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A method of differential iteration for boundary value problems in extended thermodynamics

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Abstract

The classical well-posed boundary conditions in Navier–Stokes–Fourier (NSF) theory are usually insufficient for the corresponding problems in extended theories of thermodynamics. Some additional boundary data may be needed for the uniqueness of solutions. Owing to the specific structure of systems of balance equations in extended thermodynamics, no such data will be needed in the proposed iterative method by decoupling the system into two subsystems and solving them alternatively with an iterative procedure. One of them can be solved uniquely with the classical boundary conditions, and the other determines the remaining non-equilibrium field variables by direct evaluation. The method does not rely on any criterion for uniqueness, in contrast to various physical criteria proposed for such problems recently. In Part I, the shearing flow with heat conduction is considered as an illustrative numerical example for the proposed method. The condition for convergence based on the estimated error that can easily be checked in numerical iterations is proved in Part II. Furthermore, stability and uniqueness of the numerical iterative solution are also considered. Additional examples are given to substantiate the main results on convergence, stability and uniqueness.

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Part I: General structure of iterative procedure

In extended thermodynamics, there are additional balance equations besides the usual conservation laws of mass, linear momentum, and energy. Consequently some additional boundary data may be needed to solve boundary value problems uniquely. Therefore, for uniqueness, some physical criteria have been proposed for the determination of the additional boundary data, such as minimax principle of entropy production [21,16,2], boundary layer variational principle [5], vanishing critical derivatives at the boundary [3], minimum iterative difference [11,10], and mean fluctuation theory [1]. On the other hand, similar problems have been treated in molecular dynamic simulation [18], direct Monte Carlo simulation [13], and kinetic scheme [20], with additional assumptions on wall–molecular interactions to model the molecular behaviors near the boundary.

In this paper, the problem in question consists of a system of first-order quasi-linear differential equations with boundary conditions that are generally insufficient for uniqueness. Following the idea introduced in [8], we shall

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employ a well-known straightforward numerical approach to solve a complicate system of equations, i.e., decoupling the system into simpler ones and solving alternatively with an iterative procedure. The method proposed do not require additional boundary conditions nor any particular physical or mathematical criterion. It is merely a numerical method of solving the problem mathematically avoiding the difficulties arisen from insufficient boundary conditions. We shall explain our basic idea with a simple example.

This is the example already considered in [21,5,11,20]—one-dimensional stationary heat conduction between two parallel walls. Specifically, we consider the problem in the 14-moment theory of a monatomic ideal gas at rest. In this case, as presented in [11], we have

$$\frac{\mathrm{d}p}{\mathrm{d}x} = 0, \quad \frac{\mathrm{d}q}{\mathrm{d}x} = 0, \tag{1}$$

and

$$q = -\frac{5}{2} Rp\tau \frac{\mathrm{d}\theta}{\mathrm{d}x} - \frac{1}{6}\tau \frac{\mathrm{d}\Delta}{\mathrm{d}x},$$

$$\Delta = -28R\tau \frac{\mathrm{d}(\theta q)}{\mathrm{d}x}. \tag{2}$$

The two equations in (1) are the conservation of linear momentum and energy, respectively, and hence the pressure p and the heat flux q are constants. Relation $(2)_1$ can be regarded as a generalization of Fourier law, with thermal conductivity $\kappa = (5/2)R\tau p$, while $(2)_2$ is the additional balance equation for the non-equilibrium fourth-order moment Δ in the 14-moment theory. The gas constant is denoted by R (the Boltzmann constant divided by the mass of the molecule), and θ is the temperature. The BGK model has been assumed for simplicity, the relaxation time τ is a constant.

The solution of system (1) and (2) can easily be found and it is given by

$$q = q_L,$$

$$\theta = \theta_0 - \frac{q_L}{\kappa} x - \frac{1}{15Rp}(\Delta_0 - D)(\mathrm{e}^{\gamma x} - 1),$$

$$\Delta = D + (\Delta_0 - D)\mathrm{e}^{\gamma x}, \tag{3}$$

where

$$D = \frac{56}{5}\frac{q_L^2}{p}, \quad \gamma = \frac{15}{28}\frac{1}{\tau}\frac{p}{q_L}. \tag{4}$$

In this solution, we have used the following boundary conditions:

$$\theta(0) = \theta_0, \quad q(L) = q_L, \quad \Delta(0) = \Delta_0. \tag{5}$$

With the pressure given in the gas, by prescribing the boundary values of temperature at $x = 0$ and the heat flux at $x = L$, the heat conduction problem is well-posed and it has a (unique) physically meaningful solution, in the classical Fourier theory of heat conduction. However, in the 14-moment case, the solution also depends on the boundary value Δ_0, for which an improperly assigned value may lead to physically irrelevant results. Additional data of this type are referred to as *uncontrollable* boundary data in [11,10].

Alternatively, we consider the problem which consists of the usual conservation laws and the generalized Fourier law with the classical boundary conditions,

$$\text{(I)} \quad \begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}x} = 0, \quad \dfrac{\mathrm{d}q}{\mathrm{d}x} = 0, \\ q = -\dfrac{5}{2} Rp\tau \dfrac{\mathrm{d}\theta}{\mathrm{d}x} - \dfrac{1}{6}\tau \dfrac{\mathrm{d}\Delta}{\mathrm{d}x}, \\ \theta(0) = \theta_0, \quad q(L) = q_L. \end{cases} \tag{6}$$

This boundary value problem can be uniquely solved, once the non-equilibrium moment Δ is given. We can do this by an iterative process. As the initial iterate, we take $\Delta = 0$ at the equilibrium state, and solve the above problem, then the next iterate of Δ can be calculated from the remaining Eq. $(2)_2$,

$$\Delta = -28R\tau \frac{\mathrm{d}(\theta q)}{\mathrm{d}x}. \tag{7}$$

With the new iterate of Δ, Problem (I) can be solved again, and the process can be repeated iteratively.

Indeed, with $\Delta = 0$, we obtain the first iterate for θ and q from Problem (I). It is exactly the same as the classical Fourier solution,

$$q = q_L, \quad \theta = \theta_0 - \frac{2}{5}\frac{q_L}{R\tau p}\, x. \tag{8}$$

Substituting this result into (7), we obtain the first iterate of Δ,

$$\Delta = \frac{56}{5}\frac{q_L^2}{p}. \tag{9}$$

Since the first iterate of Δ is a constant, its derivative vanishes, and the solution for the second iterate of Problem (I) remains unchanged, and so do the subsequent iterates. In other words, the iterative approximation converges trivially and we obtain the solution (8) and (9) uniquely. In particular, we have also determined the boundary value,

$$\Delta_0 = \frac{56}{5}\frac{q_L^2}{p}.$$

Note that the determination of the value Δ_0 does not rely on any additional criterion except the assumption of the initial iterate at the equilibrium state. This result has been obtained in [11] based on the criterion of minimum iterative difference.

The iterative procedure to obtain a unique solution in this problem is a trivial one. However, the idea of decoupling the system into two subsystems that can be solved with classical boundary conditions by iterative approximation can easily be adopted to more general problems in extended thermodynamics.

1. A method of differential iteration

One can always split the system of governing equations in extended thermodynamic theory into two subsystems (I) and (II). System (I) consists of the governing equations for the corresponding problem in the classical NSF theory, i.e., the conservation laws and the equations equivalent to Navier–Stokes law for the stress tensor T and the Fourier law for the heat flux $\boldsymbol{q}$. And System (II) consists of the balance equations for the remaining non-equilibrium field variables, say, $\boldsymbol{M}_a$ for $a = 1, \ldots, m$. More specifically, for boundary value problems—of time-independent processes, System (I) and (II) can be written in the form:

$$\text{(I)} \quad \begin{cases} \operatorname{div}(\rho \boldsymbol{v}) = 0, \\ \operatorname{div}(\rho \boldsymbol{v} \otimes \boldsymbol{v} - T) = 0, \\ \operatorname{div}(\rho(\varepsilon + \frac{1}{2}\boldsymbol{v}\cdot\boldsymbol{v})\boldsymbol{v} + \boldsymbol{q} - T\boldsymbol{v}) = 0, \\ T = \hat{T}(\rho, \boldsymbol{v}, \theta, \nabla\rho, \nabla\theta, \nabla\boldsymbol{v}, T, \boldsymbol{q}, \boldsymbol{M}_a, \nabla T, \nabla\boldsymbol{q}, \nabla\boldsymbol{M}_a), \\ \boldsymbol{q} = \hat{\boldsymbol{q}}(\rho, \boldsymbol{v}, \theta, \nabla\rho, \nabla\theta, \nabla\boldsymbol{v}, T, \boldsymbol{q}, \boldsymbol{M}_a, \nabla T, \nabla\boldsymbol{q}, \nabla\boldsymbol{M}_a), \end{cases}$$

$$\text{(II)} \quad \begin{cases} \text{for } a = 1, \ldots, m, \\ \boldsymbol{M}_a = \hat{\boldsymbol{M}}_a(\rho, \boldsymbol{v}, \theta, \nabla\rho, \nabla\theta, \nabla\boldsymbol{v}, T, \boldsymbol{q}, \boldsymbol{M}_a, \nabla T, \nabla\boldsymbol{q}, \nabla\boldsymbol{M}_a), \end{cases}$$

owing to the structure of additional balance equations in extended theory of thermodynamics (see Chapter 8 of [7]). And according to that, in general, the functions $\hat{T}$, $\hat{\boldsymbol{q}}$, and $\hat{\boldsymbol{M}}_a$ are linear in the gradients and the internal energy ε is a function of (ρ, θ).

1.1. Iterative approximation of the decoupled system

We shall decouple System (I) from System (II) by the following iterative scheme so that System (I) becomes a closed system of differential equations for the determination of the fields $(\rho, \boldsymbol{v}, \theta, T, \boldsymbol{q})$—similar to the classical Navier–Stokes–Fourier (NSF) theory.

$$
\text{(I)}\quad
\begin{cases}
\operatorname{div}(\overset{(n)}{\rho}\ \overset{(n)}{\boldsymbol{v}}) = 0,\\
\operatorname{div}(\overset{(n)}{\rho}\ \overset{(n)}{\boldsymbol{v}} \otimes \overset{(n)}{\boldsymbol{v}} - \overset{(n)}{T}) = 0,\\
\operatorname{div}(\overset{(n)}{\rho}(\overset{(n)}{\varepsilon} + \tfrac{1}{2}\ \overset{(n)}{\boldsymbol{v}} \cdot \overset{(n)}{\boldsymbol{v}})\ \overset{(n)}{\boldsymbol{v}} + \overset{(n)}{\boldsymbol{q}} - \overset{(n)}{T}\ \overset{(n)}{\boldsymbol{v}}) = 0,\\
\overset{(n)}{T} = \hat{T}(\overset{(n)}{\rho}, \overset{(n)}{\boldsymbol{v}}, \overset{(n)}{\theta}, \nabla\overset{(n)}{\rho}, \nabla\overset{(n)}{\boldsymbol{v}}, \nabla\overset{(n)}{\theta}, \overset{(n-1)}{T}, \overset{(n-1)}{\boldsymbol{q}}, \overset{(n-1)}{\boldsymbol{M}_a}, \nabla\overset{(n-1)}{T}, \nabla\overset{(n-1)}{\boldsymbol{q}}, \nabla\overset{(n-1)}{\boldsymbol{M}_a}),\\
\overset{(n)}{\boldsymbol{q}} = \hat{\boldsymbol{q}}(\overset{(n)}{\rho}, \overset{(n)}{\boldsymbol{v}}, \overset{(n)}{\theta}, \nabla\overset{(n)}{\rho}, \nabla\overset{(n)}{\boldsymbol{v}}, \nabla\overset{(n)}{\theta}, \overset{(n-1)}{T}, \overset{(n-1)}{\boldsymbol{q}}, \overset{(n-1)}{\boldsymbol{M}_a}, \nabla\overset{(n-1)}{T}, \nabla\overset{(n-1)}{\boldsymbol{q}}, \nabla\overset{(n-1)}{\boldsymbol{M}_a}),
\end{cases}
$$

$$
\text{(II)}\quad
\begin{cases}
\text{for } a = 1, \ldots, m,\\
\overset{(n)}{\boldsymbol{M}_a} = \hat{\boldsymbol{M}}_a(\overset{(n)}{\rho}, \overset{(n)}{\boldsymbol{v}}, \overset{(n)}{\theta}, \nabla\overset{(n)}{\rho}, \nabla\overset{(n)}{\boldsymbol{v}}, \nabla\overset{(n)}{\theta}, \overset{(n)}{T}, \overset{(n)}{\boldsymbol{q}}, \overset{(n-1)}{\boldsymbol{M}_a}, \nabla\overset{(n)}{T}, \nabla\overset{(n)}{\boldsymbol{q}}, \nabla\overset{(n-1)}{\boldsymbol{M}_a}).
\end{cases}
$$

The iterative procedure is initiated at the equilibrium state,

$$\overset{(0)}{T}_a = 0, \quad \overset{(0)}{\boldsymbol{q}}_a = 0, \quad \overset{(0)}{\boldsymbol{M}_a} = 0.$$

Note that initializing with the equilibrium state is equivalent to starting the iteration from the solution of the classical NSF theory. In this iterative scheme, at every iterative step $n = 1, 2, 3, \ldots$, the terms involving $(n-1)$th iterates in System (I) can be regarded as supply terms in the corresponding system of NSF theory. Therefore, we can assume that it can be solved uniquely for the fields $(\rho, \boldsymbol{v}, \theta, T, \boldsymbol{q})$ with the classical well-posed boundary conditions for NSF theory. Then from System (II), the non-equilibrium fields $\boldsymbol{M}_a$ can be determined by direct evaluation. In this manner, classical (NSF) boundary conditions are sufficient to solve boundary value problems in extended thermodynamics without any criterion for the determination of uncontrollable boundary data.

We emphasize that the system of differential equations are valid in the interior points only. However, we shall assume that all fields are smooth up to the boundary so that the boundary value is defined as the one-side limit from the interior points. In other words, the boundary values are not necessary the values at the walls if some slip conditions or some wall–molecular interaction assumptions are adopted.

1.2. Iterative scheme with decreasing weight

System (II) can in general be put into a fixed-point problem of the form:

$$\boldsymbol{u} = G\boldsymbol{u}, \quad \boldsymbol{u} \in X,$$

where G is a non-linear differential operator on some function space X. The iterative scheme proposed can then be written as

$$\boldsymbol{u}_n = G\boldsymbol{u}_{n-1}, \quad n = 1, 2, 3 \ldots. \tag{10}$$

It is well-known that this simple iterative scheme converges uniquely to a fixed point if the operator G is contractive, i.e., for any $\boldsymbol{u}, \boldsymbol{v} \in X$,

$$\|G\boldsymbol{u} - G\boldsymbol{v}\| \leqslant C\|\boldsymbol{u} - \boldsymbol{v}\| \quad \text{for } C < 1.$$

However, our differential operators are not contractive, and more generally, they are unbounded.

Note that the iterative scheme (10) is similar to the *Maxwellian iteration* (denominated by Truesdell who also referred to it as *differential iteration* [6,23]) in the kinetic theory of gases, to obtain approximations of Fourier law of

heat conduction and Navier–Stokes law of viscous stress from Grad's moment equations [4]. Usually only few iterations are considered without any assurance of convergence.

To circumvent the unboundedness of the differential operators, we propose a more conservative scheme with smaller corrections at each iterative step by introducing a variable weight,

$$\boldsymbol{u}_n = w_n G\boldsymbol{u}_{n-1} + (1 - w_n)\boldsymbol{u}_{n-1} \quad \text{for } 0 < w_n \leqslant 1, \quad n = 1, 2, 3, \ldots. \tag{11}$$

This scheme can also be rewritten as

$$w_n(G\boldsymbol{u}_{n-1} - \boldsymbol{u}_{n-1}) = \boldsymbol{u}_n - \boldsymbol{u}_{n-1}. \tag{12}$$

We shall take the weights w_n to be monotonically decreasing in n, specifically, $w_n = 1/n$, such that $w_n \to 0$ when $n \to \infty$.

From (12), we can define the *estimated error* of the fixed point of G at the nth approximation in some norm by

$$\text{Err}\,(n) = \|G\boldsymbol{u}_{n-1} - \boldsymbol{u}_{n-1}\| = \frac{\|\boldsymbol{u}_n - \boldsymbol{u}_{n-1}\|}{w_n}, \tag{13}$$

which estimates the error of approximate solution to the equation $G\boldsymbol{u} = \boldsymbol{u}$. Accordingly, the convergence of the scheme is to require that the following condition be verified:

$$\lim_{n\to\infty} \text{Err}\,(n) = 0. \tag{14}$$

This condition can conveniently be checked in numerical computations from the last expression of (13).

In the following we shall demonstrate the viability of the proposed iterative method to shearing flows with heat conduction, without any additional physical criteria, for the boundary value problem with insufficient boundary data, i.e., only classical boundary conditions of the NSF theory. The convergence and uniqueness of numerical iterative approximation will be considered in Part II.

2. One-dimensional shearing flow with heat conduction

We shall consider steady processes, in which all fields depend only on y, and the velocity field is in the x-direction. In the 13-moment theory (with BGK model), these have been treated in [10] and the basic equations are given by the following system of differential equations:

$$\frac{\mathrm{d}T_{\langle xy\rangle}}{\mathrm{d}y} = 0, \quad \frac{\mathrm{d}}{\mathrm{d}y}(p - T_{\langle yy\rangle}) = 0, \quad \frac{\mathrm{d}}{\mathrm{d}y}(q_y - T_{\langle xy\rangle}v_x) = 0,$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{2}{5}q_x + (p - T_{\langle yy\rangle})v_x\right) = \frac{1}{\tau}T_{\langle xy\rangle},$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{4}{15}q_y + \frac{4}{3}T_{\langle xy\rangle}v_x\right) = -\frac{1}{\tau}T_{\langle xx\rangle},$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(\frac{8}{15}q_y + \frac{2}{3}T_{\langle xy\rangle}v_x\right) = \frac{1}{\tau}T_{\langle yy\rangle},$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(7\,R\,\theta T_{\langle xy\rangle} - \frac{14}{5}q_y v_x + 3T_{\langle xy\rangle}v_x^2\right) = \frac{2}{\tau}(q_x - T_{\langle xx\rangle}v_x),$$

$$\frac{\mathrm{d}}{\mathrm{d}y}\left(5\,R\,p\,\theta - 7R\,\theta T_{\langle yy\rangle} + \frac{4}{5}q_x v_x - T_{\langle yy\rangle}v_x^2 + p\,v_x^2\right) = -\frac{2}{\tau}(q_y - T_{\langle xy\rangle}v_x), \tag{15}$$

for the determination of eight fields $(p, v_x, \theta, T_{\langle xx\rangle}, T_{\langle yy\rangle}, T_{\langle xy\rangle}, q_x, q_y)$.

2.1. NSF theory

Before trying to analyze the above system, let us first consider the corresponding problem in the NSF theory, for which the basic equations read

$$\frac{\mathrm{d}p}{\mathrm{d}y}=0,\quad \frac{\mathrm{d}T_{\langle xy\rangle}}{\mathrm{d}y}=0,\quad \frac{\mathrm{d}}{\mathrm{d}y}(q_y-T_{\langle xy\rangle}v_x)=0,$$

$$T_{\langle xy\rangle}=\mu\frac{\partial v_x}{\partial y},\quad q_y=-\kappa\frac{\partial\theta}{\partial y}.$$

These are the conservation laws of linear momentum and energy, and the laws of Navier–Stokes and Fourier, where $\mu=p\tau$ and $\kappa=(5/2)Rp\tau$.

We shall consider one-dimensional flows between two movable plates ($0\leqslant y\leqslant L$) with constant pressure P of the gas given, and supplemented with two typical types of boundary conditions:

$$\begin{aligned}&\text{Type A:}\quad \text{at } y=0:\quad v_x=v_0,\quad \theta=\theta_0;\\ &\qquad\qquad\ \text{at } y=L:\quad T_{\langle xy\rangle}=S,\quad q_y-Sv_x=Q.\end{aligned}\tag{16}$$

$$\begin{aligned}&\text{Type B:}\quad \text{at } y=0:\quad v_x=v_0,\quad \theta=\theta_0;\\ &\qquad\qquad\ \text{at } y=L:\quad v_x=v_L,\quad \theta=\theta_L.\end{aligned}\tag{17}$$

These conditions are well-posed, and the solutions for both types of the problem can easily be found.

2.2. Iterative scheme

For numerical calculations, it is convenient to introduce the dimensionless variables,

$$y'=\frac{y}{L},\quad \theta'=\frac{\theta}{\theta_0},\quad v_x'=\frac{v_x}{\sqrt{R\theta_0}},$$

$$p'=\frac{p}{P},\quad T_{\langle ij\rangle}'=\frac{T_{\langle ij\rangle}}{P},\quad q_i'=\frac{q_i}{P\sqrt{R\theta_0}},$$

and the Knudsen number,

$$\mathtt{Kn}=\frac{\tau}{L}\sqrt{R\theta_0}.$$

We can now split the system (15), in dimensionless forms (without the primes for simplicity), into two subsystems with the following iterative scheme:

$$\text{(I)}\begin{cases}\overset{(n)}{T}_{\langle xy\rangle}=S,\quad \overset{(n)}{p}-\overset{(n-1)}{T}_{\langle yy\rangle}=P,\quad \overset{(n)}{q}_y-\overset{(n)}{T}_{\langle xy\rangle}\overset{(n)}{v}_x=Q,\\ \overset{(n)}{T}_{\langle xy\rangle}=\mathtt{Kn}\dfrac{\mathrm{d}}{\mathrm{d}y}\left(P\overset{(n)}{v}_x+\dfrac{2}{5}\overset{(n-1)}{q}_x\right),\\ \overset{(n)}{q}_y=\overset{(n)}{T}_{\langle xy\rangle}\overset{(n)}{v}_x-\dfrac{1}{2}\mathtt{Kn}\dfrac{\mathrm{d}}{\mathrm{d}y}\left(5P\overset{(n)}{\theta}+P\overset{(n)}{v}_x{}^2-2\overset{(n)}{\theta}\overset{(n-1)}{T}_{\langle yy\rangle}+\dfrac{4}{5}\overset{(n-1)}{q}_x\overset{(n)}{v}_x\right),\end{cases}\tag{18}$$

$$\text{(II)}\begin{cases}\overset{(n)}{T}_{\langle xx\rangle}=-w_n\,\mathtt{Kn}\dfrac{\mathrm{d}}{\mathrm{d}y}\left(\dfrac{4}{15}\overset{(n)}{q}_y+\dfrac{4}{3}\overset{(n)}{T}_{\langle xy\rangle}\overset{(n)}{v}_x\right)+(1-w_n)\overset{(n-1)}{T}_{\langle xx\rangle},\\ \overset{(n)}{T}_{\langle yy\rangle}=w_n\,\mathtt{Kn}\dfrac{\mathrm{d}}{\mathrm{d}y}\left(\dfrac{8}{15}\overset{(n)}{q}_y+\dfrac{2}{3}\overset{(n)}{T}_{\langle xy\rangle}\overset{(n)}{v}_x\right)+(1-w_n)\overset{(n-1)}{T}_{\langle yy\rangle},\\ \overset{(n)}{q}_x-\overset{(n)}{T}_{\langle xx\rangle}\overset{(n)}{v}_x=w_n\dfrac{\mathtt{Kn}}{2}\dfrac{\mathrm{d}}{\mathrm{d}y}\left(7\overset{(n)}{\theta}\overset{(n)}{T}_{\langle xy\rangle}-\dfrac{14}{5}\overset{(n)}{q}_y\overset{(n)}{v}_x+3\overset{(n)}{T}_{\langle xy\rangle}\overset{(n)}{v}_x{}^2\right)\\ \qquad\qquad\qquad+(1-w_n)\left(\overset{(n-1)}{q}_x-\overset{(n-1)}{T}_{\langle xx\rangle}\overset{(n)}{v}_x\right),\end{cases}\tag{19}$$

and

$$\overset{(0)}{T}_{\langle xx\rangle} = 0, \quad \overset{(0)}{T}_{\langle yy\rangle} = 0, \quad \overset{(0)}{q}_x = 0.$$

Note that System (I) is equivalent to the system of NSF theory and it can be solved uniquely by the prescribed total pressure P and the boundary conditions (16) or (17).

Iterative method proceeds at every iterative step, by firstly solving System (I) for $\overset{(n)}{\theta}$, $\overset{(n)}{p}$, $\overset{(n)}{v}_x$, $\overset{(n)}{q}_y$, and $\overset{(n)}{T}_{\langle xy\rangle}$ with boundary condition (16) or (17). Then from System (II), $\overset{(n)}{T}_{\langle xx\rangle}$, $\overset{(n)}{T}_{\langle yy\rangle}$, and $\overset{(n)}{q}_x$ can be determined, noting that no additional boundary conditions are needed.

One can easily show, from $(19)_{1,2}$ by the use of $(18)_3$, that $\overset{(n)}{T}_{\langle xx\rangle} = -\frac{4}{3}\overset{(n)}{T}_{\langle yy\rangle}$. Therefore, System (II) essentially determines the fields $(\overset{(n)}{T}_{\langle xx\rangle}, \overset{(n)}{q}_x)$. Let $\boldsymbol{u} = (T_{\langle xx\rangle}, q_x)$ and

$$\|\boldsymbol{u}\| = \left(\int_0^1 (T_{\langle xx\rangle}^2 + q_x^2)\,\mathrm{d}x\right)^{1/2}$$

be the norm to be used in numerical calculations for the estimated error.

2.3. Numerical examples

For the constant total pressure P of the gas given, we shall consider two types of well-posed boundary conditions given by (16) and (17) for the NSF theory. These boundary conditions are sufficient for the determination of solutions uniquely in the 13-moment theory by the weighted iterative approximation.

The numerical computations can easily be handled. For Type A problem, System (I) can be solved by direct numerical integrations, and for Type B problem, implicit finite difference method is employed. By the smoothness assumption, extrapolation formulas from interior points are used to determine the values at the end points. In the calculation, a uniform mesh is used for the domain [0, 1] with mesh size $\frac{1}{50}$.

The following examples will be considered for comparison with the corresponding ones treated in [10] and the dimensionless data are chosen accordingly. The physical values of the reference quantities used in these examples are given by $R = 207.83\ (\mathrm{m/s})^2\mathrm{K}^{-1}$ for argon gas, $\tau = 10^{-5}$ s, $\theta_0 = 300$ K, $P = 100$ Pa, and $L = 0.02$ m. The corresponding Knudsen number is $\mathtt{Kn} = 0.124849$.

Example 1. We consider a plane shearing flow from Example 1 in [10]. The boundary conditions in dimensionless data are given by

$$v_x(0) = 0, \quad \theta(0) = 1, \quad S = 0.1, \quad Q = -0.120145.$$

Since the velocity and the temperature at $x = 1$ are treated as uncontrollable boundary data in [10], their values will be calculated together with the estimated error at various iterate steps. They are listed below.

n	$\overset{(n)}{v}_x(1)$	$\overset{(n)}{\theta}(1)$	Err (n)	$\|\boldsymbol{u}_n\|$
10	0.810055	1.253495	2.2282×10^{-5}	3.3229×10^{-2}
100	0.810061	1.253496	2.0728×10^{-6}	3.3243×10^{-2}
1000	0.810062	1.253496	2.0994×10^{-7}	3.3245×10^{-5}
2000	0.810062	1.253496	1.0561×10^{-7}	3.3245×10^{-2}

The iterative approximation seems to converge quickly and we obtain the approximated values in physical units: $v_x(L) \approx 202.27\ \mathrm{ms}^{-1}$ and $\theta(L) \approx 376.05$ K, which are in perfect agreement with $v_x(L) \approx 202.27\ \mathrm{ms}^{-1}$ and $\theta(L) \approx 376.10$ K obtained in [10].

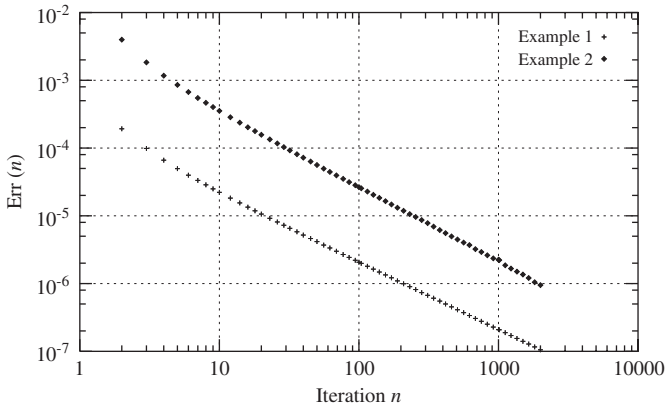

Fig. 1. Verification of numerical convergence condition: Error estimate Err (n) vs. iteration n in log–log scale.

From the above table, we note that at the iterate $n = 10$, the relative error, i.e., Err $(n)/\|\boldsymbol{u}_n\|$, of solving System (II) is less than 0.1%. Therefore, although we have carried the iterations up to very large n in order to show the tendency of convergence, a few iterations may give a satisfactory result for practical purpose.

Example 2. For the plane Couette flow from Example 2 of [10], the boundary conditions are given by

$$v_x(0) = -0.800966, \quad v_x(1) = 0.800966, \quad \theta(0) = 1, \quad \theta(1) = 1.$$

To show the sequence of the iterative approximation, we give the values of the shear stress and the heat flux at $x = 1$ in the following list:

n	$\overset{(n)}{T}_{\langle xy\rangle}(1)$	$\overset{(n)}{q}_y(1)$	Err (n)	$\|\boldsymbol{u}_n\|$
10	0.191637	0.153494	3.5345×10^{-4}	6.4675×10^{-2}
100	0.191690	0.153537	2.6528×10^{-5}	6.4434×10^{-2}
1000	0.191694	0.153541	2.2513×10^{-6}	6.4414×10^{-2}
2000	0.191694	0.153541	9.5133×10^{-7}	6.4413×10^{-2}

In terms of physical value, we obtain $S = T_{\langle xy\rangle}(L) \approx 19.17\,\text{Pa}$ and $q_y(L) \approx 3.834 \times 10^3\,\text{Wm}^{-2}$. Moreover, with $v_x(L) = 200\,\text{ms}^{-1}$ given, $Q \approx 0\,\text{Wm}^{-2}$. The results are also in perfect agreement with those obtained in [10]. Moreover, the relative error at $n = 10$ is less than 1% in this case.

Remarks. Examples 1 and 2 are taken from Ref. [10], and since we have shown that the present method leads to the same results, no detailed information about the solutions are given here. The interested reader can refer to [10] for numerical solutions.

Although the above tables might give a fair idea of numerical convergence, to be more specific, in Fig. 1 the estimated error Err (n) is plotted against the iteration n in log–log scale for both Examples 1 and 2. It shows 'numerically' that condition (14) is satisfied, i.e., Err $(n) \to 0$ as $n \to \infty$.

Furthermore, it is quite natural to argue that the iterative solution might depend on the initial iterate. In order to see that we have simulated the above problem with some non-trivial initial iterates (functions such as $(1 - x)$, $\sin(\pi x)$ or $\exp(1 - x)$, etc.) and all those results converge to the same solution with null initial iterates as the number of iterations increases. This unexpected observation enhances, beyond physical intuition, the rational of starting the iterative approximation with the null initial iterates. We shall discuss the uniqueness of numerical solution in Part II.

3. Remarks: on some previous works with continuum approach

In the pioneering paper [21] on the determination of uncontrollable boundary data in extended thermodynamics, the *minimax* principle was proposed, which as well as boundary layer variational principle [5] proposed later, is based on the assumption that the body adjusts itself in such a manner as to minimize its entropy production in a "certain" way. Such a principle not only depends on the way the minimization functional is defined, it also leads to solutions inconsistent with our physical intuition as pointed out in [11].

On the other hand, the results obtained by the use of minimum iterative difference [10] agree with the present results as seen from the examples. However, this criterion involves evaluations of the approximate solutions based on the process akin to the Maxwellian iteration in the kinetic theory, for which calculation of higher iterates become prohibitively complicated even with suitable computer software. The present method also involves similar iterative process, although of quite different nature, and is quite simple to implement in numerical algorithm, and hence it can be easily adopted in more general situations.

Part II: Convergence and uniqueness of numerical solutions

For solving boundary value problems with classical boundary conditions in extended thermodynamics, in Part I an iterative method with gradually decreasing weight is proposed. Now, convergence of iterative approximations based on the estimated errors, which can easily be checked in numerical calculations will be proved (see also [12]). Moreover, for systems of linear differential equations with constant coefficients, we shall also prove that the numerical solution is uniquely obtained in the limit, independent of any particular choice of initial iterates, provided that the iterative scheme converges.

Examples on heat conduction of ideal gases in Grad's moment theory [4] are discussed to verify convergence and uniqueness of the iterative numerical solutions. This problem has been considered in several recent studies (see [21,2,5,3,11]) of boundary value problems in moment equations by postulating some *additional* physical criteria in order to obtain a (unique) solution.

Since differential equations are valid in the interior points only, the solutions are assumed to be smooth up to the boundary, so that the boundary values are defined as the one-side limits from interior points. In other words, the boundary values are not necessary the values assigned at the wall. To account for possible slip conditions considered in Maxwell's kinetic theory, some wall conditions relating the boundary values of the solution and the values assigned at the wall will be postulated.

4. Convergence of iterative approximation

Let G be a differential operator on some function space X with norm denoted by $\|\cdot\|$. We call $\boldsymbol{u} \in X$ a *fixed point* of G, if

$$\boldsymbol{u} = G\boldsymbol{u}.$$

We have proposed the following weighted iterative scheme (11) for the above fixed point problem:

$$\boldsymbol{u}_n = w_n G\boldsymbol{u}_{n-1} + (1 - w_n)\boldsymbol{u}_{n-1}, \quad n = 1, 2, 3, \ldots, \tag{20}$$

where the weight is given by

$$w_n = \frac{1}{n^k} \quad \text{for} \quad k \geqslant 1.$$

In Part I, we have taken more specifically for $k = 1$.

The *estimated error* at the nth approximation is defined as

$$\mathrm{Err}\,(n) = \|G\boldsymbol{u}_{n-1} - \boldsymbol{u}_{n-1}\|, \tag{21}$$

which estimates the error of the approximate solution as the fixed point of the operator G. Accordingly, we have the following theorem for convergence.

Theorem 1. *Let X be a complete normed space, and G be an operator on X. For the weighted iterative approximation,*

$$\boldsymbol{u}_n = w_n G\boldsymbol{u}_{n-1} + (1 - w_n)\boldsymbol{u}_{n-1}, \tag{22}$$

with

$$w_n = \frac{1}{n^k}, \quad k > 1,$$

if $\lim_{n\to\infty} \mathrm{Err}\,(n) = 0$, *then the iterative approximation* $\{u_n\}$ *converges in* X *and* $\lim_{n\to\infty} \|G\boldsymbol{u}_n - \boldsymbol{u}_n\| = 0$.

Proof. First of all, if $\lim_{n\to\infty} \mathrm{Err}\,(n) = 0$ holds, by definition (21), it implies $\lim_{n\to\infty} \|G\boldsymbol{u}_n - \boldsymbol{u}_n\| = 0$. Therefore, we only have to show that the sequence $\{\boldsymbol{u}_n\}$ converges in X. We shall do it by proving that it is a Cauchy sequence. Let $A_n = \|\boldsymbol{u}_n - \boldsymbol{u}_{n-1}\|$.

From (13) and (21), the condition ($\lim_{n\to\infty} \mathrm{Err}\,(n) = 0$) leads to

$$\lim_{n\to\infty} \frac{A_n}{1/n^k} = \lim_{n\to\infty} \frac{\|\boldsymbol{u}_n - \boldsymbol{u}_{n-1}\|}{w_n} = 0.$$

Since the series $\sum_{n=1}^{\infty} \frac{1}{n^k}$ converges for $k > 1$, by comparison, the series $\sum_{n=1}^{\infty} A_n$ also converges. Therefore, the sequence of its partial sum $S_n = A_1 + A_2 + \cdots + A_n$ is a Cauchy sequence, i.e., $|S_m - S_n| \to 0$ when $m, n \to \infty$.

On the other hand, for $m > n > 0$, we have

$$\begin{aligned}\|\boldsymbol{u}_m - \boldsymbol{u}_n\| &= \|\boldsymbol{u}_m - \boldsymbol{u}_{m-1} + \boldsymbol{u}_{m-1} - \boldsymbol{u}_{m-2} + \cdots + \boldsymbol{u}_{n+1} - \boldsymbol{u}_n\| \\ &\leqslant \|\boldsymbol{u}_m - \boldsymbol{u}_{m-1}\| + \|\boldsymbol{u}_{m-1} - \boldsymbol{u}_{m-2}\| + \cdots + \|\boldsymbol{u}_{n+1} - \boldsymbol{u}_n\| \\ &= A_m + A_{m-1} + \cdots + A_{n+1} = S_m - S_n.\end{aligned}$$

Consequently $\|\boldsymbol{u}_m - \boldsymbol{u}_n\| \to 0$ when $m, n \to \infty$, which proves that it is a Cauchy sequence. □

The case with $k = 1$ can also be proved under a slightly restrictive condition on the limit of $\mathrm{Err}\,(n)$ (for both cases, $k > 1$ and $k = 1$, the proof is given in Theorem 3.1 of [12]). However, there are hardly any significant differences between numerical results with $k = 1$ and with k slightly greater than 1, say, $k = 1.001$ for example. Therefore, for practical purpose, in this paper, we shall only consider the iterative approximation with weight $w_n = 1/n$ from now on.

5. Differential iteration of linear differential equation

We shall show that the above numerical scheme has some interesting properties concerning stability and uniqueness of numerical solutions. To be more specific, we shall consider the following linear differential equation:

$$P(x)\boldsymbol{u}' + Q(x)\boldsymbol{u} = \boldsymbol{r}(x),$$

where $\boldsymbol{u}, \boldsymbol{r} : [a, b] \to \mathbb{R}$ and $P, Q : [a, b] \to \mathbb{R}$. The prime ($'$) denotes the derivative with respect to x. We are interested in finding a particular solution of the system with no boundary condition.

The equation can conveniently be put into a fixed-point problem of the form:

$$\boldsymbol{u} = G\boldsymbol{u} = \boldsymbol{g} + \boldsymbol{h}\,\boldsymbol{u}', \tag{23}$$

where $\boldsymbol{g}, \boldsymbol{h} : [a, b] \to \mathbb{R}$.

Theoretically if a boundary value, $\boldsymbol{u}(a)$ or $\boldsymbol{u}(b)$, is given, there exists a unique solution of the differential equation $\boldsymbol{u} = \boldsymbol{g} + D\boldsymbol{u}$. However, in the method of differential iteration, no boundary value is needed and the fixed point of G may depend on the initial iterate $\boldsymbol{u}_0$ theoretically. Nevertheless, unlike the theoretical predictions, by numerical stability analysis, we shall prove the uniqueness of numerical solutions independent of any particular choice of initial iterate.

5.1. Numerical scheme

Let $a = x_0 < x_1 < \cdots < x_{m-1} < x_m = b$ be a division of the interval $[a, b]$ into evenly spaced subintervals of length Δx and denote $\boldsymbol{u}(x_j) = \boldsymbol{u}_j$. The derivative will be approximated with a central difference scheme,

$$\boldsymbol{u}'(x_j) = \frac{1}{2\Delta x}(S_+ - S_-)\boldsymbol{u}_j,$$

where S_+ and S_- are the shift operators defined by

$$S_+\boldsymbol{u}_j = \boldsymbol{u}_{j+1}, \qquad S_-\boldsymbol{u}_j = \boldsymbol{u}_{j-1}.$$

Consider the fixed-point problem

$$\boldsymbol{u} = G\boldsymbol{u} = \boldsymbol{g} + \boldsymbol{h}\,\boldsymbol{u}',$$

with $\boldsymbol{g}$, $\boldsymbol{h} \in C^\infty([a, b], \mathbb{R})$ and $\boldsymbol{h} \neq 0$ in $[a, b]$. Denoting $\boldsymbol{u}_n(x_j) = \boldsymbol{u}_j^n$, we can write the numerical scheme of the weighted iterative approximation as

$$\boldsymbol{u}_j^n = w_n\left(\boldsymbol{g}_j + \frac{\boldsymbol{h}_j}{2\Delta x}(S_+ - S_-)\boldsymbol{u}_j^{n-1}\right) + (1 - w_n)\boldsymbol{u}_j^{n-1} = w_n\boldsymbol{g}_j + H_n\boldsymbol{u}_j^{n-1}, \tag{24}$$

where

$$H_n\boldsymbol{u}_j^{n-1} = (1 - w_n)\boldsymbol{u}_j^{n-1} + w_n\frac{\boldsymbol{h}_j}{2\Delta x}(S_+ - S_-)\boldsymbol{u}_j^{n-1}. \tag{25}$$

Note that the homogeneous operator H_n is a linear operator.

5.2. Instability of homogeneous solutions

We shall consider the case that the coefficient function $\boldsymbol{h}(x)$ is constant for $x \in [a, b]$ and the weight $w_n = 1/n$. We shall prove that any homogeneous solution, i.e., satisfying $\boldsymbol{u} = \boldsymbol{h}\,\boldsymbol{u}'$, tends to zero for any initial iterate $\boldsymbol{u}_0$ in the numerical scheme. We have the following theorem (see Theorem 4.1 in [12]),

Theorem 2. *For the homogeneous differential equation with constant coefficient, $\boldsymbol{u}(x) = \boldsymbol{h}\,\boldsymbol{u}'(x)$, $x \in [a, b]$, $\boldsymbol{h} \neq 0$, consider the numerical iterative approximation with $w_n = 1/n$,*

$$\boldsymbol{u}_n = H_n\boldsymbol{u}_{n-1}, \quad H_n = (1 - w_n) + w_n\frac{\boldsymbol{h}}{2\Delta x}(S_+ - S_-). \tag{26}$$

For any initial iterate $\boldsymbol{u}_0$, it follows that $\lim_{n\to\infty}\boldsymbol{u}_n = 0$.

Proof. We shall apply Neumann finite Fourier analysis [17,19] to the numerical scheme (26). Let the *discrete Fourier transform* of the grid function $\boldsymbol{u}$ be defined by ($i = \sqrt{-1}$)

$$\hat{\boldsymbol{u}}(\xi) = \sum_j \boldsymbol{u}_j e^{ij\xi}, \quad 0 \leqslant \xi < \pi.$$

It leads to

$$\widehat{S_+\boldsymbol{u}} = e^{-i\xi}\hat{\boldsymbol{u}}, \quad \widehat{S_-\boldsymbol{u}} = e^{i\xi}\hat{\boldsymbol{u}}.$$

From (26) it follows, with the identity $\sin\xi = (e^{i\xi} - e^{-i\xi})/2i$, that

$$\begin{aligned}\hat{\boldsymbol{u}}_n &= \left(1 - w_n + w_n\frac{\boldsymbol{h}}{2\Delta x}(e^{-i\xi} - e^{i\xi})\right)\hat{\boldsymbol{u}}_{n-1} \\ &= \left(1 - w_n - i\,w_n\frac{\boldsymbol{h}}{\Delta x}\sin\xi\right)\hat{\boldsymbol{u}}_{n-1},\end{aligned}$$

and leads to (for details see [12])

$$|\hat{\boldsymbol{u}}_n|^2 = R_n(\lambda)|\hat{\boldsymbol{u}}_0|^2,$$

where

$$R_n(\lambda) = \prod_{k=1}^{n} \frac{(k-1)^2+\lambda}{k^2}, \quad \lambda = \left(\frac{\boldsymbol{h}}{\Delta x}\sin\xi\right)^2 \geqslant 0.$$

From a numerical plot, one can easily see that $\lim_{n\to\infty} R_n(\lambda) = 0$ for any $\lambda \geqslant 0$, (for a direct proof see Lemma 4.1 of [12]). Therefore, $\lim_{n\to\infty}\hat{\boldsymbol{u}}_n = 0$, which implies $\lim_{n\to\infty}\boldsymbol{u}_n = 0$ and the theorem is proved. □

From this theorem, we may say that the only *stable* numerical solution of $\boldsymbol{u} = \boldsymbol{h}\,\boldsymbol{u}'$ is the null solution $\boldsymbol{u}(x) = 0$. Indeed, suppose that $\boldsymbol{u}_0$ is an exact solution of the equation $\boldsymbol{u} = \boldsymbol{h}\,\boldsymbol{u}'$. Since in numerical calculations the derivative is approximated by the finite difference, we may regard this as a small perturbation of the function $\boldsymbol{u}_0$, and therefore, it does not satisfy the equation exactly. In this sense, the fact that small perturbations bring the exact solution $\boldsymbol{u}_0$ down to zero as $n \to \infty$ may be stated as *instability* of homogeneous solutions in the numerical iterative approximation.

We have seen that $R_n(\lambda)$ is bounded for $\lambda \geqslant 0$ and tends to zero as n tends to infinity. However, one can see that for large values of λ the maximum value of $R_n(\lambda)$ increases rapidly at the beginning stage of the iterations. Therefore, although $R_n(\lambda)$ will eventually tends to zero as $n \to \infty$, its value may become too large too soon, resulting in great estimated errors, and spoil the subsequent iterative calculations. However, for moderate values of λ, Theorem 2 is confirmed in our numerical simulations.

5.3. Uniqueness of numerical solution

As a consequence of Theorem 2, we have the following uniqueness theorem for the numerical iterative solution, independent of any particular choice of initial iterate, of the differential equation $\boldsymbol{u} = \boldsymbol{g} + \boldsymbol{h}\boldsymbol{u}'$ with no boundary condition.

Theorem 3 (*Uniqueness*).[1] *Consider the numerical iterative scheme*

$$\boldsymbol{u}_n = G_n\boldsymbol{u}_{n-1} = w_n\boldsymbol{g} + H_n\boldsymbol{u}_{n-1},$$

where H_n is the homogeneous operator defined in (26). *Let $\boldsymbol{u}_n^*$ and $\hat{\boldsymbol{u}}_n$ be the nth iterative approximations corresponding to the initial iterates $\boldsymbol{u}_0 = 0$ and $\boldsymbol{u}_0 = \hat{\boldsymbol{u}}_0$, respectively. Then*

$$\lim_{n\to\infty}(\boldsymbol{u}_n^* - \hat{\boldsymbol{u}}_n) = 0.$$

Proof. Let $\boldsymbol{v}_n = \boldsymbol{u}_n^* - \hat{\boldsymbol{u}}_n$. By the linearity of H_n, we have

$$\begin{aligned}\boldsymbol{u}_n^* - \hat{\boldsymbol{u}}_n &= (w_n\boldsymbol{g} + H_n\boldsymbol{u}_{n-1}^*) - (w_n\boldsymbol{g} + H_n\hat{\boldsymbol{u}}_{n-1})\\ &= H_n\boldsymbol{u}_{n-1}^* - H_n\hat{\boldsymbol{u}}_{n-1} = H_n(\boldsymbol{u}_{n-1}^* - \hat{\boldsymbol{u}}_{n-1}).\end{aligned}$$

Therefore, $\boldsymbol{v}_n = H_n\boldsymbol{v}_{n-1}$ and by Theorem 2 it follows that $\lim_{n\to\infty}\boldsymbol{v}_n = 0$ (This theorem is also given in Corollary 4.2 in [12] with a different proof). □

Remark. Both Theorems 2 and 3 are proved under the assumption that the coefficient $\boldsymbol{h}$ is a constant. However, from numerical simulations, we have found that they seem to be valid for more general conditions, including the case of variable coefficient function $\boldsymbol{h}(x)$ if $|\boldsymbol{h}(x)|$ is small enough (for more information, see [17]), and perhaps more generally for the system of balance laws in extended thermodynamics (see the example of shearing flow with heat conduction in Part I). Unfortunately, we do not have a formal proof of uniqueness of numerical solution for the general structure of the subsystems (I) and (II) considered in Part I yet.

[1] This result is somehow expected by Truesdell. In Section 23 of [6] concerning the iterative approximation based on *infinite differentiation*, it is stated that "there is one particular solution which is especially important, and that for a certain [fairly broad] class of initial iterates and for small enough [coefficient] the method of differential iteration converges to that particular solution". This particular solution is referred to as the *asymptotic* solution (see the final remarks in Section 27 of [6]).

6. Heat conduction in moment theory

For ideal gases, the moment theory can be obtained either from Grad distribution for the Boltzmann equation (see e.g., [4]) or from the theory of *extended thermodynamics* [9,14]. We shall consider a problem in the 14-moment theory—one-dimensional stationary heat conduction.

Specifically, we consider the boundary value problem of heat conduction in a monatomic gas at rest between two parallel walls, $0 < x < L$. In this case, we have the following basic equations (see Part I):

$$\frac{\mathrm{d}p}{\mathrm{d}x} = 0, \quad \frac{\mathrm{d}q}{\mathrm{d}x} = 0, \tag{27}$$

and

$$-\frac{1}{\tau_q} q = \frac{5}{2} Rp \frac{\mathrm{d}\theta}{\mathrm{d}x} + \frac{1}{6} \frac{\mathrm{d}\Delta}{\mathrm{d}x},$$

$$-\frac{1}{\tau_\Delta} \Delta = 28R \frac{\mathrm{d}(\theta q)}{\mathrm{d}x}. \tag{28}$$

The equations in (27) are the conservation of linear momentum and energy, which implies that the pressure p and the heat flux q are constants. The equations in (28) are the additional balance equations for the heat flux and the fourth-order non-equilibrium moment Δ. The gas constant is denoted by R and θ is the temperature.

The relaxation times τ_q and τ_Δ depend on the nature of molecular interaction. We consider two models: the BGK model that gives constant relaxation times $\tau_q = \tau_\Delta = \tau$, and the model of Maxwellian molecules that leads to

$$\frac{1}{\tau_q} = \frac{1}{\tau_\Delta} = \frac{2}{3} \sigma\rho = \frac{2}{3} \sigma \frac{p}{R\theta}, \tag{29}$$

where σ is a constant, i.e., for constant pressure the relaxation time is proportional to the temperature.

6.1. Boundary value problem in BGK model

Let us first consider the BGK model and introduce the following dimensionless variables:

$$x' = \frac{x}{L}, \quad \theta' = \frac{\theta}{\theta_0}, \quad q' = \frac{q}{p\sqrt{R\theta_0}}, \quad \Delta' = \frac{\Delta}{pR\theta_0}. \tag{30}$$

Omitting the prime for simplicity, (28) can be written in dimensionless form:

$$q = -\frac{5}{2} \,\mathrm{Kn}\, \frac{\mathrm{d}\theta}{\mathrm{d}x} - \frac{1}{6} \,\mathrm{Kn}\, \frac{\mathrm{d}\Delta}{\mathrm{d}x},$$

$$\Delta = -28 \,\mathrm{Kn}\, q \frac{\mathrm{d}\theta}{\mathrm{d}x}, \tag{31}$$

where the Knudsen number is defined as

$$\mathrm{Kn} = \sqrt{R\theta_0}\, \tau / L.$$

We shall consider the following boundary conditions:

$$\theta(1) = 1, \quad q(0) = q_0.$$

In this case, since $q(x) = q_0$, we are left with only one boundary condition for two unknown integration constants of the two equations of (31).

We can eliminate the temperature from system (31) and obtain

$$\Delta(x) = \frac{56}{5} q_0^2 + \frac{28}{15} \,\mathrm{Kn}\, q_0 \frac{\mathrm{d}\Delta}{\mathrm{d}x}. \tag{32}$$

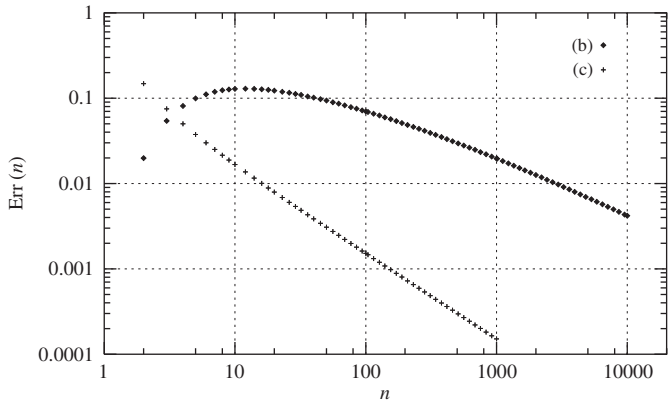

Fig. 2. The plot of estimated error Err(n) in log–log scale for initial iterates of cases (b) and (c).

This linear differential equation with constant coefficients takes the form of the fixed-point problem (23) with constant coefficients. No boundary value of Δ will be given, because, in the kinetic theory, it is the higher moments that we know nothing about physically.

This simple problem has been used as a motivating example for the proposed method of differential iteration in Part I and will be used here again to substantiate the main results concerning convergence and uniqueness of the iterative numerical solutions.

6.1.1. Numerical iterative solutions

At each iteration, $\Delta_n(x)$ at the interior mesh points are calculated from the iterative scheme (24), and by continuity, extrapolation formulas with interior mesh points are used to determine the value of $\Delta_n(x)$ at the end points. The mesh points are evenly spaced with length Δx. The norm is defined as $\|f\| = \sup|f(x)|$.

For the numerical calculations the following data are used:

$$\mathrm{Kn} = 0.1, \quad q_0 = 0.25, \quad \Delta x = \frac{1}{50}, \quad w_n = \frac{1}{n}.$$

Three initial iterates are considered:

$$\text{(a) } \Delta_0(x) = 0, \quad \text{(b) } (\Delta_0(x) = \frac{56}{5} q_0^2 - \exp\left(\frac{15}{28}\,\frac{x-1}{\mathrm{Kn}\, q_0}\right), \quad \text{(c) } \Delta_0(x) = \sin \pi x.$$

The initial state (a) for $\Delta_0(x) = 0$ is the trivial one considered as a motivating example in Part I for introducing the method of differential iteration. The iteration converge trivially after the first iteration (theoretically and numerically for $n = 1, 2, 3, \ldots$) leading to the solution,

$$\Delta(x) = \lim_{n\to\infty} \Delta_n(x) = \frac{56}{5} q_0^2, \tag{33}$$

and the classical Fourier solution for the temperature,

$$\theta(x) = \theta(1) - \frac{2}{5}\,\frac{q_0}{\mathrm{Kn}}\,(x-1).$$

The initial iterate (b) is in fact an exact solution of Eq. (32) with non-trivial homogeneous part. Therefore, theoretically it is already a fixed point and should remain unchanged in every iteration. However, numerically, according to the uniqueness Theorem 3, it should converge to the same numerical solution given by (33). Moreover, as an example of an arbitrary initial iterate, the state (c) is considered. It does not correspond to any meaningful physical state at all, yet we also expect that it should converge to the same numerical solution. The numerical results of both cases (b) and (c) are given in Figs. 2 and 3.

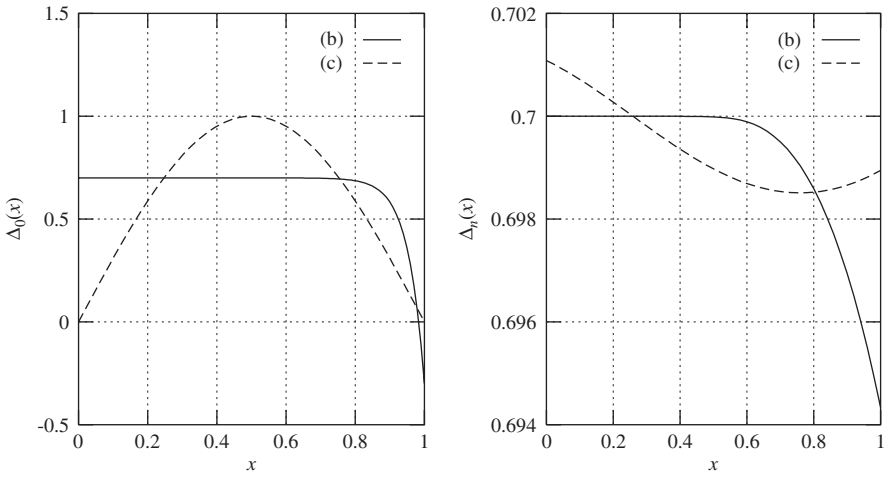

Fig. 3. The initial iterate (left) and the nth iterate (right) of cases (b) and (c) at $n = 10\,000$ and 100, respectively. The solution for $\Delta_0(x) = 0$ is a constant $(56/5)q_0^2 = 0.7$ in this example.

Fig. 2 shows the estimated error Err(n) vs. n in log–log scale. Note that at the beginning, the error is much smaller for case (b) because it starts with an exact solution. However, the instability of the homogeneous part sets in as n increases and the decreasing rate of the estimated error becomes much slower than that of case (c). Nevertheless, numerically, it is evident that Err (n) will go to zero as $n \to \infty$. Therefore, by Theorem 1 the convergence of the approximation sequence $\{\Delta_n\}$ is assured for both cases.

On the right side of Fig. 3, we plot the numerical solutions for case (b) at $n = 10\,000$ and case (c) at $n = 100$. The corresponding initial states are plotted on the left side for comparison (please note the difference in scale). The numerical results show that the approximate solutions $\Delta_n(x)$ are not constant but they are within 1% of the constant solution given by (33) with value equal to 0.7 in the present example. Note that for more or less the same precision, case (c) converges 100 times much faster. However, it shows sooner or later both converge to the same solution. This confirms Theorem 3 for uniqueness as expected.

Remark. This problem can also be solved following the procedure of the method proposed in Part I by decoupling the system into two subsystems and solve alternatively with differential iteration. This procedure will be considered in the next example.

6.2. Model of Maxwellian molecules and slip boundary conditions

In the second example, we shall consider the same problem with the model of Maxwellian molecules and a different type of boundary condition.

For the classical Fourier theory, in addition to the boundary conditions of Dirichlet type (temperature prescribed) and Neumann type (normal heat flux prescribed), one can also prescribe a condition of mixed type:

$$\theta - \alpha(\boldsymbol{q} \cdot \boldsymbol{n}) = \theta_{\mathrm{W}}, \tag{34}$$

where $\boldsymbol{n}$ is the outward normal at the boundary.

The prescribed value θ_{W} will be referred to as the *wall temperature*, because we can write the condition at the wall as

$$\theta - \theta_{\mathrm{W}} = \alpha(\boldsymbol{q} \cdot \boldsymbol{n}).$$

In other words, there is a difference between the temperature of the gas at the wall and the wall temperature, and the difference is proportional to the outflow of heat flux (for $\alpha > 0$) similar to the Newton's law of cooling.

With this interpretation, the wall is not merely regarded as a mathematical boundary and rather as a physical wall, between the gas in its interior and the exterior environment, with possible cooling through the wall due to temperature difference. This interpretation seems to be consistent with the *slip boundary conditions* resulting from Maxwell's simple model of solid wall, depicting the distribution function with kinetic boundary conditions of incident and reflected molecules at the wall (see [23,20]).

6.2.1. Exact iterative solutions

For the model of Maxwellian molecules, with (29), Eq. (28) become

$$q = -\frac{5}{2}\,\mathrm{Kn}\,\theta\,\frac{\mathrm{d}\theta}{\mathrm{d}x} - \frac{1}{6}\,\mathrm{Kn}\,\theta\,\frac{\mathrm{d}\Delta}{\mathrm{d}x},$$

$$\Delta = -28\,\mathrm{Kn}\,q\,\theta\,\frac{\mathrm{d}\theta}{\mathrm{d}x}, \tag{35}$$

where the Knudsen number is defined as

$$\mathrm{Kn} = \frac{3}{2}\,\frac{(R\theta_0)^{3/2}}{p\,\sigma L}.$$

Moreover, from (27), the pressure and the heat flux are constant. System (35) is non-linear.

According to the iterative procedure proposed in Part I, we shall decouple the system and take the initial state $\Delta(x)=0$ for Eq. $(35)_1$, which can then be simplified to

$$\frac{\mathrm{d}^2(\theta^2)}{\mathrm{d}x^2} = 0.$$

It gives the following solutions:

$$\theta^2(x) = \theta_0^2 + (\theta_1^2 - \theta_0^2)x,$$

$$q = -\tfrac{5}{4}\,\mathrm{Kn}(\theta_1^2 - \theta_0^2), \tag{36}$$

where $\theta_0 = \theta(0)$ and $\theta_1 = \theta(1)$ are the gas temperatures at the wall. Let the prescribed wall temperatures be noted by T_0 and T_1 at $x = 0$ and 1, respectively. Then the boundary condition (34) gives

$$\theta_0 = T_0 - \alpha q, \quad \theta_1 = T_1 + \alpha q,$$

which can be solved easily and we obtain

$$\theta_0 = \frac{1}{1+2s}((1+s)T_0 + sT_1), \quad \theta_1 = \frac{1}{1+2s}((1+s)T_1 + sT_0), \tag{37}$$

where

$$s = \tfrac{5}{4}\,\alpha\,\mathrm{Kn}(T_0 + T_1).$$

After obtaining the solutions $\theta(x)$ and q, we can then evaluate the first iterative solution for $\Delta(x)$ from $(35)_2$,

$$\Delta(x) = -28\,\mathrm{Kn}\,q\,\frac{\mathrm{d}(\theta^2)}{\mathrm{d}x} = \frac{56}{5}\,q^2. \tag{38}$$

Note that this is the same as $\Delta(x)$ in (33) for the BGK model. Since $\Delta(x)$ is a constant, its derivative vanishes and therefore, the subsequent iterative solutions from $(35)_1$ for $\theta(x)$ remain unchanged. Consequently, the iteration converges trivially at the first iteration just like the example with BGK model in Section 6.1.

6.2.2. Uniqueness of numerical iterative solutions

We shall follow the procedure of Part I by splitting system (35) into two subsystems with the following numerical iterative scheme.

System (I):

$$q_n = -\frac{5}{2}\,\mathrm{Kn}\,\theta_{n-1}\frac{\mathrm{d}\theta_n}{\mathrm{d}x} - \frac{1}{6}\,\mathrm{Kn}\,\theta_{n-1}\frac{\mathrm{d}\Delta_{n-1}}{\mathrm{d}x}, \quad \frac{\mathrm{d}q_n}{\mathrm{d}x} = 0,$$
$$\theta_n(0) = T_0 - \alpha\, q_n(0), \quad \theta_n(1) = T_1 + \alpha\, q_n(1). \tag{39}$$

System (II):

$$\Delta_n = w_n\left(-28\,\mathrm{Kn}\,q_n\theta_n\frac{\mathrm{d}\theta_n}{\mathrm{d}x}\right) + (1 - w_n)\Delta_{n-1}. \tag{40}$$

The wall temperatures T_0 and T_1 are given at $x = 0$ and 1, respectively.

In this scheme, the boundary value problem of System (I) can easily be solved because the differential equation has been linearized. Finite difference method will be used. The differential iteration of System (II) with $w_n = 1/n$ can be carried out from the solutions of System (I) by a straightforward numerical evaluation.

For the numerical calculations the following data are used:

$$T_0 = 1.0, \quad T_1 = 1.2, \quad \alpha = 1.5, \quad \Delta x = \frac{1}{50}, \quad w_n = \frac{1}{n},$$

for several values of Knudsen number, $\mathrm{Kn} = 0.01, 0.03, 0.05, 0.10$.

Two different initial iterates are considered:

(a) $\Delta_0(x) = 0$, (b) $\Delta_0(x) = \sin \pi x$.

We shall also take $\theta_0(x) = T_0$ initially.

Even though the initial state (a) corresponds to the problem with null initial iterate, unlike the exact solution obtained in (36), the iterative numerical solution does not converge trivially. However, it will be shown that it approaches the exact solution in the numerical iteration with linearized differential equation in the scheme (39).

In order to show that the numerical iterative solution is independent of the choice of initial iterate, a typical non-trivial state (b) is considered.

For all the cases considered with different initial states and different Knudsen numbers, convergence of iterations has been checked numerically. The results show that for $n > 100$, the estimated error $\mathrm{Err}\,(n) < \varepsilon$ with $\varepsilon < 10^{-6}$ for all cases, and decreases as n increases. The running time for the number of iterations n up to 1000 or more is only a few seconds. We regard this as numerical evidence for convergence.

On the left side of Fig. 4 the iterated solution $\Delta_n(x)$ with $\mathrm{Kn} = 0.05$ for initial states (a) and (b) are plotted at $n = 1000$. It shows that for both the null initial state (a) and the non-trivial state (b), $\Delta_n(x)$ differs from the exact solution $\Delta(x) = 4.24528 \times 10^{-3}$ given in (38) by less than 0.02%. In other words, the linearized problem (I) in (39) does lead to the same solution of the original non-linear one in (35) for null initial iterate. On the other hand, the non-trivial initial state (b) leading to the same solution is quite interesting. The fact that we do obtain the same solution with different initial states seems to suggest uniqueness of numerical solutions similar to the BKG model considered in Section 6.1. We have also remarked in Part I that for shearing flows with heat conduction, the uniqueness has also been verified numerically. Nevertheless, unlike the example of BGK model in Section 6.1, we do not have a formal proof yet.

On the right side of Fig. 4, the profiles of $\theta_n(x)$ show temperature jumps at the walls for various values of the Knudsen number, $\mathrm{Kn} = 0.01,\ 0.03,\ 0.05,\ 0.10$ (with Kn increasing upward on the left part of the curves). The wall temperatures are $T_0 = 1.0$ and $T_1 = 1.2$. After large enough number of iterations, the numerical results (with insignificant differences) confirm the same temperature profiles as well as the exact solutions given by (36) for the two initial states (a) and (b) and for each values of Kn—another numerical evidence of uniqueness.

The temperature jumps at the walls in these results are qualitatively consistent with the results from kinetic theory with Maxwell-type boundary condition, in [20] for Grad's moment equations via kinetic scheme, and in [15] for Boltzmann equation. There are slight differences near the walls between our results and those with Maxwell-type assumptions in

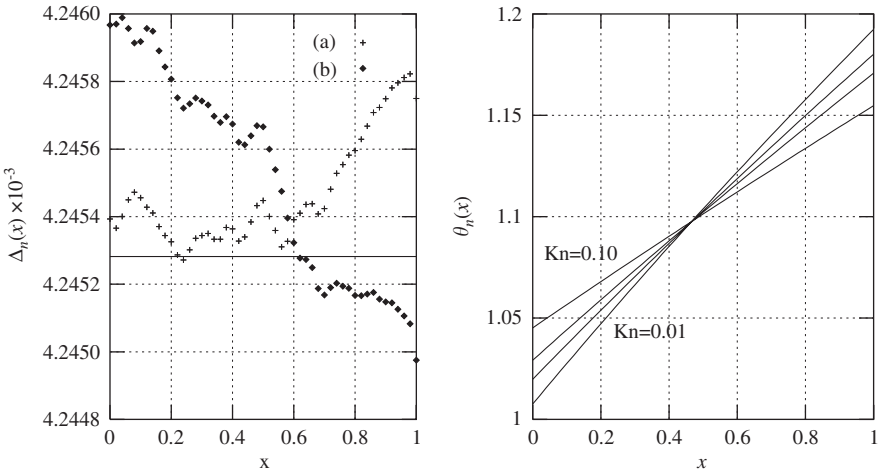

Fig. 4. Left side: $\Delta_n(x)$ at $n = 1000$ and $\mathrm{Kn} = 0.05$ for cases (a) and (b), solid straight line is the exact solution. Right side: $\theta_n(x)$ for $\mathrm{Kn} = 0.01,\ 0.03,\ 0.05,\ 0.10$. Temperature slip for wall temperatures $T_0 = 1.0$ and $T_1 = 1.2$.

the so called Knudsen boundary layers, which are absent from our results. In our numerical simulations, the constant $\alpha = 1.5$ and various Kn are chosen conveniently with no attempt for quantitative comparison.

Since for constant pressure, the temperature is inversely proportional to the density, we can also compare our results with the experimental data of the density distribution in [22] (also cited in [15]). We note that in [22] the data do not include points in the immediate vicinity of the wall and the agreement with ours is qualitatively more satisfactory.

The Maxwell-type boundary conditions in the kinetic theory, concerning the distribution functions of incident and reflected molecules together with some accommodation coefficient in the *vicinity* of the wall, give rise to the Knudsen-type boundary layers in the solutions of Boltzmann equation. On the other hand, in the continuum approach, the solutions are governed by a system of partial differential equations with proper boundary conditions. They are valid in the interior and are assumed to be continuous up to the boundary. Consequently, no such boundary layers can be obtained in our results. Therefore, in order to take into account the presence of such boundary layers, some similar assumptions have to be made into the system of governing equations concerning the behavior of the gas in the vicinity of the wall.

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