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Generalized heat conduction model involving imperfect thermal contact surface: Application of the GSSSS-1 differential-algebraic equation time integration

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ABSTRACT

A number of contributions have been made to model thermal contact problems involving perfect/imperfect thermal interfaces. The Fourier-, Cattaneo-, and *Jeffreys*-types of thermal flux modes have been exploited to govern the heat transfer processes of adjacent regions. However, most of the existing studies consider using only one type of these thermal flux models to describe the thermal physics of the entire system such that the mathematical model may fail to precisely describe the physics within the multi-domain system, especially, when the mean free paths of different adjacent domains span in a large range with respect to the characteristic dimension of the material. To circumvent this issue, a generalized heat conduction model, termed C- and F-processes heat conduction model, with the consideration of perfect/imperfect thermal interface is proposed and formulated under the expression of a first-order time dependent differential-algebraic equation in which the interface conditions are treated as algebraic equations. The unified time integration of GSSSS-1 is extended to solve the resulting differential-algebraic system with Index 2 constraints. The numerical results illustrate *that* the proposed framework has *a* better capacity of describing the thermal contacts with/without the thermal resistance of Fourier-Fourier, Fourier-Cattaneo, and other general cases.

1. Introduction

For the coupling of different scales/materials within a solid, of either *multilayered* nano-scale films, micro devices or macro systems, the interfaces connecting adjacent domains play an important role in the thermal response of the entire system. In the ideal situation, the adjacent domains contact perfectly such that the temperature and the flux perform no jumps across the interface due to the energy conservation law. The interface of the perfect contacting case is classified as *Perfect Interface*. However, in the general practical applications, the adjacent domains usually do not contact well and there exist gaps between the contacting domains. In such a way, this *Imperfect Interface* leads a discontinuity of the temperature while the thermal flux retains *a continuity* across the interface. Specifically, the relationships with respect to the temperature T and the thermal flux $\boldsymbol{q}$ for the imperfect interfaces [1–3] are given by:

$$\begin{aligned} [\![T]\!] &= -R\{\{\boldsymbol{q}\}\}\cdot\boldsymbol{n} \\ [\![\boldsymbol{q}]\!]\cdot\boldsymbol{n} &= 0 \end{aligned} \tag{1}$$

where $[\![T]\!]$ represents $T|_{\Gamma_1} - T|_{\Gamma_2}$ and $\{\{\boldsymbol{q}\}\}$ represents $\frac{1}{2}\left(\boldsymbol{q}|_{\Gamma_1} + \boldsymbol{q}|_{\Gamma_2}\right)$. The *coefficient* $R \geqslant 0$ *represents* the thermal (Kapitza) resistance, when $R = 0$ the thermal contact is associated with the perfect interface while $R \neq 0$ the thermal contact is associated with the imperfect interface. Γ_1 and Γ_2 are the surfaces in contact and $\boldsymbol{n}$ is the normal direction from Γ_2 to Γ_1. It is worth noting that Eq. (1) represents the *lowly-conducting* interface, which is classically modeled using Kapitza's assumption of thermal resistance. A more general formulation regarding the interface conditions has been proposed in [4], both the lowly-conducting and the highly-conducting interfaces are covered in this general imperfect interface theory. However, the general imperfect interface assumes that the interface is a zero-thickness material and has its own heat transfer process such that it may introduce more numerical problems. For simplicity, the lowly-conducting interface is of interest to this article.

Numerous analytical, experimental, and numerical models have been done regarding the thermal contact and the treatments of the

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interface condition. In some thermal contact problems, the adjacent regions are governed by the Fourier' s heat conduction model. The weak-form based numerical approaches such as FEM, XFEM are applied to capture the strong discontinuity caused by the thermal resistance [5,1,3]. In the engineering applications of thermal wave theory involving thermal *interfaces*, the thermal contact is usually considered in the framework of the hyperbolic heat conduction model. The thermal resistance *was* treated as a jump boundary conditions in [6,7]. Additionally, remarkable studies regarding the theoretical analysis with respect to the thermal contact with/without resistance in the framework of hyperbolic model have been done in [8,9]. Note that the numerical approaches applied in the hyperbolic-type system should be able to capture the discontinuities in each domain and also works well under the condition of thermal resistance. The thermal contact has also been extended to the field of bio-engineering, such as the thermal processes in the multi-layer bio-tissues. Both the *Fourier*-type heat conduction and dual-phase-lag heat conduction model[1] have been done with respect to this particular aspect [11,12]. Instead of the linear thermal resistance between the temperature and the flux at the interface, the heat flux across the interface of two layers is assumed to proportionally change with the difference between the fourth powers of the temperatures on the two sides of the interface, which is similar to the radiation heat transfer model. The specific expression of R [8] is as follows:

$$R = \frac{T|_{\Gamma_1} - T|_{\Gamma_2}}{\bar{h}\left(T^4|_{\Gamma_1} - T^4|_{\Gamma_2}\right)} \tag{2}$$

where $\bar{h}$ is a thermal contact parameter related to the surface roughness [13].

The overview described earlier indicates that the existing works consider implementing only one certain thermal flux model to govern the thermal transfer over the entire multi-domain system, which seems to be not precise and cannot be considered as a complete theory when the mean free paths of different adjacent domains span in a large range with respect to the characteristic dimension of the material. For example, [6] utilized the hyperbolic heat conduction model in all the adjacent regions to formulate the thermal contact of the practical electronic *device*, which are comprised by conducting film and substrate composite. However, the proper thermal flux models for the film and the subtract are *necessary to be* determined by the relationship between the mean free path (λ) and the characteristic dimension of the material (L). Specifically,

1. When $\lambda \gg L$, the pure ballistic transport dominates the transport process;
2. When $\lambda \approx L$, the transport process is governed by a diffusive-ballistic nature;
3. When $\lambda \ll L$, the heat transport is treat to be macroscopic and is governed by a purely diffusive nature.

In other words, using a single heat conduction model cannot fulfill the requirement of precisely describing the thermal process over the entire system. In order to achieve it, different types of heat conduction models are coupled by the interface, which turns out to be a numerical challenge for the previous studies. The specific reasons include that:

(i) different orders of time-dependent systems are needed to describe the thermal contact between the Fourier-type flux and the Cattaneo-/*Jeffreys*-type flux;

(ii) the flux models of the Cattaneo-type and the *Jeffreys*-type involve the partial time derivative and are not explicitly given, which implies that the interface condition of thermal flux is not easy to be fulfilled;

(iii) the existing numerical treatments with respect to both the perfect and imperfect interfaces also seem to be a numerical challenge in different approaches, specifically, the interface is usually handled as a boundary condition that are embedded in the time stepping of the governing equation. Consequently, in most of the previous studies the governing equations of each domain have to be evaluated separately and the time stepping strategies to the associated numerical simulations are designed in the framework of staggering methodology, which may have the issue of violating the interface conditions.

Therefore, increasing application and necessity regarding the treatment of interface, the modeling of the heat conduction within adjacent regions, and the thermal performance at different scales have motivated the objective of this work to develop a general framework of describing the complex thermal contact physics and a decent approach to deal with the perfect/imperfect interface condition.

To circumvent these issues, a two-field (both the temperature and the thermal flux are primary variables) generalized heat conduction model, the C- and F-processes heat conduction model, is utilized to depict the heat conduction of the adjacent regions. The C- and F-processes heat conduction model is originally developed in [14] and is based *upon* the assumption that the Cattaneo-type thermal flux associated with *a* finite sound speed and the Fourier-type thermal flux associated with *an* infinite sound speed co-exist in a heat process simultaneously. Therefore, the C- and F-heat conduction model is acknowledged to cover various heat conduction models. Though the hyperbolic- and *Jeffreys*-types of heat conduction are acknowledged as second-order time systems in terms of single-field formulation (only the temperature is the primary variable), the governing equation of the proposed C-F heat conduction is presented in a first-order two-field form with considering both the temperature and the thermal flux as the primary physical fields of interest. In the framework of the two-field C-and F-model, the thermal flux model in each adjacent region can be switched easily and all the governing equations can be expressed in a unified formulation. Different from the past efforts, we treat the interface condition, Eq. (1), as an algebraic equation such that coupling the interface algebraic equation with the generalized two-field C- and F-heat conduction equation formulates a first-order time dependent *Differential Algebraic Equation*. The principal contributions emanating from such a generalized framework are summarized as follows:

1. A simple computational framework to model the thermal contact between either the Fourier-type and/or Cattaneo-type and/or *Jeffreys*-type, without having to resort to the individual governing equation.
2. A perfect preservation of the perfect/imperfect thermal interface condition in a machine error (1E-16).

Additionally, we also present the formalism of a unified second-order accurate time integration, GS4 (generalized single step single solve)[15–17], to solve this first order DAEs system in terms of GS4-1 DAE Index-2. Note that the Index 2 is the highest constraint index existing in the first-order time dependent DAE system and naturally arises from the interface condition in this particular thermal contact problem.

[1] The underlying physics of the dual-phase-lag has been proved to be the same as the *Jeffreys*' conduction model. More details can be found in [10].