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A monolithic approach toward coupled electrodynamic–thermomechanical problems with regard to weak formulations

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Abstract Weak formulations of boundary value problems are the basis of various numerical discretization schemes. They are classically derived applying the method of weighted residuals or a variational principle. For electrodynamic and caloric problems, variational approaches are not straightforwardly obtained from physical principles like in mechanics. Weak formulations of Maxwell’s equations and of energy or charge balances thus are frequently derived from the method of weighted residuals or tailored variational approaches. Related formulations of multiphysical problems, combining mechanical balance equations and the axioms of electrodynamics with those of heat conduction, however, raise the additional issue of lacking consistency of physical units, since fluxes of charge and heat intrinsically involve time rates and temperature is only included in the heat balance. In this paper, an energy-based approach toward combined electrodynamic–thermomechanical problems is presented within a classical framework, merging Hamilton’s and Jourdain’s variational principles, originally established in analytical mechanics, to obtain an appropriate basis for a multiphysical formulation. Complementing the Lagrange function by additional potentials of heat flux and electric current and appropriately defining generalized virtual powers of external fields including dissipative processes, a consistent formulation is obtained for the four-field problem and compared to a weighted residuals approach.

1 Introduction

The understanding of multiphysical processes nowadays is of increasing importance in many fields of engineering. Phenomena based on the coupling of mechanics, electrodynamics and heat generation and conduction are essential in many classes of smart materials employed in batteries, energy harvesters, sensors or actuators. Their deep understanding is crucial for the design of efficient and reliable devices. Modeling and simulation, in this context, play a prominent role, relying on the continuously increasing computing power.

Weak formulations of boundary value problems are required as a starting point of various numerical discretization approaches, which are indispensable for the solution of application-oriented problems. They can be obtained from variational principles if applicable to the considered problem. In mechanics, classical principles, such as the one of virtual displacements or Hamilton’s principle [9], are often exploited and can straightforwardly be extended toward problems of electro- or magnetostatics [2, 18].

This does not hold for problems of heat conduction, however, whereupon the method of weighted residuals is commonly employed as a basis to derive weak formulations, starting from the differential equation and strong formulation, respectively [15, 26]. Introducing a virtual temperature change as generalization of virtual displacements as a test function, the basis of a Galerkin approach is obtained. A few possibilities to establish variational principles for problems of heat conduction are found in the literature. One approach replaces

the parabolic differential equation by a hyperbolic one, e.g., by introducing extended independent variables [21,33]. Alternatively, a variational functional can be constructed to obtain the parabolic differential equation, e.g., by adding an additional term containing the temperature gradient [29].

Maxwell's equations, as the fundamental axioms of electrodynamics, are not intrinsically represented by an equivalent variational principle as is the case in mechanics. The method of weighted residuals provides a weak formulation appropriate for numerical solution, employing virtual changes of a scalar and a vector potential as test functions [13,32]. Variational approaches of electrodynamics have been elaborated predominantly by the physics and electrical engineering communities so far [3,8,23,28,36], constructing electrodynamic Lagrangians matching Maxwell's differential equations, often adapted to specific applications. Mostly, parts of the differential equations in terms of the strong formulation are already included in the Lagrangian density, thus resembling a weighted residual approach rather than a classical variational one based on pure energetic considerations. However, it is exactly the formulation based on a thermodynamical potential, matched with an appropriate virtual work, which is sought for the extension of an electrodynamic variational approach toward multifield coupled problems, involving mechanical and caloric fields, and providing natural boundary conditions besides the governing differential equations.

Weak formulations of thermomechanical problems can be established by weighted residuals, based on the balance equations of momentum and energy, with virtual displacements and temperature as independent test functions. Due to incompatible physical units, however, dimensional factors lacking physical interpretations have to be introduced [24], making the approach somewhat unattractive, although the factors disappear in a finite element implementation. In the case of a three-field problem involving electric currents, a further dimensional factor would have to be incorporated. A monolithic variational approach toward thermomechanical problems has to cope with the issue that time rates are intrinsically involved in the heat flux and a further problem is that energies exhibit a gradient in the mechanical displacement, however, not in the temperature. A time integration is another requirement in a variational principle of thermomechanics and electrodynamics.

A variational approach to thermoelastic problems, including electrostatics, has recently been published in [39]. Variational formulations for thermomechanically coupled inelastic material behavior have been established in [5,11,30,35]. In [40], an integration factor is introduced in connection with the distinction of equilibrium and external temperatures, in order to remedy the problem of lacking natural variational structure in thermomechanics of general dissipative continua. Consequently, comprehensive functionals are identified, including all conservative and dissipative changes of state, whose critical points provide solutions of the coupled boundary value problem in both its rate and incremental forms. Further approaches based on stored energy functions generalized from mechanics, incorporating a dissipation function in order to overcome the fundamental problem of combining principles established for conservative systems with dissipative processes such as heat or charge diffusion, are presented in [25] for inelastic magnetomechanics. In [27,34], non-dissipative magneto- or electromechanical problems are considered on the basis of suitable potential energy functionals.

In this paper, classical variational principles of rational mechanics are exploited and generalized to obtain a weak formulation for a coupled four-field problem, including Maxwell's equations of electrodynamics, heat and charge diffusion as well as arbitrary irreversible material response within the framework of small deformations. The principles of Jourdain and Hamilton, the first one introducing time rates, the second one incorporating the essential time integration, are merged to one joint principle, constituting the basis of a monolithic approach. Contemporary incremental variational principles, which are proved to be absolutely appropriate for numerical implementation as referenced exemplarily above, require the introduction of tailored dissipation functions and potentials, respectively. The Hamilton–Jourdain approach involves conservative and dissipative processes intrinsically, including the fluxes of heat and electric current in the Lagrangian, while any kind of irreversible mechanical or magnetoelectric material-related response is incorporated in the virtual power of external forces. The latter have to be formulated appropriately, to finally match the balance equations and natural boundary conditions in their strong form. The separation of the virtual power of non-conservative forces and a functional, as known from Hamilton's classical principle, constitutes a major difference compared to [40], sparing a dissipation potential and not providing one comprehensive functional as known from sophisticated variational theories of general dissipative solids. To our best knowledge, previously published work on variational principles including dissipative processes does not cover fully coupled electrodynamics and thermomechanics of deformable dielectrics in a monolithic framework.

The strong form of the problem will be outlined first in the following section. In Sect. 3, a weak formulation of the combined four-field problem is developed based on the method of weighted residuals, in order to demonstrate the issue of unphysical scaling factors. Section 4 finally presents the monolithic variational formulation.

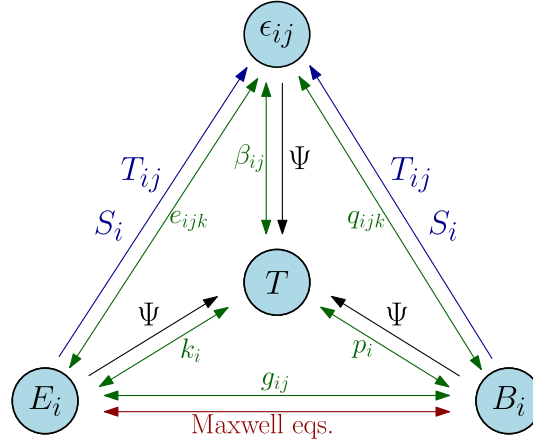


Fig. 1 Interactions between magnetic (B_i), electric (E_i), mechanical (ϵ_{ij}) and caloric (T) fields due to constitutive relations ($q_{ijk}, e_{ijk}, g_{ij}, \beta_{ij}, k_i, p_i$), electromagnetic forces (T_{ij}, S_i), dissipation (Ψ) and Maxwell's equations

2 Coupling phenomena and strong formulation of the boundary value problem

The essential coupling phenomena in a mechanical–electrodynamic–caloric four-field problem are illustrated in Fig. 1. Transient electric and magnetic fields are coupled intrinsically, in a local formulation described by the famous Maxwell equations [37]

$$\dot{B}_i = -\epsilon_{ijk} E_{k,j}, \quad (1)$$

$$\dot{D}_i + J_i = \epsilon_{ijk} H_{k,j}, \quad (2)$$

$$B_{i,i} = 0, \quad (3)$$

$$D_{i,i} = \omega_V, \quad (4)$$

where Eqs. (1) and (3) emanate from Faraday's law of induction and Eqs. (2) and (4) from Ampère's circuital law, thus not being independent. The analytical and index notation, respectively, is applied here as in the following. In this connection, the number of single indices indicates the order of a tensor, while repeated indices imply a summation. A comma denotes a partial spatial derivative, and ϵ_{ijk} are the coordinates of the Levi-Civita tensor, whose permutations convey the vector product, whereupon the right-hand sides of Eqs. (1) and (2) exhibit the curls of electric and magnetic fields E_k and H_k , respectively. The dots on the associated quantities electric displacement D_i and magnetic induction B_i denote partial time derivatives. Finally, in Eq. (2) J_i is the electric current density and ω_V in Eq. (4) is the volumetric density of free charges, which are both zero in a dielectric body. In electric conductors, on the other hand, a charge balance yields the equation of continuity of electrodynamics, claiming the conservation of charges within an arbitrary control volume:

$$J_{i,i} + \dot{\omega}_V = 0. \quad (5)$$

In multifunctional materials, constitutive relations in the most general case couple all four kinds of fields, i.e., electric, magnetic, mechanical and caloric, the latter being represented by the strain tensor ϵ_{ij} and the absolute thermodynamic temperature T . The constitutive relations of infinitesimal changes of state can be written as [6]

$$d\sigma_{ij} = C_{ijkl} d\epsilon_{kl} - e_{lij} dE_l + q_{lij} dB_l - \beta_{ij} dT, \quad (6)$$

$$dD_i = e_{ikl} d\epsilon_{kl} + \kappa_{ij} dE_j + g_{ij} dB_j + k_i dT, \quad (7)$$

$$dH_i = q_{ikl} d\epsilon_{kl} - g_{ij} dE_j + \mu_{ij} dB_j + p_i dT, \quad (8)$$

$$ds = \beta_{kl} d\epsilon_{kl} + k_j dE_j - p_j dB_j + \gamma dT. \quad (9)$$

The coupling tensors

$$\begin{aligned} e_{lij} &= -\frac{\partial^2 F}{\partial \epsilon_{ij} \partial E_l}, & q_{lij} &= \frac{\partial^2 F}{\partial \epsilon_{ij} \partial B_l}, & \beta_{ij} &= -\frac{\partial^2 F}{\partial \epsilon_{ij} \partial T}, \\ g_{ij} &= -\frac{\partial^2 F}{\partial E_i \partial B_j}, & k_i &= -\frac{\partial^2 F}{\partial E_i \partial T} & \text{and} & p_i = \frac{\partial^2 F}{\partial B_i \partial T} \end{aligned} \quad (10)$$

describe the piezoelectric, piezomagnetic, thermomechanical, magnetoelectric, pyroelectric and pyromagnetic effects, based on the Helmholtz free energy $F(\epsilon_{ij}, E_i, B_i, T)$ as thermodynamical potential, while

$$C_{ijkl} = \frac{\partial^2 F}{\partial \epsilon_{ij} \partial \epsilon_{kl}}, \quad \kappa_{ij} = -\frac{\partial^2 F}{\partial E_i \partial E_j}, \quad \mu_{ij} = \frac{\partial^2 F}{\partial B_i \partial B_j} \quad \text{and} \quad \gamma = -\frac{\partial^2 F}{\partial T \partial T} \quad (11)$$

represent the stiffness as well as the dielectric and magnetic permeability coefficients and the temperature-related specific heat capacity. Within a nonlinear constitutive framework including ferroelectric, ferroelastic or magnetostrictive effects, they are functions of the independent variables, which have been chosen as strain, electric field, magnetic induction and temperature in Eqs. (6) to (9) and have to be interpreted as material tangents for finite changes of state. The σ_{ij} in Eq. (6) are the stresses, and s in Eq. (9) denotes the specific entropy.

Most of the materials exhibit just one or two of the above-mentioned coupling effects. In particular, the magnetoelectric coupling is scarcely found in natural matter [14] and hard to handle from an engineering point of view. Equations (6) to (9), however, may represent the constitutive behavior of a magnetoelectric composite on a macroscopic scale [4, 22].

Another type of field coupling, in Fig. 1 indicated by the Maxwell stress tensor

$$T_{ij} = E_i D_j + H_i B_j - \frac{1}{2} (D_l E_l + B_l H_l) \delta_{ij} \quad (12)$$

and the Poynting vector

$$S_i = \epsilon_{ijk} E_j H_k, \quad (13)$$

is mediated by the electromagnetic force [16, 17]

$$F_i^{EM} = - \int_V \frac{\dot{S}_i}{c_M^2} dV + \int_V T_{ij,j}^M dV + \int_{\partial V} (T_{ij}^E - T_{ij}^M) n_j dA \quad (14)$$

acting in the domain V of a material body and on its boundary with unit normal n_j . In Eq. (12), the identity tensor is introduced in terms of the Kronecker symbol δ_{ij} . In Eq. (14), the phase velocity of electromagnetic waves is denoted by c_M , in an isotropic medium being known as $c_M = 1/\sqrt{\kappa\mu}$ with κ and μ as isotropic coefficients of dielectric and magnetic permeabilities. The superscripts M and E refer to the fields in the material and the surrounding environment, respectively. According to Eq. (14), the tractions $t_i = (T_{ij}^E - T_{ij}^M) n_j$ at the boundary Γ come along with a jump of the Maxwell stress tensor with dielectric and magnetic properties of environment and material, respectively.

In a multifield problem involving electric and magnetic fields, mechanical equilibrium is thus governed by the momentum balance

$$\rho \ddot{u}_i = \sigma_{ij,j} + T_{ij,j}^M + f_i^V - \frac{\dot{S}_i}{c_M^2}, \quad (15)$$

where ρ and f_i^V represent the mass and body force densities, respectively. The Cauchy stress tensor has been employed referring to the current configuration or the limit of infinitely small deformations, the latter taken as a basis in Eqs. (6) to (9). The mass density $\rho = \rho_0$ thus being constant, an additional equation for the conservation of mass is redundant. The vector of mechanical displacement u_i in this case is related to the strain according to

$$\epsilon_{ij} = \frac{1}{2} (u_{i,j} + u_{j,i}) = u_{i,j} - \Omega_{ij}, \quad (16)$$

where Ω_{ij} is the skew-symmetric part of the displacement gradient.

One further issue of small versus large deformations, which is often overlooked in electrodynamics of deformable continua, is that the fundamental equations of non-relativistic mechanics and electrodynamics possess different invariance properties [19], i.e., Galilean and Lorentz, respectively. As one consequence, the assumption of electromagnetic fields experienced by a moving material point is not unique. This aspect, however, is irrelevant within a small deformations approximation.

A further mechanical–electrodynamic coupling mechanism prevails just for finite deformations, where the strain controls the domain V for the solution of Eqs. (1) to (4). The same holds for the impact of large mechanical deformations on the temperature field, which is governed by the energy balance of non-equilibrium thermodynamics [39,40]

$$T\dot{s} = -q_{i,i}^A + \dot{q}_V + \dot{\chi}(\dot{E}_i, \dot{B}_i, \dot{\epsilon}_{ij}), \quad (17)$$

depicted in its entropy formulation. The specific dissipation rate here is denoted by $\dot{\chi}$. For ferroelectric domain switching with irreversible strain and polarization rates $\dot{\epsilon}_{ij}^{\text{irr}}$ and \dot{P}_i^{irr} , it is commonly specified as [20]

$$\dot{\chi} = T\dot{s}^i = \sigma_{ij}\dot{\epsilon}_{ij}^{\text{irr}} + E_i\dot{P}_i^{\text{irr}} \quad (18)$$

and basically is proportional to the time rate of the irreversible part of the specific entropy at a given temperature. \dot{q}_V in Eq. (17) is a volumetric heat source, whereas the heat flux related to a local reference surface A is often given by Fourier's law, i.e.,

$$q_i^A = -\lambda_{ij}T_{,j}, \quad (19)$$

with the second-order tensor of heat conduction λ_{ij} . Dissipation, as internal heat source, is controlled by the mechanical and the electromagnetic fields, physically being attributed to friction and irreversible transitions in terms of phase transitions and domain switching [12]. In Fig. 1, a dissipative power Ψ indicates the one-sided field coupling changing the temperature. The material coefficients of Eqs. (6) to (9), on the other hand, are partly considerably temperature-dependent, basically depending on the mechanical, electric and magnetic variables of state as well. The same holds for Ohm's law, relating the electric current in Eq. (2) to the independent variables:

$$J_i = \varrho_{ij}(T, E_i, B_i, \epsilon_{ij}) E_j. \quad (20)$$

Equations (1) to (5), (15) and (17) represent a set of partial differential equations, in conjunction with boundary conditions and additional Eqs. (12), (13), (19) and (20) basically constituting strong formulations of thermomechanical–electrodynamic boundary value problems. Incorporating the constitutive equations Eqs. (6) to (9), solutions in terms of the independent variables u_i , E_i , B_i and T are obtained, where Eq. (16) has to be taken into account and ω_V is a further unknown in electric conductors. In the special case of electrostatics ($\dot{B}_i, \dot{D}_i, J_i = 0$), scalar potentials are introduced according to $E_k = -\phi_{,k}$ and $H_k = -\psi_{,k}$, trivially satisfying Eqs. (1) and (2) and leaving Eqs. (3) and (4) for further consideration [16]. In electrodynamics, the set of equations and independent variables is likewise reduced, introducing a scalar potential ϕ and a vector potential A_i according to

$$B_i = \varepsilon_{ijk}A_{k,j}, \quad (21)$$

$$E_i = -\phi_{,i} - \dot{A}_i, \quad (22)$$

intrinsically satisfying Eqs. (1) and (3). A boundary value problem is then formulated in terms of the eight independent variables ϕ , A_i , u_i and T . A set of mechanical–electrodynamic equations, incorporating all couplings within a framework of small deformations, is found in [31], where gauge transformations are furthermore introduced, in order to decouple the differential equations of electrodynamics.

3 Method of weighted residuals for the multifield problem

Applying the method of weighted residuals to a mechanical problem, the strong formulation, represented by the local formulation of the momentum balance Eq. (15), is taken as a basis, complemented by the natural boundary condition with prescribed tractions \bar{t}_i . Introducing virtual displacements δu_i as test or weighting functions, respectively, the weak formulation of the mechanical boundary value problem is obtained:

$$\int_V (\sigma_{ij,j} + b_i^V - \rho\ddot{u}_i) \delta u_i dV + \int_{\partial V} (\bar{t}_i - t_i) \delta u_i dA = 0. \quad (23)$$

The specific volume force b_i^V comprises both mechanical and electrodynamic forces, according to Eq. (15) reading

$$b_i^V = f_i^V + T_{ij,j}^M - \frac{\dot{S}_i}{c_M^2}. \quad (24)$$

The tractions \bar{t}_i are composed of classical mechanical boundary loads \tilde{t}_i and electromagnetic tractions, see Eq. (14):

$$\bar{t}_i = \tilde{t}_i + (T_{ij}^E - T_{ij}^M) n_j. \quad (25)$$

For a caloric boundary value problem, the weak formulation of Eq. (17) is obtained likewise, introducing a virtual change of temperature δT as test function and natural boundary conditions in terms of the heat flux:

$$\int_V (T\dot{s} + q_{i,i}^A - \dot{q}_V - \dot{\chi}) \delta T \, dV + \int_{\partial V} (\bar{q}_i^A - q_i^A) n_i \delta T \, dA = 0. \quad (26)$$

The Maxwell equations Eqs. (2) and (4) in connecti on with the two potentials introduced in Eqs. (21) and (22) constitute the strong formulation of an electrodynamic boundary value problem, complemented by the natural boundary conditions $(D_i^M - D_i^E) n_i = -\bar{\omega}_A$ and $\varepsilon_{ijk} n_j H_k = \varepsilon_{ijk} n_j \bar{H}_k$, where $\bar{\omega}_A$ is a prescribed surface charge density. Disregarding the dielectric properties of the commonly surrounding air with regard to typically much larger dielectric coefficients of the solid, the environmental D_i^E is neglected in the following. Choosing virtual changes of scalar and vector potentials as test functions, the weak formulation of electrostatics is obtained as

$$\begin{aligned} & \int_V [(\varepsilon_{ijk} H_{k,j} - \dot{D}_i - J_i) \delta A_i - (D_{i,i} - \omega_V) \delta \phi] \, dV \\ & + \int_{\partial V} [\varepsilon_{ijk} (\bar{H}_k - H_k) n_j \delta A_i + (\bar{\omega}_A + D_i n_i) \delta \phi] \, dA = 0, \end{aligned} \quad (27)$$

being complemented by the condition of conservation of charges, according to Eq. (5), i.e.,

$$\int_V (J_{i,i} + \dot{\omega}_V) \delta \phi \, dV + \int_{\partial V} (\bar{J}_i - J_i) n_i \delta \phi \, dA = 0, \quad (28)$$

where the natural boundary condition is incorporated in terms of the normal component of the electric current density.

Considering the physical units of Eqs. (23) to (28), the mechanical and electrodynamic equations, Eqs. (23) and (27), hold the unit [J], whereas the caloric balance Eq. (26) holds [JK/s] and the charge balance Eq. (28) [J/s]. Not being an issue for the separated mechanical, caloric and electrodynamic problems at all, assembling Eqs. (23), (26), (27) and (28) to obtain a monolithic formulation for coupled four-field problems, however, requires an unsatisfactory trick. Dimensional scaling factors Λ , Ω , Γ have to be introduced [24] meeting the conditions

$$\frac{\Lambda}{\Omega} = 1 \frac{K}{s}, \quad \frac{\Lambda}{\Gamma} = \frac{1}{s}, \quad \frac{\Omega}{\Gamma} = \frac{1}{K}, \quad (29)$$

finally leading to the weak formulation of the coupled multifield problem:

$$\begin{aligned}
& \left\{ \int_V \left[(\sigma_{ij,j} + b_i^V - \rho \ddot{u}_i) \delta u_i + (\varepsilon_{ijk} H_{k,j} - \dot{D}_i - J_i) \delta A_i - (D_{i,i} - \omega_V) \delta \phi \right] dV \right. \\
& \quad \left. + \int_{\partial V} [(\bar{t}_i - t_i) \delta u_i + \varepsilon_{ijk} (\bar{H}_k - H_k) n_j \delta A_i + (\bar{\omega}_A + D_i n_i) \delta \phi] dA \right\} \Lambda \\
& \quad + \left\{ \int_V (J_{i,i} + \dot{\omega}_V) \delta \phi dV + \int_{\partial V} (\bar{J}_i - J_i) n_i \delta \phi dA \right\} \Gamma \\
& \quad + \left\{ \int_V (T \dot{s} + q_{i,i}^A - \dot{q}_V - \dot{\chi}) \delta T dV + \int_{\partial V} (\bar{q}_i^A - q_i^A) n_i \delta T dA \right\} \Omega = 0.
\end{aligned} \tag{30}$$

Being unphysical on the one hand side, the factors Λ , Ω and Γ , on the other, vanish in a finite element approach derived from Eq. (30). Alternatively, the scaling factors could be circumvented, in the test functions replacing δu_i by $\delta \dot{u}_i$, δT by $\delta T/T$, thus considering entropy instead of energy, and finally replacing the electrodynamic potentials by their time rates, except for the third row in Eq. (30), where $\delta \phi$ has to remain unchanged. This adaption, however, appears just as arbitrary as the retroactive introduction of scaling factors.

4 Variational formulation of electrodynamics–thermomechanics

One of the most exploited variational principles of mechanics probably is the principle of virtual work

$$\delta \Pi^i = \delta W^e, \tag{31}$$

which, for conservative systems, is equivalent to the principle of the minimum of the total potential, merging the internal and external potentials Π^i and $\Pi^e = -W^e$. Within the framework of variational calculus, δ in Eq. (31) denotes the first variation. For dissipative systems, δW^e is the virtual work, being identical to the first variation of W^e just for a conservative system. Distinguished notations of δ , however, will not be introduced here. For non-mechanical problems, the potential Π^i and conjugated virtual work δW^e have to be adapted to the specific physical process.

Alternatively, Eq. (31) can be formulated in terms of velocities and time rates, respectively, constituting the principle of virtual power, classically known as Jourdain's principle [9]

$$\delta \dot{\Pi}^i = \delta P^e. \tag{32}$$

The virtual work in Eq. (31) is replaced by the virtual power of both external loads and dissipative forces δP^e . Kinematic constraints in Eq. (32) are formulated on Dirichlet boundaries in terms of velocities, thus, e.g., $\delta \dot{u}_i = 0$ or $\delta \dot{\phi} = 0$. Due to the time rate formulation and in contrast to Eq. (31), $\delta u_i = 0$ and $\delta \phi = 0$, etc., hold on the whole boundary. For holonomic constraints, essential boundary conditions in Eq. (32) may likewise be formulated either as displacements, electric potentials, etc., or as their time rates.

A dissipative power Ψ can be introduced, separating conservative from non-conservative contributions to the total virtual power:

$$\delta P^e = \delta \Psi - \delta \dot{\Pi}^e. \tag{33}$$

The kinetic energy K is incorporated in Hamilton's principle

$$\delta \int_{t_0}^{t_1} (K - \Pi^i) dt + \int_{t_0}^{t_1} \delta W^e dt = 0 \tag{34}$$

integrating in a time interval $[t_0, t_1]$, whereupon the first variations of the independent variables, e.g., δu_i or $\delta \phi$, disappear at t_0 and t_1 following a basic postulate of the Lagrangian embedding theorem (Lagrangian variation)

of variational calculus [10]. The kinetic and potential energies are commonly merged in the Lagrange function $L = K - \Pi^i$.

One major issue of caloric problems in a variational principle is that in the internal potential of Hamilton's principle Eq. (34), i.e.,

$$\delta \Pi^i = \delta F = \int_V (\sigma_{ij} \delta \epsilon_{ij} - D_i \delta E_i + H_i \delta B_i - s \delta T) dV, \quad (35)$$

the temperature T is involved without a gradient, whereas strain, electric field and magnetic induction are related to the displacements and electrodynamic potentials applying differential operators following Eqs. (16), (21) and (22). Not involving the gradient of a variable, the divergence theorem cannot be applied in order to separate contributions of domain and boundary, as it is done with mechanical and electrodynamic terms. The Helmholtz free energy F is employed in Eq. (35) as thermodynamical potential, introducing B_i instead of H_i as independent variable, thus being able to directly introduce the vector potential A_i in the following derivations.

Two further issues arise with combined mechanical/electrodynamic–caloric problems. Firstly, time rates are intrinsically involved in the heat flux and electric current and, however, do not appear in the mechanical stress, electric displacement or magnetic field. Secondly, some terms in the Lagrange function require time integration by parts in order to end up in an appropriate weak formulation, finally providing the governing differential equations of Sect. 2. In the electrodynamics part, the latter aspect evolves from Eqs. (21), (22) and (35), whereupon δB_i and δE_i are associated with δA_i on the one hand side and $\delta \dot{A}_i$ on the other. While mechanical problems are equivalently governed by the principles of virtual work or by those of Jourdain or Hamilton [9], combined problems of mechanics and electrodynamics thus require the time integration associated with Hamilton's principle, whereupon Eqs. (31) and (32) are not applicable. Caloric aspects being involved in mechanical or electrodynamic calculations or both, none of the variational principles outlined above is appropriate, requiring both time integration and a rate dependent formulation.

A modified variational formulation has to be introduced in this case, combining the classical principles of Jourdain and Hamilton, Eqs. (32) and (34):

$$\delta \int_{t_0}^{t_1} \dot{\mathcal{L}} dt + \int_{t_0}^{t_1} \delta P^e dt = 0. \quad (36)$$

From now on, Eq. (36) shall be denoted as principle of Hamilton–Jourdain which, just as Hamilton's principle, seeks solutions from a stationarity condition. For mechanical problems, it is equivalent to the principles of virtual work, Jourdain and Hamilton, providing identical differential equations as associated strong formulations, accounting for the constraints of generalized virtual displacements and velocities outlined in connection with Eq. (32). The letter L for the Lagrange function has been replaced by an \mathcal{L} in Eq. (36) to indicate the possibility of generalized definitions.

For caloric problems, the time derivative of the Lagrange function has to be extended by an additional term as follows:

$$\dot{\mathcal{L}} = \dot{K} - \dot{F} - \frac{H}{T} = \dot{L} - \frac{H}{T}. \quad (37)$$

The Helmholtz free energy is employed as thermodynamical potential, and the kinetic energy rate of a continuum reads

$$\dot{K} = \int_V \rho \dot{u}_i \dot{u}_i dV. \quad (38)$$

The additional term in Eq. (37) is denoted as heat flux potential [29], being defined as

$$H(T, j) = \frac{1}{2} \int_V \lambda_{ij} T_{,i} T_{,j} dV = -\frac{1}{2} \int_V q_i^A T_{,i} dV, \quad (39)$$

where Eq. (19) has been inserted for the second identity. Its formal structure reminds of the Helmholtz free energy, e.g., for a piezoelectric problem reading

$$F(\epsilon_{ij}, E_i) = \int_V \left(\frac{1}{2} C_{ijkl} \epsilon_{ij} \epsilon_{kl} - e_{lij} E_l \epsilon_{ij} - \frac{1}{2} \kappa_{ij} E_i E_j \right) dV, \quad (40)$$

replacing C_{ijkl} or κ_{ij} by λ_{ij} and ϵ_{ij} or E_i by T_i . It incorporates temperature gradients, in view of spatial derivatives of displacements and electrodynamic potentials providing a unitary mathematical basis.

A further extension of the Lagrange function is required in regard to the electric current J_i , involved in the Maxwell equations and the balance equation Eq. (5). An electric current potential is introduced in the style of the heat flux potential Eq. (39), i.e.,

$$C(E_i) = \frac{1}{2} \int_V \varrho_{ij} E_j E_i dV = \frac{1}{2} \int_V J_i E_i dV, \quad (41)$$

where Ohm's law according to Eq. (20) has been inserted for the second identity. The first variation of the time rate of the extended Lagrange function Eq. (37), adding the electric current potential Eq. (41), is thus obtained inserting Eqs. (38), (39) and (35):

$$\begin{aligned} \delta \dot{\mathcal{L}} &= \delta \dot{K} - \delta \dot{F} - \delta C - \delta \left(\frac{H}{T} \right) \\ &= \int_V \left(\rho \ddot{u}_i \delta \dot{u}_i + \rho \dot{u}_i \delta \ddot{u}_i - \sigma_{ij} \delta \dot{\epsilon}_{ij} + D_i \delta \dot{E}_i - H_i \delta \dot{B}_i + s \delta \dot{T} - J_i \delta E_i + \frac{q_j^A}{T} \delta T_{,j} \right) dV. \end{aligned} \quad (42)$$

The temperature T in the denominator has been included in the integrand as a constant quantity, thus not being subject to variation. It is interpreted as reference temperature for an incremental change of state. Further discussion and some details on the derivation of Eq. (42) are depicted in the Appendix.

The contributions of external tractions, charges, magnetic and heat fluxes as well as electric currents to the virtual power δP^e can be separated in such a way that the electromagnetic part is represented by

$$\delta P_{\omega/H}^e = - \int_V \omega_V \delta \dot{\phi} dV - \int_{\partial V} (\bar{\omega}_A \delta \dot{\phi} + \varepsilon_{ijk} \bar{H}_k \delta \dot{A}_i n_j) dA \quad (43)$$

and

$$\delta P_J^e = - \int_V \dot{\omega}_V \delta \phi dV - \int_{\partial V} \bar{J}_i \delta \phi n_i dA, \quad (44)$$

while the mechanical and caloric parts are given as follows:

$$\delta P_t^e = \int_V b_i^V \delta \dot{u}_i dV + \int_{\partial V} \bar{t}_i \delta \dot{u}_i dA, \quad (45)$$

$$\delta P_q^e = \dot{S}^e \delta T = \frac{\dot{Q}^e}{T} \delta T = \int_V \frac{\dot{q}_V}{T} \delta T dV - \int_{\partial V} \frac{\bar{q}_i^A}{T} \delta T n_i dA. \quad (46)$$

The caloric virtual power δP_q^e is based on the flux of exchange entropy \dot{S}^e which, in turn, is associated with the external heat flux \dot{Q}^e , incorporating the absolute thermodynamic temperature. For a system with material-related dissipative response, e.g., in terms of domain switching, see Eq. (18), or phase transition, the dissipative power introduced in Eq. (33) is involved, its first variation yielding

$$\delta \Psi = \dot{S}^i \delta T = \int_V \frac{\dot{\chi}}{T} \delta T dV. \quad (47)$$

Akin to Eq. (46), there is a relation to the entropy flux; however, the part of irreversible entropy production is incorporated at this point.

The total virtual power of generalized external conservative and dissipative forces finally is assembled from Eqs. (43) to (47):

$$\delta P^e = \delta P_t^e + \delta P_{\omega/H}^e + \delta P_J^e + \delta P_q^e + \delta \Psi. \quad (48)$$

Equations (36), (42) and (48) constitute a weak formulation of the electrodynamic–thermomechanical problem. To be suitable for applications toward numerical discretization schemes or to obtain associated strong formulations, however, time integrations by parts are indispensable. Details are depicted in the Appendix. The principle of Hamilton–Jourdain then yields

$$\begin{aligned} & \int_{t_0}^{t_1} \left\{ \int_V \left[(b_i^V - \rho \ddot{u}_i) \delta \dot{u}_i - \sigma_{ij} \delta \dot{\epsilon}_{ij} + D_i \delta \dot{E}_i - H_i \delta \dot{B}_i - J_i \delta E_i - \omega_V \delta \dot{\phi} \right. \right. \\ & \quad \left. \left. - \dot{\omega}_V \delta \phi + \left(\frac{\dot{\chi}}{T} - \dot{s} + \frac{\dot{q}_V}{T} \right) \delta T + \frac{q_j^A}{T} \delta T_{,j} \right] dV \right. \\ & \quad \left. + \int_{\partial V} \left[\bar{t}_i \delta \dot{u}_i - \bar{\omega}_A \delta \dot{\phi} - \varepsilon_{ijk} \bar{H}_k \delta \dot{A}_i n_j - \left(\bar{J}_i \delta \phi + \frac{\bar{q}_i^A}{T} \delta T \right) n_i \right] dA \right\} dt = 0. \end{aligned} \quad (49)$$

Introducing Eqs. (16), (21) and (22), virtual strain, electric field and magnetic induction are replaced by virtual displacements δu_i and the virtual electrodynamic potentials $\delta \phi$ and δA_i , yielding

$$\begin{aligned} & -\sigma_{ij} \delta \dot{\epsilon}_{ij} + D_i \delta \dot{E}_i - H_i \delta \dot{B}_i - J_i \delta E_i + \frac{q_j^A}{T} \delta T_{,j} \\ & = -\sigma_{ij} \delta \dot{u}_{i,j} - D_i (\delta \dot{\phi}_{,i} + \delta \dot{A}_i) + J_i (\delta \phi_{,i} + \delta \dot{A}_i) - \varepsilon_{ijk} H_i \delta \dot{A}_{k,j} + \frac{q_j^A}{T} \delta T_{,j} \\ & = \left(-\sigma_{ij} \delta \dot{u}_i - D_j \delta \dot{\phi} + J_j \delta \phi - \varepsilon_{ijk} H_i \delta \dot{A}_k + \frac{q_j^A}{T} \delta T \right)_{,j} \\ & \quad + \sigma_{i,j} \delta \dot{u}_i + D_{j,j} \delta \dot{\phi} - J_{j,j} \delta \phi - D_i \delta \dot{A}_i + J_i \delta \dot{A}_i + \varepsilon_{ijk} H_{i,j} \delta \dot{A}_k - \frac{q_{j,j}^A}{T} \delta T. \end{aligned} \quad (50)$$

As in Eq. (42), the temperature T in the denominators is not subject to differentiation, see the Appendix. Equation (50) can now be inserted into Eq. (49). Taking into account that $\varepsilon_{ijk} H_i \delta \dot{A}_k = -\varepsilon_{ijk} H_k \delta \dot{A}_i$, applying Gauß integral theorem and introducing Cauchy's theorem $t_i = \sigma_{ij} n_j$ with its generalization toward charges, see the Appendix, the principle of Hamilton–Jourdain finally yields

$$\begin{aligned} & \int_{t_0}^{t_1} \left\{ \int_V \left[(b_i^V - \rho \ddot{u}_i + \sigma_{ij,j}) \delta \dot{u}_i + (D_{j,j} - \omega_V) \delta \dot{\phi} - (J_{j,j} + \dot{\omega}_V) \delta \phi \right. \right. \\ & \quad \left. \left. + (\varepsilon_{ijk} H_{i,j} + \dot{D}_k + J_k) \delta \dot{A}_k + \left(\frac{\dot{\chi}}{T} - \dot{s} + \frac{\dot{q}_V}{T} - \frac{q_{j,j}^A}{T} \right) \delta T \right] dV \right. \\ & \quad \left. + \int_{\partial V} \left[(\bar{t}_i - t_i) \delta \dot{u}_i - (\bar{\omega}_A - \omega_A) \delta \dot{\phi} - (\bar{J}_j - J_j) n_j \delta \phi \right. \right. \\ & \quad \left. \left. - \varepsilon_{ijk} (\bar{H}_k - H_k) n_j \delta \dot{A}_i - \left(\frac{\bar{q}_j^A}{T} - \frac{q_j^A}{T} \right) n_j \delta T \right] dA \right\} dt = 0. \end{aligned} \quad (51)$$

A time integration by parts applied to the term $D_i \delta \dot{A}_i dt$ is prerequisite for the derivation of the weak form according to Eq. (51). The principle of Jourdain thus cannot be the basis of a variational approach in electrodynamics, lacking the time integration. Hamilton's principle, on the other hand, is not appropriate either, lacking the time rates which are essential for caloric problems and electric currents.

Taking into account the relation $\varepsilon_{ijk}H_{i,j} = -\varepsilon_{kij}H_{j,i}$ and applying the fundamental lemma of variational calculus, Eq. (51) yields the strong formulation of an electrodynamic–thermomechanical boundary value problem in terms of the differential equations Eqs. (2), (4), (5), (15) and (17), where the volume forces in the momentum balance are given in Eq. (24), as well as the natural boundary conditions

$$t_i = \bar{t}_i \text{ on } A_t, \quad (52)$$

$$\omega_A = \bar{\omega}_A \text{ on } A_\omega, \quad (53)$$

$$J_j n_j = \bar{J}_j n_j \text{ on } A_J, \quad (54)$$

$$q_i^A n_i = \bar{q}_i^A n_i \text{ on } A_q, \quad (55)$$

$$\varepsilon_{ijk} n_j H_k = \varepsilon_{ijk} n_j \bar{H}_k \text{ on } A_H, \quad (56)$$

with the tractions \bar{t}_i depicted in Eq. (25). Equation (51) in this respect is an alternative approach of Eq. (30), where unphysical scaling factors Λ , Ω and Γ or arbitrary adaptations of test functions are redundant, and a power functional with associated virtual work rates constitutes the basis, rather than a set of differential equations. Concerning a finite element implementation starting from the weak forms, discretized algebraic systems of equations are accomplished likewise by introducing interpolation functions in connection with nodal (virtual) variables $\delta \hat{A}_i$, $\delta \hat{\phi}$, $\delta \hat{u}_i$, $\delta \hat{T}$ and their time derivatives, respectively.

5 Conclusion

A monolithic energy-based approach, covering fully coupled electrostatics and thermomechanics of deformable dielectrics, has been presented, based on a combination of the classical variational principles of Jourdain and Hamilton. Electrodynamic problems alone could be based on Hamilton’s principle, if the Lagrange function and the virtual work are chosen appropriately. Coupled caloric–mechanical or caloric–electrodynamic problems, however, require a time rate formulation. Time rates and time integration being inherently included in the merged principle of Hamilton–Jourdain dissipative processes are readily incorporated, extending the Lagrange function by heat and electric current flux potentials. Non-conservative material-related processes, being intrinsically involved in ferroelectrics and ferromagnets due to domain wall motions, respectively, are incorporated in the virtual power of external forces. The introduction of electromagnetic scalar and vector potentials besides mechanical displacements and temperature as independent variables reduces the problem to a minimum of unknowns, whereupon the weak formulation obtained is valid for any kind of isotropic or anisotropic multiphysically coupled constitutive behavior.

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6 Appendix

In [29,38], a heat flux potential according to Eq. (39) is introduced in conjunction with a functional, where the temperature is not involved in the denominator as in Eq. (42). Consequently, the assumption of a constant temperature is not applicable; however, an ”isotropic variation” has to be applied instead.

Alternatively, $G_i = T_{,i}/T$ could be introduced as independent variable [7,40], whereupon

$$\hat{h}(G_i) = -\lambda_{ij} T_{,j} \frac{T_{,i}}{T} = \dot{q}_i^A G_i \quad (57)$$

constitutes a specific Fourier potential and replaces h/T ($h = H/V$) in Eq. (42). Its first variation

$$\delta \hat{h}(G_i) = \frac{\partial \hat{h}(G_i)}{\partial G_i} \delta G_i = \dot{q}_i^A \delta \left(\frac{T_{,i}}{T} \right) = \dot{q}_i^A \left(\frac{\delta T}{T} \right)_{,i} \quad (58)$$

eventually yields Eq. (50) without further specification regarding the temperature T . Finally, it is noted that this also applies if heat flux is included in the irreversible entropy production of Eq. (47) in terms of $-\dot{q}_i^A T_{,i}/T^2$, as basically suggested in [1,21].

The time derivatives in Eq. (42) are derived starting from the specific Helmholtz potential in Eq. (35) in rate-dependent formulation, i.e.,

$$\delta \dot{f}(\epsilon_{ij}, \dot{\epsilon}_{ij}, E_i, \dot{E}_i, B_i, \dot{B}_i, T, \dot{T}) = \underbrace{\frac{\partial \dot{f}}{\partial \dot{\epsilon}_{ij}} \delta \dot{\epsilon}_{ij}}_{\frac{\partial f}{\partial \epsilon_{ij}} = \sigma_{ij}} + \underbrace{\frac{\partial \dot{f}}{\partial \dot{E}_i} \delta \dot{E}_i}_{-D_i} + \underbrace{\frac{\partial \dot{f}}{\partial \dot{B}_i} \delta \dot{B}_i}_{H_i} + \underbrace{\frac{\partial \dot{f}}{\partial \dot{T}} \delta \dot{T}}_{-s}, \quad (59)$$

and from Eq. (38):

$$\delta \dot{K}(\dot{u}_i, \ddot{u}_i) = \frac{\partial \dot{K}}{\partial \dot{u}_i} \delta \dot{u}_i + \frac{\partial \dot{K}}{\partial \ddot{u}_i} \delta \ddot{u}_i = \int_V \rho \ddot{u}_i \delta \dot{u}_i \, dV + \int_V \rho \dot{u}_i \delta \ddot{u}_i \, dV. \quad (60)$$

Time integration by parts of the first volume integral in Eq. (60) yields

$$\int_{t_0}^{t_1} \int_V \rho \ddot{u}_i \delta \dot{u}_i \, dV dt = \int_V \left[\rho \dot{u}_i \delta u_i \right]_{t_0}^{t_1} dV - \int_{t_0}^{t_1} \int_V \rho \dot{u}_i \delta u_i \, dV dt = 0, \quad (61)$$

vanishing due to the general requirement of Jourdain's principle, i.e., $\delta u_i = 0$, and of the second volume integral

$$\int_{t_0}^{t_1} \int_V \rho \dot{u}_i \delta \ddot{u}_i \, dV dt = \int_V \underbrace{\left[\rho \dot{u}_i \delta \dot{u}_i \right]_{t_0}^{t_1}}_{=0} dV - \int_{t_0}^{t_1} \int_V \rho \ddot{u}_i \delta \dot{u}_i \, dV dt, \quad (62)$$

where the first term on the right-hand side vanishes at the boundaries t_0 and t_1 due to $\delta \dot{u}_i(t_0) = \delta \dot{u}_i(t_1) = 0$, following a basic postulate of the Lagrangian embedding theorem of variational calculus.

Further integrations by parts are required in Eqs. (49) and (51):

$$\int_{t_0}^{t_1} \int_V s \delta \dot{T} \, dV dt = \int_V \underbrace{\left[s \delta T \right]_{t_0}^{t_1}}_{=0} dV - \int_{t_0}^{t_1} \int_V \dot{s} \delta T \, dV dt, \quad (63)$$

$$\int_{t_0}^{t_1} \int_V D_i \delta \ddot{A}_i \, dV dt = \int_V \underbrace{\left[D_i \delta \dot{A}_i \right]_{t_0}^{t_1}}_{=0} dV - \int_{t_0}^{t_1} \int_V \dot{D}_i \delta \dot{A}_i \, dV dt. \quad (64)$$

With the Cauchy theorem of charges, as a generalization of the mechanical theorem relating the stress tensor and traction vector via the unit normal n_j of the body cut, i.e.,

$$D_j n_j = -\omega_A, \quad (65)$$

and Gauß's integral theorem applied to Eq. (50), i.e.,

$$\begin{aligned} & \int_V \left(-\sigma_{ij} \delta \dot{u}_i - D_j \delta \dot{\phi} - J_j \delta \phi - \varepsilon_{ijk} H_i \delta \dot{A}_k + \frac{q_j^A}{T} \delta T \right) dV \\ & = \int_{\partial V} \left(-\sigma_{ij} n_j \delta \dot{u}_i - D_j n_j \delta \dot{\phi} - J_j n_j \delta \phi - \varepsilon_{ijk} H_i n_j \delta \dot{A}_k + \frac{q_j^A n_j}{T} \delta T \right) dA, \end{aligned} \quad (66)$$

Eq. (51) is straightforwardly derived.

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