

# Heat conduction in microstructured solids under localised pulse loading

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## Abstract

The influence of a microstructure on heat conduction in solids is studied numerically using the internal variable approach. Two variants of the internal variable treatment are compared by means of the numerical simulation of two-dimensional heat conduction in a plate under a localised thermal pulse loading. Computations of the same problem by the different internal variable descriptions produce qualitatively dissimilar results. The single internal variable approach leads to a diffusional type of the internal variable evolution. In contrast, dual internal variable technique provides a wave-like evolution of the internal variables, and, as the consequence, the corresponding wave-like heat transfer. The results are obtained in the dimensionless form, and parameters of models are chosen to emphasize the features of each model.

*Keywords:* Heat conduction, Internal variables, Microstructured solids, Numerical simulation

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## 1. Introduction

The Fourier law is the cornerstone of heat transfer theory and practice (Carslaw and Jaeger, 1992, e.g.). Being well applicable for homogeneous continua, it is not sufficient for the description of heat conduction in inhomogeneous solids (Kaminiski, 1990; Özişik and Tzou, 1994). Moreover, an inner microstructure in a solid can be the source of a hyperbolic character of heat conduction (Mariano, 2017).

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A variety of phenomenological hyperbolic heat conduction models has been proposed as discussed in (Joseph and Preziosi, 1989; Tzou, 1995; Roetzel et al., 2003; Straughan, 2011; Ván and Fülöp, 2012; Sellitto et al., 2016; Liu et al., 2017; Rogolino et al., 2018, e.g.). The most popular are the Cattaneo–Vernotte model, Guyer-Krumhansl model (Guyer and Krumhansl, 1966), and dual-phase lag model (Tzou, 1995). Among others, Coleman et al. model (Coleman et al., 1982), Gurtin-Pipkin model (Gurtin and Pipkin, 1968), double temperature model (Sobolev, 2016), temperature gradient model (Nguyen, 2010), thermomass model (Guo and Hou, 2010), micromorphic model (Liu et al., 2017), should be mentioned. The common feature of many hyperbolic heat conduction models is the extension of the thermodynamic state space by heat flux and/or entropy flux. The extension of the thermodynamic state space by heat flux has been employed and discussed by several researchers (Coleman et al., 1982, 1986; Bai and Lavine, 1995; Lebon and Grmela, 1996; Barletta and Zanchini, 1997; Jou et al., 2004; Rogolino et al., 2018). The dependence of entropy on temperature and heat flux is the main constitutive postulate in the extended irreversible thermodynamics (Jou et al., 2010).

It is known that the thermodynamic state space can be extended in a more general manner (Cimmelli, 2009; Ván and Fülöp, 2012; Cimmelli et al., 2014; Carlomagno et al., 2016; Liu et al., 2017, e.g.). The consecutive and thermodynamically consistent method of such an extension is provided by the internal variable theory (Coleman and Gurtin, 1967; Rice, 1971; Maugin and Muschik, 1994a). Internal variables are used to describe how the influence of a possible material microstructure can be taken into account. This approach can be implemented in the finite volume framework for numerical simulations of the transient heat conduction in solids with a microstructure.

It should be noted that the conventional internal variable thermodynamic theory (Maugin and Muschik, 1994a) has been extended recently by the dual internal variable concept (Ván et al., 2008; Berezovski et al., 2011; Berezovski and Ván, 2017). In the paper, both kinds of the internal variable theory are compared on the example of transient heat conduction in a thin plate of a microstructured material under localised pulse loading at a boundary. The goal of the study is to examine possible similarities and/or differences in the application of internal variables for the description of the microstructure influence on heat conduction in rigid solids.

Classical representation of heat conduction in rigid solids is reminded briefly in Section 2. Section 3 contains the derivation of governing equations and results of numerical simulations of heat conduction in microstructured solids under localised pulse loading in the framework of the single internal variable theory. For

the dual internal variables approach, the corresponding governing equations and results of numerical simulations are given in Section 4. Conclusions are formulated in Section 5.

## 2. Classical heat conduction in rigid solids

The conduction of heat in rigid solids is governed by the local balance law for energy (in the absence of body sources) (Gurtin et al., 2010, e.g.)

$$\frac{\partial E}{\partial t} + \nabla \cdot \mathbf{q} = 0, \quad (1)$$

and by the second law of thermodynamics

$$\frac{\partial S}{\partial t} + \nabla \cdot \left( \frac{\mathbf{q}}{T} \right) \geq 0. \quad (2)$$

Here  $E$  is the internal energy per unit volume,  $\mathbf{q}$  is the heat flux,  $S$  is the entropy per unit volume,  $T$  is the absolute temperature.

The corresponding free energy density  $W = E - TS$  depends on temperature only (Gurtin et al., 2010)

$$W = W(T), \quad (3)$$

and the entropy density is calculated as follows

$$S = -\frac{\partial W}{\partial T}. \quad (4)$$

Due to the definition of entropy density, the time derivative of energy can be calculated by chain rule

$$\begin{aligned} \frac{\partial E}{\partial t} &= \frac{\partial(W + TS)}{\partial t} = \frac{\partial W}{\partial t} + \frac{\partial(TS)}{\partial t} = \frac{\partial W}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial(TS)}{\partial t} = \\ &= -S \frac{\partial T}{\partial t} + S \frac{\partial T}{\partial t} + T \frac{\partial S}{\partial t} = T \frac{\partial S}{\partial t}, \end{aligned} \quad (5)$$

and balance of energy (1) can be rewritten as

$$T \frac{\partial S}{\partial t} + \nabla \cdot \mathbf{q} = 0. \quad (6)$$

Multiplying second law (2) by  $T$  and comparing the result with balance of energy (6), we arrive at the inequality

$$-\mathbf{q} \nabla T \geq 0. \quad (7)$$

The latter inequality leads to the classical constitutive equation for heat flux which is called the Fourier law

$$\mathbf{q} = -k\nabla T, \quad (8)$$

with the thermal conductivity  $k$  considered here as a positive constant.

The quadratic free energy density of the form

$$W = -\frac{\rho c_p}{2T_0}(T - T_0)^2, \quad (9)$$

where  $\rho$  is the matter density and  $c_p$  is the heat capacity, determines the heat conduction equation for small deviations from the reference temperature  $T_0$

$$\rho c_p T_t - k\nabla^2 T = 0. \quad (10)$$

Classical heat conduction equation (10) is valid for homogeneous materials obeying the Fourier law. It is clear that this equation should be generalized to include the influence of a possible inhomogeneity of a material in the description of the heat conduction. Such a generalization can be achieved in many ways as it is demonstrated in (Liu et al., 2017; Berezovski, 2019, e.g.).

### 2.1. Heat flux as independent variable

The simplest step in the generalization is the inclusion of heat flux into the thermodynamic state space

$$W = W(T, \mathbf{q}). \quad (11)$$

Keeping the definition of the entropy density

$$S = -\frac{\partial W}{\partial T}, \quad (12)$$

we can calculate the time derivative of the internal energy

$$\begin{aligned} \frac{\partial E}{\partial t} &= \frac{\partial(W + TS)}{\partial t} = \frac{\partial W}{\partial t} + \frac{\partial(TS)}{\partial t} = \frac{\partial W}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial W}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t} + \frac{\partial(TS)}{\partial t} = \\ &= -S \frac{\partial T}{\partial t} + \frac{\partial W}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t} + S \frac{\partial T}{\partial t} + T \frac{\partial S}{\partial t} = T \frac{\partial S}{\partial t} + \frac{\partial W}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t}. \end{aligned} \quad (13)$$

Correspondingly, balance of energy (1) obtains the form

$$T \frac{\partial S}{\partial t} + \frac{\partial W}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t} + \nabla \cdot \mathbf{q} = 0. \quad (14)$$

Comparing the latter equation with the second law of thermodynamics multiplied by  $T$

$$T \frac{\partial S}{\partial t} + T \nabla \cdot \left( \frac{\mathbf{q}}{T} \right) \geq 0, \quad (15)$$

we arrive at the dissipation inequality in the form

$$-\frac{\partial W}{\partial \mathbf{q}} \frac{\partial \mathbf{q}}{\partial t} - \frac{\mathbf{q}}{T} \nabla T \geq 0. \quad (16)$$

Using a quadratic dependence for the free energy density

$$W = W(T, \mathbf{q}) = -\frac{\rho c_p}{2T_0} (T - T_0)^2 + \frac{1}{2} B \mathbf{q}^2, \quad (17)$$

we can rewrite the dissipation inequality as follows:

$$-\mathbf{q} (BT \frac{\partial \mathbf{q}}{\partial t} + \nabla T) \geq 0. \quad (18)$$

It is clear that the choice for heat flux

$$\mathbf{q} = -k (BT \frac{\partial \mathbf{q}}{\partial t} + \nabla T), \quad k \geq 0, \quad (19)$$

satisfies the dissipation inequality.

The latter equation can be represented in the form of the Cattaneo–Vernotte equation for small deviation from the reference temperature  $T_0$

$$\mathbf{q} + \tau \frac{\partial \mathbf{q}}{\partial t} = -k \nabla T, \quad k \geq 0, \quad (20)$$

with  $\tau = kBT_0$ .

Thus, the extension of the thermodynamic state space by heat flux allows to derive the Cattaneo–Vernotte equation in a thermodynamically consistent way. It should be noted that the corresponding heat conduction equation cannot be reduced to the telegrapher equation due to the presence of the second term in balance of energy (14). This has been noticed already by Coleman et al. (1982, 1986). A similar situation appears in the framework of the extended irreversible thermodynamics (Lebon et al., 2011) where the telegrapher equation is obtained only under assumption of the independence of internal energy of heat flux. Such an assumption is inconsistent with the main constitutive postulate of the dependence of entropy (and, therefore, internal energy) on temperature and heat flux (Jou et al., 2010).

This is why a more systematic way of the extension of the thermodynamic state space is described in what follows.

### 3. Single internal variable

It is supposed that the use of an internal variable will take into account the influence of microstructural processes on the global behavior of a material (Rice, 1971; Maugin and Muschik, 1994a). The internal variable theory has a long history (Coleman and Gurtin, 1967; Rice, 1971; Lubliner, 1973; Day, 1976; Maugin, 1990; Muschik, 1991; Kestin, 1993; Maugin and Muschik, 1994a; McDowell, 2005; Ván et al., 2008; Horstemeyer and Bammann, 2010; Maugin, 2015). Its comprehensive presentation for mechanical problems is given in (Maugin, 2006, 2010). The specification of the theory to heat conduction in microstructured solids is provided in (Berezovski, 2016, 2019). Here the main concepts needed for the derivation of governing equations for heat conduction in rigid solids with a microstructure are reminded.

We start with a weakly nonlocal theory of internal variable including an internal variable  $\alpha$  and its gradient into the thermodynamic state space (Lebon and Grmela, 1996; Valanis, 1996, cf.). In the simplest variant of such a theory (for rigid heat conductors), the free energy per unit volume  $W$  is specified as a function of the absolute temperature  $T$ , the internal variable  $\alpha$ , and its gradient  $\nabla\alpha$  (Maugin, 2006). In the case of a quadratic free energy density, we have

$$W = -\frac{\rho c_p}{2T_0}(T - T_0)^2 + \frac{1}{2}B\alpha^2 + \frac{1}{2}C(\nabla\alpha)^2, \quad (21)$$

where  $B$  and  $C$  are material parameters. The energy balance in terms of the free energy can be represented as (Maugin, 2006)

$$\frac{\partial(ST)}{\partial t} + \nabla \cdot \mathbf{q} = -\frac{\partial W}{\partial t}, \quad (22)$$

where body forces are neglected for simplicity.

Since the free energy depends on an internal variable, its time derivative is calculated by chain rule

$$\begin{aligned} -\frac{\partial W}{\partial t} &= -\frac{\partial W}{\partial T} \frac{\partial T}{\partial t} - \frac{\partial W}{\partial \alpha} \frac{\partial \alpha}{\partial t} - \frac{\partial W}{\partial \nabla \alpha} \frac{\partial \nabla \alpha}{\partial t} = \\ &= ST_t - B\alpha : \alpha_t - C\nabla\alpha : (\nabla\alpha_t)^T. \end{aligned} \quad (23)$$

Substituting expression (23) into Eq. (22), we can rewrite the balance of energy as follows:

$$(ST)_t + \nabla \cdot (\mathbf{q} + C\nabla\alpha : \alpha_t) = ST_t + (C\nabla^2\alpha - B\alpha) : \alpha_t. \quad (24)$$

### 3.1. Dissipation inequality

Having in mind the presence of the internal variable we can write the second law of thermodynamics in the form

$$\frac{\partial S}{\partial t} + \nabla \cdot \mathbf{S} \geq 0, \quad \mathbf{S} = \frac{\mathbf{q}}{T} + \mathbf{K}, \quad (25)$$

with the entropy flux  $\mathbf{S}$  containing an extra entropy flux  $\mathbf{K}$  (Müller, 1967, 1985; Maugin, 1990; Grmela et al., 1998; Maugin, 2006, cf.). The extra entropy flux vanishes in most cases, but this is not a basic requirement.

Multiplying second law (25) by temperature and taking into account energy balance equation (24) we can rewrite the dissipation inequality as

$$(C\nabla^2\alpha - B\alpha) : \alpha_t + \nabla \cdot (-C\nabla\alpha : \alpha_t + T\mathbf{K}) - \mathbf{S} \cdot \nabla T \geq 0. \quad (26)$$

Selecting the extra entropy flux following the idea by Maugin (1990)

$$\mathbf{K} = \frac{1}{T}(C\nabla\alpha) : \alpha_t, \quad (27)$$

we can eliminate the divergence term in the dissipation inequality

$$T(C\nabla^2\alpha - B\alpha) : \alpha_t - (\mathbf{q} + C\nabla\alpha : \alpha_t) \cdot \nabla T \geq 0. \quad (28)$$

Now the left-hand side of the dissipation inequality consists from the products of thermodynamic fluxes and forces.

### 3.2. Evolution equation for the single internal variable

The solution of dissipation inequality (28) is provided by the representation thermodynamic fluxes  $\alpha_t$  and  $(\mathbf{q} + C\nabla\alpha : \alpha_t)$  as linear functions of conjugated thermodynamic forces following the standard thermodynamic approach (De Groot and Mazur, 1962)

$$\begin{pmatrix} \alpha_t \\ (\mathbf{q} + C\nabla\alpha : \alpha_t) \end{pmatrix} = \mathbf{M} \begin{pmatrix} T(C\nabla^2\alpha - B\alpha) \\ -\nabla T \end{pmatrix}, \quad (29)$$

with

$$\mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}, \quad (30)$$

and components  $M_{ij}$  of the matrix  $\mathbf{M}$  are considered as constants for simplicity. The symmetric part of the matrix  $\mathbf{M}$  should be positive semidefinite to ensure the

non-negativity of the entropy production, which requires (Johnson, 1970; Horn et al., 1990)

$$M_{11} \geq 0, \quad M_{22} \geq 0, \quad M_{11}M_{22} - \frac{(M_{12} + M_{21})^2}{2} \geq 0. \quad (31)$$

Therefore, the evolution equation for the internal variable  $\alpha$  has the form

$$\alpha_t = M_{11}T (C\nabla^2\alpha - B\alpha) - M_{12}\nabla T. \quad (32)$$

Accordingly, for the generalized heat flux we have

$$\mathbf{q} + C\nabla\alpha : \alpha_t = M_{21}T (C\nabla^2\alpha - B\alpha) - M_{22}\nabla T. \quad (33)$$

Eliminating the heat flux from energy conservation equation (24) using Eq. (33), we arrive at the heat conduction equation in the framework of the single internal variable approach

$$TS_t - M_{22}\nabla^2T = (C\nabla^2\alpha - B\alpha) : \alpha_t - M_{21}\nabla \cdot [T(C\nabla^2\alpha - B\alpha)]. \quad (34)$$

### 3.3. Heat flux as internal variable

Now we are able to make a certain interpretation of the internal variable. It is noteworthy that choosing heat flux as the internal variable we obtain for its evolution from Eq. (32)

$$\mathbf{q}_t = M_{11}T(C\nabla^2\mathbf{q} - B\mathbf{q}) - M_{12}\nabla T. \quad (35)$$

It is clear that in the absence of internal variables (i.e., for zero values of  $B$  and  $C$ ) we have the classical Fourier law

$$\mathbf{q}_t = -M_{12}\nabla T. \quad (36)$$

If the free energy density does not depend on the gradient of the internal variable (i.e.,  $C = 0$ ), then the evolution equation for heat flux is reduced to a Cattaneo-Vernotte-type equation

$$\frac{1}{M_{11}TB}\mathbf{q}_t + \mathbf{q} = -\frac{M_{12}}{M_{11}TB}\nabla T. \quad (37)$$

If, vice versa, the free energy density depends only on the gradient of the internal variable and independent of the internal variable itself (i.e.,  $B = 0$ ), then we arrive at the Green-Naghdi-type equation for heat flux

$$\frac{1}{M_{11}TC}\mathbf{q}_t = -\frac{M_{12}}{M_{11}TC}\nabla T + \nabla^2\mathbf{q}. \quad (38)$$



Entire equation (35) can be interpreted as the Guyer-Krumhansl-type equation

$$\frac{1}{M_{11}TB} \mathbf{q}_t + \mathbf{q} = -\frac{M_{12}}{M_{11}TB} \nabla T + \frac{C}{B} \nabla^2 \mathbf{q}. \quad (39)$$

As noted in Section 2, the generalized evolution equations for heat flux do not ensure a hyperbolic character of the heat conduction equation. It is worth therefore to examine the complete system of equations (32) and (34). In the absence of analytical solution, we do this numerically.

### 3.4. Numerical test

#### 3.4.1. Governing equations

Considering small deviations of temperature from the reference value  $T_0$ , we neglect nonlinear terms which reduces heat conduction equation (34) to

$$T_t - k \nabla^2 T = -k_1 \nabla \cdot (\nabla^2 \boldsymbol{\alpha}) + k_2 \nabla \cdot \boldsymbol{\alpha}, \quad (40)$$

with  $k = M_{22}/\rho c_p$  and coupling coefficients  $k_1 = M_{21}T_0C/\rho c_p$  and  $k_2 = M_{21}B/\rho c_p$ . Accordingly, evolution equation for the internal variable (32) is represented as

$$\boldsymbol{\alpha}_t = a_1 \nabla^2 \boldsymbol{\alpha} - a_2 \boldsymbol{\alpha} - a_3 \nabla T, \quad (41)$$

with model parameters  $a_1 = M_{11}T_0C$ ,  $a_2 = M_{11}T_0B$ , and  $a_3 = M_{12}$ . Last two equations are similar to those presented in (Grot, 1969; Ieşan, 2002).

#### 3.4.2. Formulation of the problem

As an example, the transient heat conduction from a heat source localized at the boundary of a thin plate is considered. The sketch of the problem is shown in Fig. 1. The plate is made from a homogeneous isotropic material with a possible inner microstructure. The length of the plate is denoted by  $L$  and its width is equal to  $d$ .

Initially, the plate has uniform temperature  $T_0$ . The thermal loading  $T_l(x, t)$  is nonzero only at the bottom boundary for  $x \in [-h/2, h/2]$ . All other parts of plate boundaries are keeping at the ambient temperature  $T_0$ . The shape of the loading  $T_l(x, t)$  is a smooth cosine pulse of duration  $t_l$  with the amplitude  $T_1$  changing according to cosine function in  $x$ , namely,

$$T(x, t) = \frac{T_1}{2} \cos\left(\frac{\pi x}{2h}\right) \left(1 - \cos\frac{2\pi t}{t_l}\right) [H(t) - H(t - t_l)], \quad (42)$$

where  $H(t)$  denotes the Heaviside step function.

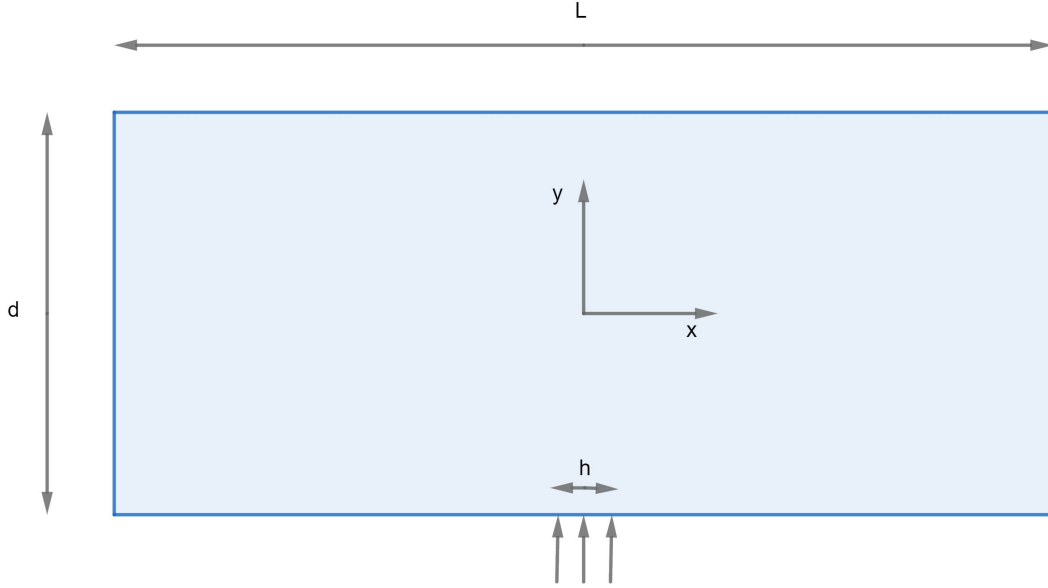


Figure 1: Sketch of the problem.

### 3.4.3. Dimensionless variables

To reduce the number of coefficients it is useful to introduce dimensionless variables. Let  $t_0$  is a characteristic time of a process and  $l_0 = L$  is its characteristic length. Dimensionless variables (denoted by primes) are introduced as follows:

$$t' = \frac{t}{t_0}, \quad \mathbf{x}' = \frac{\mathbf{x}}{l_0}, \quad T' = \frac{T}{T_0}, \quad \boldsymbol{\alpha}' = \frac{\boldsymbol{\alpha}}{A_0}, \quad (43)$$

with the reference temperature  $T_0$  and the reference magnitude of the internal variable  $A_0$ . Substitution of definitions (43) into Eqs. (40) and (41) provides

$$\frac{A_0}{t_0} \boldsymbol{\alpha}'_{t'} = \frac{A_0 a_1}{l_0^2} \nabla'^2 \boldsymbol{\alpha}' - A_0 a_2 \boldsymbol{\alpha}' - \frac{T_0 a_3}{l_0} \nabla' T', \quad (44)$$

and

$$\frac{T_0}{t_0} T'_{t'} - \frac{k T_0}{l_0^2} \nabla'^2 T' = -\frac{k_1 A_0}{l_0^3} \nabla' \cdot (\nabla'^2 \boldsymbol{\alpha}') + \frac{k_2 A_0}{l_0} \nabla' \cdot \boldsymbol{\alpha}'. \quad (45)$$

The choice of characteristic values  $t_0$  and  $A_0$  is dictated by the conservation of the same order of magnitude for first three terms in heat conduction equation (45)

$$t_0 = \frac{l_0^2}{k}, \quad A_0 = l_0 T_0. \quad (46)$$

Such a choice results in the dimensionless heat conduction equation

$$T'_{,t} - \nabla'^2 T' = -\frac{k_1}{k} \nabla' \cdot (\nabla'^2 \alpha') + \frac{k_2 l_0^2}{k} \nabla' \cdot \alpha'. \quad (47)$$

The dimensionless evolution equation for the internal variable obtains the form

$$\alpha'_{,t} = \frac{a_1}{k} \nabla'^2 \alpha' - \frac{a_2 l_0^2}{k} \alpha' - \frac{a_3}{k} \nabla' T'. \quad (48)$$

For a clear demonstration of the effect of the internal variable, we choose the value of parameters  $k = 1$ ,  $k_1 = 10$ ,  $k_2 l_0^2 = 0.5$ , the equality of coefficients  $a_1$  and  $k$ , and  $a_2$  and  $k_2$ , and the small value of  $a_3 = 0.005$ .

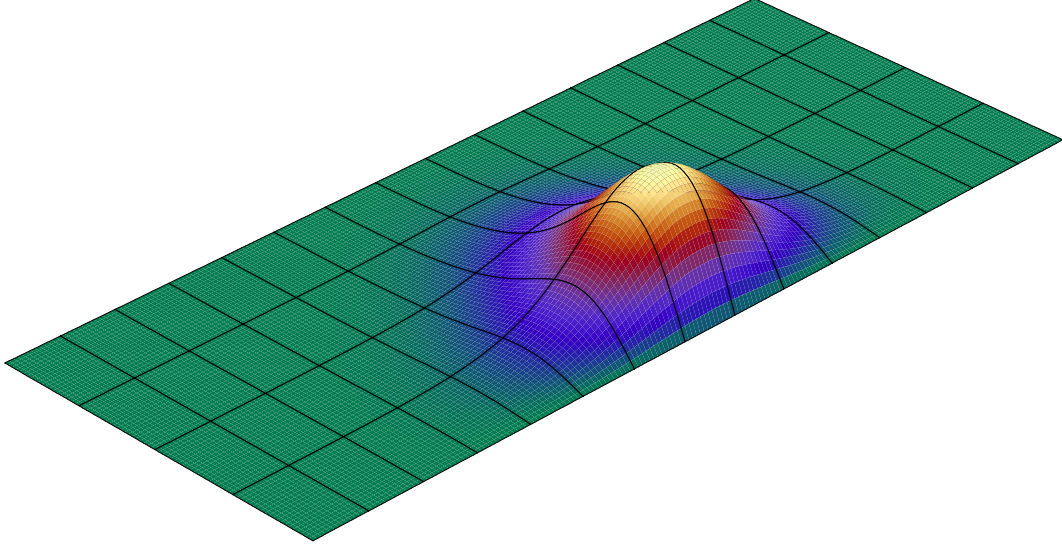


Figure 2: Temperature distribution in the plate at 1000 time steps.

#### 3.4.4. Results of the simulation

Computations in the two-dimensional case are performed by means of the finite-volume numerical scheme (Berezovski et al., 2008) with the dimensionless space step  $\Delta x' = 5 \cdot 10^{-3}$  and the dimensionless time step  $\Delta t' = 8.33 \cdot 10^{-6}$ . The length of the computational domain is equal to  $200\Delta x$  and its width is  $80\Delta x$ . The pulse duration is  $50\Delta t$ , its width  $h = 20\Delta x$ , and the initial amplitude is equal to  $5T_0$  (expressed in Celsius degrees). Typical result of the simulation is presented

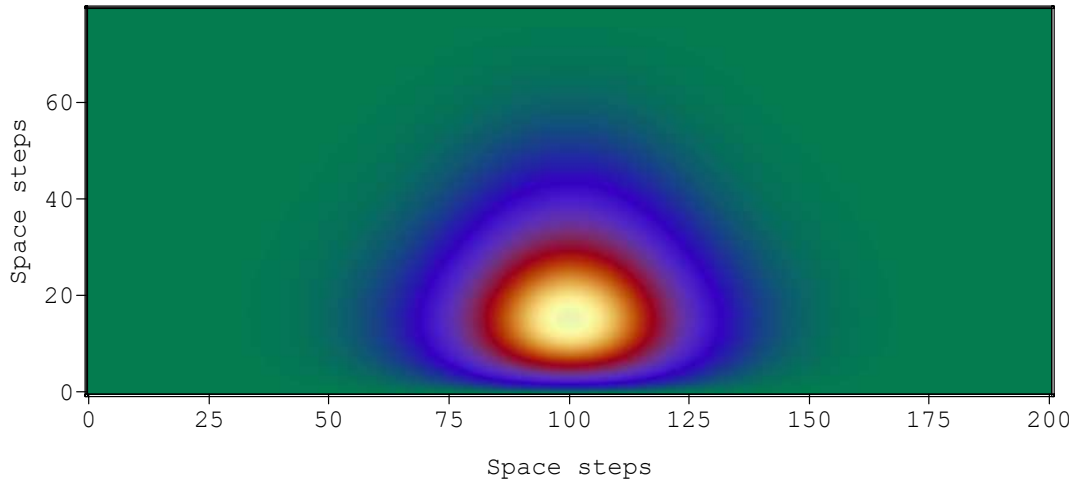


Figure 3: Contour plot of temperature distribution in the plate with microstructure at 1000 time steps.

in Fig. 2 in terms of the distribution of the excess of dimensionless temperature at 1000 time steps. The corresponding contour plot is shown in Fig. 3.

As one can see, the microstructure influence changes the distribution of temperature in the plate only slightly in comparison with the more symmetrical temperature distribution in the homogeneous plate without microstructure shown in Fig. 4. This is due to the parabolicity of the evolution equation for the internal variable.

It seems that the single internal variable technique is unable to describe a wave-like thermal response to the localised heating. The single internal variable theory provides the generalization of governing equations of heat conduction in microstructured solids but does not change the mathematical structure of the description. Governing equations (40) and (41) remain parabolic in this framework both for heat conduction and the internal variable evolution.

However, the internal variable theory does not exhausted by the single internal variable case. The dual internal variable approach (Ván et al., 2008; Berezovski et al., 2011; Berezovski and Ván, 2017) affords a more general description ensuring a hyperbolic behavior of internal variables even in the heat conduction case (Berezovski, 2016, 2019).

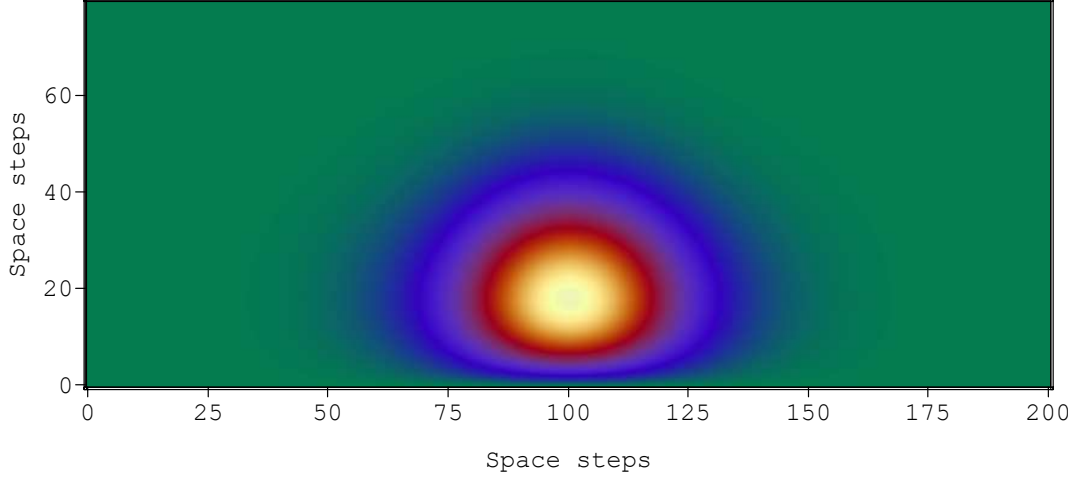


Figure 4: Contour plot of temperature distribution in the plate without microstructure at 1000 time steps.

#### 4. Dual internal variables

The dual internal variable approach is the generalization of the single internal variable theory (Ván et al., 2008; Berezovski et al., 2011; Berezovski and Ván, 2017). For heat conduction in solids, it has been specified in (Berezovski, 2016, 2019). In this approach it is supposed that the free energy depends on internal variables  $\alpha, \beta$ , and their space gradients.

##### 4.1. Quadratic free energy

Specifying the free energy density as a quadratic function of its arguments

$$W = -\frac{\rho c_p}{2T_0}(T - T_0)^2 + \frac{1}{2}B\alpha^2 + \frac{1}{2}C(\nabla\alpha)^2 + \frac{1}{2}D\beta^2 + \frac{1}{2}F(\nabla\beta)^2, \quad (49)$$

we can calculate the time derivative of the free energy

$$\begin{aligned} -\frac{\partial W}{\partial t} &= -\frac{\partial W}{\partial T} \frac{\partial T}{\partial t} - \frac{\partial W}{\partial \alpha} \frac{\partial \alpha}{\partial t} - \frac{\partial W}{\partial \nabla \alpha} \frac{\partial \nabla \alpha}{\partial t} - \frac{\partial W}{\partial \beta} \frac{\partial \beta}{\partial t} - \frac{\partial W}{\partial \nabla \beta} \frac{\partial \nabla \beta}{\partial t} = \\ &= ST_t - B\alpha : \alpha_t - C\nabla\alpha : (\nabla\alpha_t)^T - D\beta : \beta_t - F\nabla\beta : (\nabla\beta_t)^T. \end{aligned} \quad (50)$$

Balance of energy (Eq. (22)) is then rewritten with the obtained expression for time rate of the free energy

$$\begin{aligned} (ST)_t + \nabla \cdot \mathbf{q} &= ST_t - B\alpha : \alpha_t - C\nabla\alpha : (\nabla\alpha_t)^T - \\ &\quad - D\beta : \beta_t - F\nabla\beta : (\nabla\beta_t)^T. \end{aligned} \quad (51)$$

It can be further transformed to

$$\begin{aligned} (ST)_t + \nabla \cdot (\mathbf{q} + C\nabla\alpha : \alpha_t + F\nabla\beta : \beta_t) &= \\ &= ST_t + (C\nabla^2\alpha - B\alpha) : \alpha_t + (F\nabla^2\beta - D\beta) : \beta_t. \end{aligned} \quad (52)$$

Accordingly, the dissipation inequality reads

$$\begin{aligned} (C\nabla^2\alpha - B\alpha) : \alpha_t + (F\nabla^2\beta - D\beta) : \beta_t + \\ + \nabla \cdot (C\nabla\alpha : \alpha_t + F\nabla\beta : \beta_t + T\mathbf{K}) - \\ - \frac{1}{T}(\mathbf{q} - C\nabla\alpha : \alpha_t - F\nabla\beta : \beta_t) \cdot \nabla T \geq 0. \end{aligned} \quad (53)$$

The elimination of the divergence term in the dissipation inequality is achieved using the idea of Maugin (1990)

$$\mathbf{K} = -\frac{1}{T}(C\nabla\alpha : \alpha_t + F\nabla\beta : \beta_t). \quad (54)$$

This choice of the extra entropy flux reduces the dissipation inequality to the sum of products of thermodynamic fluxes and forces

$$\begin{aligned} (C\nabla^2\alpha - B\alpha) : \alpha_t + (F\nabla^2\beta - D\beta) : \beta_t - \\ - \frac{1}{T}(\mathbf{q} - C\nabla\alpha : \alpha_t - F\nabla\beta : \beta_t) \cdot \nabla T \geq 0. \end{aligned} \quad (55)$$

#### 4.2. Evolution equations for internal variables

Similarly to the case of single internal variable we can represent a linear solution of the dissipation inequality as

$$\begin{pmatrix} \alpha_t \\ \beta_t \\ (\mathbf{q} - C\nabla\alpha : \alpha_t - F\nabla\beta : \beta_t) \end{pmatrix} = \mathbf{L} \begin{pmatrix} (C\nabla^2\alpha - B\alpha) \\ (F\nabla^2\beta - D\beta) \\ -\frac{1}{T}\nabla T \end{pmatrix}, \quad (56)$$

where

$$\mathbf{L} = \begin{pmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{pmatrix}, \quad (57)$$

with the similar condition of semidefiniteness of the matrix  $\mathbf{L}$  as mentioned above.

It follows that evolution equations for internal variables  $\alpha$  and  $\beta$  have the form

$$\alpha_t = L_{11}(C\nabla^2\alpha - B\alpha) + L_{12}(F\nabla^2\beta - D\beta) - L_{13}\frac{1}{T}\nabla T, \quad (58)$$

$$\beta_t = L_{21}(C\nabla^2\alpha - B\alpha) + L_{22}(F\nabla^2\beta - D\beta) - L_{23}\frac{1}{T}\nabla T, \quad (59)$$

and the modified heat flux is calculated similarly

$$\begin{aligned} \mathbf{q} - C\nabla\alpha : \alpha_t - F\nabla\beta : \beta_t &= L_{31}(C\nabla^2\alpha - B\alpha) + \\ &+ L_{32}(F\nabla^2\beta - D\beta) - L_{33}\frac{1}{T}\nabla T. \end{aligned} \quad (60)$$

Correspondingly, the heat conduction equation reads

$$\begin{aligned} (ST)_t + \nabla \cdot (L_{31}(C\nabla^2\alpha - B\alpha) + L_{32}(F\nabla^2\beta - D\beta) - L_{33}\frac{1}{T}\nabla T) &= \\ = ST_t + (C\nabla^2\alpha - B\alpha) : \alpha_t + (F\nabla^2\beta - D\beta) : \beta_t. \end{aligned} \quad (61)$$

Equations (58) – (61) compose the complete system of equations for the calculation of the evolution of internal variables and temperature. However, one of the internal variables (say,  $\beta$ ) can be eliminated.

#### 4.3. Elimination of one internal variable

Neglecting the nonlinear contributions for small deviations of temperature from its reference value  $T_0$  we can calculate the time derivative of the evolution equation for the internal variable  $\alpha$

$$\alpha_{tt} = L_{11}(C\nabla^2\alpha_t - B\alpha_t) + L_{12}(F\nabla^2\beta_t - D\beta_t) - L_{13}\frac{1}{T_0}\nabla T_t, \quad (62)$$

and express the time rate of  $\beta$  in terms of  $\alpha$

$$\beta_t = \frac{\widehat{L}_{21}}{L_{12}}(C\nabla^2\alpha - B\alpha) + \frac{L_{22}}{L_{12}}\alpha_t + \frac{\widehat{L}_{23}}{L_{12}}\frac{1}{T_0}\nabla T, \quad (63)$$

as well as the time rate of the Laplacian  $\beta$

$$\nabla^2\beta_t = \frac{\widehat{L}_{21}}{L_{12}}\nabla^2(C\nabla^2\alpha - B\alpha) + \frac{L_{22}}{L_{12}}\nabla^2\alpha_t + \frac{\widehat{L}_{23}}{L_{12}}\frac{1}{T_0}\nabla(\nabla^2T), \quad (64)$$

with  $\widehat{L}_{21} = L_{21}L_{12} - L_{11}L_{22}$ ,  $\widehat{L}_{23} = L_{13}L_{22} - L_{23}L_{12}$ .

The single evolution equation for the internal variable  $\alpha$  is obtained by substitution the relationships for the time derivatives of  $\beta$  and its Laplacian in the expression for the second time derivative of  $\alpha$

$$\begin{aligned}\alpha_{tt} = & \widehat{L}_{21}BD\alpha - \widehat{L}_{21}(CD + BF)\nabla^2\alpha - (L_{22}D + L_{11}B)\alpha_t + \\ & + (L_{11}C + L_{22}F)\nabla^2\alpha_t - \widehat{L}_{23}D\frac{1}{T_0}\nabla T - L_{13}\frac{1}{T_0}\nabla T_t + \\ & + CF\widehat{L}_{21}\nabla^2(\nabla^2\alpha) + F\widehat{L}_{23}\frac{1}{T_0}\nabla(\nabla^2T).\end{aligned}\quad (65)$$

#### 4.4. Simplifications

To reduce the complexity of the obtained evolution equation, we consider its simplified version with vanishing values of coefficients  $B$  and  $F$  in the free energy dependence

$$\begin{aligned}\alpha_{tt} = & -\widehat{L}_{21}(CD)\nabla^2\alpha - (L_{22}D)\alpha_t + (L_{11}C)\nabla^2\alpha_t - \\ & -\widehat{L}_{23}D\frac{1}{T_0}\nabla T - L_{13}\frac{1}{T_0}\nabla T_t.\end{aligned}\quad (66)$$

Avoiding viscous dissipation, i.e.,  $L_{13} = 0$ ,  $L_{22} = 0$ , we arrive at

$$\alpha_{tt} = -\widehat{L}_{21}(CD)\nabla^2\alpha + (L_{11}C)\nabla^2\alpha_t - \widehat{L}_{23}D\frac{1}{T_0}\nabla T.\quad (67)$$

Single hyperbolic equation (67) for the internal variable  $\alpha$  can be represented in the form

$$\alpha_{tt} = a_4^2\nabla^2\alpha + a_5\nabla^2\alpha_t + a_6\nabla T,\quad (68)$$

with obvious relations for the values of coefficients, i.e.,  $a_4^2 = -\widehat{L}_{21}(CD)$ ,  $a_5 = L_{11}C$ ,  $a_6 = -\widehat{L}_{23}DT_0^{-1}$ . Accordingly, the heat conduction equation can be rewritten as

$$T_t - k\nabla^2T = k_3\nabla \cdot (\nabla^2\alpha) + k_4\nabla \cdot (\alpha_t),\quad (69)$$

with  $k = (\rho c_p L_{12} T_0)^{-1}(L_{33}L_{12} - L_{32}L_{13})$ ,  $k_3 = C(\rho c_p L_{12})^{-1}(L_{11}L_{32} - L_{31}L_{12})$ , and  $k_4 = (\rho c_p L_{12})^{-1}L_{32}$ .

Thus, the heat conduction equation remains parabolic, but the evolution equation for the internal variable  $\alpha$  is hyperbolic. Now we will examine the influence of the microstructure on the transient heat conduction in the framework of dual internal variables. Solution of the system of equations (68)–(69) will be obtained numerically.



#### 4.5. Dimensionless variables

As in the case of single internal variable, it is useful to introduce the dimensionless variables in the same way. Definitions of dimensionless variables (43) provide the equations for internal variable

$$\frac{A_0}{t_0^2} \alpha'_{t't'} = a_4^2 \frac{A_0}{l_0^2} \nabla'^2 \alpha' + a_5 \frac{A_0}{l_0^2 t_0} \nabla'^2 \alpha'_{t'} + a_6 \frac{T_0}{l_0} \nabla T', \quad (70)$$

and for heat conduction

$$\frac{T_0}{t_0} T'_{t'} - k \frac{T_0}{l_0^2} \nabla'^2 T = k_3 \frac{A_0}{l_0^3} \nabla' \cdot (\nabla'^2 \alpha') + k_4 \frac{A_0}{l_0 t_0} \nabla' \cdot (\alpha'_{t'}). \quad (71)$$

In this case we make another characteristic choice keeping the same order of magnitude for two first terms in the evolution equation for the internal variable and for the temperature coupling term

$$t_0 = \frac{l_0}{a_4}, \quad A_0 = l_0 T_0. \quad (72)$$

Due to this choice, the dimensionless evolution equation for the internal variable obtains the form

$$\alpha'_{t't'} = \nabla'^2 \alpha' + \frac{a_5}{a_4 l_0} \nabla'^2 \alpha'_{t'} + \frac{a_6}{a_4^2} \nabla T', \quad (73)$$

and the heat conduction equation reads, respectively,

$$T'_{t'} - \frac{k}{a_4 l_0} \nabla'^2 T' = \frac{k_3}{a_4 l_0} \nabla' \cdot (\nabla'^2 \alpha') + k_4 \nabla' \cdot (\alpha'_{t'}). \quad (74)$$

#### 4.6. Numerical test

Computations of the problem formulated in Section 3.4.2 are performed using the explicit finite-volume numerical scheme (Berezovski et al., 2008) with the same values of dimensionless space step  $\Delta x' = 5 \cdot 10^{-3}$  and the dimensionless time step  $\Delta t' = 8.33 \cdot 10^{-6}$  as previously. Initial and boundary conditions did not changed. The values of used dimensionless model parameters are the following:  $a_5/a_4 l_0 = 10^{-3}$ ,  $a_6 = a_4^2$ ,  $k/a_4 l_0 = 0.1$ ,  $k_3/a_4 l_0 = 5 \cdot 10^{-3}$ , and  $k_4 = 1.5$ . Results of simulation are presented in Fig. 5 in terms of the distribution of the excess temperature normalized by initial temperature  $T_0$ . Due to the difference in time scales for single and dual internal variables, the temperature distribution in Fig. 5 corresponds to only 100 time steps. A clear wave-like behavior of temperature is

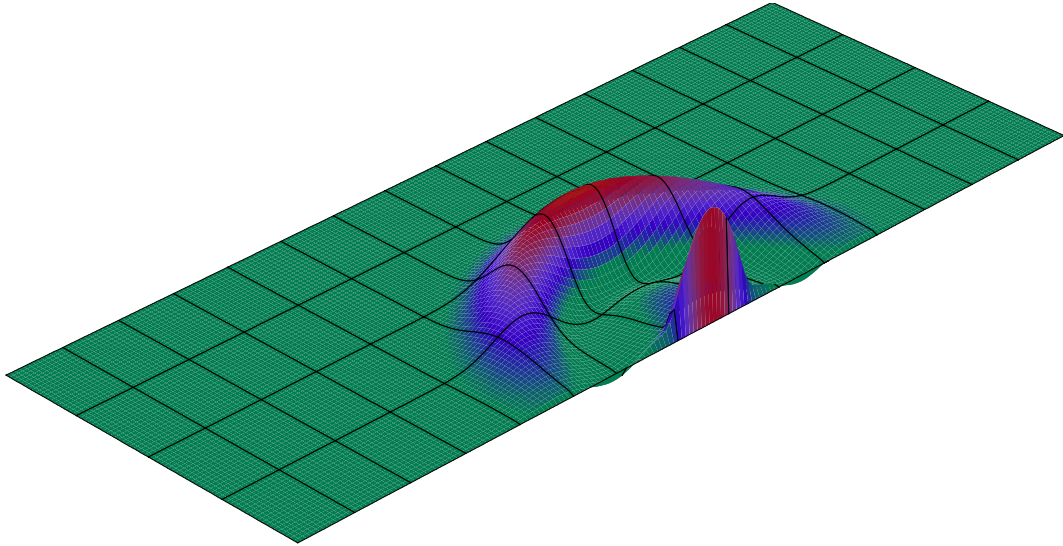


Figure 5: Temperature distribution in the plate with microstructure at 100 time steps.

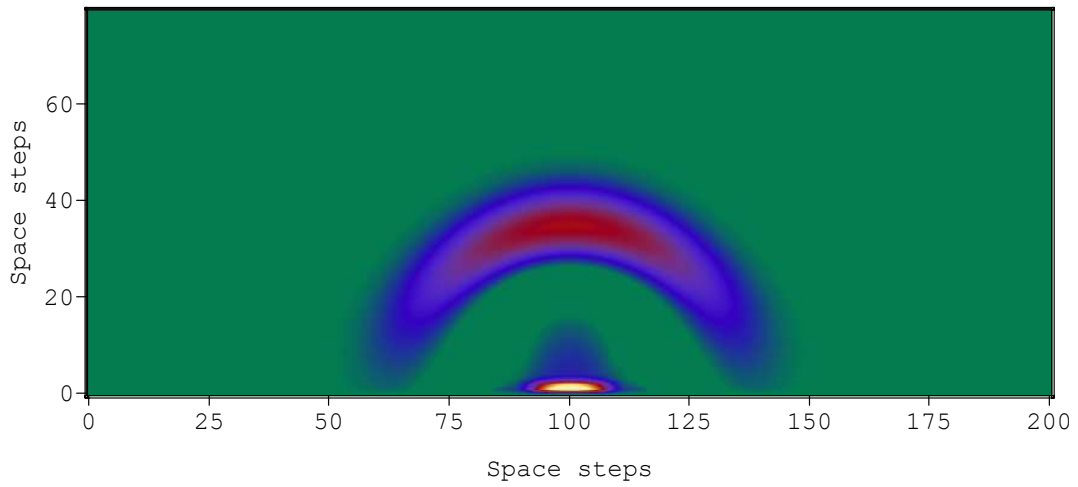


Figure 6: Contour plot of temperature distribution in the plate with microstructure at 100 time steps.

observed complemented by a narrow diffusional zone close to the thermal loading location. It is confirmed by the contour plot shown in Fig. 6.

The obtained result follows from the hyperbolic character of the evolution equation of the internal variable  $\alpha$  which is reflected in the behavior of temperature due to the coupling of governing equations. Since the internal variable  $\alpha$  represents the influence of the microstructure, it can be associated with the microtemperature (Grot, 1969).

## 5. Conclusions

The extension of the thermodynamic state space is a paradigmatic method in the non-equilibrium thermodynamics (Müller, 1985; Müller and Ruggeri, 1998; Maugin, 1999; Jou et al., 2010; Cimmelli et al., 2014). The thermodynamics with internal variables (Coleman and Gurtin, 1967; Maugin and Muschik, 1994a; Cimmelli and Rogolino, 2001) provides a formalization of such an extension. The single internal variable method is broadly employed for a long time (Maugin and Muschik, 1994b; Horstemeyer and Bammann, 2010; Maugin, 2015, e.g.). Its application to heat conduction results in the coupled parabolic equations both for heat conduction and internal variable evolution (Berezovski, 2016). The more recent dual internal variable concept (Ván et al., 2008; Berezovski et al., 2011; Berezovski and Ván, 2017) provides a hyperbolic equation for the behavior of internal variables keeping the parabolic nature for heat conduction equation.

In the paper, both approaches are compared by means of the numerical simulation of two-dimensional heat conduction in a plate under a localised thermal pulse loading. Computations of the same problem by the different internal variable descriptions produce qualitatively dissimilar results. The single internal variable approach leads to a diffusional type of the internal variable evolution. In contrast, dual internal variable technique provides a wave-like evolution of the internal variables, and, as the consequence, the corresponding wave-like heat transfer. The results are obtained in the dimensionless form, and parameters of models are chosen to emphasize the features of each model.

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