

A note on construction of continuum mechanics and thermodynamics

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Abstract The standard way towards continuum thermodynamics based on conservation laws is discussed. Modelling of complex materials, where detailed state variables are necessary, requires insight beyond the conservation laws to determine the evolution equations for the detailed variables in a unique way. Several such approaches are discussed, including the natural configurations, SHTC equations and GENERIC.

1 Introduction

When teaching continuum mechanics, e.g. [26, 44], one typically starts with a reference configuration and a mapping to the actual configuration (inertial reference frame). The mapping expresses kinematics of mass points and, consequently, of material volumes. To obtain dynamics of material volumes, the laws of conservation of mass, linear momentum and energy are invoked. By means of the Reynolds transport theorem one obtains the integral versions of equation of continuity, balance of momentum and balance of energy of the volume situated in the actual configuration (Eulerian inertial frame). The balance of momentum contains a priori unknown surface terms, which using the Cauchy theorem, are expressed by a second-order tensor field. Balance of energy contains unknown heat flux. The balances are then localized by shrinking the material volume to infinitesimal size, which yields the

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partial differential equations (balance laws with unknown Cauchy stress and heat flux) in the Eulerian inertial frame. A General balance equation can be seen as

$$\partial_t \Phi = -\partial_i J_\Phi^i, \quad (1)$$

where J_Φ^i is the flux of quantity Φ .

Because there are some unspecified fields present in the balance equations (Cauchy stress and heat flux, and possibly others), thermodynamics is used to find suitable constitutive relations for them. Firstly, the set of state variables is declared, on which the entropy density (or free energy density) depends. Derivatives of the entropy potential (or free energy) with respect to the state variables (energy density, density, velocity, and extra state variables) are denoted as temperature, pressure, etc., using the assumption of local thermodynamic equilibrium for interpretation. This is called a Gibbs relation. Time-derivative of entropy density is then calculated by means of chain rule and, using the balances of mass, momentum and energy, it is rewritten into a form of divergence of entropy flux, while the remaining terms interpreted as the entropy production. The remaining terms contain the so far unspecified quantities and suitable constitutive relations (for instance linear force-flux relations) are sought so that entropy production be non-negative. This ensures validity of the second law of thermodynamics.

When seeking the constitutive relations, further axioms are often invoked, like objectivity or material frame indifference, Galilean invariance, Curie principle and Onsager-Casimir reciprocal relations [23]. Because the entropy is allowed to depend on some extra state variables (not only mass, momentum and energy densities), their time-derivatives are present in the formula for entropy production, and their evolution equations are thus part of the closure relations. This way a closed set of evolution equations for the state variables is obtained.

Let us refer to this last step (seeking suitable constitutive relations) as the modelling step because actual modelling and creativity is needed in that step. In the case of simple fluids (Navier-Stokes-Fourier system), there is not much freedom in the modelling, since there are no extra state variables. However, in non-equilibrium thermodynamics beyond the Classical Irreversible Thermodynamics (formulated in [26, 6]), some extra state variables (fluxes of other variables, internal variables, etc.) are typically present, and their evolution equations are to be found in the modelling step. If an extra variable is a scalar quantity, it is usually clear that the substantial derivative (including convection) expresses evolution of the variable. On the other hand, in case of tensorial variables, one has the freedom to choose any objective time-derivative (upper-or-lower-convective, Jaumann, etc.) with no theoretical lead which to choose. The conservation laws with the additional requirements above are typically not enough to fully specify the complex kinematics of tensorial state variables, and additional insight is needed. Let us make a non-exhaustive review of several possibilities.

2 Some sources of additional insight into modelling

Further insight can be gained from kinetic theory, e.g. the Grad hierarchy [19, 42] for the Boltzmann equation or the BBGKY hierarchy, results of which can be implemented into non-equilibrium thermodynamics [6, 22, 33]. In the case of dense gases, a new double hierarchy was proposed in [39].

One can also exploit the Liu procedure for generating the closure relations, [28, 27].

Additional insight can be obtained by introducing another configurations like the natural configuration [37, 24] or relaxed metric [12, 4]. In the case of natural configurations, evolution is split into plastic processes from the reference configuration to the natural configuration (irreversible) and elastic processes from the natural to the actual configuration (reversible). Dynamics of the natural configuration (pure elasticity) then provides the additional insight, namely the evolution for deformation tensor or its variant.

One can also exploit the space-time formulations of kinematics, see e.g. [25, 12], which provides additional leads for choosing time-derivatives.

Another source of additional insight is provided by the requirement that the evolution equations be symmetric hyperbolic, quasilinear first-order, dissipative and obey certain gauge invariance (w.r.t. rotations, etc.) [15, 18, 17, 14, 16, 11, 29, 38, 45]. This line of research is culminating with the Symmetric Hyperbolic Thermodynamically Compatible equations (SHTC) [36, 8, 7], a simplified version of which is

$$\partial_t \rho = -\partial_i(\rho E_{m_i}) \quad (2a)$$

$$\begin{aligned} \partial_t m_i &= -\partial_j(m_i E_{m_j}) - \rho \partial_i E_\rho - m_j \partial_i E_{m_j} - s \partial_i E_s - A^L_l \partial_i E_{A^L_l} \\ &\quad + \partial_i(A^L_l E_{A^L_l}) - \partial_l(A^L_l E_{A^L_l}) \end{aligned} \quad (2b)$$

$$\partial_t s = -\partial_i(s E_{m_i}) + \frac{E_{A^L_l}}{E_s} M_{li}^{LI} \frac{E_{A^L_l}}{E_s}, \quad (2c)$$

$$\partial_t A^L_l = -\partial_i(A^L_l E_{m_i}) + (\partial_t A^L_l - \partial_i A^L_l) E_{m_i} - M_{li}^{LI} \frac{E_{A^L_l}}{E_s}. \quad (2d)$$

These equations express evolution of density, total momentum density, entropy density (per volume) and distortion \mathbf{A} , which can be interpreted as inverse deformation gradient (at least in the absence of irreversible terms, see below). The symmetric positive definite tensor \mathbf{M} is typically considered isotropic, in which case it can be interpreted as inverse relaxation time and typically depends on the state variables $(\rho, \mathbf{m}, s, \mathbf{A})$. These evolution equations represent a set of first-order quasilinear symmetric hyperbolic equations that conserve energy, produce entropy and are Galilean invariant. Note that irreversible terms (those with the time-reversal behavior opposite to the corresponding left-hand side [32]) are present only in the equation for the distortion.

Hyperbolicity of the SHTC equations is advantageous in numerical simulations. In Fig. 1 a simple one-dimensional finite string at three subsequent time instants is shown. The numerical results were obtained using publicly available code [21] in [43].

Further insight into the modelling step can be found in geometry. For instance one can take advantage of variational principles [41, 13, 9], which yields evolution equations for the chosen state variables once a Lagrangian is specified.

Finally, another possibility is to formulate the evolution equations as Hamiltonian mechanics. For instance on the material manifold (sometimes also called reference configuration) each continuum particle is equipped with a label \mathbf{X} . The state variables are then the field of positions in an inertial frame (actual configuration) of the particles and the field of their momenta, $\mathbf{x}(\mathbf{X})$ and $\mathbf{M}(\mathbf{X})$. The canonical Poisson bracket expressing kinematics of these fields is

$$\{F, G\}^{(L)} = \int d\mathbf{X} \left(\frac{\delta F}{\delta x^i(\mathbf{X})} \frac{\delta G}{\delta M_i(\mathbf{X})} - \frac{\delta G}{\delta x^i(\mathbf{X})} \frac{\delta F}{\delta M_i(\mathbf{X})} \right), \quad (3)$$

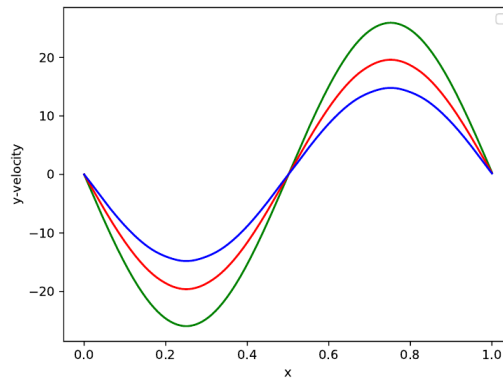
where F and G are two arbitrary functionals and subscripts stand for functional derivatives. The Hamilton canonical equations implied by this bracket are

$$\partial_t x^i(\mathbf{X}) = \frac{\delta E}{\delta M_i(\mathbf{X})}, \quad \partial_t M_i(\mathbf{X}) = -\frac{\delta E}{\delta x^i(\mathbf{X})}. \quad (4)$$

Once the energy is known, a closed set of reversible evolution equations is obtained. A transformation of the canonical Poisson bracket to the Eulerian fields $(\rho, \mathbf{m}, s, \mathbf{A})$ then leads to a non-canonical Poisson bracket for the fields, which leads to the reversible part of SHTC evolution equations (2), see [35, 34]. This Lagrange-to-Euler transformation, c.f. [5], can be used to derive boundary conditions for free surfaces [1]. The reversible part of SHTC equations is Hamiltonian.

The irreversible part of the SHTC equations, which provides dissipative algebraic terms, can be seen as a particular instance of gradient dynamics as shown in [35, 33].

Fig. 1 Vertical vibrations in an elastoplastic solid with parameters specified in [43]. The figure shows y -velocity profiles times $t = 0.00005$ (green), $t = 0.00005 + P$ (red) and $t = 0.00005 + 2P$ (blue), where $P = 1/2141$ is the period of the linearized elastic problem. Dissipation gradually diminishes the velocity.



SHTC equations are thus fully compatible with the framework of General Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC) [20, 30, 31, 33].

Yet further insight can be gained by firstly formulating the motion as an infinite-dimensional Lie group as in [3, 2, 40]. For instance, the SHTC equations then possess the structure of a semidirect product, which has further mathematical implications about hyperbolicity, gauge invariance, etc., see [34]. Finally, one can also formulate evolution equations for fluid dynamics and Grad's hierarchy in differential geometry without Lie groups [10], which leads to sort of GENERIC without Poisson brackets.

3 Conclusion

In this note, several approaches to continuum thermodynamics have been briefly recalled. It was emphasized that only balance laws are not sufficient for modeling complex materials, where extra state variables (not only density, momentum and energy density) are necessary. Indeed, their kinematics is often too complex to be derived based just on the conservation laws, entropy principle and objectivity. Several approaches that go beyond the conservation laws were then discussed. The framework of Symmetric Hyperbolic Thermodynamically Compatible equations has been recalled and illustrated on a simple numerical example. Finally, geometric techniques based on Poisson geometry and Lie groups were mentioned and the Hamiltonian origin of SHTC equations was exposed.

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