frac{\partial}{\partial x_{i}} [(p + \Pi)\delta_{ij} + \rho v_{i}v_{j}] = 0,$$

$$\frac{\partial}{\partial t} (2\rho\varepsilon + \rho v^{2}) + \frac{\partial}{\partial x_{i}} \left\{ \left[2(p + \Pi) + 2\rho\varepsilon + \rho v^{2} \right] v_{i} \right\} = 0,
\frac{\partial}{\partial t} \left[3(p + \Pi) + \rho v^{2} \right] + \frac{\partial}{\partial x_{i}} \left\{ \left[5(p + \Pi) + \rho v^{2} \right] v_{i} \right\} = \hat{P}_{II}.$$
(35)

with

$$\hat{P}_{II} = -\frac{2}{\nu} \frac{(D-3)^2 \rho^3 \Pi}{D(\rho+\Pi)((D-3)\rho-3\Pi)}.$$
(36)



The non equilibrium entropy have the following expression:

$$k = -\frac{p}{2T} \log \left(\frac{p^{D}}{(p+\Pi)^{3} \left(p - \frac{3\Pi}{D-3} \right)^{D-3}} \right).$$
(37)

The argument of log in (37) depends on a single variable Π/p . For D > 3, k exists and is bounded in the domain that contains the equilibrium state:

$$-1 < \frac{\Pi}{p} < \frac{D-3}{3},\tag{38}$$

in which $k(\rho, \varepsilon, \Pi) < 0, \forall \Pi \neq 0$ and k has a global maximum $k(\rho, \varepsilon, 0) = 0$ at the equilibrium state.





Figure: Nonequilibrium entropy density k as the function of Z for different values of D.

The main field for which the system became symmetric hyperbolic have the following components:

$$\lambda = -\frac{g}{T} + k + \frac{v^2}{2T} \left(1 + \frac{\Pi}{p} \right)^{-1},$$

$$\lambda_i = -\frac{v_i}{T} \left(1 + \frac{\Pi}{p} \right)^{-1},$$

$$\mu_{II} = \frac{1}{2T} \left(1 - \frac{3}{D-3} \frac{\Pi}{p} \right)^{-1},$$

$$\lambda_{II} = -\frac{1}{2T} \frac{D}{D-3} \frac{\Pi}{p} \left(1 + \frac{\Pi}{p} \right)^{-1} \left(1 - \frac{3}{D-3} \frac{\Pi}{p} \right)^{-1}.$$
(39)

Notice that, in equilibrium where $\Pi = 0$, the first five components of the main field (39) coincide with those obtained by Godunov for the Euler fluid [21]:

$$\lambda|_E = -rac{1}{T}\left(g-rac{v^2}{2}
ight), \quad \lambda_i|_E = -rac{v_i}{T}, \quad \mu_{II}|_E = rac{1}{2T},$$

while $\lambda_{II}|_E = 0$ according to the fact that the Euler fluid is a *principal subsystem* of the 6-moment system.

The field equations for linear production become:

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0,$$

$$\rho \dot{v}_i + \frac{\partial}{\partial x_i} (\rho + \Pi) = 0,$$

$$\rho \dot{\varepsilon} + (\rho + \Pi) \operatorname{div} \mathbf{v} = 0,$$

$$\tau \dot{\Pi} + \left(\nu + \tau \frac{5D - 6}{3D} \Pi\right) \operatorname{div} \mathbf{v} = -\Pi,$$
(40)

where the bulk viscosity $\nu \propto D - 3$. When $D \rightarrow 3$ (monatomic gas) the previous system have the same solution of the Euler fluid provided $\Pi(\mathbf{x}, 0) = 0$.



The parabolic case $\tau \rightarrow 0$:

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0,$$

$$\rho \dot{\mathbf{v}}_i + \frac{\partial}{\partial x_i} (\rho + \Pi) = 0,$$

$$\rho \dot{\varepsilon} + (\rho + \Pi) \operatorname{div} \mathbf{v} = 0,$$

$$\nu \operatorname{div} \mathbf{v} = -\Pi,$$

(41)

was studied in same papers, e.g. :

- P. Secchi Rend. Sem. Padova (1984)
- V. Shelukhin Journal of Differential Equations (2000)
- H. Frid & V. Shelukhin Siam J. Math. Anal. (2000)



Comparison between the nonlinear systems of the ET6 theory and of Meixner's theory

The Meixner theory may be regarded as the prototype of the theories of internal variables, but it is still frequently applied to various nonequilibrium phenomena. The simplest version of Meixner's theory composed of the Euler equations and only one relaxation equation for an internal variable ξ :

$$\dot{\rho} + \rho \frac{\partial v_k}{\partial x_k} = 0,$$

$$\rho \dot{v}_i + \frac{\partial \mathcal{P}}{\partial x_i} = 0,$$

$$\rho \dot{\mathcal{E}} + \mathcal{P} \frac{\partial v_k}{\partial x_k} = 0,$$

$$\dot{\xi} = -\beta \mathcal{A},$$

(42)

where \mathcal{P} , \mathcal{E} and \mathcal{A} are, respectively, the pressure, the specific internal energy and the affinity of relaxation processes, and β is a positive phenomenological coefficient.

The generalized Gibbs relation in Meixner's theory is assumed to be:

$$\mathcal{T}d\mathcal{S} = d\mathcal{E} - \frac{\mathcal{P}}{\rho^2}d\rho - \mathcal{A}d\xi,$$
 (43)

where \mathcal{T} is the temperature and \mathcal{S} is the specific entropy. Note that the quantities \mathcal{T} , \mathcal{S} , \mathcal{P} and \mathcal{A} depend not only on the mass density ρ and the specific internal energy \mathcal{E} but also on the internal variable ξ . From (43), taking into account (42), we obtain:

$$\dot{S} = \beta \frac{\mathcal{A}^2}{\mathcal{T}}.$$
(44)

Comparing the system of the ET6 theory (41) and $(\ref{eq:system})$ with the system of Meixner's theory (42) and (44), we obtain the perfect correspondence provided that

$$\xi = \frac{p+\Pi}{\rho} - \frac{2}{3}\varepsilon, \quad \mathcal{P} = p+\Pi$$

$$\mathcal{E} = \varepsilon, \quad \mathcal{A} = -\mathcal{T}k_{\Pi}, \qquad (45)$$

$$\mathcal{S} = \mathbf{s} + \frac{k}{\rho}, \quad \beta = \frac{\alpha}{3\rho\mathcal{T}},$$

where \mathcal{T} is given by

$$\frac{1}{\mathcal{T}} = \frac{1}{\mathcal{T}} + \left\{ \frac{1}{\rho} k_{\varepsilon} + \left(\frac{2}{3} - \frac{p_{\varepsilon}}{\rho} \right) k_{\Pi} \right\}.$$



In the general theory of hyperbolic conservation laws and hyperbolic-parabolic conservation laws, the existence of a strictly convex entropy function, which is a generalization of the physical entropy, is a basic condition for the well-posedness (K. O. Friedrichs & P. D. Lax, Proc. Nat. Acad. Sci. U.S.A. 68 (1971), S. Kawashima, Proc. Roy. Soc. Edinburgh 106A (1987)). In fact if \mathbf{F}^{α} and the production \mathbf{f} are smooth enough, in a suitable convex open set $D \in \mathbb{R}^n$ it is well known that the Cauchy problem has a unique local (in time) smooth solution for smooth initial data.

However, in the general case, and even for arbitrarily small and smooth initial data, there is no global continuation for these smooth solutions, which may develop singularities, shocks or blow up, in finite time, see for instance Majda - 1978 and C. M. Dafermos, *Hyperbolic conservation laws in continuum physics*, Springer-Verlag, Berlin, 2000.

On the other hand, in many physical examples, thanks to the interplay between the dissipation due to the source term and the hyperbolicity there exist global smooth solutions for a suitable set of initial data.

Example : $u_t + uu_x = -\nu u$ Inviscid Burgers' equation with friction term ($\nu = const. \ge 0$).



Figure: a) $\nu = 0$, b) ν small,c) ν large.



In physical dissipative case the hyperbolic systems are of mixed type, some equations are conservation laws and other ones are real balance laws, i.e., we are in the case in which

$$\mathbf{u}_t + \partial_i \mathbf{F}^i(\mathbf{u}) = \mathbf{F}(\mathbf{u})$$

with

$$\mathbf{F}(\mathbf{u}) \equiv \left(egin{array}{c} 0 \ \mathbf{g}(\mathbf{u}) \end{array}
ight); \qquad \mathbf{g} \in \mathbb{R}^{N-M}.$$

In this case the coupling condition discovered for the first time by Kawashima and Shizuta (K-condition) such that the dissipation present in the second block have effect also to the first block of equation plays a very important role in this case for global existence of smooth solutions.



In fact, if the system of balance law is endowed with a convex entropy law, and it is dissipative, then the K-condition becomes a sufficient condition for the existence of global smooth solutions provided that the initial data are sufficiently smooth (Hanouzet and Natalini 2003, Wen-An Yong 2004, Bianchini, Hanouzet and Natalini 2007)

Theorem (Global Existence)

Assume that the system of balance laws is strictly dissipative and the K-condition is satisfied. Then there exists $\delta > 0$, such that, if $\|\mathbf{u}(x,0)\|_2 \leq \delta$, there is a unique global smooth solution, which verifies

$$\mathsf{u}\in\mathcal{C}^{0}\left([0,\infty);\;H^{2}(\mathbb{R})\cap\mathcal{C}^{1}\left([0,\infty);H^{1}(\mathbb{R}).
ight)$$



Moreover Ruggeri and Serre have proved in the one-dimensional case that the constant states are stable:

Theorem (Stability of Constant State)

Under natural hypotheses of strongly convex entropy, strict dissipativeness, genuine coupling and "zero mass" initial for the perturbation of the equilibrium variables, the constant solution stabilizes

$$\|\mathbf{u}(t)\|_2 = O\left(t^{-1/2}\right).$$

Lou and Ruggeri have observed that the weaker K-condition in which we require the K-condition only for the right eigenvectors corresponding to genuine non linear is a necessary (but not sufficient) condition for the global existence of smooth solutions.



The shock wave structure in a rarefied polyatomic gas is, under some conditions, quite different from the shock wave structure in a rarefied monatomic gas due to the presence of the microscopic internal modes in a polyatomic molecule such as the rotational and vibrational modes. For examples: 1) The shock wave thickness in a rarefied monatomic gas is of the order of the mean free path. On the other hand, owing to the slow relaxation process involving the internal modes, the thickness of a shock wave in a rarefied polyatomic gas is several orders larger than the mean free path. 2) As the Mach number increases from unity, the profile of the shock wave structure in a polyatomic rarefied gas changes from the nearly symmetric profile (Type A) to the asymmetric profile (Type B), and then changes further to the profile composed of thin and thick layers (Type C)



Schematic profiles of the mass density are shown in Figure 3. Such change of the shock wave profile with the Mach number cannot be observed in a monatomic gas.



Figure: Schematic representation of three types of the shock wave structure in a rarefied polyatomic gas, where ρ and x are the mass density and the position, respectively. As the Mach number increases from unity, the profile of the shock wave structure changes from Type A to Type B, and then to Type C that consists of the thin layer Δ and the thick layer Ψ .



In order to explain the shock wave structure in a rarefied polyatomic gas, there have been two well-known approaches. One was proposed by Bethe and Teller and the other is proposed by Gilbarg and Paolucci. Although the Bethe-Teller theory can describe qualitatively the shock wave structure of Type C, its theoretical basis is not clear enough. The Gilbarg-Paolucci theory, on the other hand, cannot explain asymmetric shock wave structure (Type B) nor thin layer (Type C). Recently it was shown that the ET_{14} theory can describe the shock wave structure of all Types A to C in a rarefied polyatomic gas In other words the ET_{14} theory has overcome the difficulties encountered in the previous two approaches. This new approach indicates clearly the usefulness of the ET theory for the analysis of shock wave phenomena.



Shock structure in ET_{14}



S. Taniguchi, T. Arima, T. Ruggeri, and M. Sugiyama Phys. Rev. E (2014), Phys. of Fluids (2014).



Riemann Problem in ET₆



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T. Ruggeri, M. Sugiyama Rational Extended Thermodynamics beyond the Monatomic Gas

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Rational extended thermodynamics (RET) is a thermodynamic theory that is applicable to non-equilibrium phenomena. It is described by differential hyperbolic systems of balance laws with local constitutive equations. As RET has been strictly related to the kinetic theory through the closure method of moment hierarchy associated to the Boltzmann equation, the applicability range of the theory has been restricted within arefele monatomic gases.

This books is dedicated to the recent developments in RET with the aim to explore polyatomic gas, dense gas, and mitture of gases in non-equilibrium. In particular we present the theory of dense gases with 14 fields, which reduces to the Navier-Stokes foruire classical theory in the parabolic limit. Molecular BET with an arbitrary number of field-variables for polyatomic gases is also discussed and the theory is proved to be perfectly compatible with the kinetic theory in which the distribution function depends on a extra variable that takes into account a molecule's internal degrees of freedom. Recent results on mixtures of gases with multi-temperature are presented together with a natural definition of the average temperature. The qualitative analysis and, in particular, the existence of the global smooth solution and the convergence to equilibrium are also studied by taking into account the results are compared in bygether with light statering and heat conduction, and the results are compared with experimental data.

The book represents a valuable resource for applied mathematicians, physicists and engineers, offering powerful models for potential applications like satellites reentering the atmosphere, semiconductors, and nano-scale phenomena.



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