Convolved energy variational principle in heat diffusion

B.T. Darrall, G.F. Dargush*

Department of Mechanical & Aerospace Engineering, University at Buffalo, The State University of New York, Buffalo, NY 14260

ABSTRACT

One of the major, long-standing challenges in analytical mechanics involves the inability to address systems with dissipation in a rigorous manner. In this paper, we overcome that difficulty by formulating a novel temperature-based stationary variational action principle for transient heat diffusion based upon a temporal convolution operator and fractional derivatives. The associated Euler-Lagrange equations provide the governing heat equation, along with the initial conditions on temperature and specified heat flux boundary conditions. A further integration-by-parts then leads to a formulation that is somewhat less symmetric but can be written without introducing fractional calculus. Finally, the resulting principle is used to solve two basic one-dimensional problems, as an illustration of a Ritz-type approach.

Keywords: Heat diffusion; Variational methods; Hamilton's principle; Euler-Lagrange equations; Fractional calculus; Convolved energy

1. Introduction

Analytical mechanics, which began with the work of Lagrange [1] and Hamilton [2, 3], brought powerful new ideas to the study of dynamical problems. However, these original forms were unable to address problems with dissipation. Furthermore, Hamilton's principle treats the initial value problem from a boundary value problem perspective by constraining the variations to be zero at both the beginning and end of the interval of time. However, in a dynamical system, the response at the end of the time interval is not known and often is the most important objective of the entire analysis. The first major attempt to address damped systems is attributed to Rayleigh [4] through his introduction of what is now called the Rayleigh dissipation function. Fundamental work by Biot [5, 6] along these lines for heat diffusion is particularly noteworthy.

* Corresponding author. Tel.: 1 716 645 2315.
E-mail addresses: gdargush@buffalo.edu (G.F. Dargush), bdarrall@buffalo.edu (B.T. Darrall)

Modern work on the application of this idea led to the development of the mixed Lagrangian formalism (MLF) originally by Sivaselvan and Reinhorn [7] and Sivaselvan *et al*. [8]. Subsequent research extended MLF to fracture [9], contact [10] and thermomechanics [11-14]. Although this approach can provide useful solutions as noted above, the Rayleigh dissipation formulation does not adhere to rigorous operations of variational calculus for action principles, as the dissipation functional enters the first variation in an *ad hoc* manner. Additionally, one can no longer construct an action in explicit form; only the first variation can be written. Several less elegant solutions also were proposed to write Lagrangians for dissipative systems, including those approaches that involve additional variables and mirror systems [15, 16]. Other notable work to create functionals for dissipative systems includes that by Kaufman [17], Morrison [18], Grmela [19], Anthony [20], Cresson *et al*. [21], Kim *et al*. [22] and more recently by Guo and colleagues [23-25]. Nevertheless, none of these proposed formulations truly break the fundamental result presented by Bauer in his 1931 paper, which states "The equations of motion of a dissipative linear dynamical system with constant coefficients are not given by a variational principle" [26].

A major step forward to counter that statement was proposed by Gurtin [27-29] and Tonti [30-32] with the introduction of the convolution operator to replace the usual inner product in the temporal integral of Hamilton's principle. However, the Gurtin formulation produces integral forms of the Euler-Lagrange equations with no restrictions on the variations, while the Tonti formalism misstates the initial conditions for dissipative systems. Riewe [33, 34] proposed the use of fractional derivatives in an inner product action integral. This was a particularly good idea and Podlubny [35] has provided some physical interpretations of fractional calculus. However, an appearance of fractional derivatives in the functional by themselves is unable to recover the governing differential equations for a dissipative system. To resolve the issues, Dargush and Kim [36] present a principle of mixed convolved action using fractional derivatives. This formulation can address both conservative and dissipative contributions, recovers the governing differential equations as the associated Euler-Lagrange equations and restricts variations consistently with the specified initial conditions. The principle was subsequently extended to fractional single degree of freedom dynamical systems [37], continuum elastodynamics [38], dynamic poro- and thermo-elasticity [39, 40] and heat diffusion [41]. These are true variational methods that solve the two main long-standing issues by addressing dissipative dynamical systems with proper variations consistent with the specified initial conditions. Note that all this more recent work uses mixed

impulsive variables. As an alternative, Kalpakides and Charalambopoulos [42] built upon the ideas of convolution and fractional derivatives to present a displacement-based formulation for elastodynamics. On the other hand, the primary objective of the present paper on heat diffusion is to write a novel temperature-based convolved action variational principle in three dimensions, which also may be reformulated to eliminate the need for fractional calculus, a previously unanticipated result. To illustrate the new variational principle, several simple one-dimensional thermal problems are addressed.

The remainder of the paper is organized as follows. In Section 2, we provide a review of the necessary preliminary relations and previously derived results to develop novel variational principles for the continuum heat diffusion problem. One of these principles, based upon convolved energy, is developed in Section 3. Included is the convolved functional with semi-derivatives, its first variation and the corresponding Euler-Lagrange equations. Then, after invoking a fractional integration-by-parts identity, the functional is rewritten without the need for fractional calculus. In Section 4, a new approach is presented to leverage this variational method towards solving heat diffusion problems. The approach is inspired by Ritz methods, which typically are used to solve for exact or approximate solutions to boundary values problems. Here a Ritz-type method is developed, which will be used to obtain solutions to the time-dependent one-dimensional continuum heat diffusion problem. Finally, in Section 5, some general conclusions are outlined.

2. Preliminary Relations

This section is reserved for concisely presenting key equations that will be necessary for developing the stationary action principle for transient heat conduction in the following section. Full derivations are not included here, and instead readers are referred to [36, 37] for details. Throughout this work standard tensor notation is used, with indices i, j and k ranging from 1 to 3, or x to z. Any subscripts other than i, j and k are just for notational purposes and should not be treated as ranging indices. The standard Einstein summation convention is also taken advantage of here. The primary variable throughout is temperature T, which when not clear, is always assumed to be a function of three-dimensional space and time. Also, dots will be used to represent

partial derivatives with respect to time, breve symbols to denote temporal semi-derivatives, and overbars to signify "known" or specified quantities.

The governing equation for transient heat transfer via conduction, also known as the "Heat Equation" is given as

$$\nabla_i \left(\kappa_{ij} \nabla_j T \right) = \rho_o \, c_\epsilon \dot{T} \qquad \text{in volume } \Omega \tag{1}$$

For a well posed initial boundary value problem we also have initial conditions

$$T(0) = \bar{T}_0 \qquad \text{in volume } \Omega \tag{2}$$

as well as the standard boundary conditions on heat flux and temperature, respectively,

$$-\kappa_{ij} \nabla_j T \; n_i = \bar{q} \qquad \text{on surface } \Gamma_q \tag{3a}$$

$$T = \bar{T} \qquad \text{on surface } \Gamma_T \tag{3b}$$

In the above, $\bar{T}_0$ represents the specified initial temperature, $\bar{T}$ is the given boundary temperature, and $\bar{q}$ is the specified normal component of the heat vector, as shown in Fig. 1, with $\bar{q} = 0$ as the default boundary condition at any point. Furthermore, ρ_o is density, κ_{ij} is the thermal conductivity tensor, c_ϵ is the heat capacity, n_i is a unit outward normal vector to the surface, and ∇_i is the gradient operator. Additionally, for a well posed problem $\Gamma_q \cup \Gamma_T = \Gamma$ and $\Gamma_q \cap \Gamma_T = \varnothing$.

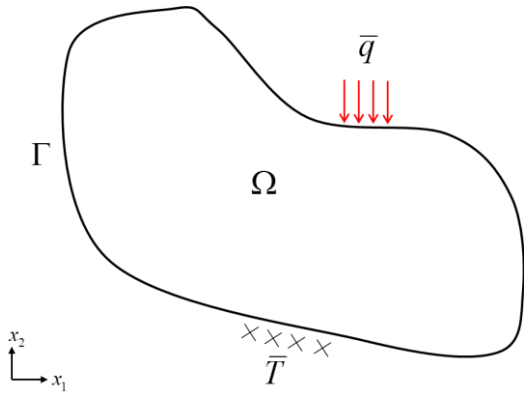

Fig. 1. Heat diffusion problem definition

The convolution of two functions, which is central to the energy principle defined in the following section, is given as

$$\left(u * v\right)(t) = \int_0^t u(\tau)v(t-\tau)d\tau \tag{4}$$

In the above it is assumed that functions $u(t)$ and $v(t)$ are Lebesgue integrable. One specific convolution that is important in this work is the left Riemann-Liouville fractional derivative of order α, defined as

$$\left(\mathscr{D}_{0^+}^{\alpha}u\right)(t) \equiv +\frac{1}{\Gamma(1-\alpha)}\frac{d}{dt}\int_0^t \frac{u(\tau)}{\left(t-\tau\right)^{\alpha}}d\tau \qquad \text{for } 0<\alpha<1 \tag{5}$$

The semi-derivative, having $\alpha = ½$, plays a central role in the development to follow. This will be denoted by a breve symbol and is defined explicitly as

$$\breve{u}(t) = \left(\mathscr{D}_{0^+}^{1/2}u\right)(t) \equiv +\frac{1}{\Gamma(1/2)}\frac{d}{dt}\int_0^t \frac{u(\tau)}{\left(t-\tau\right)^{1/2}}d\tau \tag{6}$$

Crucial to the developments throughout this work are integration-by-parts operations, including integration-by-parts of terms containing fractional derivatives. The usual temporal integration-by-parts operation on the inner product of two functions is

$$\int_0^t \dot{u}(\tau)v(\tau)d\tau = -\int_0^t u(\tau)\dot{v}(\tau)d\tau + u(t)v(t) - u(0)v(0) \tag{7}$$

On the other hand, the temporal integration-by-parts operation of two convolved functions, which is even more useful here than the prior relation, is given by

$$\left(\dot{u} * v\right)(t) = \left(u * \dot{v}\right)(t) + u(t)v(0) - u(0)v(t) \tag{8}$$

Next, the fractional integration-by-parts relation for the convolution of fractional derivatives can be written

$$\left(\left(\mathcal{D}_{0^+}^{1-\alpha}u\right)*\left(\mathcal{D}_{0^+}^{\alpha}v\right)\right)(t)=\left(u*\dot{v}\right)(t)+u(t)v(0) \tag{9}$$

which reduces in the specific case of semi-derivatives with $\alpha=½$ to the following form:

$$\left(\breve{u}*\breve{v}\right)(t)=\left(u*\dot{v}\right)(t)+u(t)v(0) \tag{10}$$

Detailed derivation of these fractional derivative relations can be found in References [36, 37].

Finally, we have the following for spatial integration-by-parts over the domain Ω having bounding surface Γ

$$\int_{\Omega}\left[\left(\nabla_i u\right)v\right]\,d\Omega=\int_{\Gamma}\left[u\,v\right]n_i\,\,d\Gamma-\int_{\Omega}\left[u\left(\nabla_i v\right)\right]\,d\Omega \tag{11}$$

where use is made of the classical divergence theorem of Gauss.

3. Convolved Energy Principle for the Transient Heat Problem

In this section we present a new functional, I_{C_H}, that is posed purely in terms of temperature as the primary variable. We will prove that this functional serves as a viable base for a novel variational principle for the transient heat problem. In other words, the Euler-Lagrange equations derived by setting the variation of this functional to zero, and performing necessary integration-by-parts operations, will correspond directly to the correct governing heat equation, boundary conditions, and initial conditions. While it is tempting to refer to I_{C_H} as an action, because it results in a variational principle for a time-dependent problem, we should be careful, because it turns out that the dimensions are of energy, not action, thus we will refer to I_{C_H} as a "convolved energy". Several other closely related convolved action variational principles also can be developed. As noted above, mixed versions have already appeared in References [40, 41]. In general, convolved action or energy principles can be developed using a semi-implicit construction methodology that resembles the process employed to build classical explicit solutions to boundary value problems. However, so as not to distract from the primary objective of this paper, the new, purely

temperature-based convolved energy variational principle for the heat problem will remain the focus of this section.

With a semi-implicit approach for the transient heat problem with Fourier conduction, one begins by writing the required set of Euler-Lagrange equations governing the problem, defined above in (1)-(3). Then, by developing an understanding of the anticipated outcomes of temporal and spatial integration-by-parts operations from (7)-(11), one can iteratively construct an appropriate functional form. With that background in mind, let us now present the new convolved energy functional for the transient heat conduction problem:

$$\begin{aligned} I_{C_H}\left(T,\breve{T}\,;t\right) &= \int_\Omega \tfrac{1}{T_o}\Big[\tfrac{1}{2}\left(\breve{T} * \rho_o c_\epsilon \breve{T}\right)(t) + \tfrac{1}{2}\left(\nabla_i T * \kappa_{ij}\nabla_j T\right)(t)\Big]d\Omega \\ &\quad - \int_\Omega \tfrac{1}{T_o}\Big[\rho_o c_\epsilon T(t)\bar{T}_0\Big]d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\Big[\left(T * \bar{q}\right)(t)\Big]d\Gamma \end{aligned} \tag{12}$$

where T_o represents the absolute temperature at the free stress state, which should not be confused with the initial temperature distribution throughout the domain $\bar{T}_0$. Now, via taking variations of (12), and applying the appropriate temporal and spatial integration-by-parts relations, we will show that the stationarity of this energy functional will provide a solution to the transient heat problem as given by (1)-(3). Let us start by taking the first variation and setting this equal to zero:

$$\begin{aligned} \delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta\breve{T} * \rho_o c_\epsilon \breve{T} + \tfrac{1}{2}\nabla_i \delta T * \kappa_{ij}\nabla_j T + \tfrac{1}{2}\nabla_i T * \kappa_{ij}\nabla_j \delta T\Big]d\Omega \\ &\quad - \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\,\rho_o c_\epsilon\,\bar{T}_0\Big]d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\Big[\delta T * \bar{q}\Big]d\Gamma = 0 \end{aligned} \tag{13}$$

(Notice that in (13), and in all equations to follow, the explicit reference to time t in the convolutions is dropped.) Next, we apply spatial and temporal integration-by-parts operations to the first three terms, with the goal of removing all derivatives from the variational quantities. Here we are also accounting for the symmetry of κ_{ij}, and considering separately the parts of the boundary Γ_q, where heat flux is specified and Γ_T, on which temperature is given. Then,

$$\begin{aligned} \delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta T * \rho_o c_\epsilon \dot{T} - \delta T * \nabla_i\left(\kappa_{ij}\nabla_j T\right)\Big]d\Omega \\ &\quad + \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\rho_o c_\epsilon\left(T(0)-\bar{T}_0\right)\Big]d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\Big[\delta T * \left(\kappa_{ij}\nabla_j T\ n_i + \bar{q}\right)\Big]d\Gamma \\ &\quad + \int_{\Gamma_T} \tfrac{1}{T_o}\Big[\delta T * \kappa_{ij}\nabla_j T\ n_i\Big]d\Gamma = 0 \end{aligned} \tag{14}$$

(The detailed mathematical steps required to arrive at (14), starting from (13) are provided in Appendix A.) At this point it is imperative to point out that the variations are arbitrary, except that we must restrict these variations, such that along the boundary where temperature is specified, $\delta T = 0$. Thus, the final integral in (14) vanishes. Now, looking at the three remaining square bracketed terms, we are left with Euler-Lagrange equations corresponding to the heat equation (1), the initial conditions on temperature (2), and the heat flux boundary conditions (3a), respectively. Meanwhile, the fixed temperature boundary conditions (3b) are handled explicitly.

Thus, we have successfully established a *Principle of Stationary Convolved Energy for Transient Heat Diffusion*, based upon the functional I_{C_H}, defined in (12). Notice that the current approach resolves the difficulty with dissipative processes inherent in variational formulations based upon Hamilton's principle, while also avoiding the disturbing end point constraint issue associated with those classical statements. Consequently, this represents the first true variational principle for dissipative heat conduction, written exclusively in terms of temperature-based variables. Here, we emphasize that previous contributions by Gurtin [27] on the related viscoelastic problem used extraneous convolutions that led to principles involving the time integration of action and the work by Tonti [30, 31] produced incorrect initial conditions. On the other hand, the work by Darrall and Dargush [40] and Dargush *et al.* [41] are mixed formulations written in terms of impulse variables. Thus, the work presented in this section is advantageous in several ways over all existing true variational approaches for the problem of heat conduction. In particular, the convolved energy functional I_{C_H} is written in terms of temperature, rather than the less familiar concept of temperature impulse. However, the functional in (12) still depends upon the semi-derivative of temperature $\breve{T}$, as do the mixed convolved action functionals in References [40, 41]. Is this necessary? Does breaking the limitations stated by Bauer [26] require the introduction of fractional derivatives?

To address these questions, let us present an alternative, equivalent form of the convolved energy functional I_{C_H} by applying the integration-by-parts relation (9) to the first integral in (12). Specifically, we write

$$\breve{T} * \rho_o c_\epsilon \breve{T} = T * \rho_o c_\epsilon \dot{T} + T(t) \rho_o c_\epsilon T(0) \tag{15}$$

Substituting (15) into (12) produces the following convolved energy functional:

$$I_{C_H}\left(T,\dot{T};t\right)=\int_\Omega \tfrac{1}{T_o}\Big[\tfrac{1}{2}T*\rho_o c_\epsilon \dot{T}+\tfrac{1}{2}\nabla_i T*\kappa_{ij}\nabla_j T\Big]d\Omega$$
$$+\int_\Omega \tfrac{1}{T_o}\Big[\tfrac{1}{2}T(t)\rho_o c_\epsilon T(0)\Big]d\Omega-\int_\Omega \tfrac{1}{T_o}\Big[T(t)\rho_o c_\epsilon \overline{T}_0\Big]d\Omega+\int_{\Gamma_q}\tfrac{1}{T_o}\Big[T*\bar{q}\Big]d\Gamma \tag{16}$$

which involves only ordinary calculus. Alternatively, if one satisfies the initial conditions exactly, such that $T(0)=\overline{T}_0$ throughout the domain Ω as an essential condition, then this can be rewritten in a simplified form as

$$I_{C_H}\left(T,\dot{T};t\right)=\int_\Omega \tfrac{1}{T_o}\Big[\tfrac{1}{2}T*\rho_o c_\epsilon \dot{T}+\tfrac{1}{2}\nabla_i T*\kappa_{ij}\nabla_j T\Big]d\Omega$$
$$-\int_\Omega \tfrac{1}{T_o}\Big[\tfrac{1}{2}T(t)\rho_o c_\epsilon T(0)\Big]d\Omega+\int_{\Gamma_q}\tfrac{1}{T_o}\Big[T*\bar{q}\Big]d\Gamma \tag{17}$$

The functional (16) is equivalent to that expressed in (12), but without fractional derivatives. By enforcing the stationarity of (16), and then using appropriate temporal and spatial integration-by-parts operations, the governing equations for dissipative heat diffusion in (1), (2) and (3a) are recovered as its Euler-Lagrange equations. Relation (3b) is enforced as an essential condition. For the functional defined by (17), both (3b) and (2) become essential conditions.

Note that in all preceding relations there are no terms related to volumetric heating. However, if one wishes to include body heating, then one can simply add a term $\int_\Omega \frac{1}{T_o}\Big[T*\overline{\Psi}\Big]d\Omega$, where $\overline{\Psi}$ is the specified heat rate per volume, to any of the energy functionals.

The convolved energy functional presented in (12) provides a most elegant symmetry for the transient heat problem. An entire family of non-symmetric formulations can be derived by using the more general integration-by-parts relation (9) with $\alpha \neq ½$. Clearly, however, with the alternative variational functionals (16) and (17), fractional calculus is not required to break the limitations presented by Bauer for dissipative variational statements [26]. Only convolution is necessary, along with suitable initial condition integrals.

Before concluding this section, we should compare the present temperature-based convolved energy principle with the previous mixed convolved action functional I_{C_F} appearing as equation (22) in [41] for classical Fourier heat diffusion. First and foremost, the corresponding Euler-

Lagrange equations are not identical. In particular, the mixed convolved action enforces the Fourier law of heat conduction in a variational sense, whereas the present functional (12) assumes that law embedded within the heat equation. This results in the appearance of different boundary integrals and prevents one from deriving (12) directly from the convolved action I_{C_F} of [41]. Furthermore, the convolved action I_{C_F} is written in terms of temperature impulse $\theta(t)$, while the present formulation uses the more familiar temperature variable $T(t)$, where $\theta(t)=\int_0^t T(\tau)d\tau$. One advantage of temperature impulse is that allows the formulation of ballistic heat transfer in addition to classical heat diffusion in a common framework. Furthermore, it provides an elegant symmetry to the equations of dynamic thermoelasticity [40].

Finally, as the main results from this section, in (12) and (16), we have developed temperature-based variational principles, which involve the convolution operator. The first of these takes a beautifully symmetric form in terms of semi-derivatives. Most importantly, in the second form, there is no need for fractional derivatives. This latter form will prove to be useful immediately in the proceeding section, where taking semi-derivatives may prove to be tedious.

4. A Ritz-type Method for Solving the 1D Problem

We now turn our attention to leveraging the new variational principle presented in the previous section to solve one dimensional transient heat conduction problems. The key idea here is to select assumed solution forms that generally depend on both the spatial coordinate x, where $0\le x\le L$, and time t. While the spatial and temporal functional form will be assumed, unknown coefficients will be determined by enforcing the stationarity of the convolved energy, as written in the form of (16). In general, we will label these unknown coefficients a_n and b_n, depending on how they appear in the assumed solution form, and then we can write any assumed solution as $T_a=T_a(x,t,a_n,b_n)$. Note that generally the assumed solution forms can be infinite series, finite series, or not series at all.

Upon substitution of an assumed solution form T_a into (16), and further evaluation of all convolution integrals, standard time integrals, time derivatives, spatial derivatives, and spatial integration, all processes that can be easily coded with a symbolic type toolbox (*i.e.*, Matlab symbolic toolbox [43] or Mathematica [44]), we will be left with a function that is solely dependent on the coefficients a_n and b_n. Thus, the variation of the resulting energy will be fully governed by the variation of these coefficients, and stationarity boils down to the resulting simpler equations, involving only first partial derivatives:

$$\frac{\partial I_{C_H}}{\partial a_n} = 0, \quad \frac{\partial I_{C_H}}{\partial b_n} = 0 \tag{18}$$

If not already clear, this approach is extremely reminiscent of a Ritz method to solving boundary value problems approximately [45, 46]. The approach here however involves both space and time, and involves stationarity of a time-dependent energy functional, as opposed to minimization of a time-independent total potential energy functional. Of course, the jump to a time-dependent version of this type of solution method is by no means trivial and presents certain obstacles. Namely, while it is simple to setup a Ritz method solution with quadratic potentials such that all the final resulting equations to be solved are linear with respect to the unknown coefficients, in general we will find that when using the Ritz-type approach presented here, the resulting equations to be solved can generally be sets of nonlinear equations. Despite this added complexity, we will show in the proceeding subsections that this new type of time-dependent Ritz method can still be quite useful.

Before moving on to problem solving, a few more notes should be made on the outlined approach. First, it is important to highlight a powerful feature of the proposed time-dependent variational approach. In particular, one need not know the actual form of the solution *a priori* to get a reasonably accurate approximate solution. Also, as most specific problems will not have a closed form analytical solution, the method here becomes all the more important, as we can in theory still arrive at useful approximate solutions. On the other hand, just as with similar variational approaches to non-time dependent problems, quality intuition about what types of assumed solution forms will work well goes a long way. In other words, the better the initial guess of an assumed solution form, the better one can expect the final approximate solution to be.

4.1 Assumed solution as Fourier series in space and exponential in time

Let us proceed forward with the time-dependent variational approach outlined above. For boundary conditions, we will assume the homogeneous case, such that $T(0,t)=T(L,t)=0$, and for initial conditions we will assume generally that for $0<x<L$, $T(x,0)=\bar{T}_0$, where $\bar{T}_0$ is some constant. This problem of course has the well-known analytical solution [47]:

$$T(x,t)=\sum_{n=1}^{\infty}-\left(\frac{2\bar{T}_0}{n\pi}\left((-1)^n-1\right)\right)\sin\left(\frac{n\pi}{L}x\right)e^{-\left(\frac{\kappa}{\rho_o c_c}\frac{n^2\pi^2}{L^2}\right)t} \tag{19}$$

Let us then assume a solution form that is a Fourier sine series in space, and exponential in time:

$$T_a(x,t,\mathbf{a},\mathbf{b})=\sum_{n=1}^{\infty}a_n\sin\left(\frac{n\pi}{L}x\right)e^{b_n t} \tag{20}$$

where **a** and **b** are the vectors of unknown coefficients. Now our job is to substitute (20) into (16) and evaluate the resulting convolved energy associated with this solution form. First the relevant temporal and spatial derivatives are evaluated as, respectively:

$$\dot{T}(x,t)=\sum_{n=1}^{\infty}a_n\sin\left(\frac{n\pi}{L}x\right)b_n e^{b_n t} \tag{21}$$

and for this spatially one-dimensional case

$$\nabla_1 T=\frac{\partial T}{\partial x}=\sum_{n=1}^{\infty}a_n\frac{n\pi}{L}\cos\left(\frac{n\pi}{L}x\right)e^{b_n t} \tag{22}$$

Meanwhile the relevant convolution for computing the energy here is

$$e^{b_n t}*e^{b_n t}=t\,e^{b_n t} \tag{23}$$

Next, we proceed forward evaluating all the remaining temporal and spatial integrations as instructed by (16). We handle each of the four terms separately here for clarity. Note the importance of the orthogonality of the sine functions here, as this allows us to completely disregard any terms coming from the cross multiplication of summation terms, or in other words terms coming from multiplication of terms with summation subscripts $m\neq n$. Computing integrals for the first terms yield:

$$\int_\Omega \left[\tfrac{1}{2} T * \rho_o c_\epsilon \dot{T}\right] d\Omega = \frac{\rho_o c_\epsilon}{2} \int_0^L \left[\sum_{n=1}^{\infty} a_n^2 \sin^2\left(\frac{n\pi}{L} x\right) b_n t e^{b_n t}\right] dx$$
$$= \frac{\rho_o c_\epsilon L}{8\pi} \sum_{n=1}^{\infty} \frac{1}{n} a_n^2 \left(2\pi n - \sin\left(2n\pi\right)\right) b_n t e^{b_n t}$$
$$= \frac{\rho_o c_\epsilon L}{4} \sum_{n=1}^{\infty} a_n^2 \; b_n t e^{b_n t}$$

while for the second term:

$$\int_\Omega \left[\tfrac{1}{2} \nabla_i T * \kappa_{ij} \nabla_j T\right] d\Omega = \frac{\kappa}{2} \int_0^L \left[\sum_{n=1}^{\infty} \frac{a_n^2 n^2 \pi^2}{L^2} \cos^2\left(\frac{n\pi}{L} x\right) t e^{b_n t}\right] dx$$
$$= \frac{\kappa L}{8\pi} \sum_{n=1}^{\infty} \frac{a_n^2 n^2 \pi^2}{n L^2} \left(2\pi n + \sin\left(2n\pi\right)\right) t e^{b_n t}$$
$$= \frac{\kappa}{4L} \sum_{n=1}^{\infty} a_n^2 n^2 \pi^2 t e^{b_n t}$$

and for the combination of the third and fourth terms:

$$\int_\Omega \left[\rho_o c_\epsilon T(t)\left(\tfrac{1}{2} T(0) - \bar{T}_0\right)\right] d\Omega = \rho_o c_\epsilon \int_0^L \left[\sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi}{L} x\right) e^{b_n t} \left(\frac{1}{2} a_n \sin\left(\frac{n\pi}{L} x\right) - \bar{T}_0\right)\right] dx$$
$$= \rho_o c_\epsilon e^{b_n t} \left[\sum_{n=1}^{\infty} a_n^2 \frac{L}{8n\pi} \left(2\pi n - \sin(2\pi n)\right) + a_n \frac{\bar{T}_0 L}{n\pi} \left(\cos\left(n\pi\right) - 1\right)\right]$$
$$= \rho_o c_\epsilon e^{b_n t} \left[\sum_{n=1}^{\infty} a_n^2 \frac{L}{4} + a_n \frac{\bar{T}_0 L}{n\pi} \left(\left(-1\right)^n - 1\right)\right]$$

Finally, the fifth term is simply zero, because for this problem, there is no boundary with prescribed heat flux. Then, collecting all terms, we have the following for convolved energy

$$I_{C_H}\left(\mathbf{a}, \mathbf{b}; t\right) = \sum_{n=1}^{\infty} \tfrac{1}{T_o} \left[a_n^2 b_n \frac{\rho_o c_\epsilon L}{4} t + a_n^2 \frac{\kappa}{4L} n^2 \pi^2 t + a_n^2 \frac{\rho_o c_\epsilon L}{4} + a_n \rho_o c_\epsilon \frac{\bar{T}_0 L}{n\pi} \left(\left(-1\right)^n - 1\right)\right] e^{b_n t} \qquad (24)$$

Now, in accordance with (18), we set the first partial derivative of this expression with respect to the unknown coefficients to zero. Let us begin by taking derivatives with respect to a_n. Thus,

$$\frac{\partial I_{C_H}}{\partial a_n} = 0 = \tfrac{1}{T_o} \left[a_n b_n \frac{\rho_o c_\epsilon L}{2} t + a_n \frac{\kappa}{2L} n^2 \pi^2 t + a_n \frac{\rho_o c_\epsilon L}{2} + \rho_o c_\epsilon \frac{\bar{T}_0 L}{n\pi} \left(\left(-1\right)^n - 1\right)\right] e^{b_n t} \qquad (25)$$

Dividing out the exponential term $e^{b_n t}$, $\frac{1}{T_o}$ and factoring out time:

$$\left(-a_n b_n \frac{\rho_o c_\epsilon L}{2} + a_n \frac{\kappa}{2L} n^2\pi^2\right) t + \left(a_n \frac{\rho_o c_\epsilon L}{2} + \rho_o c_\epsilon \frac{\bar{T}_0 L}{n\pi}\left((-1)^n - 1\right)\right) = 0 \tag{26}$$

Now, clearly for the above expression to reduce to zero, we must have each of the bracketed terms vanish independently. Interestingly, this provides us with $2n$ linear equations to solve for all $2n$ unknown coefficients without ever actually taking derivatives with respect to b_n. From the equation coming from setting the second bracketed term to zero:

$$a_n = -\left(\frac{2\bar{T}_0}{n\pi}\left((-1)^n - 1\right)\right) \tag{27a}$$

and from setting the first bracketed term to zero:

$$b_n = -\left(\frac{\kappa}{\rho_o c_\epsilon}\frac{n^2\pi^2}{L^2}\right) \tag{27b}$$

Upon substitution of these newly solved for coefficients into the assumed solution form of (20) we find that we have recovered the exact analytical solution of (19). While, this could be expected, simply by the developments in Section 3, it should not go unnoticed that we have recovered the exact solution to this initial-boundary value problem (I-BVP) in a very different manner than the typical separation of variables approach.

Finally, we should check what will happen if we do indeed take partial derivatives of (24) with respect to the coefficients b_n, and set this to zero. Then,

$$\frac{\partial I_{C_H}}{\partial b_n} = 0 = \tfrac{1}{T_o}\left[a_n^2(b_n t + 1)\frac{\rho_o c_\epsilon L}{4} t + a_n^2 \frac{\kappa}{4L} n^2\pi^2 t^2 + a_n^2 \frac{\rho_o c_\epsilon L}{4} t + a_n \rho_o c_\epsilon \frac{\bar{T}_0 L}{n\pi}\left((-1)^n - 1\right) t\right] e^{b_n t}$$

Factoring out time t and dividing by the exponential term and $\frac{1}{T_o}$ yields:

$$\left[a_n^2 b_n \frac{\rho_o c_\epsilon L}{4} + a_n^2 \frac{\kappa}{4L} n^2\pi^2\right] t^2 + \left[a_n^2 \frac{\rho_o c_\epsilon L}{2} + a_n \rho_o c_\epsilon \frac{\bar{T}_0 L}{n\pi}\left((-1)^n - 1\right)\right] t = 0$$

Now setting independently these bracketed terms to zero, we recover the same results for a_n and b_n as before, and thus the analytical solution has again been realized.

4.2 Assumed solution as quadratic in space and exponential in time

In the previous example, we were able to recover the exact solution to our transient heat problem via the new temperature based variational principle, and a wisely selected assumed series solution form. But the variational method posed here is also capable of producing reasonably accurate approximate solutions. The goal now is to show that this does occur. Again, for boundary conditions, we will assume the homogeneous case, such that $T(0,t)=T(L,t)=0$. But now, for initial conditions we have $T(x,0)=\bar{T}_0\sin\left(\frac{\pi}{L}x\right)$. This problem has analytical solution:

$$T(x,t)=\bar{T}_0\sin\left(\frac{\pi}{L}x\right)e^{-\left(\frac{\kappa}{\rho_o c_\epsilon}\frac{\pi^2}{L^2}\right)t} \tag{28}$$

Now, rather than selecting the spatial dependency of the assumed solution to be sinusoidal, which would result in recovering the exact analytical solution, we instead choose the spatial dependency to be quadratic, such that

$$T_a(x,t,a_1,b_1)=a_1\,x\left(x-L\right)e^{b_1 t} \tag{29}$$

Substituting this into (16), and computing all necessary derivatives and integrals, as in the previous section, yields the following for I_{C_H}:

$$I_{C_H}\left(a_1,b_1;t\right)=\frac{L^3 c_\epsilon\rho_o}{60T_o}a_1\left(L^2a_1b_1t+10a_1\frac{\kappa}{c_\epsilon\rho_o}t+L^2a_1+\frac{240\bar{T}_0}{\pi^3}\right)e^{b_1t} \tag{30}$$

Now, applying (18) and solving for the unknown coefficients gives

$$a_1=-\frac{120\bar{T}_0}{L^2\pi^3},\quad b_1=-\frac{10\kappa}{L^2c_\epsilon\rho_o} \tag{31a,b}$$

The following plots, corresponding to Figs. 2 and 3, show comparisons of the approximate quadratic temperature solution T_a and the exact analytical solution T_{exact} given by (28), respectively. For problem parameters we use unit non-dimensional numeric values for ρ_o, c_ϵ, L and $\bar{T}_0$ with $\kappa=0.1$. Then, in Fig. 4 the mean error $e_1=\frac{1}{L}\int_0^L\left(T_a-T_{exact}\right)dx$ is plotted versus time, while Fig. 5 provides the mean square error $e_2=\frac{1}{L}\int_0^L\left(T_a-T_{exact}\right)^2dx$ versus time. From observing these plots, the approximate solution is quite accurate, both in space and time! For this case, from

Fig. 5 we see that the square error is maximum at the initial time, but actually decreases exponentially to zero with time.

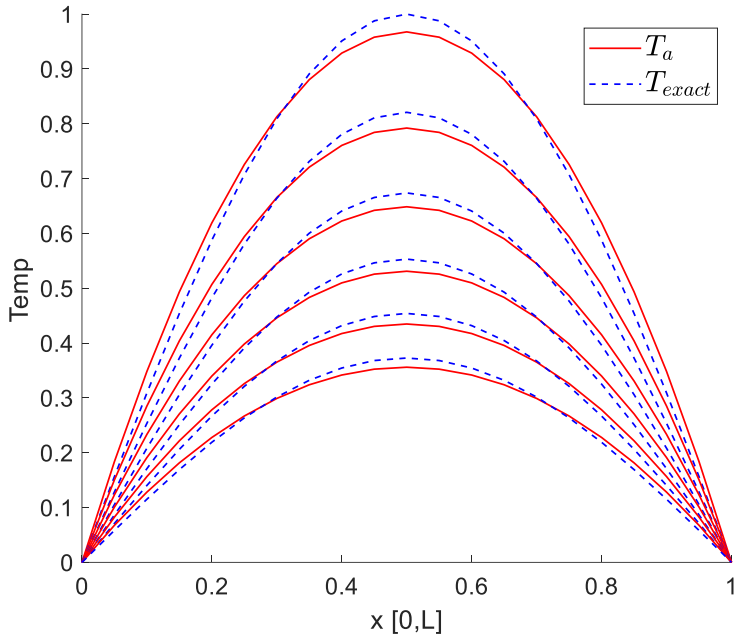

Fig. 2. Temperature profiles for approximate and exact solutions at times $t = [0, 0.2, 0.4, 0.6, 0.8, 1]$

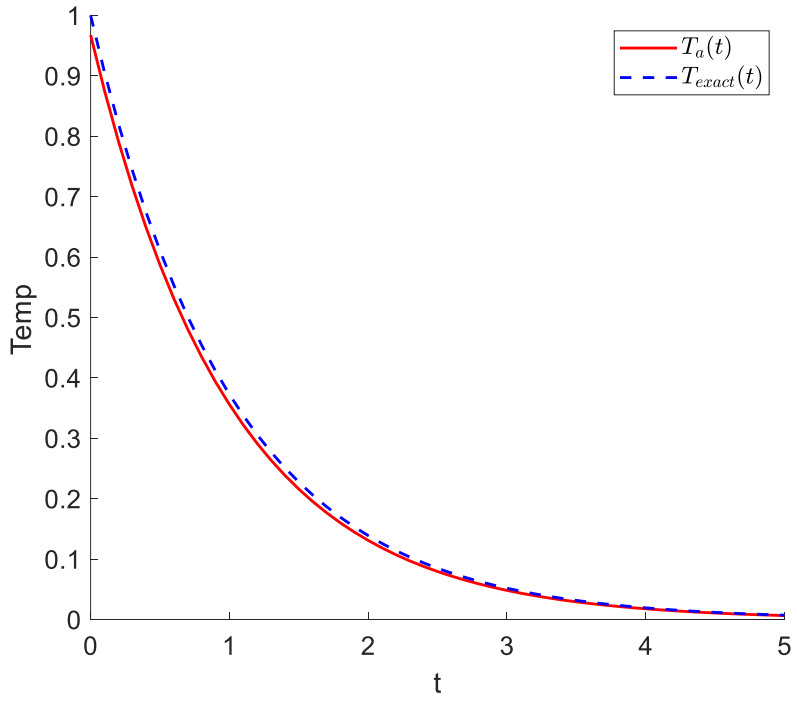

Fig. 3. Centerline temperature for approximate and exact solutions versus time

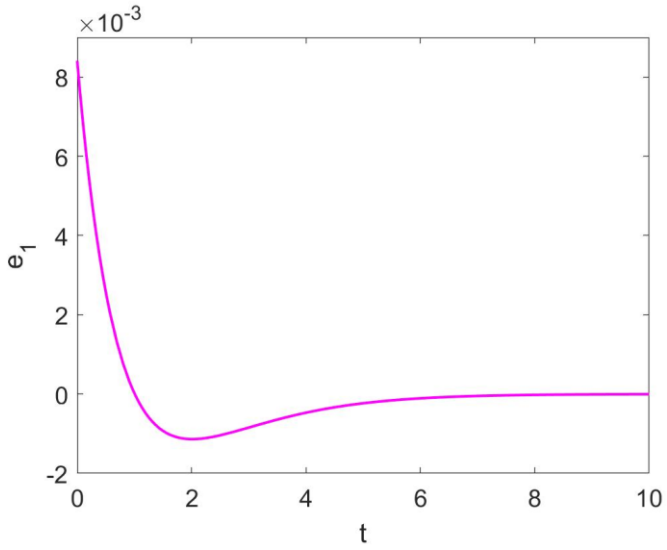

Fig. 4. Mean error in temperature versus time

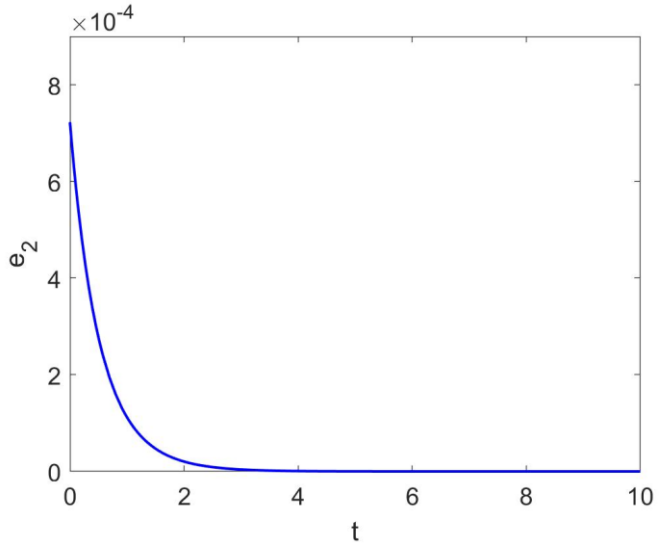

Fig. 5. Mean square error in temperature versus time

At this point we will conclude our discussion of using the new temperature based variational principle developed in Section 3 to derive approximate solutions to transient heat problems. We could continue, namely by solving problems with different boundary conditions, initial conditions, or assumed solution forms, but at some point, we would be detracting from the true highlight of this paper, which is the new variational principle itself. Further, we are making no suggestion that the method of solving problems presented in this section is extraordinarily powerful, in fact if one assumes solution forms significantly more complex than the ones here, for example with many

more unknown coefficients, then the resulting, generally non-linear, equations to be solved may quickly become unsolvable in closed form. Instead, we suspect that the true power of this new variational principle lies in the fact that it serves as an ideal base to develop new time-space numerical methods, using basis functions with compact support, such as has been done recently for the mixed convolved action papers [38-41].

5. Conclusions

In this paper, we have developed, for the first time, a true variational principle for the dissipative problem of heat diffusion in terms of the temperature field. An initial beautifully symmetric formulation employs temporal convolutions and semi-derivatives, while a second reformulated convolved action is written without the need for fractional calculus. Both stationary variational statements recover the governing heat equation, temperature initial conditions and specified heat flux boundary conditions, as the associated Euler-Lagrange equations. A Ritz-type method is then introduced to provide solutions to two simple one-dimensional transient heat diffusion examples.

References

[1] J-L. Lagrange, Mecanique Analytique, Gauthier-Villars et fils, Paris, 1788.

[2] W.R. Hamilton, On a general method in dynamics, Philosophical Transactions of the Royal Society of London 124 (1834) 247-308.

[3] W.R. Hamilton, Second essay on a general method in dynamics, Philosophical Transactions of the Royal Society of London 125 (1835) 95-144.

[4] J.W.S. Rayleigh, The Theory of Sound. I & II, Dover Publications, New York, NY, 1877 (Second edition, reprint 1945).

[5] M.A. Biot, New methods in heat flow analysis with application to flight structures, Journal of the Aeronautical Sciences 24 (1957) 857-873.

[6] M.A. Biot, Variational Principles in Heat Transfer – A Unified Lagrangian Analysis of Dissipative Phenomena, Clarendon Press, Oxford, UK, 1970.

[7] M.V. Sivaselvan, A.M. Reinhorn, Lagrangian approach to structural collapse simulation, Journal of Engineering Mechanics ASCE 132 (2006) 795-805.

[8] M.V. Sivaselvan, O. Lavan, G.F. Dargush, H. Kurino, Y. Hyodo, R. Fukuda, K. Sato, G. Apostolakis, A.M. Reinhorn, Numerical collapse simulation of large-scale structural systems using an optimization-based algorithm, Earthquake Engineering and Structural Dynamics 38 (2009) 655-677.

[9] O. Lavan, M.V. Sivaselvan, A.M. Reinhorn, G.F. Dargush, Progressive collapse analysis through strength degradation and fracture in the Mixed Lagrangian Formulation, Earthquake Engineering and Structural Dynamics, 38 (2009) 1483-1504.

[10] O. Lavan, Dynamic analysis of gap closing and contact in the Mixed Lagrangian Framework: Toward progressive collapse prediction, Journal of Engineering Mechanics, ASCE, 136 (2010) 979-986.

[11] G. Apostolakis, G.F. Dargush, Mixed Lagrangian formulation for linear thermoelastic response of structures, Journal of Engineering Mechanics ASCE 138 (2012) 508-518.
[12] G. Apostolakis, G.F. Dargush, Mixed variational principles for dynamic response of thermoelastic and poroelastic continua, International Journal of Solids and Structures 50 (2013) 642-650.
[13] G. Apostolakis, G.F. Dargush, Variational methods in irreversible thermoelasticity: Theoretical developments and minimum principles for the discrete form, Acta Mechanica 224 (2013) 2065–2088.
[14] G. Apostolakis, Mixed variational one-dimensional dynamic thermo-viscoplasticity for wave propagation, European Journal of Mechanics – A/Solids, 85 (2021) 104086.
[15] H. Bateman, On dissipative systems and related variational principles, Physical Review 38 (1931) 815-819.
[16] P.M. Morse, H. Feshbach, Methods of Theoretical Physics, McGraw-Hill, New York, NY, 1953.
[17] A.N. Kaufman, Dissipative Hamiltonian systems: A unifying principle, Physics Letters 100A (1984) 419–422.
[18] P.J. Morrison, Bracket formulation for irreversible classical fields, Physics Letters 100A (1984) 423–427.
[19] M. Grmela, Bracket formulation of dissipative fluid mechanics equations, Physics Letters 102A (1984) 355–358.
[20] K.H. Anthony. Hamilton's action principle and thermodynamics of irreversible processes – a unifying procedure for reversible and irreversible processes, Journal of Non-Newtonian Fluid Mechanics 96 (2001) 291–339.
[21] J. Cresson, I. Greff, P. Inizan, Lagrangian for the convection–diffusion equation, Mathematical Methods in the Applied Sciences 35 (2012) 1885-1895.
[22] J. Kim, G.F. Dargush, Y-K. Ju, Extended framework of Hamilton's principle for continuum dynamics, International Journal of Solids and Structures 50 (2013) 3418–3429.
[23] Y-C. Hua, Z-Y. Guo, The least action principle for heat conduction and its optimization application, International Journal of Heat and Mass Transfer 105 (2017) 697-703.
[24] Y-C. Hua, T. Zhao, Z-Y. Guo, Irreversibility and action of the heat conduction process, Entropy 20 (2018**)** 206.
[25] T. Zhao, Y-C. Hua, Z-Y. Guo, The principle of least action for reversible thermodynamic processes and cycles, Entropy 20 (2018) 542.
[26] P.S. Bauer, Dissipative dynamical systems I, Proceedings of the National Academy of Sciences 17 (1931) 311-314.
[27] M.E. Gurtin, Variational principles in the linear theory of viscoelasticity, Archive for Rational Mechanics and Analysis 13 (1963) 179-191.
[28] M.E. Gurtin, Variational principles for linear initial-value problems, Quarterly of Applied Mathematics 22 (1964) 252-256.
[29] M.E. Gurtin, Variational principles for linear elastodynamics, Archive for Rational Mechanics and Analysis 16 (1964) 34-50.
[30] E. Tonti, On the variational formulation for linear initial value problems, Annali di Matematica Pura ed Applicata XCV (1973) 331-360.
[31] E. Tonti, A general solution of the inverse problem of the calculus of variations, Hadronic Journal 5 (1982) 1404-1450.
[32] E. Tonti, Variational formulation for every nonlinear problem, International Journal of Solids and Structures 22 (1984) 1343-1371.
[33] F. Riewe, Nonconservative Lagrangian and Hamiltonian mechanics, Physical Review E 53 (1996) 1890-1899.

[34] F. Riewe, Mechanics with fractional derivatives, Physical Review E 55 (1997) 3581-3592.
[35] I. Podlubny, Geometric and physical interpretation of fractional integration and fractional differentiation, arXiv math/0110241, 2001.
[36] G.F. Dargush, J. Kim, Mixed convolved action, Physical Review E 85 (2012) 066606.
[37] G.F. Dargush, Mixed convolved action for classical and fractional-derivative dissipative dynamical systems, Physical Review E 86 (2012) 066606.
[38] G.F. Dargush, B.T. Darrall, J. Kim, G. Apostolakis, Mixed convolved action principles in linear continuum dynamics, Acta Mechanica 226 (2015) 4111-4137.
[39] B.T. Darrall, G.F. Dargush, 2016, Mixed convolved action variational methods for poroelasticity, Journal of Applied Mechanics, ASME 83 (2016) 091011-1-12.
[40] B.T. Darrall, G.F. Dargush, Variational principle and time-space finite element method for dynamic thermoelasticity based on mixed convolved action, European Journal of Mechanics – A/Solids 71 (2018) 351-364.
[41] G.F. Dargush, G. Apostolakis, B.T. Darrall, J. Kim, 2016, Mixed convolved action variational principles in heat diffusion, International Journal of Heat and Mass Transfer 100 (2016) 790-799.
[42] V.K. Kalapakides, A. Charalambopoulos, On Hamilton's Principle for discrete and continuous media, arXiv:1912.08490v1 [math-ph], 2019.
[43] Matlab, Release 2020b, The MathWorks, Inc., Natick, Massachusetts, 2020.
[44] Wolfram Research, Inc., Mathematica, Version 12.2, Champaign, Illinois, 2020.
[45] W. Ritz, Über eine neue Methode zur Lösung gewisser Variationsprobleme der mathematischen Physik, Journal für die Reine und Angewandte Mathematik 135 (1909) 1–61.
[46] S.G. Mikhlin. Variational Methods in Mathematical Physics, Pergamon Press, Oxford, 1964.
[47] H.S. Carslaw, J.C. Jaeger, Conduction of Heat in Solids, Oxford University Press, Oxford, 1959.

Appendix A: Detailed derivation of Euler-Lagrange equations

In this appendix, we outline the mathematical steps necessary to arrive at (14) starting from (13). These steps were mentioned in Section 3, but not explicitly written out, as to not distract from the key results of that section, and the paper as whole. Nonetheless, for the interested reader the steps are presented here. We begin by rewriting (13):

$$\begin{aligned}\delta I_{C_H} = &\int_\Omega \tfrac{1}{T_o}\Big[\delta\breve{T} * \rho_o c_\epsilon \breve{T} + \tfrac{1}{2}\nabla_i \delta T * \kappa_{ij}\nabla_j T + \tfrac{1}{2}\nabla_i T * \kappa_{ij}\nabla_j \delta T\Big] d\Omega \\ &- \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\,\rho_o c_\epsilon\, \bar{T}_0\Big] d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\big[\delta T * \bar{q}\big] d\Gamma = 0\end{aligned} \tag{A.1}$$

Let us now move κ_{ij} in the 3rd term to the left side of the convolution and then, recognizing the commutativity of the convolution operator, symmetry of κ_{ij}, and swapping i and j in the third term, we combine terms two and three to obtain:

$$\begin{aligned}\delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta\breve{T} * \rho_o c_\epsilon \breve{T} + \nabla_i \delta T * \kappa_{ij}\nabla_j T\Big] d\Omega \\ &\quad - \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\,\rho_o c_\epsilon\, \bar{T}_0\Big] d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\big[\delta T * \bar{q}\big] d\Gamma = 0\end{aligned} \tag{A.2}$$

Now, with the goal of removing derivatives from the variations, we perform spatial integration-by-parts via (11) on the second term:

$$\begin{aligned}\delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta\breve{T} * \rho_o c_\epsilon \breve{T} - \delta T * \nabla_i\big(\kappa_{ij}\nabla_j T\big)\Big] d\Omega \\ &\quad - \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\,\rho_o c_\epsilon\, \bar{T}_0\Big] d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\big[\delta T * \bar{q}\big] d\Gamma \\ &\quad + \int_\Gamma \tfrac{1}{T_o}\Big[\delta T * \kappa_{ij}\nabla_j T\, n_i\Big] d\Gamma = 0\end{aligned} \tag{A.3}$$

Next, let us proceed to temporal integration-by-parts operations, with the goal of removing time derivatives from the variations. Using (10) on the 1st term, and combining the resulting additional term with the previous 3rd term yields

$$\begin{aligned}\delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta T * \rho_o c_\epsilon \dot{T} - \delta T * \nabla_i\big(\kappa_{ij}\nabla_j T\big)\Big] d\Omega \\ &\quad + \int_\Omega \tfrac{1}{T_o}\Big[\delta T\,\rho_o c_\epsilon\,\big(T(0) - \bar{T}_0\big)\Big] d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\big[\delta T * \bar{q}\big] d\Gamma \\ &\quad + \int_\Gamma \tfrac{1}{T_o}\Big[\delta T * \kappa_{ij}\nabla_j T\, n_i\Big] d\Gamma = 0\end{aligned} \tag{A.4}$$

Finally, dividing the boundary integral into two parts, one over the temperature specified boundary, and one over the flux specified boundary, and combining the flux boundary integral with the 4th term above, results in the previously presented (14), that is

$$\begin{aligned}\delta I_{C_H} &= \int_\Omega \tfrac{1}{T_o}\Big[\delta T * \rho_o c_\epsilon \dot{T} - \delta T * \nabla_i\big(\kappa_{ij}\nabla_j T\big)\Big] d\Omega \\ &\quad + \int_\Omega \tfrac{1}{T_o}\Big[\delta T(t)\,\rho_o c_\epsilon\,\big(T(0) - \bar{T}_0\big)\Big] d\Omega + \int_{\Gamma_q} \tfrac{1}{T_o}\Big[\delta T * \big(\kappa_{ij}\nabla_j T\; n_i + \bar{q}\big)\Big] d\Gamma \\ &\quad + \int_{\Gamma_T} \tfrac{1}{T_o}\Big[\delta T * \kappa_{ij}\nabla_j T\; n_i\Big] d\Gamma = 0\end{aligned} \tag{A.5}$$

As in Section 3, at this point we note that variations on temperature should be set to zero on Γ_T, and thus the 4th term vanishes. Meanwhile, noting the arbitrary nature of the variations, the remaining three bracketed terms can easily be recognized as Euler-Lagrange equations corresponding to the heat equation (1), the initial conditions on temperature (2), and the heat flux boundary conditions (3a), respectively.