Boundary Conditions, Nonequilibrium Thermodynamics Equations

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In this entry, we present a systematical review on boundary conditions (BCs) for partial differential equations (PDEs) from nonequilibrium thermodynamics. From a stability point of view, such PDEs should satisfy the structural stability condition. In particular, they constitute hyperbolic systems, for which the generalized Kreiss condition (UKC) is a sufficient and essentially necessary condition for the well-posedness of the corresponding models (PDEs with BCs).

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

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][3][4][5][6][7][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.

For such first-order PDEs, the first fundamental requirement corresponds to the hyperbolicity of Equation (2) [10][11]. 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 [12][13]. See [13][14].

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][15]). On the other hand, formulating proper BCs for hyperbolic systems of PDEs is mathematically a tough issue [16]. 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) [17] 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. 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): (5) U t + ∑ j = 1d A j U x j = 1ϵ Q U , together with homogeneous boundary conditions (6) B U (0,x ^ ,t) = 0 for x = (x 1, x ^) = (x 1, x 2, ⋯ , x d) with x 1> 0. Here, A j (j = 1, 2, ⋯ , d) and Q are n × n constant matrices and B is a full-rank constant p × n -matrix with p the number of positive eigenvalues of A 1.

Following [17][18][19], we consider the corresponding eigenvalue problem: (7) ξ U ^ + A 1U ^ x 1− i ∑ j = 2d ω j A j U ^ = Q U ^ ,B U ^ (0) = 0 for complex number ξ with R e ξ > 0 and ω = (ω 2, ⋯ , ω d) ∈ R d − 1. Let U ^ = U ^ (x 1) be a bounded solution to the above problem. It is not difficult to verify that U ϵ (x ,t) : = exp ξ t ϵ − i ω · x ^ ϵ U ^ x 1ϵ solves (5) and (6) with a bounded initial value. Since R e ξ > 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.

If there exists ξ with R e ξ > 0 such that the p × p -matrix B R M S (ξ ,ω ,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.

Motivated by this, the following condition was proposed in [18]:

Generalized Kreiss Condition. There exists a constant c K > 0, such that det B R M S (ξ ,ω ,η) ≥ c K det { R M S * (ξ ,ω ,η) R M S (ξ ,ω ,η) } for all η ≥ 0, ω ∈ R d − 1 and ξ with R e ξ > 0.

3. 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 [13]. 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.

In this regard, it was established in [18][20] that

Under the structural stability condition and the GKC, there exists a p 1× p -matrix B p , unique up to an invertible p 1× p 1-matrix multiplying B p from left, such that relation (12) B p B u u (0 , x ^ , t) = B p b (x ^ , t) 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 [21] and subtle matrix analysis. The key is to analyze the limit of right-stable matrix R M S (ξ ,ω ,η) as η → ∞ . According to the GKC, B R M S (ξ ,ω ,+ ∞) is a p × p invertible matrix. Then, B p can be chosen as the p 1× p -matrix consisting of the first p 1 rows of [B R M S (ξ ,ω ,+ ∞)] − 1. Such a matrix B p is independent of ξ and ω . We omit the details here, and the interested reader is referred to [18][20].

By a standard procedure [20], the outer solution solves equilibrium system (10) with reduced BC (12), while the other terms in (13) can also be determined.

4. Construction of BCs

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.

Moreover, the given BC for the equilibrium system is B ^ u v (0,t) = b ^ (t) with B ^ = (B 1^ ,B 2^) being a constant full-rank matrix. The number of rows of B ^ is equal to the number of positive eigenvalues of coefficient matrix A 11≡ α − 1− G α .

This matrix has eigenvalues α ± G , while coefficient matrix A 1≡ α − 10− G α − 10G − E α has eigenvalues α ± E and α .

To be precise and simple, we chose α ∈ (− E ,− G) , while other choices can be found in [22]. For such an α , boundary x = 0 is noncharacteristic for both (17) and (16), boundary matrix B ^ is void, and we need to construct one BC of the form (18) B u (0,t) v (0,t) p (0,t) = b ϵ (t) for the relaxation system (16).

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