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Numerical modeling of thermoelectric coupling

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Abstract. *A thermoelectric device creates a temperature gradient due to the applied voltage and produces a voltage due to a temperature gradient. This thermoelectric coupling is referred to as the* PELTIER-SEEBECK *effect. We start from the balance equations for a material with electric charge and deduce the constitutive equations necessary for modeling. After insertion of the constitutive relations into the balance equations coupled nonlinear field equations result. We implement and solve them by using open-source codes. A simulation of a thermoelectric device validates the performed thermodynamically consistent continuum mechanics approach.*

Keywords: finite element method; electromagnetic interaction; thermoelectric coupling

1 GOVERNING EQUATIONS

In rational mechanics the balance equations are stated without further discussion. Unfortunately for balance equations including electromagnetic interactions many different formalisms exist, see [7, §286]. Even the MAXWELL equations, which provide the connection between the electromagnetic fields, occur in various formulations, see [6] and [3, §II]. Hence we present explicitly our derivation of the governing equations. We apply the EINSTEIN summation convention to all repeated indices and use a comma notation, $_{,i}$ for partial derivatives in space, x_i. We start from the balance of (total) energy with energy density ρe and the balance of (linear) momentum with momentum density ρv_i written in (fixed) Cartesian coordinates:

$$\rho \dot{e} - F_{j,j} - \rho S = \rho f_i^{\text{Lor.}} v_i^{\text{e}} \,, \quad \rho \dot{v_i} - \sigma_{ji,j} - \rho f_i = \rho f_i^{\text{Lor.}} \,, \tag{1}$$

respectively, where the flux of energy, F_i, as well as the specific supply term, S, need to be defined. The flux of momentum, σ_{ji}, is nothing else but CAUCHY's stress. The supply term of momentum, f_i, includes body forces stemming from a potential such as gravitational forces. The production of energy is given by the product between the velocity of a charged particle, v_i^{e}, and the LORENTZ force density:

$$\rho f_i^{\text{Lor.}} = \rho z E_i + \epsilon_{ijk} J_j B_k \,, \tag{2}$$

where z denotes the specific electric charge, ρ the mass density, and J_i the electric current. The motion of atomic charged particles is difficult to measure. However, the electric current, $J_i = \rho z v_i^{\text{e}}$, represents their motion in macroscopic terms. Hence, the production term for total energy becomes

$$\rho f_i^{\text{Lor.}} v_i^{\text{e}} = \big(\rho z E_i + \epsilon_{ijk} \rho z v_j^{\text{e}} B_k\big) v_i^{\text{e}} = \rho z E_i v_i^{\text{e}} = J_i E_i \,, \tag{3}$$

since $\epsilon_{ijk} = -\epsilon_{jik}$ leads to $\epsilon_{ijk} v_i^{\text{e}} v_j^{\text{e}} = 0$. The total energy is the sum of internal and kinetic energies. By multiplying the balance of momentum by v_i we obtain the balance of kinetic energy. After subtracting it from the balance of total energy we obtain the balance of internal energy:

$$\rho \dot{u} - \big(F_j - \sigma_{ji} v_i\big)_{,j} - \rho(S - f_i v_i) = J_i E_i + \sigma_{ji} v_{i,j} - \rho f_i^{\text{Lor.}} v_i \,. \tag{4}$$

The supply term of the internal energy is called the internal heating, r, and its flux term is known as the heat flux, q_i. By convention it is positive if the system gains energy. Hence:

$$-q_j = F_j - \sigma_{ji} v_i \ , \quad r = S - f_i v_i \ . \tag{5}$$

The production term can be rewritten by using $J_i = \rho z v_i + \jmath_i$ and the definition of the LORENTZ force density:

$$\begin{aligned} J_i E_i - \rho f_i^{\text{Lor.}} v_i = J_i E_i - (\rho z E_i + \epsilon_{ijk} J_j B_k) v_i = E_i (J_i - \rho z v_i) - \epsilon_{ijk} (\jmath_j + \rho z v_j) B_k v_i = \\ = E_i \jmath_i - \epsilon_{ijk} \jmath_j B_k v_i = \jmath_j (E_j + \epsilon_{jik} v_i B_k) \ . \end{aligned} \tag{6}$$

The electric current measured on the moving body, $\jmath_i$, will be defined by a constitutive equation. The electromotive intensity, $\mathfrak{E}_i = E_i + \epsilon_{ijk} v_j B_k$, allows us to rewrite the balance of internal energy as follows

$$\rho \dot{u} + q_{i,i} - \rho r = \jmath_i \mathfrak{E}_i + \sigma_{ji} v_{i,j} \ . \tag{7}$$

For an unpolarized solid body the GIBBS equation reads

$$\rho \, \mathrm{d}u = \rho T \, \mathrm{d}\eta + {}^{\mathrm{e}}\sigma_{ij} \mathrm{d}\varepsilon_{ij} \ , \tag{8}$$

where the specific entropy, η, and the elastic part of stress, ${}^{\mathrm{e}}\sigma_{ij}$, have been introduced. The stress tensor is additively separated, $\sigma_{ij} = {}^{\mathrm{e}}\sigma_{ij} + {}^{\mathrm{d}}\sigma_{ij}$, into an elastic term, ${}^{\mathrm{e}}\sigma_{ij}$, and into a dissipative term, ${}^{\mathrm{d}}\sigma_{ij}$. We use a linearized strain measure $\varepsilon_{ij} = 1/2(u_{i,j} + u_{j,i}) = u_{(i,j)}$, where u_i is the displacement field in space and time, which will be computed from the balance of momentum. Then by inserting the GIBBS equation (8) into the balance of internal energy (7) we obtain the balance of entropy:

$$\rho \dot{\eta} + \left(\frac{q_i}{T} \right)_{,i} - \rho \frac{r}{T} = \Sigma \ , \quad \Sigma = -\frac{q_i}{T^2} T_{,i} + \frac{\jmath_i}{T} \mathfrak{E}_i + \frac{{}^{\mathrm{d}}\sigma_{ji}}{T} v_{i,j} \ , \tag{9}$$

where the entropy production, Σ, has to be positive according to the 2nd law of thermodynamics, $\Sigma \geq 0$. Tensors of different rank will not depend on each other—this principle is known as the CURIE principle. For simplicity we neglect any viscous deformations in the continuum body, ${}^{\mathrm{d}}\sigma_{ij} = 0$, and propose the following relations for an isotropic material:

$$-\frac{q_i}{T^2} = \lambda T_{,i} + \gamma \mathfrak{E}_i \ , \quad \frac{\jmath_i}{T} = \beta T_{,i} + \theta \mathfrak{E}_i \ . \tag{10}$$

Since the 2nd law has to hold for any process:

$$-\frac{q_i}{T^2} T_{,i} + \frac{\jmath_i}{T} \mathfrak{E}_i \geq 0 \ , \quad \lambda T_{,i} T_{,i} + (\gamma + \beta) T_{,i} \mathfrak{E}_i + \theta \mathfrak{E}_i \mathfrak{E}_i \geq 0 \ , \tag{11}$$

we conclude that:

$$\lambda \geq 0 \ , \quad \gamma + \beta = 0 \ , \quad \theta \geq 0 \ . \tag{12}$$

The second relation is referred to as ONSAGER's relation.[1] By renaming $\kappa = \lambda T^2$, $\pi = T\beta/\varsigma$, and $\varsigma = \theta T$ we obtain

$$q_i = -\kappa T_{,i} + \varsigma \pi T \mathfrak{E}_i \ , \quad \jmath_i = \varsigma \pi T_{,i} + \varsigma \mathfrak{E}_i \ . \tag{13}$$

The constitutive equations are linear if all coefficients are constant, *viz.*, the heat conduction parameter, κ, the electrical conductivity, ς, and the thermoelectric coupling, π, are constants. For materials without thermoelectric coupling, $\pi = 0$, we obtain the well-known laws of FOURIER and OHM. In every conductor even a small temperature gradient induces an electric current—this phenomenon is called the SEEBECK effect and is used by thermocouples. The same relation also results in a heat conduction due to an electric field—this effect is named after PELTIER.

Now by introducing the specific free energy, $f = u - T\eta$, and by inserting it in the GIBBS equation we obtain:

$$\mathrm{d}f = -\eta \, \mathrm{d}T + {}^{\mathrm{e}}\sigma_{ij} v \, \mathrm{d}\varepsilon_{ij} \Rightarrow f = f(T, \varepsilon_{ij}) \ , \tag{14}$$

According to the equipresence principle the conjugated variables, η and ${}^{\mathrm{e}}\sigma_{ij}$, depend on the same set of arguments as the energy, so that they become

$$\mathrm{d}\eta = \frac{c}{T} \, \mathrm{d}T - \tilde{m}_{ij} v \, \mathrm{d}\varepsilon_{ij} \ , \quad \mathrm{d}\, {}^{\mathrm{e}}\sigma_{ij} = \tilde{m}_{ij} \, \mathrm{d}T + C_{ijkl} \, \mathrm{d}\varepsilon_{kl} \ , \tag{15}$$

[1] In the literature the ONSAGER relation is motivated by atomistic arguments. Herein we reach the same conclusion by using thermodynamics.

where we have readily used the so-called MAXWELL relations and the fact that the measurement of entropy is realized by controlling the heat pumped into the system. For a more detailed outline of these steps we refer the interested reader to [1, §5]. The specific heat capacity, c, is measured at a constant strain and the stiffness tensor, C_{ijkl}, is determined at a constant temperature. Such measurements are well-known in the literature, however, the thermal stress coefficient, $\tilde{m}_{ij}$, is difficult to determine. For a constant stress we obtain:

$$0 = \tilde{m}_{ij}\,\mathrm{d}T + C_{ijkl}\,\mathrm{d}\varepsilon_{kl} \Rightarrow \tilde{m}_{ij} = -C_{ijkl}\frac{\partial \varepsilon_{kl}}{\partial T}\bigg|_{\boldsymbol{\sigma}} = -C_{ijkl}\alpha_{kl}\ , \tag{16}$$

where the thermal expansion coefficient, α_{ij}, is known for many materials. For a linear material with constant parameters, C_{ijkl}, α_{ij}, we obtain the stress for an elastic material as well as the entropy after an integration from the stress- and entropy-free states at $\boldsymbol{\varepsilon} = 0$, $T = T_{\text{ref.}}$ to the present ones:

$$\eta = c\ln\Big(\frac{T}{T_{\text{ref.}}}\Big) + C_{ijkl}\alpha_{kl}v\varepsilon_{ij}\ ,\ \ \sigma_{ij} = {}^{\circ}\sigma_{ij} = -C_{ijkl}\alpha_{kl}(T - T_{\text{ref.}}) + C_{ijkl}\varepsilon_{kl}\ . \tag{17}$$

For the electromagnetic fields, namely the electric field, E_i, and the magnetic flux (areal) density, B_i, we declare two potentials, *viz.*, the scalar potential ϕ in V $\hat{=}$ J/C, and the vector potential A_i in Wb/m $\hat{=}$ T m $\hat{=}$ J/(A m), as follows

$$E_i = -\phi_{,i} - \frac{\partial A_i}{\partial t}\ ,\ \ B_i = \epsilon_{ijk}A_{k,j}\ . \tag{18}$$

For a conductor the scalar potential, ϕ, is calculated by satisfying the balance of (electric) charge:

$$\jmath_{i,i} = 0\ , \tag{19}$$

under the assumption that no static load occurs, $z = 0$. In other words, we assume that the number of charged particles flowing into the material from one end flow out through the other end simultaneously, such that the net charge remains zero. In order to calculate the vector potential, A_i, we use one of MAXWELL's equations:

$$-\frac{\partial D_i}{\partial t} + \epsilon_{ijk}H_{k,j} = J_i\ , \tag{20}$$

where the charge potential, D_i, and current potential, H_i, are given by the MAXWELL-LORENTZ aether relations:

$$D_i = \varepsilon_0 E_i\ ,\ \ H_i = \frac{1}{\mu_0}B_i\ ,\ \ \varepsilon_0 = 8.85\cdot 10^{-12}\,\mathrm{A\,s\,/\,(V\,m)}\ ,\ \ \mu_0 = 12.6\cdot 10^{-7}\,\mathrm{V\,s\,/\,(A\,m)}\ . \tag{21}$$

2 COMPUTATION

The objective is to compute the displacement u_i from Eq. $(1)_2$, the (absolute) temperature T from Eq. (9), and the scalar and vector potentials, ϕ and A_i, from Eqs. (19) and (20), respectively. Since we model a solid body a formulation in the LAGRANGEan configuration is more beneficial. For simplicity we approximate the deformation gradient as the identity, in other words, we allow only small deformations. Then the governing equations remain the same and the partial derivatives are in the space of initial positions of particles. For a numerical computation we generate the weak form with the following steps:

- Discretize in time by using EULER backwards finite difference method, for example $v_i = \dfrac{\partial u_i}{\partial t} = \dfrac{u_i - u_i^0}{\Delta t}$,
- Multiply the governing equations with test functions, δu_i, δT, $\delta\phi$, δA_i, and integrate over one finite element,
- Bring them to the same unit (herein we choose the unit of energy in J) and sum them up,
- Employ partial integrations in order to reduce the order in space derivatives in each term.

After applying these steps we obtain:

$$\begin{aligned}
\mathrm{F}_{\boldsymbol{u}} &= \int_\Omega \Big(\rho\frac{v_i - v_i^0}{\Delta t}\delta u_i + \sigma_{ji}\delta u_{i,j} - \rho f_i\delta u_i - \rho f_i^{\text{Lor.}}\delta u_i\Big)\,\mathrm{d}v - \int_{\partial\Omega}\sigma_{ji}\delta u_i n_j\,\mathrm{d}a\ ,\\
\mathrm{F}_T &= \int_\Omega \Big(\rho(\eta-\eta^0)\delta T - \Delta t\frac{q_i}{T}\delta T_{,i} - \Delta t\frac{\rho r}{T}\delta T + \Delta t\frac{q_i}{T^2}T_{,i}\delta T - \Delta t\frac{\jmath_i}{T}\mathfrak{E}_i\delta T - \Delta t\frac{{}^{\mathrm{d}}\sigma_{ji}}{T}v_{i,j}\delta T\Big)\,\mathrm{d}v +\\
&\quad + \int_{\partial\Omega}\Delta t\frac{q_i}{T}\delta T n_i\,\mathrm{d}a\ ,\ \ \mathrm{F}_\phi = \int_{\mathcal{B}_0}\big(-\Delta t\jmath_i\delta\phi_{,i}\big)\,\mathrm{d}V + \int_{\partial\mathcal{B}_0}\Delta t\jmath_i\delta\phi N_i\,\mathrm{d}A\ ,\\
\mathrm{F}_{\boldsymbol{A}} &= \int_\Omega\Big(-\frac{D_i - D_i^0}{\Delta t}\delta A_i - \epsilon_{ijk}H_k\delta A_{i,j} - \jmath_i\delta A_i - \rho_0 z v_i\delta A_i\Big)\,\mathrm{d}v + \int_{\partial\Omega}\epsilon_{ijk}H_k\delta A_i n_j\,\mathrm{d}a\ ,
\end{aligned} \tag{22}$$

where Form $= \mathrm{F}_{\boldsymbol{u}} + \mathrm{F}_T + \mathrm{F}_\phi + \mathrm{F}_{\boldsymbol{A}}$ is a nonlinear integral form. We choose the functional space for the *primitive* variables u_i, T, ϕ, A_i and their corresponding *test* functions δu_i, δT, $\delta\phi$, δA_i from the same SOBOLEV space as usual in the GALERKIN-type finite element method. We program and solve in Python by using the novel open-source packages developed under the FEniCS project, see [5].

Consider a wire with a rectangular cross section made of chromel (nickel-chromium alloy). This wire works as a thermocouple (type E), such that a temperature difference at its both ends is measured as a (scalar) potential difference. We clamp the wire of length $\ell = 0.1$ m at one end and increase the ambient temperature at the other end linearly in time, see the results in Figs. 1.

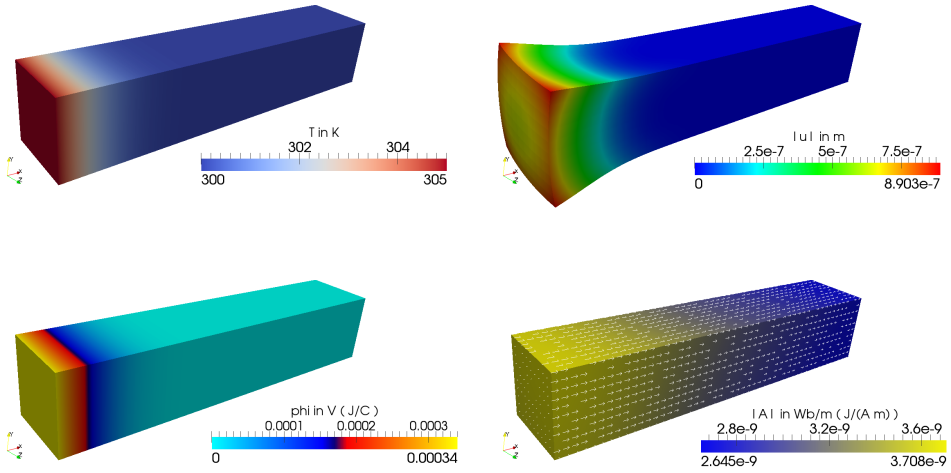

Figure 1: Distributions of primitive variables, T, u_i, ϕ, A_i, colors indicate the magnitude, the deformation is 5000 times enlarged for a better visualization.

3 CONCLUSIONS

We have presented a multiphysical phenomenon well-known from thermocouples. As a consequence of the SEEBECK effect different temperatures at both ends of a wire produce a potential difference leading to an electric current in a closed circuit. Hence, by measuring the potential difference in V we can detect the temperature. For the computation of this phenomenon all necessary constitutive equations have been derived by using thermodynamics. The weak form is solved by using the finite element method in space and the finite difference method in time. In order to encourage further studies we publish the code in [2] under GNU Public license as in [4].

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