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A symbolic computation framework for constitutive modelling based on entropy principles

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ABSTRACT

The entropy principle in the formulation of Müller and Liu is a common tool used in constitutive modelling for the development of restrictions on the unknown constitutive functions describing material properties of various physical continua.

In the current work, a symbolic software implementation of the Liu algorithm, based on `Maple` software and the `GeM` package, is presented. The computational framework is used to algorithmically perform technically demanding symbolic computations related to the entropy principle, to simplify and reduce Liu identities, and ultimately to derive explicit formulas describing classes of constitutive functions that do not violate the entropy principle. Detailed physical examples are presented and discussed.

1. Introduction

Entropy principles are used in continuum mechanics in order to investigate the material behavior. For a given model, the universal balance laws, such as those for mass, momentum and energy, are commonly given by a system of partial differential equations (PDEs). The specific material behavior is defined by a *constitutive model*, through the specification of *constitutive functions* present in the system. While the set of balance equations holds for a wide class of physical settings, for example, gases, ideal and non-ideal fluids, elastic and plastic solids, etc., the constitutive functions prescribe individual material behavior. From the mathematical point of view, they provide closure conditions for the system of balance equations, so that its fields can be uniquely determined. For an overview of constitutive modelling in the context of continuum mechanics, see, e.g., Hutter and Jöhnk's extensive work [1].

The principles of constitutive modelling may vary depending on the application; they can be based on theoretical considerations, experimental data, and/or heuristic assumptions. Fundamental theoretical principles for the formulation of material models include the requirements of *material objectivity*, *material symmetry* and *thermodynamic consistency*. The first requirement determines that material behavior, and therefore the constitutive equations, must be independent of the observer, that is, Galilei-invariant. The second rule points towards the fact that the material laws must also satisfy the symmetric properties of a body, such as invariance under rotations, translations, etc.

In this work, following the ideas of Müller [2,3] and Liu [4], we focus on the third requirement, which demands that the constitutive functions are restricted in such a way that an *entropy principle* holds for all solutions of the model, thus are consistent with thermodynamics. The entropy principle is formulated in terms of an entropy inequality expressing the

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second law of thermodynamics (SL). The requirement that the entropy production inequality holds for every solution yields a set of constraints on the model's constitutive functions. Müller's approach is based on the fact that the generalized entropy inequality is linear with respect to a set of independent higher derivatives of field variables; the constraints arise as coefficients of such derivatives set to zero.

Multiple alternative approaches to constitutive modelling exist. For example, constitutive modelling approaches can also be based on the descriptions of material behavior by balance equations. For this, an additional class of fields is considered, called the *internal variables*, accounting for an internal state of the material. Such variables represent the microstructure and physical mechanisms within the body, and their evolution is described by respective balance equations. An example is given by the volume fraction (e.g., [5]), which accounts for the microstructure and the distribution of a granular material. In such approaches, the entropy principle of Müller and Liu provides an additional useful insight into the possible interdependence between those newly introduced internal variables and the general constitutive functions of a system.

Another approach used in micromechanical modelling is based on scale differences. There, microscale models are used to derive macroscale constitutive functions through the method of homogenization. This approach was employed, for example, in [6,7], to describe anistropic micropolar continua, i.e., structured solids, in the context of continuum mechanics, but without a reference to the entropy principle.

As there exist a wide range of definitions of entropy, there are also multiple entropy principles. With the *Maximum Entropy Principle*, coming from statistical mechanics, the parameter distribution for problems, in particular, in gas dynamics, can be derived. An example of an application of this principle to fluid dynamics is given in Ref. [8], while its connection with the Extended Thermodynamics for gases, established by Müller and Liu in [9], is discussed in Ref. [10]. In the context of continuum mechanics, it is important to mention the approach of Coleman and Noll [11] which provides an entropy principle based on the Clausius–Duhem inequality. Wang and Hutter [12] pointed out, however, that for mixtures, for structured continua and for polar continua like solids or liquid crystals, the entropy principle of Müller and Liu is to be favored. To the present day, the entropy principle of Müller and Liu is applied in many different fields of modelling, with applications ranging from chemical processes [13] to granular flows [14].

Liu [4] (also see [15]) systematized Müller's procedure, applying the method of Lagrange multipliers. Liu algorithm is significantly more general, and can be applied to a wide range of models, without the requirement that external supply terms be related. It can also be used for models that do not involve the physical entropy. In Section 2, we review the details of the problem of constitutive modelling based on entropy principles, and the main steps of Müller's approach and the Liu algorithm, illustrating them for a specific example of an anisotropic heat-conducting fluid.

The Liu algorithm [4] is based on the following lemma, formulated for linear algebraic equations and a linear inequality (see also [15] and [16]).

Lemma 1 (Liu). *Let $z \in \mathbb{R}^p$, and let M be a $p \times n$ real matrix. Consider a linear system $MY + z = 0$ of p equations on the components of the unknown vector $Y \in \mathbb{R}^n$, with a non-empty solution set S. Let also $\mu \in \mathbb{R}^n$, $\mu \neq 0$, and $\zeta \in \mathbb{R}$ be given. Then the following statements are equivalent:*

1. $\forall Y \in S$, $\mu^T Y + \zeta \geq 0$;
2. $\exists \lambda \in \mathbb{R}^p$ *such that* $\forall Y \in \mathbb{R}^n$, $\mu^T Y + \zeta - \lambda^T (MY + z) \geq 0$;
3. $\exists \lambda \in \mathbb{R}^p$ *such that* $\mu = M^T \lambda$, *and* $\zeta \geq \lambda^T z$.

As pointed out in [16], Lemma 1 is related to the fundamental inequality lemma of Farkas and Minkowski. The latter plays a key role in linear programming, and is in turn related to the general Hahn–Banach separation theorem.

Lemma 1 has a flavor different from the Lagrange multiplier approach to constrained optimization of nonlinear functions. In particular, both the equations and the inequality in the problem are linear. Moreover, the geometrical meaning of the Lemma can be understood as follows: since the inequality $F = \mu^T Y + \zeta \geq 0$ must hold for *all* points Y in the set defined by $MY + z = 0$, that set (a line, a hyperplane, etc.) must be, in a certain sense, *parallel* to isosurfaces $F = \text{const}$.

The technical computations related to the execution of the Müller–Liu procedure can be time consuming, and equations that arise tend to be quite lengthy. While simplest examples can be carried out within minutes by an experienced researcher, generally, the derivation of constraints on the constitutive functions can become error-prone, especially for complicated settings, such as mixture models involving multiple phases and internal variables, governed by additional balance equations, and/or having complex material behavior. One of the goals of the current paper is the application of modern symbolic software to facilitate computations related to the Liu algorithm, in particular, lengthy chain rule differentiations, computation of coefficients at higher-order derivatives, and efficient reduction and solution of overdetermined systems of partial differential equations for the unknown constitutive functions. The computations are based on a symbolic package `GeM` for `Maple`, developed in [17–19] for symmetry and conservation law computations. Significant similarities between the nature of those problems and the algorithm of Liu, and the capabilities of `GeM` software to efficiently handle linear and nonlinear PDEs, partial derivatives of field variables, and constitutive functions that may involve derivatives, make `Maple` and `GeM` a natural computational platform choice. It should be noted that this kind of treatment can be transferred to other applications in the context of constitutive modeling, for example to the aforementioned entropy principle of Coleman and Noll.