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## CLOSE-TO-FOURIER HEAT CONDUCTION EQUATION FOR SOLIDS: MOTIVATION AND SYMBOLIC-NUMERICAL ANALYSIS

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ABSTRACT. Heat conduction close-to-Fourier means, that we look for a minimal extension of heat conduction theory using the usual Fourier expression of the heat flux density and modifying that of the internal energy as minimal as possible by choosing the minimal state space. Applying Liu's procedure results in the class of materials and a differential equation both belonging to the close-to-Fourier case of heat conduction. A symbolicnumerical computing method is applied to approximate the numerical solutions of 2 special heat conduction equations belonging to the close-to-Fourier class.

### 1. Introduction

As it is well-known, one of other shortcomings of the classical Fourier heat conduction theory is caused by a parabolic differential equation which allows indefinite propagation of energy. This unphysical fact can be avoided, if the parabolic heat conduction equation is replaced by an hyperbolic one [1–4]. Here the question is investigated, if a minimal change of Fourier heat conduction results in an hyperbolic differential equation of first order in time.

By use of Fourier's expression for the heat flux density and the minimal state space spanned by the temperature and its gradient, Liu's procedure is applied for exploiting the second law systematically. The Liu procedure results in coupled differential equations for the specific internal energy, the specific entropy, the heat flux density and the entropy flux density. One result is, that the internal energy and the entropy depend on only one variable which is a state function and which transforms to the thermostatic temperature in the thermostatic limit. An other result is, that an hyperbolic heat conduction equation is compatible with the Fourier expression for the heat flux density.

### 2. The balances

In solids of constant mass density  $\rho$ , an observer exists for which the field of velocity v vanishes

(1) 
$$\varrho = \text{const}, \quad v \equiv 0.$$

Consequently, the balance equations of the specific internal energy  $\varepsilon$  and the specific entropy *s* result in

(2) 
$$\varrho \partial_t \varepsilon + \nabla \cdot \boldsymbol{q} = 0, \qquad \varrho \partial_t s + \nabla \cdot \boldsymbol{\Phi} = \sigma \geq 0.$$

Here q is the heat flux density,  $\Phi$  the entropy flux density and  $\sigma$  is the entropy production density. The inequality in  $(2)_2$  characterizes the second law of thermodynamics. As minimal possible state space, we choose that which is spanned by the temperature T and its gradient  $\nabla T$ 

$$z = (T, \nabla T).$$

Using the chain rule for calculating the derivatives in the balance equations (2) we obtain the so-called balances on the state space [5]

(4) 
$$\varrho \left[ \frac{\partial \varepsilon}{\partial T} \partial_t T + \frac{\partial \varepsilon}{\partial \nabla T} \cdot \partial_t \nabla T \right] + \frac{\partial \mathbf{q}}{\partial T} \cdot \nabla T + \frac{\partial \mathbf{q}}{\partial \nabla T} : \nabla \nabla T = 0$$

(5) 
$$\varrho \left[ \frac{\partial s}{\partial T} \partial_t T + \frac{\partial s}{\partial \nabla T} \cdot \partial_t \nabla T \right] + \frac{\partial \Phi}{\partial T} \cdot \nabla T + \frac{\partial \Phi}{\partial \nabla T} : \nabla \nabla T = \sigma$$

The higher derivatives belonging to the state space (3) are

(6) 
$$\boldsymbol{y} = (\partial_t T, \nabla \partial_t T, \nabla \nabla T).$$

Using them, the balance equations on the state space (4) and (5) can be written down in matrix formulation

0

(7) 
$$\left( \begin{array}{c} \varrho \frac{\partial \varepsilon}{\partial T} & \varrho \frac{\partial \varepsilon}{\partial \nabla T} & \frac{\partial \boldsymbol{q}}{\partial \nabla T} \end{array} \right) \cdot \boldsymbol{y} = -\frac{\partial \boldsymbol{q}}{\partial T} \cdot \nabla T,$$

(8) 
$$\left( \begin{array}{c} \varrho \frac{\partial s}{\partial T} & \varrho \frac{\partial s}{\partial \nabla T} & \frac{\partial \Phi}{\partial \nabla T} \end{array} \right) \cdot \boldsymbol{y} \geq -\frac{\partial \Phi}{\partial T} \cdot \nabla T$$

This inequality, named dissipation inequality, has to be exploited by taking into account the energy balance (7). This will be done in the next section.

#### 3. The Liu procedure

For exploiting the balance equations with respect to the second law, we apply Liu's well-known procedure [6–8]. This procedure is based on the following theorem:

 $\Box$  If

(9) 
$$\mathbf{A} \cdot \boldsymbol{y} = \boldsymbol{B}, \quad \boldsymbol{\alpha} \cdot \boldsymbol{y} \ge \boldsymbol{\beta}, \quad \mathbf{A}(\boldsymbol{z}), \, \boldsymbol{B}(\boldsymbol{z}), \, \boldsymbol{\alpha}(\boldsymbol{z}), \, \boldsymbol{\beta}(\boldsymbol{z})$$

are the balance equations and the dissipation inequality in matrix formulation, a state space function  $\Lambda(z)$  exists which satisfies the so-called Liu equations and the residual inequality

(10) 
$$\mathbf{\Lambda} \cdot \mathbf{A} = \boldsymbol{\alpha}, \quad \mathbf{\Lambda} \cdot \boldsymbol{B} \geq \boldsymbol{\beta}$$

The higher derivatives y (6) are eliminated by the Liu procedure.

According to (7) and (8), in our case a comparison with (9) results in

(11) 
$$\left( \varrho \frac{\partial \varepsilon}{\partial T} \quad \varrho \frac{\partial \varepsilon}{\partial \nabla T} \quad \frac{\partial \mathbf{q}}{\partial \nabla T} \right) \stackrel{\wedge}{=} \mathbf{A}, \quad -\frac{\partial \mathbf{q}}{\partial T} \cdot \nabla T \stackrel{\wedge}{=} \mathbf{B},$$

(12) 
$$\left( \begin{array}{cc} \varrho \frac{\partial s}{\partial T} & \varrho \frac{\partial s}{\partial \nabla T} & \frac{\partial \Phi}{\partial \nabla T} \end{array} \right) \stackrel{\wedge}{=} \alpha, \qquad -\frac{\partial \Phi}{\partial T} \cdot \nabla T \stackrel{\wedge}{=} \beta.$$

Using (11) and (12), we obtain the Liu equations and the residual inequality (10). In our case, the Liu equations run as follows

(13) 
$$\lambda \varrho \frac{\partial \varepsilon}{\partial T} = \varrho \frac{\partial s}{\partial T} \longrightarrow \lambda = \frac{\partial s/\partial T}{\partial \varepsilon/\partial T} = \left(\frac{ds}{d\varepsilon}\right)_{\nabla T},$$

(14) 
$$\lambda \varrho \frac{\partial \varepsilon}{\partial \nabla T} = \varrho \frac{\partial s}{\partial \nabla T},$$

(15) 
$$\lambda \frac{\partial q}{\partial \nabla T} = \frac{\partial \Phi}{\partial \nabla T}.$$

The residual inequality is

(16) 
$$-\lambda \frac{\partial \boldsymbol{q}}{\partial T} \cdot \nabla T \geq -\frac{\partial \boldsymbol{\Phi}}{\partial T} \cdot \nabla T \longrightarrow \frac{\partial}{\partial T} (\lambda \boldsymbol{q} - \boldsymbol{\Phi}) \cdot \nabla T \leq \frac{\partial \lambda}{\partial T} \boldsymbol{q} \cdot \nabla T$$

Liu's equations and the residual inequality represent constraints for the partial derivatives of the constitutive mappings  $\varepsilon$ , s, q and  $\Phi$ .

From (13) and (14) we obtain

(17) 
$$\lambda \partial_t \varepsilon = \partial_t s,$$

and from (15) and (16)

(18) 
$$\lambda \nabla \cdot \boldsymbol{q} \leq \nabla \cdot \boldsymbol{\Phi} \longrightarrow -\boldsymbol{q} \cdot \nabla \lambda \leq \nabla \cdot (\boldsymbol{\Phi} - \lambda \boldsymbol{q}).$$

From (13) and (14) the second derivatives result in

(19) 
$$\frac{\partial^2 s}{\partial \nabla T \partial T} = \frac{\partial}{\partial \nabla T} \left( \lambda \frac{\partial \varepsilon}{\partial T} \right) = \frac{\partial}{\partial T} \left( \lambda \frac{\partial \varepsilon}{\partial \nabla T} \right),$$

(20) 
$$\frac{\partial^2 \varepsilon}{\partial \nabla T \partial T} = \frac{\partial}{\partial \nabla T} \left( \frac{1}{\lambda} \frac{\partial s}{\partial T} \right) = \frac{\partial}{\partial T} \left( \frac{1}{\lambda} \frac{\partial s}{\partial \nabla T} \right).$$

Consequently, we obtain from the second equations by straight forward calculation

(21) 
$$\frac{\partial \lambda}{\partial \nabla T} \frac{\partial \varepsilon}{\partial T} = \frac{\partial \lambda}{\partial T} \frac{\partial \varepsilon}{\partial \nabla T},$$

(22) 
$$\frac{\partial(1/\lambda)}{\partial\nabla T}\frac{\partial s}{\partial T} = \frac{\partial(1/\lambda)}{\partial T}\frac{\partial s}{\partial\nabla T}.$$

The differential of the internal energy follows by the choice of the state space (3)

(23) 
$$d\varepsilon = \frac{\partial \varepsilon}{\partial T} dT + \frac{\partial \varepsilon}{\partial \nabla T} \cdot \nabla T = \frac{\partial \varepsilon}{\partial T} dT + \frac{\partial \varepsilon}{\partial T} \frac{\partial \lambda / \partial \nabla T}{\partial \lambda / \partial T} \cdot \nabla T.$$

Here, the second equation comes out by inserting (21). From (23) follows

(24) 
$$\frac{\partial\lambda}{\partial T}d\varepsilon = \frac{\partial\varepsilon}{\partial T}\left[\frac{\partial\lambda}{\partial T}dT + \frac{\partial\lambda}{\partial\nabla T}\cdot\nabla T\right] = \frac{\partial\varepsilon}{\partial T}d\lambda,$$

and therefore

(25) 
$$d\varepsilon = \frac{\partial \varepsilon / \partial T}{\partial \lambda / \partial T} d\lambda.$$

Totally analogous, (22) results in

(26) 
$$ds = \frac{\partial s/\partial T}{\partial (1/\lambda)/\partial T} d(1/\lambda) = \frac{\partial s/\partial T}{\partial \lambda/\partial T} d\lambda.$$

By (25) and (26), we obtain that the internal energy and the entropy depend on only one variable which is a state function

(27) 
$$\varepsilon = \varepsilon(\lambda(T, \nabla T)), \quad s = s(\lambda(T, \nabla T))$$

This result cannot be derived for the heat flux density and the entropy flux density, because the equation analogous to (13) does not exist and is replaced by the inequality (16). Thus we obtain from (13) and (14) the relation

(28) 
$$\lambda \frac{\partial \varepsilon}{\partial \lambda} = \frac{\partial s}{\partial \lambda} \longrightarrow \varepsilon = \frac{\partial}{\partial \lambda} (\lambda \varepsilon - s)$$

The influence of the constraints on the constitutive mappings by the Liu equations and the residual inequality is investigated in the next section.

### 4. Close-to-Fourier constitutive equations

In the frame of the chosen state space (3), we assume for the heat flux density and for the rate of the specific internal energy

(29) 
$$\boldsymbol{q} = -\kappa(\boldsymbol{z})\nabla T,$$

(30) 
$$\partial_t \varepsilon = C(z) \partial_t T + D(z) \nabla T \cdot \partial_t \nabla T$$

From the last equation follows

(31) 
$$C(\mathbf{z}) = \frac{\partial \varepsilon(\mathbf{z})}{\partial T} = \frac{\partial \varepsilon}{\partial \lambda} \frac{\partial \lambda}{\partial T},$$

(32) 
$$D(z)\nabla T = \frac{\partial \varepsilon(z)}{\partial \nabla T} = \frac{\partial \varepsilon}{\partial \lambda} \frac{\partial \lambda}{\partial \nabla T}$$

A relation follows from both the last equations for D and C

(33) 
$$D\nabla T = C \frac{\partial \lambda / \partial \nabla T}{\partial \lambda / \partial T}.$$

Inserting this into (30), we obtain

(34) 
$$\partial_t \varepsilon = C \left( \partial_t T + \frac{\partial \lambda / \partial \nabla T}{\partial \lambda / \partial T} \cdot \partial_t \nabla T \right).$$

Using the Liu equations (13) to (15) and the dissipation inequality (16), the partial derivatives of s and  $\Phi$  satisfy

(35) 
$$\frac{\partial s}{\partial T} = \frac{\partial s}{\partial \lambda} \frac{\partial \lambda}{\partial t} = \lambda C, \qquad \frac{\partial s}{\partial \nabla T} = \frac{\partial s}{\partial \lambda} \frac{\partial \lambda}{\partial \nabla T} = \lambda D \nabla T,$$

(36) 
$$\frac{\partial \Phi}{\partial T} \cdot \nabla T \ge -\lambda \frac{\partial \kappa}{\partial T} \nabla T \cdot \nabla T, \qquad \frac{\partial \Phi}{\partial \nabla T} = -\lambda \left( \frac{\partial \kappa}{\partial \nabla T} \nabla T + \kappa \mathbf{1} \right)$$

#### 5. Close-to-Fourier heat conduction equation

Inserting the constitutive equations (29) and (30) into the balance of energy  $(2)_1$ , we obtain the following close-to-Fourier heat conduction equation

(37) 
$$\varrho(C\partial_t T + D\nabla T \cdot \partial_t \nabla T) = \frac{\partial\kappa}{\partial T} \nabla T \cdot \nabla T + \frac{\partial\kappa}{\partial \nabla T} \nabla T : \nabla \nabla T + \kappa \nabla \cdot \nabla T$$

This heat conduction equation is of first order in time, a fact which is essential for the initial conditions. Dependent on the values of its coefficients, this differential equation is parabolic or hyperbolic. This demonstrate that the ansatz (29) allows hyperbolic heat conduction, if the expression for the internal energy, modified by (30), is chosen according to the minimal state space (3). If  $D \equiv 0$ , (37) becomes parabolic according to usual Fourier heat conduction.

### 6. Mathematical classification of close-to-Fourier heat conduction equation

Nonlinear partial differential equations of second order can be classified according to the eigenvalues of the coefficient matrix of the second derivatives. The classification is as follows:

- non-vanishing defect<sup>1</sup> ( $\delta > 0$ ): parabolic
- vanishing defect and inertia index<sup>2</sup> equal one: hyperbolic
- vanishing defect and inertia index zero or two: elliptic

The eigenvalues of this partial differential equation are

$$\lambda_{1} = -\frac{\sqrt{\left(D^{2}\varrho^{2} + \left(\frac{d}{dT}\kappa\right)^{2}\right)\left(\frac{d}{dx}T\right)^{2} + 2\kappa\left(\frac{d}{dT}\kappa\right)\left(\frac{d}{dx}T\right) + \kappa^{2} - \frac{d}{dT}\kappa\left(\frac{d}{dx}T\right) - 2}{2}}{\sqrt{\left(D^{2}\varrho^{2} + \left(\frac{d}{dT}\kappa\right)^{2}\right)\left(\frac{d}{dx}T\right)^{2} + 2\kappa\left(\frac{d}{dT}\kappa\right)\left(\frac{d}{dx}T\right) + \kappa^{2}} + \frac{d}{dT}\kappa\left(\frac{d}{dx}T\right) + \kappa}{2}}$$

$$\lambda_2$$

From this results that the defect is zero, if  $D \neq 0$ . This means the PDE is hyperbolic.

### 7. Introduction to Symbolic-Numerical approximation

The close-to-Fourier heat conduction equation (37) contains three different parameters C, D and  $\hat{\kappa} = \frac{\kappa}{\rho}$ .

For further investigation we will restrict to the 1-space-dimensional case. Furthermore we will assume C = const. = 1 and  $\hat{\kappa} = \text{const.}$  or  $\hat{\kappa} = T$  in the next sections, this means the second term of the right hand side in (37) vanishes.

Symbolic-Numerical approximation means we are using a finite element full discretisation with linear ansatz functions ( $P_1$ -FEM). However, the geometric structure of the discrete solutions might be more complicated than the analytic ones. In contrast to usual numeric evaluation of the finite element equation, the ansatz functions would be computed

 $\kappa$ 

<sup>&</sup>lt;sup>1</sup>The defect is the number of vanishing eigenvalues.

<sup>&</sup>lt;sup>2</sup>The inertia index is the number of negative eigenvalues.

symbolically on a reasonable initial grid. This enables us to leave parameters unspecified. By this we can also determine for which ranges of a parameter the solution of the PDE is isomorphic, and for which range there exists more than one solution so that the Newton type methods might go to a wrong destination (or even diverge). Those ansatz functions obtained by symbolic computing method are called the preprocessed solutions, which own the main structure of finite element solutions. In order to obtain the more accurate numerical solutions, we could chose these preprocessed solutions as the starting values for further re-correction on the refined grids. That will save the total Newton steps and make the numerical approach on the refined grid works more stable.

#### 8. Symbolic-Numerical approximation with $\hat{\kappa} = \text{const.}$

Considering the model problem

(40) 
$$\partial_t T + D\nabla T \cdot \partial_t \nabla T = \kappa \nabla \cdot \nabla T,$$

on space domain [0,1] with initial boundary condition T(0,t) = 1, T(1,t) = 0 and  $T(\cdot,0) = (1-x)^2$ , the exact result  $T(\cdot,1)$  is expected to be a linear function 1-x. To compute the numerical solution  $T_h(\cdot,1)$  we discretize (40) in the linear finite element space  $S_h([0,1]$  combined with backward Euler scheme associated to the time variable t. The numerical solutions satisfies the following discrete form:

Look for  $T_h^N$ , satisfies

(41) 
$$\int_{0}^{1} Kv(U_{h}^{n} - U_{h}^{n-1} + \frac{D(U_{h}^{'n} - 1)^{2}}{2} - \frac{D(U_{h}^{'n-1} - 1)^{2}}{2}) + v'U_{h}^{'n} = 0,$$
  
$$\forall v \in S_{h}([0, 1]), \ n = 1, ..N,$$

where K is the average mesh size with respect to time variable t, KN = 1,  $U_h^0 = x - x^2$ , and  $T_h^N = U_h^N + 1 - x$ . Form (41) appears as a system of polynomial equations, so that the D-parameter dependent solutions can be computed by the symbolic computing software [10] if all the domain partition sizes are determined. E.g. if the average partition to the space [0, 1] generates 4 inner variables and the mesh size K = 1/16, Figure 1 roughly shows the geometric structure of finite element solution  $U_h^1$  at space grid 4/5 after the first backward Euler iteration (e.g. t = 1/16).

In Figure 1 we see that only for parameter D close to 1, there exist "a-most" unique finite element solution so that the followed iteration for backward Euler scheme will work stable. On other range of D, there exists more than one iterative starting points which lead to different destinations. On that case, we should chose which iterative procedure approaches more close to the real result by further analysis. For specific D = 6/7 in (41), we obtain the finite element solution  $T_h$  in Figure 2, which is sufficiently close to the exact solution.



FIGURE 1. The D-dependent function curve of  $U_h^1$  at grid 4/5



FIGURE 2.  $T_h(\cdot, t = 1)$  on the whole range [0,1]

# 9. Symbolic-Numerical approximation with $\hat{\kappa} = T$

We consider another model problem

(42) 
$$\partial_t T + D\nabla T \cdot \partial_t \nabla T = \nabla T \cdot \nabla T + T \nabla \cdot \nabla T.$$

on domain [0,1] with initial boundary condition T(0,t) = 1, T(1,t) = 0 and  $T(\cdot,0) = (1-x)^2$ . The analytic result  $T(\cdot,1)$  is expect to be a "fading-wave" function.

In the finite element space  $S_h[0,1]$ , the discrete solution  $T_h^N$  should satisfies

(43) 
$$\int_{0}^{1} Kv(U_{h}^{n} - U_{h}^{n-1} + D(U_{h}^{'n} - 1)^{2}/2 - D(U_{h}^{'n-1} - 1)^{2}/2) + v'(U_{h}^{'n} - x + 1)(U_{h}^{'n} - 1) = 0, \ \forall v \in S_{h}([0, 1]), \ n = 1, ..N,$$

where K is the average mesh size with respect to time variable t, KN = 1,  $U_h^0 = x - x^2$ , and  $T_h^N = U_h^N + 1 - x$ .

Again, the *D*-parameter dependent solution can be computed symbolically since the form (43) is a system of polynomial equations. Divide the space [0, 1] by average which generates 4 inner variables and set the mesh size K = 1/14, Figure 3 shows the geometric structure of finite element solution  $U_h^1$  around the range D = 1, after the first backward Euler iteration step.



FIGURE 3. The D-dependent function curve of  $U_h^1$  at grid 4/5

Set specific D = 1, there exist two separated numerical results, so that the backward Euler scheme also generates more than one numerical solutions at t = 1. By further analysis, we chose one of the solutions (Figure 4) as the more reasonable preprocessed result. In order to reach the higher accuracy, we take this function in Figure 4 as the starting value for further Newton iterative re-correction on refined grid, so that the numerical approach on the fine grid will work efficient.

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FIGURE 4. One of the preprocessed function curve of  $T_h(\cdot, t = 1)$ 

#### 10. Summary

Close-to-Fourier heat conduction is characterized by two items: Choice of a minimal state space and choice of Fourier's ansatz for the heat flux density. By Liu's procedure, we obtain a close-to-Fourier heat conduction equation which is hyperbolic and parabolic in the thermostatic limit. This result demonstrates that close-to-Fourier heat conduction is hyperbolic beyond the thermostatic limit, thus avoiding one of the shortcomings of Fourier heat conduction.

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