Recent Advances on Boundary Conditions for Equations in Nonequilibrium Thermodynamics

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Abstract: This paper is concerned with modeling nonequilibrium phenomena in spatial domains with boundaries. The resultant models consist of hyperbolic systems of first-order partial differential equations with boundary conditions (BCs). Taking a linearized moment closure system as an example, we show that the structural stability condition and the uniform Kreiss condition do not automatically guarantee the compatibility of the models with the corresponding classical models. This motivated the generalized Kreiss condition (GKC)—a strengthened version of the uniform Kreiss condition. Under the GKC and the structural stability condition, we show how to derive the reduced BCs for the equilibrium systems as the classical models. For linearized problems, the validity of the reduced BCs can be rigorously verified. Furthermore, we use a simple example to show how thus far developed theory can be used to construct proper BCs for equations modeling nonequilibrium phenomena in spatial domains with boundaries.

Keywords: hyperbolic relaxation system; structural stability condition; generalized Kreiss condition

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1. Introduction

Irreversible thermodynamics is a theory in physics for the mathematical modeling of nonequilibrium processes. The resultant models are usually time-dependent partial differential equations (PDEs) [1]. So far, the theory is still developing, and there are no well-accepted rules in establishing the equations. Therefore a number of different theories exist [2–8], leading to various PDEs. It is a challenging issue to evaluate the reasonableness of the different equations. To do so, four fundamental requirements were proposed and expounded in [9]. They are the observability of physical phenomena, time irreversibility, long-time tendency to equilibrium, and compatibility with possibly existing classical theories.

Recall well-known theories extended irreversible thermodynamics (EIT) [4,5], rational extended thermodynamics (RET) [6], and conservation–dissipation formalism (CDF) [8]. Irreversible processes can be described with PDEs of the form:

$$U_t + \sum_{j=1}^d F_j(U)_{x_j} = \tilde{Q}(U). \quad (1)$$

Here, $U = U(x, t) \in G \subset \mathbb{R}^n$ is the unknown function of $x = (x_1, x_2, \dots, x_d)$ with d (=1, 2 or 3) for the spatial dimension and $t > 0$, G is an open set called the state space, $F_j(U)$ is the flux along the x_j -direction, source term $\tilde{Q}(U)$ represents the thermodynamical force, and subscripts t, x_j denote partial derivatives with respect to the corresponding variables. Very often, the source term can be written as

$$\tilde{Q}(U) = \begin{pmatrix} 0 \\ q(U) \end{pmatrix}.$$

Accordingly, we partition

$$U = \begin{pmatrix} u \\ v \end{pmatrix}, \quad F_j(U) = \begin{pmatrix} f_j(u, v) \\ g_j(u, v) \end{pmatrix}.$$

With this partition, $u \in \mathbb{R}^{n-r}$ stands for the conserved variables, and $v \in \mathbb{R}^r$ is referred to as nonequilibrium variables. To cover more equations from EIT [4,5] and general equation for nonequilibrium reversible–irreversible coupling (GENERIC) [7,10]), we also consider the following equation.

$$U_t + \sum_{j=1}^d A_j(U) U_{x_j} = \tilde{Q}(U), \quad (2)$$

which is more general than (1). Indeed, (1) can be written as (2) with $A_j(U) = \frac{\partial F_j}{\partial U}(U)$.

For such first-order PDEs, the first fundamental requirement corresponds to the hyperbolicity of Equation (2) [11,12]. To see the other requirements, thermodynamic force $Q(U)$ contains a relaxation time ϵ in general, and we explicitly write it as $\tilde{Q}(U) = Q(U)/\epsilon$. The requirements are closely related to the limit as the relaxation time ϵ tends to zero—the so-called zero relaxation limit. Without considering the boundary conditions, the four requirements are fulfilled by (2) if the PDEs satisfy the structural stability condition proposed in [13,14]. See [14,15].

When the nonequilibrium phenomena occur in a spatial domain with boundaries, the PDEs alone cannot completely describe the physical processes, and proper boundary conditions (BCs) are indispensable. However, it is a challenging task to have such BCs, since the physical meaning of the nonequilibrium variables is often unclear (e.g., the higher-order moments in moment-closure systems [6,16]). On the other hand, formulating proper BCs for hyperbolic systems of PDEs is mathematically a tough issue [17]. For example, the number of BCs for (2) should be equal to the number of positive eigenvalues of coefficient matrix $A_1(U)$ in case that the boundary is $x_1 = 0$; moreover, the BCs should satisfy the uniform Kreiss condition (UKC) [18] to ensure the well-posedness of the complete model (PDEs together with BCs)—the first fundamental requirement. Furthermore, the rest requirements also apply to the complete model. This suggests to study the zero relaxation limit of initial-boundary-value problems (IBVPs) for hyperbolic systems (1) or (2). The resultant results are expected to be useful in providing reasonable constraints for the possible BCs and in developing a systematical method to construct the required BCs.

The paper presents the first author's considerations in the past two decades and recent results on these issues. It is organized as follows. Section 2 contains some basic knowledges about relaxation system (3) and boundary conditions. In Section 3, we show that the structural stability condition and the UKC do not automatically guarantee compatibility, and present a strengthened version of the UKC—the generalized Kreiss condition (GKC). Section 4 is devoted to the derivation of the boundary condition for the zero relaxation limit under the GKC and the structural stability condition. In Section 5, we use an example to show how the theory presented above can be used to construct BCs for the PDEs (3). Some concluding remarks are given in Section 6.

2. Preliminaries

To address the long-term tendency and compatibility requirements, we explicitly introduce relaxation time ϵ and write Equation (3) as

$$U_t + \sum_{j=1}^d A_j(U) U_{x_j} = \frac{1}{\epsilon} Q(U). \quad (3)$$

For such a small parameter problem, the most fundamental is the following structural stability condition proposed in [13,14]:

- (i) There is an invertible $n \times n$ -matrix $P(U)$ and an invertible $r \times r$ -matrix $S(U)$ ($0 < r \leq n$), defined on equilibrium manifold $\mathcal{E} = \{U \in G : Q(U) = 0\}$, such that

$$P(U)Q_U(U) = \begin{pmatrix} 0 & 0 \\ 0 & S(U) \end{pmatrix} P(U) \quad \text{for } U \in \mathcal{E};$$

- (ii) As a hyperbolic system, (1) is symmetrizable, that is, there is a positive definite symmetric matrix $A_0(U)$, such that

$$A_0(U)A_j(U) = A_j^*(U)A_0(U) \quad \text{for } U \in G;$$

- (iii) The hyperbolic part and the source term are coupled in the following sense.

$$A_0(U)Q_U(U) + Q_U^*(U)A_0(U) \leq -P^*(U) \begin{pmatrix} 0 & 0 \\ 0 & I_r \end{pmatrix} P(U) \quad \text{for } U \in \mathcal{E}.$$

Here and below, Q_U denotes the Jacobian matrix of $Q = Q(U)$, I_k denotes the unit matrix of order k , and superscript $*$ denotes the (conjugate) transpose of a matrix.

In the structural stability condition, (i) is just the usual assumption in the corresponding theory for ordinary differential equations [14], that is, only for the source term; (ii) is for the part of spatial derivatives and means that (3) is symmetrizable hyperbolic; and (iii) is a coupling condition that involves the both parts. As observed in [14,19], the structural stability condition is fulfilled by many classical models from mathematical physics. It is related to the Onsager reciprocal relation and can be viewed as a stability criterion for nonequilibrium thermodynamics. Regarding the Onsager relation, matrix $A_0(U)Q_U(U)$ is often symmetric. For simplicity, this symmetry is assumed throughout the paper.

Under the structural stability condition, it was proved in [13,14] that the solution to the initial-value problem of (3) converges to that of the corresponding equilibrium system as ϵ goes to zero. For the case where

$$Q(U) = \begin{pmatrix} 0 \\ q(U) \end{pmatrix}$$

with $q = q(U) \in \mathbb{R}^r$, we write

$$U = \begin{pmatrix} u \\ v \end{pmatrix}, \quad A_j(U) = \begin{pmatrix} A_{j11} & A_{j12} \\ A_{j21} & A_{j22} \end{pmatrix}(U).$$

In this case, it is reasonable to assume that $q(U) = 0$ if and only if $v = h(u)$. Then, the equilibrium system can be expressed as

$$v = h(u),$$

$$u_t + \sum_{j=1}^d A_{j11}(u, h(u))u_{x_j} + \sum_{j=1}^d A_{j12}(u, h(u))h(u)_{x_j} = 0.$$

Under the structural stability condition, it was also proved in [13,20] that the equilibrium system is symmetrizable hyperbolic.

When Equation (3) is given in a spatial domain with boundaries, proper boundary conditions (BCs) should be prescribed to solve the equations. By referring to [21], it is adequate to consider that the spatial domain is half-space

$$(x_1, x_2, \dots, x_d) \equiv (x_1, \hat{x}) \in [0, +\infty) \times \mathbb{R}^{d-1}.$$

For this domain, assume that coefficient matrix $A_1(U)$ has p positive eigenvalues. According to the classical theory of hyperbolic equations [17,22], p independent BCs

$$B(U(0, \hat{x}, t); t) = 0 \quad (4)$$

should be prescribed at boundary $x_1 = 0$. Moreover, they should satisfy the uniform Kreiss condition (UKC) [18] to ensure the well-posedness, namely, there is a positive constant c_K , such that

$$\left| \det \{ B_U R_M^S(\xi, \omega) \} \right| \geq c_K \sqrt{\det \{ R_M^{S*}(\xi, \omega) R_M^S(\xi, \omega) \}}$$

for all $\omega \in \mathbb{R}^{d-1}$ and all complex number ξ with $\operatorname{Re} \xi > 0$. To decode this UKC, we assume that $A_1(U)$ is invertible, and know from [18] that matrix

$$\tilde{M}(\xi, \omega) := A_1^{-1} \left(-\xi I + i \sum_{j=2}^d \omega_j A_j \right),$$

has p stable eigenvalues (eigenvalues with negative real parts) for $\operatorname{Re} \xi > 0$ and $\omega = (\omega_2, \dots, \omega_d) \in \mathbb{R}^{d-1}$. Then, there is a full-rank $n \times p$ -matrix $R_M^S(\xi, \omega)$ (so-called right-stable matrix of $\tilde{M}$ [23]) satisfying

$$\tilde{M}(\xi, \omega) R_M^S(\xi, \omega) = R_M^S(\xi, \omega) \tilde{\Lambda}(\xi, \omega)$$

with $\tilde{\Lambda}(\xi, \omega)$ a $p \times p$ -matrix having p stable eigenvalues.

When $A_1(U)$ is not invertible, boundary $x_1 = 0$ is referred to as characteristic. In this case, a modified UKC was formulated in [21] as a sufficient and essentially necessary condition for well-posedness. In addition, it was indicated in [21] that the boundary condition should not involve characteristic modes corresponding to the zero eigenvalue.

3. Generalized Kreiss Condition

This section shows that the structural stability condition together with the UKC do not automatically guarantee a well-behaved zero relaxation limit. To do this, we start with the linearized version of PDEs in (3):

$$U_t + \sum_{j=1}^d A_j U_{x_j} = \frac{1}{\epsilon} Q U, \quad (5)$$

together with homogeneous boundary conditions

$$B U(0, \hat{x}, t) = 0 \quad (6)$$

for $x = (x_1, \hat{x}) = (x_1, x_2, \dots, x_d)$ with $x_1 > 0$. Here, $A_j (j = 1, 2, \dots, d)$ and Q are $n \times n$ constant matrices and B is a full-rank constant $p \times n$ -matrix with p the number of positive eigenvalues of A_1 .

Following [18,23,24], we consider the corresponding eigenvalue problem:

$$\begin{cases} \xi \hat{U} + A_1 \hat{U}_{x_1} - i \sum_{j=2}^d \omega_j A_j \hat{U} = Q \hat{U}, \\ B \hat{U}(0) = 0 \end{cases} \quad (7)$$

for complex number ξ with $\operatorname{Re} \xi > 0$ and $\omega = (\omega_2, \dots, \omega_d) \in \mathbb{R}^{d-1}$. Let $\hat{U} = \hat{U}(x_1)$ be a bounded solution to the above problem. It is not difficult to verify that

$$U^\epsilon(x, t) := \exp \left(\frac{\xi t}{\epsilon} - \frac{i \omega \cdot \hat{x}}{\epsilon} \right) \hat{U} \left(\frac{x_1}{\epsilon} \right)$$

solves (5) and (6) with a bounded initial value. Since $\operatorname{Re} \xi > 0$, such a solution exponentially increases as ϵ goes to zero for any $t > 0$. Apparently, the zero relaxation limit is not well-behaved or does not exist in this situation.

In order to see when problem (7) has bounded solutions, we assume A_1 to be invertible and rewrite (7) as

$$\frac{d\hat{U}}{dx_1} = M(\xi, \omega, 1)\hat{U} \quad (8)$$

with

$$M(\xi, \omega, \eta) = A_1^{-1} \left(\eta Q - \xi I + i \sum_{j=2}^d \omega_j A_j \right).$$

Here, $\eta \geq 0$ was introduced to cover the case without source term Q , namely, $M(\xi, \omega, 0) = \tilde{M}(\xi, \omega)$ in Section 2.

According to Lemma 2.3 in [23], under the structural stability condition, matrix $M = M(\xi, \omega, \eta)$ has precisely p stable eigenvalues (with negative real parts) and $(n - p)$ unstable eigenvalues. Then, there is a full-rank $n \times p$ -matrix $R_M^S = R_M^S(\xi, \omega, \eta)$ satisfying

$$MR_M^S = R_M^S \Lambda$$

with Λ a $p \times p$ -matrix having p stable eigenvalues. If the $p \times p$ -matrix $BR_M^S(\xi, \omega, 1)$ is not invertible, then there is a nonzero p -vector ζ , such that $BR_M^S(\xi, \omega, 1)\zeta = 0$. With $\hat{U}(0) = R_M^S(\xi, \omega, 1)\zeta$ as initial value, the ordinary differential Equation (8) has a bounded solution for $x_1 > 0$.

Consequently, we obtain

Proposition 1. *If there exists ξ with $\operatorname{Re} \xi > 0$ such that the $p \times p$ -matrix $BR_M^S(\xi, \omega, 1)$ is singular, then the problem in (5) and (6), with a bounded initial value, admits an exponentially increasing solution for $t > 0$ as ϵ goes to zero.*

The above discussion can be illustrated with the one-dimensional linearized moment closure system [16,25]:

$$\begin{cases} U_t + A_1 U_x = QU/\epsilon, \\ BU(0, t) = 0 \end{cases} \quad (9)$$

with $Q = \operatorname{diag}(0, 0, 0, -1)$ and

$$A_1 = \begin{pmatrix} 0 & \rho_0 & 0 & 0 \\ \theta_0/\rho_0 & 0 & 1 & 0 \\ 0 & 2\theta_0 & 0 & 6/\rho_0 \\ 0 & 0 & \rho_0\theta_0/2 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \chi\rho_0\sqrt{\theta_0} & -1 \end{pmatrix}.$$

Here, $U = (\rho, u, \theta, f)$ is the unknown. ρ, u, θ are fluid density, velocity, and temperature, respectively, while f is related to the heat flux. Constants ρ_0 and θ_0 in coefficient matrix A_1 denote density and temperature at the equilibrium. Constant χ in the BC is a positive parameter. Obviously, the moment-closure system satisfies the structural stability condition with symmetrizer

$$A_0 = \begin{pmatrix} 2\theta_0^3 & 0 & 0 & 0 \\ 0 & 2\rho_0^2\theta_0^2 & 0 & 0 \\ 0 & 0 & \rho_0^2\theta_0 & 0 \\ 0 & 0 & 0 & 12 \end{pmatrix}.$$

It was shown in [25] that the BC in (9) satisfies the UKC if and only if

$$\chi \neq \frac{\sqrt{3+\sqrt{6}} + \sqrt{3-\sqrt{6}}}{2(3+\sqrt{3})}.$$

Moreover, Proposition 3.3 in [25] says that if

$$\chi \in (0, \frac{\sqrt{3+\sqrt{6}} + \sqrt{3-\sqrt{6}}}{2(3+\sqrt{3})}),$$

there is a positive ξ such that $BR_M^S(1, \xi)$ is singular. According to Proposition 1, the structural stability condition and the UKC do not automatically imply the existence of the zero relaxation limit.

Proposition 1 and the example above indicate the following necessary condition for the existence of zero relaxation limit:

$$\det\{BR_M^S(\xi, \omega, 1)\} \neq 0, \quad \text{for any } \operatorname{Re}\xi > 0, \omega \in \mathbb{R}^{d-1}.$$

Motivated by this, the following condition was proposed in [23]:

Generalized Kreiss Condition. There exists a constant $c_K > 0$, such that

$$\left| \det\{BR_M^S(\xi, \omega, \eta)\} \right| \geq c_K \sqrt{\det\{R_M^{S*}(\xi, \omega, \eta) R_M^S(\xi, \omega, \eta)\}}$$

for all $\eta \geq 0, \omega \in \mathbb{R}^{d-1}$ and ξ with $\operatorname{Re}\xi > 0$.

Clearly, this GKC does not depend on the special choice of $R_M^S(\xi, \omega, \eta)$. It recovers the standard UKC when $\eta = 0$. Unlike the UKC, the GKC involves parameters even for one-dimensional problems. Moreover, it was shown in [23] that the GKC holds if the BCs are strictly dissipative in the following sense:

Definition 1. The boundary condition is referred to as strictly dissipative with respect to symmetrizer A_0 and A_1 , if there is a positive constant c_d , such that

$$y^* A_0 A_1 y \leq -c_d |y|^2 + c_d^{-1} |By|^2$$

for all $y \in \mathbb{R}^n$.

We conclude this section with the following remark:

Remark 1. In studying IBVPs for hyperbolic systems, it is important to distinguish whether the boundary is characteristic or not [21], that is, whether A_1 is invertible or not. In the above discussions, the invertibility of A_1 plays the role of the starting point. When A_1 is not invertible, a modified GKC was proposed in [26]. It covers the above GKC for noncharacteristic problems.

4. Reduced Boundary Conditions

Besides the GKC, deriving reduced boundary conditions is another crucial issue in studying the zero relaxation limit for the initial-boundary-value problems. The relaxation limit satisfies the equilibrium system under the structural stability condition [14]. When the problem is given in the half-space, the equilibrium system alone can not determine the limit. It must be supplemented with proper boundary conditions. As part of the system determining the limit, such BCs should be completely derived from the relaxation system and its BCs. BCs thus derived are called reduced boundary conditions.

For linearized system (3) satisfying the structural stability condition, we assume without loss of generality that $Q = \text{diag}(0, S)$ with S being a negative definite matrix. Corresponding to the partition of Q , we write coefficient matrix A_j as

$$A_j = \begin{pmatrix} A_{j11} & A_{j12} \\ A_{j21} & A_{j22} \end{pmatrix}.$$

Thus, the aforementioned equilibrium system reads as

$$\begin{cases} v = 0, \\ u_t + \sum_{j=1}^d A_{j11} u_{x_j} = 0. \end{cases} \quad (10)$$

Recall that coefficient matrices A_{j11} are symmetrizable.

Let p_1 be the number of positive eigenvalues for matrix A_{111} . According to the classical theory of IBVPs for hyperbolic systems [17,22], equilibrium system (10) needs p_1 BCs satisfying the UKC to be well-posed. As mentioned before, these BCs should be completely determined from the relaxation system and its BCs:

$$BU(0, \hat{x}, t) = (B_u, B_v) \begin{pmatrix} u \\ v \end{pmatrix} (0, \hat{x}, t) = b(t). \quad (11)$$

In this regard, it was established in [23,27] that

Theorem 1. *Under the structural stability condition and the GKC, there exists a $p_1 \times p$ -matrix B_p , unique up to an invertible $p_1 \times p_1$ -matrix multiplying B_p from left, such that relation*

$$B_p B_u u(0, \hat{x}, t) = B_p b(\hat{x}, t) \quad (12)$$

satisfies the UKC as a BC for the equilibrium system. Moreover, if boundary $x_1 = 0$ is characteristic for the equilibrium system, BC (12) does not involve the characteristic modes corresponding to the zero eigenvalue.

The equilibrium system with the reduced BC (12) consist of a well-posed IBVP since the reduced BC satisfies the UKC. The proof of this theorem involves the perturbation theory of linear operators [28] and subtle matrix analysis. The key is to analyze the limit of right-stable matrix $R_M^S(\xi, \omega, \eta)$ as $\eta \rightarrow \infty$. According to the GKC, $BR_M^S(\xi, \omega, +\infty)$ is a $p \times p$ invertible matrix. Then, B_p can be chosen as the $p_1 \times p$ -matrix consisting of the first p_1 rows of $[BR_M^S(\xi, \omega, +\infty)]^{-1}$. Such a matrix B_p is independent of ξ and ω . We omit the details here, and the interested reader is referred to [23,27].

Regarding this theorem:

Remark 2.

- For nonlinear problems, reduced BCs are quite complicated, but can be derived by considering boundary-layer equations

$$A_1(U)U_y = Q(U), \quad y = \frac{x_1}{\epsilon} \geq 0.$$

For the details, the interested reader is referred to [23].

- In case the boundary is characteristic (for the relaxation system), a similar result can be found in [26].

To see the validity of the reduced BCs, we consider asymptotic solutions of the form:

$$\begin{pmatrix} u_\epsilon \\ v_\epsilon \end{pmatrix}(x_1, \hat{x}, t; \epsilon) = \begin{pmatrix} \bar{u} \\ \bar{v} \end{pmatrix}(x_1, \hat{x}, t) + \begin{pmatrix} \mu_0 \\ \nu_0 \end{pmatrix}\left(\frac{x_1}{\epsilon}, \hat{x}, t\right) \\ + \begin{pmatrix} \mu_1 \\ \nu_1 \end{pmatrix}\left(\frac{x_1}{\sqrt{\epsilon}}, \hat{x}, t\right) + \sqrt{\epsilon} \begin{pmatrix} \mu_2 \\ \nu_2 \end{pmatrix}\left(\frac{x_1}{\sqrt{\epsilon}}, \hat{x}, t\right) \quad (13)$$

for relaxation system (5) and its BC (11). Here, $(\bar{u}, \bar{v})$ is the outer solution, and (μ_i, ν_i) ($i = 0, 1, 2$) are boundary-layer corrections satisfying matching conditions

$$(\mu_i, \nu_i)(\infty, \hat{x}, t) = 0, \quad i = 0, 1, 2.$$

By a standard procedure [27], the outer solution solves equilibrium system (10) with reduced BC (12), while the other terms in (13) can also be determined.

If the boundary is not characteristic for the equilibrium system, there is no boundary-layer with length $\sqrt{\epsilon}$. In other words, the last two terms in (13) are void, and the three scales in the expansion degenerate to two scales.

The validity of the reduced BC (12) is verified with the following theorem.

Theorem 2 ([27]). *Assuming that the structural stability condition and the GKC hold, the initial data are given at the equilibrium, and the BC is compatible with the initial condition, there exists a constant $K > 0$, such that the exact solution (u^ϵ, v^ϵ) fulfils the following estimate.*

$$\|(u^\epsilon - u_\epsilon, v^\epsilon - v_\epsilon)(\cdot, \cdot, t)\|_{L^2(\mathbb{R}^+ \times \mathbb{R}^{d-1})} \leq K\epsilon^{1/2}$$

for all time $t \in [0, T]$.

Next, we return to one-dimensional linearized moment closure system (9) to illustrate the reduced BCs. For this model, we have

$$A_1 = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \left(\begin{array}{ccc|c} 0 & \rho_0 & 0 & 0 \\ \theta_0/\rho_0 & 0 & 1 & 0 \\ 0 & 2\theta_0 & 0 & 6/\rho_0 \\ \hline 0 & 0 & \rho_0\theta_0/2 & 0 \end{array} \right),$$

and

$$B = (B_u, B_v) = \left(\begin{array}{ccc|c} 0 & 1 & 0 & 0 \\ 0 & 0 & \chi\rho_0\sqrt{\theta_0} & -1 \end{array} \right), \quad b(t) = 0.$$

As shown in [25], coefficient matrix A_1 has two positive eigenvalues, $\sqrt{3 \pm \sqrt{6}}\sqrt{\theta_0}$, and A_{11} has one positive eigenvalue $\sqrt{3\theta_0}$, that is, $p = 2$ and $p_1 = 1$. Thus equilibrium system

$$\begin{pmatrix} \bar{\rho} \\ \bar{u} \\ \bar{\theta} \end{pmatrix}_t + \begin{pmatrix} 0 & \rho_0 & 0 \\ \theta_0/\rho_0 & 0 & 1 \\ 0 & 2\theta_0 & 0 \end{pmatrix} \begin{pmatrix} \bar{\rho} \\ \bar{u} \\ \bar{\theta} \end{pmatrix}_{x_1} = 0$$

needs one reduced boundary condition. On the other hand, in this case, we have

$$BR_M^S(\xi, +\infty) = \begin{pmatrix} \sqrt{3\theta_0}/\rho_0 & 0 \\ 2\chi\theta_0\sqrt{\theta_0} & -\chi\theta_0\sqrt{\theta_0} \end{pmatrix}.$$

This matrix is obviously invertible, and its inverse is a lower-triangular matrix. Therefore, B_p can be chosen as the 1×2 -matrix $(1, 0)$, and the reduced BC is

$$B_p B \bar{U}(0, t) = (1, 0) \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & \chi \rho_0 \sqrt{\theta_0} & -1 \end{pmatrix} \bar{U}(0, t) = B_p b(t) = 0$$

with $\bar{U} = (\bar{\rho}, \bar{u}, \bar{\theta}, \bar{f})$. That is, just no-slip velocity BC

$$\bar{u}(0, t) = 0.$$

5. Construction of BCs

In this section, we show how the theory presented above can be used to construct BCs for PDEs (2). Usually, the relaxation system is derived by augmenting certain classical equations to take account into more refined physical processes. However, proper BCs for the relaxation systems are not always available, since the physical meaning of the nonequilibrium variables is often unclear (e.g., the higher-order moments in moment-closure systems [6,16]). Because of this, no physical means can be expected to obtain the BCs for certain relaxation systems.

For our construction of the BCs, we assume that both the relaxation systems and the well-posed BCs for the corresponding equilibrium systems are given. This assumption is reasonable because there already exist many well-known approaches to construct the relaxation systems, and much knowledge on equilibrium systems and their BCs exists.

We illustrate the construction with the following simple model.

$$\begin{aligned} \partial_t u - \partial_x v &= 0, \\ \partial_t v - \partial_x \sigma &= 0, \\ \partial_t (\sigma - Eu) &= (g(u) - \sigma)/\epsilon. \end{aligned} \quad (14)$$

This model was proposed in [29] for the isothermal motions of a viscoelastic material, and can be viewed as an augmentation of classical equations of isothermal elastodynamics:

$$\begin{aligned} \partial_t u - \partial_x v &= 0, \\ \partial_t v - \partial_x g(u) &= 0. \end{aligned} \quad (15)$$

Here, u and σ denote strain and stress, v is related to particle velocity, E is a positive constant called dynamic Young's modulus, ϵ is the relaxation time, and $g(u)$ is a given function of u . For this model, the structural stability condition reads as

$$0 < g'(u) < E.$$

For simplicity, we assume that the model was defined in the domain where $x \geq -\alpha t$ and $g(u) = Gu$, with $G > 0$ a constant and α a parameter. Under change in variables $(x, t) \rightarrow (x + \alpha t, t)$, the system (14) becomes

$$\begin{pmatrix} u \\ v \\ p \end{pmatrix}_t + \begin{pmatrix} \alpha & -1 & 0 \\ -G & \alpha & -1 \\ 0 & G - E & \alpha \end{pmatrix} \begin{pmatrix} u \\ v \\ p \end{pmatrix}_x = \frac{1}{\epsilon} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} u \\ v \\ p \end{pmatrix} \quad (16)$$

with $p = \sigma - Gu$ and (15) reads as

$$\begin{pmatrix} u \\ v \end{pmatrix}_t + \begin{pmatrix} \alpha & -1 \\ -G & \alpha \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}_x = 0. \quad (17)$$

Moreover, the given BC for the equilibrium system is

$$\hat{B} \begin{pmatrix} u \\ v \end{pmatrix} (0, t) = \hat{b}(t)$$

with $\hat{B} = (\hat{B}_1, \hat{B}_2)$ being a constant full-rank matrix. The number of rows of $\hat{B}$ is equal to the number of positive eigenvalues of coefficient matrix

$$A_{11} \equiv \begin{pmatrix} \alpha & -1 \\ -G & \alpha \end{pmatrix}.$$

This matrix has eigenvalues $\alpha \pm \sqrt{G}$, while coefficient matrix

$$A_1 \equiv \begin{pmatrix} \alpha & -1 & 0 \\ -G & \alpha & -1 \\ 0 & G - E & \alpha \end{pmatrix}$$

has eigenvalues $\alpha \pm \sqrt{E}$ and α .

To be precise and simple, we chose $\alpha \in (-\sqrt{E}, -\sqrt{G})$, while other choices can be found in [30]. For such an α , boundary $x = 0$ is noncharacteristic for both (17) and (16), boundary matrix $\hat{B}$ is void, and we need to construct one BC of the form

$$B \begin{pmatrix} u(0, t) \\ v(0, t) \\ p(0, t) \end{pmatrix} = b_\epsilon(t) \quad (18)$$

for the relaxation system (16).

To find such a nonzero vector $B \in \mathbb{R}^3$, we consider the asymptotic solution of form

$$\begin{pmatrix} u_\epsilon \\ v_\epsilon \\ p_\epsilon \end{pmatrix} (x, t; \epsilon) = \begin{pmatrix} \bar{u} \\ \bar{v} \\ \bar{p} \end{pmatrix} (x, t) + \begin{pmatrix} \mu \\ \nu \\ \pi \end{pmatrix} \left(\frac{x}{\epsilon}, t \right)$$

and require it to satisfy the BC (18):

$$B \begin{pmatrix} \bar{u} + \mu \\ \bar{v} + \nu \\ \bar{p} + \pi \end{pmatrix} (0, t) = b_0(t).$$

In this way, we obtain some algebraic relations or restrictions on B , from which we deduce that

$$B^* = \begin{pmatrix} 1 + \frac{C_1}{\alpha^2 - G} \\ \sqrt{G} + \frac{\alpha C_1}{\alpha^2 - G} \\ C_1 \end{pmatrix} \times \begin{pmatrix} 1 + \frac{C_2}{\alpha^2 - G} \\ -\sqrt{G} + \frac{\alpha C_2}{\alpha^2 - G} \\ C_2 \end{pmatrix}$$

with C_1, C_2 two free parameters. BCs thus constructed are not unique, which is expected.

It was shown in [30] that, when C_1, C_2 are both sufficiently small, the constructed BCs are strictly dissipative. Thus, they satisfy the GKC. On this basis, the validity of the constructed BCs was rigorously proved in [30].

6. Concluding Remarks

In this paper, we presented a systematical review on boundary conditions (BCs) for partial differential equations (PDEs) from nonequilibrium thermodynamics. From a stabil-

ity point of view, such PDEs should satisfy the structural stability condition. In particular, they constitute hyperbolic systems, for which the uniform Kreiss condition (UKC) is a sufficient and essentially necessary condition for the well-posedness of the corresponding models (PDEs with BCs). Taking a linearized moment closure system as an example, we showed that the structural stability condition and UKC do not automatically guarantee the compatibility of the models with the corresponding classical models. This motivated the generalized Kreiss condition (GKC)—a strengthened version of the UKC. It is expected that the GKC and the structural stability condition are the very criteria to verify the four fundamental requirements when modeling nonequilibrium phenomena in spatial domains with boundaries.

The compatibility and long-time tendency requirements suggest to study the zero relaxation limit of the PDEs with BCs. It is trivial to obtain the equilibrium system for the limit. However, the equilibrium system alone cannot determine the limit, and proper BCs are needed. The needed BCs are referred to as reduced BCs, and they should be completely determined by the PDEs with the given BCs. The derivation of the reduced BCs is by no means trivial.

Under the GKC and the structural stability condition, we showed how to derive the reduced BCs for general relaxation models. For linearized problems, the validity of the reduced BCs was rigorously verified. For nonlinear problems, such a verification is open. Furthermore, we used a simple example to show how the thus far developed theory can be used to construct proper BCs accompanying PDEs modeling nonequilibrium phenomena in spatial domains with boundaries.

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