

RESEARCH ARTICLE

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Symmetry analysis and equivalence transformations for the construction and reduction of constitutive models

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Abstract

A methodology based on Lie analysis is proposed to investigate the mechanical behavior of materials exhibiting experimental master curves. It is based on the idea that the mechanical response of materials is associated with hidden symmetries reflected in the form of the energy functional and the dissipation potential leading to constitutive laws written in the framework of the thermodynamics of irreversible processes. In constitutive modeling, symmetry analysis lets one formulate the response of a material in terms of so-called master curves, and construct rheological models based on a limited number of measurements. The application of symmetry methods leads to model reduction in a double sense: in treating large amounts number of measurements data to reduce them in a form exploitable for the construction of constitutive models, and by exploiting equivalence transformations extending point symmetries to efficiently reduce the number of significant parameters, and thus the computational cost of solving boundary value problems (BVPs). The symmetry framework and related conservation law analysis provide invariance properties of the constitutive models, allowing to predict the influence of a variation of the model parameters on the material response or on the solution of BVPs posed over spatial domains. The first part of the paper is devoted to the presentation of the general methodology proposed in this contribution. Examples of construction of rheological models based on experimental data are given for setting up a reduced model of the uniaxial creep and rupture behaviour of a Chrome-Molybdenum alloy (9Cr1Mo) at different temperatures and stress levels. Constitutive equations for creep and rupture master responses are identified for this alloy, and validated based on experimental data. Equivalence transformations are exemplified in the context of parameter reduction in fully nonlinear anisotropic fiber-reinforced elastic solids.

Keywords: Experimental data, Symmetry and similarity methods, Constitutive modeling, Master Curves, Equivalence transformations, Creep and rupture invariants, Time-temperature equivalence, model reduction

Introduction

The notion of symmetry is a fundamental scientific concept present in many disciplines, from biology to mathematics and theoretical physics. Independently from its aesthetic

attraction, the symmetry intrinsically contained in physical systems allows to concisely describe their invariance properties, classify and synthesize their mathematical structure and physical properties, and systematically derive exact solutions. Invariance properties of physical systems described by algebraic or differential equations emerge from these symmetries, including scale transformations, time, parity and charge inversions, gauge symmetries, dynamical symmetries, nonlocal symmetries.

Generalizing the discrete symmetry classification of crystals ([1–3]), the notion of continuous symmetries, in particular, Lie groups of point symmetries introduced by Sophus Lie (e.g., [4]), with multiple further generalizations (e.g., [5,6] and references therein). Noether [7] provided a connection between conservation laws (energy, momentum, etc.) and local symmetries for models arising from a variational principle (see, e.g., [5,6]). The majority of field theories built in the twentieth century heavily rely on Lie symmetries, which are reflected in the form taken by the Lagrangian function [8]. In continuum mechanics, symmetries play a major role in the construction of the constitutive laws of materials, formulated from tensor valued functionals, objective (invariance of the material's response under the group of rotations in the three dimensional Euclidean space) and invariant under the action of the material symmetry group (discrete symmetries) [9,10]. The thermodynamics of irreversible processes (abbreviated as TIP in the sequel) is the natural framework for writing rheological models of dissipative and non dissipative materials, relying on thermodynamic potentials - namely the free energy and a dissipation or pseudo-dissipation potential. These potentials have to reflect the symmetry properties of the material being analyzed. Thereby, our approach relies on the postulate that the mechanical response of materials is associated with hidden symmetries, and our objective is precisely to reveal those symmetries from a set of measurements, and to write appropriate constitutive laws from them.

The consideration of Lie symmetries and equivalence transformations in the mechanics of materials is an emergent topic in the literature [11]. Recent works from the literature underline the interest of using Lie symmetries to obtain invariance properties of materials relying on experimental data; furthermore, Lie symmetries is a predictive methodology to predict the response of materials when the parameters inherent to their constitutive law change.

Invariance relations, together with master curves that constitute their graphical representation, are currently used in experimental rheology to synthesize the constitutive response of various materials subject to thermomechanical loadings. A typical example of such an empirical construction is the well-known time-temperature equivalence principle, stating an equivalence between the effect of time and of temperature, as proposed originally by Williams, Landel and Ferry in the so-called WLF model. In the same spirit, power laws in fatigue have been formulated in [12,13] (also [14] and references therein), using arguments of dimensional analysis in combination with similarity principles. These relationships are of a high practical interest, and it the aim of this contribution to highlight Lie symmetries and equivalence transformations as the underlying mathematical background.

From the point of view of solutions of the mechanical problem formulated in terms of differential equations, a symmetry is any transformation preserving the solution set, i.e., mapping solutions into solutions. In particular, solutions that are mapped into themselves, called the invariant solutions, can be algorithmically computed, and often have a clear

physical meaning. This includes, for example, traveling waves and self-similar (scaling-invariant) solutions. While the full set of symmetries admitted by a model is a rather general geometrical object, Lie groups of point symmetries can be calculated using the local form of these symmetries, in terms of symmetry generators [5,6]. From a geometrical point of view, finding the symmetries of a given BVP allows to define a surface in the extended space of variables and parameters (when considering equivalence transformations), on which the solution is living.

The majority of contemporary mathematical models, in particular, physical models written in terms of partial or ordinary differential equations (PDEs, ODEs), involve constant or variable parameters. These parameters, also called arbitrary or constitutive elements, appear in the equations in the form of arbitrary constants (*constitutive parameters*) that assume values in certain ranges, and/or arbitrary functions (*constitutive functions*) belonging to certain classes. Equivalent formulations of a model at hand, involving fewer constitutive parameters and/or reduced forms of constitutive functions, can lead to a significant simplification of the analysis of the model, in particular, when such analysis involves classifications, such as local symmetry or conservation law classifications. Equivalent formulations of a class of models may be systematically sought using *equivalence transformations* [15,16]. Equivalence transformations are used to simplify classifications of mathematical models, relate models with seemingly different forms of constitutive functions and/or parameters, and simplify families of models by reducing the forms and number of such constitutive functions and/or parameters.

Lie symmetries, equivalence transformations, conservation laws, and other related analytical properties of nonlinear equations (cf. [6]) can be efficiently computed and classified using symbolic software, for example, the GeM package for Maple [17–19]. In particular, GeM can be used for systematic computation of equivalence transformations [16].

Another approach in constitutive modeling that is related to symmetry ideas, both philosophically and mathematically, is the use of entropy principles to predict and reduce the dependencies of constitutive functions. The approach consists in requiring that the admissible processes correspond to nonnegative entropy production, and yields constraints on the general postulated forms of constitutive functions. This constitutive modeling idea has been introduced pioneered by Ingo Müller's [20–24], and subsequently modified by Liu [25]; the result was called the Müller-Liu procedure. In the recent work [26,27], the entropy principle methodology was reformulated in terms of the solution set of the model equations, and a systematic procedure was suggested to use leading derivatives to compute constitutive function constraints; the approach was implemented in Maple symbolic software using the capabilities of the GeM package [27].

Recall that two main classes of approaches combining Lie symmetry methods and constitutive modeling have arisen in the literature, which will be referred to as the *direct* and the *inverse problem* or *method*, in the vocabulary used in [28]. The direct problem consists in finding Lie symmetries of a given set of constitutive equations, as developed by several authors in the field of mechanics of materials (see, e.g., [29,30]). It allows *a priori* the calculation of all symmetries and associated invariances of those equations, which may lead to geometrical transformation rules revealing (graphical) superpositions of the material responses (the superposition of those responses in a given space of variables gives the master curve). The methodology at the root of this construction consists of three main steps, which entail an algorithm for the determination of the constitutive law and

master curves. In the first step, one looks for one or several Lie symmetries formulated from experimental master curves. Next, the subsequent symmetry conditions are applied to a general expression of the constitutive equations involving some unknown functions, resulting in a PDE system satisfied by these unknown functions. The comparison of the constructed constitutive model with experimental results allows to validate or refine the model if needed. As a last step, the inverse problem is linked to the direct problem: once a possible material constitutive law has been constructed, the material's response can be predicted outside the range of variation of the control variables involved in the measurements for varying experimental conditions, hence using Lie symmetries inherent to the obtained constitutive law as an extrapolation technique. Thereby, Lie symmetries leads to reduced constitutive models based on invariants having a true physical meaning, allowing to efficiently predict the response of materials with a complex rheological behavior when parameters change.

The paper is organized as follows. Section 2 describes in a synthetic manner the methodology of the application of Lie groups of symmetries to construct and simplify constitutive models. Section 3 presents an example of a computation of master curves and invariant constitutive equations modeling the creep and rupture behavior of metallic alloys. In Section 4, invariance relations and master responses associated to a rheological model are discussed. An example of the computation of equivalence transformations and parameter reduction in a model of nonlinear S-waves propagating in a hyperelastic fiber-reinforced material is presented in Section 5. The paper is concluded with a discussion in Section 6.

Methodology

For physical continuum systems, in particular, ones involving the mechanics of solids and fluids, the governing balance/evolution equations, as well as constitutive/rheological models, are commonly described by a set of algebraic and/or differential equations (ordinary, ODE, or partial, PDE). Symmetry ideas provide insights and rational methodologies to describe and study such models, revealing their intrinsic structure. For an experimental data set, the use of Lie group ideas is therefore not a simple interpolation of data, since the constitutive laws that can be constructed from a set of data based on a postulated Lie group structure allow both to interpolate within the data set and to extrapolate beyond the experimental parameter domains used to build the constitutive model.

The use of Lie groups in combination with experimentally recorded responses of a given material to formulate its constitutive law has been initiated in [11] and [31] (see also [26,27]). The aim of this contribution is to provide an overview of the Lie symmetry method in constitutive modeling. The generalized methodology proposed in this contribution is organized into the following steps:

- Formulation of Lie symmetries from measurements;
- Formulation of constitutive equations in terms of invariants;
- Computation of the Lie algebra and predictions of the material response for a range of variation of the parameters;
- Computation of equivalence transformations of constitutive models;
- Model simplification based on its admitted equivalence transformations.

In subsequent developments, the above methodology is used to construct constitutive models describing the creep and rupture behavior of metallic alloys, both phenomena being highly stress- and temperature-dependent. In order to set the stage, we provide the non specialist with a comprehensive and synthetic overview of Lie symmetries, that will prove useful in subsequent developments.

Lie symmetries: a basic summary

Suppose a mathematical model formulated as a system of ordinary and/or partial differential equations \mathcal{R}

$$R^\sigma(\mathbf{x}, \mathbf{u}) = 0, \quad \sigma = 1, \dots, N, \tag{2.1}$$

of differential order $k \geq 1$, with $s \geq 1$ independent variables $\mathbf{x} = (x_1, \dots, x_s)$ and $n \geq 1$ dependent variables $\mathbf{u}(\mathbf{x}) = (u_1(\mathbf{x}), \dots, u_n(\mathbf{x}))$. For brevity, we will denote any derivatives of dependent variables $\mathbf{u}(\mathbf{x})$ by subscript symbols

$$\frac{\partial^p u_\nu(\mathbf{x})}{\partial x_{i_1} \dots \partial x_{i_p}} \equiv (u_\nu)_{i_1 \dots i_p}.$$

For the independent and dependent variables $\mathbf{x}, \mathbf{u}(\mathbf{x})$, one can consider the *jet space* $J^q(\mathbf{x}|\mathbf{u})$: a multi-dimensional space of variables \mathbf{x}, \mathbf{u} , and all derivatives of \mathbf{u} up to and including the order $q \geq k$. Then the DEs (2.1) (and possibly their differential consequences), treated as algebraic equations in $J^q(\mathbf{x}|\mathbf{u})$, define a manifold \mathcal{S} in that space. This is the *solution manifold* of the system (2.1); indeed, any solution of (2.1) $\mathbf{u}(\mathbf{x})$ and its derivatives, for all admissible x , define a point on \mathcal{S} .

Lie groups of point transformations provide a mathematically sound tool to deform the solution manifold \mathcal{S} of a given DE system to map its solutions to solutions of some other model; Lie point transformations preserving \mathcal{S} yield *Lie point symmetries* of a given system (2.1). The admissible symmetry groups contain coordinate-independent, geometrical information about the solution set of a given model, enabling one to systematically construct exact invariant solutions and conservation laws, map known solutions and conservation laws to new ones, etc. (see, e.g., [6] for more details). vast literature is available on the topic, ranging from introductory and practically-oriented textbooks to more mathematically advanced and specialized (see, e.g., [5,6,32] and references therein). We now summarize the basic points required for the subsequent presentation.

A Lie group of point symmetries of a DE system (2.1) is a group of transformations of dependent and independent variables

$$\begin{aligned} \tilde{x}_i &= f_i(\mathbf{x}, \mathbf{u}; \mu) = x_i + \mu \xi^i(\mathbf{x}, \mathbf{u}) + O(\mu^2), \quad i = 1, \dots, s, \\ \tilde{u}_\nu &= g_\nu(\mathbf{x}, \mathbf{u}; \mu) = u_\nu + \mu \eta^\nu(\mathbf{x}, \mathbf{u}) + O(\mu^2), \quad \nu = 1, \dots, n, \end{aligned} \tag{2.2}$$

additive in the continuous parameter μ , with the property that if (2.1) is a solution of $\mathbf{u}(\mathbf{x})$, then so is the transformed function $\tilde{\mathbf{u}}(\tilde{\mathbf{x}})$. For example, the scaling transformation

$$\begin{aligned} \tilde{x} &= e^\mu x = x + \mu x + O(\mu^2), \\ \tilde{t} &= e^{2\mu} t = t + 2\mu t + O(\mu^2), \\ \tilde{u} &= u \end{aligned} \tag{2.3}$$

leaves invariant the diffusion equation $u_t = u_{xx}$, and maps its every solution $u = f(x, t)$ into a new solution $\tilde{u} = f(e^{-\mu} \tilde{x}, e^{-2\mu} \tilde{t})$, or removing bars and changing the sign of the parameter, simply into a solution $u_1(x, t) = f(e^\mu x, e^{2\mu} t)$ with re-scaled space and time dependence.

To every one-parameter Lie group of point transformations (2.2) there corresponds a unique infinitesimal generator (also known as the tangent vector field to the solution manifold of the system in the (\mathbf{x}, \mathbf{u}) -space), given by

$$\mathbf{v} = \xi^i \frac{\partial}{\partial x_i} + \eta^v \frac{\partial}{\partial u_v} \tag{2.4}$$

(here and below, summation in repeated indices is assumed). For example, for the scaling transformation (2.3), one has

$$\mathbf{v} = x \frac{\partial}{\partial x} + 2t \frac{\partial}{\partial t} + 0 \cdot \frac{\partial}{\partial u}. \tag{2.5}$$

The local generator (2.4), in turn, uniquely determines the global transformation (2.2), through the solution of an ODE system initial-value problem

$$\begin{aligned} \frac{d\tilde{x}_i}{d\mu} &= \xi^i(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}), & \tilde{x}_i|_{\mu=0} &= x_i, & i &= 1, \dots, s, \\ \frac{d\tilde{u}_v}{d\mu} &= \eta^v(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}), & \tilde{u}_v|_{\mu=0} &= u_v, & v &= 1, \dots, n, \end{aligned} \tag{2.6}$$

or briefly in the operator exponent notation,

$$\tilde{x}_i = e^{\mu v} x_i, \quad \tilde{u}_v = e^{\mu v} u_v.$$

A one-parameter Lie group of point transformations (2.2) induces one-parameter Lie groups of point transformations acting on the derivatives of $\mathbf{u}(\mathbf{x})$ in the jet space $J^q(\mathbf{x}|\mathbf{u})$, as follows:

$$(\tilde{u}_v)_i = u_i^v + \mu \eta_i^{(1)v} + O(\mu^2), \tag{2.7a}$$

⋮

$$(\tilde{u}_v)_{i_1 \dots i_q} = (u_v)_{i_1 \dots i_q} + \mu \eta_{i_1 \dots i_q}^{(q)v} + O(\mu^2); \tag{2.7b}$$

here the extended infinitesimals given by

$$\begin{aligned} \eta_i^{(1)v} &= D_i \eta^v - (D_i \xi^j) u_j^v, \\ \eta_{i_1 \dots i_k}^{(k)v} &= D_{i_k} \eta_{i_1 \dots i_{k-1}}^{(k-1)v} - (D_{i_k} \xi^j) u_{i_1 \dots i_{k-1} j}^\mu \end{aligned} \tag{2.8}$$

with $v = 1, \dots, n, i, i_j = 1, \dots, s$ for $j = 1, \dots, k$ with $k = 2, 3, \dots, q$. The q^{th} prolongation of the transformation generator (2.4) is given by

$$\mathbf{v}^{(q)} = \xi^i \frac{\partial}{\partial x_i} + \eta^v \frac{\partial}{\partial u_v} + \eta_i^{(1)v} \frac{\partial}{\partial u_i^v} + \dots + \eta_{i_1 \dots i_q}^{(q)v} \frac{\partial}{\partial (u_v)_{i_1 \dots i_q}}. \tag{2.9}$$

The main mathematical tool used to systematically seek Lie groups of point transformations (2.2) that are symmetries of a DE system (2.1) is the infinitesimal invariance condition

$$\mathbf{v}^{(k)} R^\alpha(x, u, \partial u, \dots, \partial^k u) = 0 \tag{2.10}$$

holding on all solutions of (2.1). The invariance condition expresses the fact that the mapping generated by the transformation is locally tangent to the solution set of the DE system (2.1), and upon splitting, yields a set of linear determining PDEs that define the unknown symmetry components ξ^i, η^v of admissible symmetry generators (2.4) (e.g., [5,6]). The substitution of solution space conditions and splitting of the determining equations can often be efficiently accomplished in symbolic software, such as the GeM package for Maple [17–19].

Another important notion related to Lie symmetries of differential equations, or more generally, to Lie group of point transformations, is that of an invariant, or a differential invariant. A function $F(\mathbf{x}, \mathbf{u})$ is called invariant under the group of transformations (2.2) when

$$F(\bar{\mathbf{x}}, \bar{\mathbf{u}}) = F(\mathbf{x}, \mathbf{u}).$$

Locally, the invariance condition is given by the vanishing action of the transformation generator (2.4), as a differential operator, on F :

$$\mathbf{v} F(\mathbf{x}, \mathbf{u}) = 0.$$

One of the simplest methods to find invariants of a given one-parameter Lie group of transformations (2.2) is through the solution of the characteristic system

$$\frac{dx_1}{\xi^1} = \dots = \frac{dx_s}{\xi^s} = \frac{du_1}{\eta^1} = \dots = \frac{du_n}{\eta^n},$$

yielding a solution that can be written in the form

$$I^1(\mathbf{x}, \mathbf{u}) = c_1, \dots, I^{n+s-1}(\mathbf{x}, \mathbf{u}) = c_{n+s-1}, \tag{2.11}$$

where c_i are arbitrary integration constants, and I^i are $n + s - 1$ functionally independent functions that do not involve any free integration constants. The functions $\{I^i\}$ are the elementary transformation invariants; more general invariants can be obtained as arbitrary functions of $\{I^i\}$.

Seeking invariants (2.11) forms an essential part of the procedure of seeking canonical coordinates that are used to produce symmetry-reduced versions of physical models (e.g., [5,6]).

In a fashion similar to that for invariant functions, *differential invariants* of the group of transformations (2.2) $F[\mathbf{u}]$, differential functions that may depend on \mathbf{x}, \mathbf{u} , and derivatives of \mathbf{u} to some order k , satisfy the invariance condition

$$\mathbf{v}^{(k)} F[\mathbf{u}] = 0.$$

As an example, the scaling transformation (2.3) has invariants arising from solving the system

$$\frac{dx}{x} = \frac{dt}{2t} = \frac{du}{0},$$

for example, $I^1 = x/\sqrt{t}, I^2 = u$, which allows one to seek symmetry-invariant solutions of the diffusion equation in the form $u(x, t) = f(x/\sqrt{t})$. Differential invariants corresponding to the scaling transformation (2.3) include $x^2 u_t, u_t/u_{xx}, u_{tt}/u_{xxxx}$, etc.

Equivalence transformations and their computation

In many cases, it is important to consider a class of mathematical models consisting of governing dynamic equations and constitutive relations as a whole. Such models are often given by systems of ordinary and/or partial differential equations, and/or algebraic equations, forming a family \mathcal{R}_p

$$R^\sigma(\mathbf{x}, \mathbf{u}, \mathbf{p}) = 0, \quad \sigma = 1, \dots, N, \tag{2.12}$$

involving s independent variables $\mathbf{x} = (x_1, \dots, x_s)$, n dependent variables $\mathbf{u}(\mathbf{x}) = (u_1(\mathbf{x}), \dots, u_n(\mathbf{x}))$, and m arbitrary elements (constitutive functions and/or parameters)

$\mathbf{p} = (p_1, \dots, p_m)$. The expressions R^σ in (2.12) may involve derivatives of \mathbf{u} and functions within \mathbf{p} as necessary.

An *equivalence transformation* for a DE family $\mathcal{R}_{\mathbf{p}}$ is commonly defined as a change of variables and arbitrary elements

$$(\mathbf{x}, \mathbf{u}, \mathbf{p}) \rightarrow (\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{p}}) \tag{2.13}$$

that maps every system of equations (2.12) into a system of equations in the same family $\mathcal{R}_{\mathbf{p}}$ (see, e.g., [6, 16] and references therein).

Generally, no systematic procedure exists to compute explicit formulas of the transformations (2.13). However, equivalence transformations that form Lie groups, such as point equivalence transformations

$$\begin{aligned} \tilde{x}_i &= f_i(\mathbf{x}, \mathbf{u}; \mu) = x_i + \mu \xi^i(\mathbf{x}, \mathbf{u}) + O(\mu^2), \quad i = 1, \dots, s, \\ \tilde{u}_v &= g_v(\mathbf{x}, \mathbf{u}; \mu) = u_v + \mu \eta^v(\mathbf{x}, \mathbf{u}) + O(\mu^2), \quad v = 1, \dots, n, \\ \tilde{p}_\lambda &= G_\lambda(\mathbf{Q}_\lambda; \mu) = p_\lambda + \mu \theta^\lambda(\mathbf{Q}_\lambda) + O(\mu^2), \quad \lambda = 1, \dots, m, \end{aligned} \tag{2.14}$$

can be computed systematically, and therefore are commonly used in practice [15, 16, 33]. In (2.14), the form of the argument \mathbf{Q}_λ of the transformation G_λ and the tangent vector field component θ^λ depends on the nature of the arbitrary element p_λ , $\lambda = 1, \dots, m$. For example, if p_ℓ is a constitutive parameter, \mathbf{Q}_λ may be a set of constitutive parameters of the model; if p_λ is a constitutive function, then \mathbf{Q}_λ may involve quantities that p_λ depends on, and/or other constitutive functions with compatible dependencies. In the above definition, the transformations form a group on the (\mathbf{x}, \mathbf{u}) space; in particular, the transformations for \mathbf{x}, \mathbf{u} do not involve arbitrary elements. The infinitesimal generator for (2.14) takes the form

$$\mathbf{v} = \xi^i \frac{\partial}{\partial x_i} + \eta^v \frac{\partial}{\partial u_v} + \theta^\lambda \frac{\partial}{\partial p_\lambda}. \tag{2.15}$$

Lie groups of equivalence transformations (2.14) are closely related to Lie groups (2.2) of point symmetries mapping the model equations (2.12) into themselves, without change of the parameters [5, 6].

As an elementary example of equivalence transformations (2.14), one can consider the non-dimensionalization of (1+1)-dimensional linear wave equation

$$u_{tt} = c^2 u_{xx}, \quad c = \text{const}, \tag{2.16}$$

for the unknown $u(x, t)$. It is evident that the PDE family (2.16) clearly admits scaling and translation-type equivalence transformations

$$\tilde{x} = A_3 x + A_1, \quad \tilde{t} = A_4 t + A_2, \quad \tilde{u}(\tilde{x}, \tilde{t}) = A_5 u(x, t), \quad \tilde{c} = \frac{A_3}{A_4} c, \tag{2.17}$$

where A_1, \dots, A_5 are arbitrary nonzero constants. Indeed, if $u(x, t)$ is a solution of the PDE (2.16) with a constitutive parameter c , then $\tilde{u}(\tilde{x}, \tilde{t})$ is a solution of a PDE

$$\tilde{u}_{\tilde{t}\tilde{t}} = \tilde{c}^2 \tilde{u}_{\tilde{x}\tilde{x}}, \tag{2.18}$$

a member of the family (2.16) with a different constitutive parameter, \tilde{c} . In particular, if $A_3 = L$ and $A_5 = u_0$ are the characteristic size and wave amplitude, then one can choose $A_4 = A_3 c$ as the characteristic time of the model, and the PDE (2.18) will become

$$\tilde{u}_{\tilde{t}\tilde{t}} = \tilde{u}_{\tilde{x}\tilde{x}},$$

that is, dimensionless, and involving no parameters. This is the basic idea of parameter reduction; similarly, when constitutive functions are involved, their forms may be simplified using equivalence transformations. We note that in the form of Lie groups, the transformations (2.17) include five one-parameter groups of equivalence transformations

$$x^* = e^{\mu_3}x + \mu_1, \quad t^* = e^{\mu_4}t + \mu_2, \quad u^*(x^*, t^*) = e^{\mu_5}u(x, t), \quad c^*(u^*) = e^{\mu_3 - \mu_4}c(u), \tag{2.19}$$

with group parameters $\mu_i, i = 1, \dots, 5$, and infinitesimal generators

$$v_1 = \frac{\partial}{\partial x}, \quad v_2 = \frac{\partial}{\partial t}, \quad v_3 = x \frac{\partial}{\partial x} + c \frac{\partial}{\partial c}, \quad v_4 = t \frac{\partial}{\partial t} - c \frac{\partial}{\partial c}, \quad v_5 = u \frac{\partial}{\partial u}. \tag{2.20}$$

Various extensions of the notion of equivalence transformations (2.14) exist (see, e.g., [16] for a brief review). A natural extension arises when the transformation components for the independent and/or dependent variables ξ^i, η^v are allowed to additionally depend on arbitrary elements:

$$v = \xi^i(x, u, p) \frac{\partial}{\partial x_i} + \eta^v(x, u, p) \frac{\partial}{\partial u_v} + \theta^\lambda(x, u, p) \frac{\partial}{\partial p_\lambda}. \tag{2.21}$$

These are referred to as groups of *generalized equivalence transformations* [15,34,35].

Lie groups of generalized equivalence transformations for a family of models \mathcal{R}_p (2.12) can be constructed in the following manner. (Here for simplicity we assume that if the set p involves arbitrary functions, these functions do not depend on derivatives of u .)

1. Replace the constitutive functions and/or parameters p by new dependent variables $(p_1(x), \dots, p_m(x))$. Thus consider a new model given by a system of equations $\tilde{\mathcal{R}}$ with $n + m$ dependent variables and no arbitrary elements.
2. Seek point symmetries of $\tilde{\mathcal{R}}$, with infinitesimal generators (2.21). Obtain the split system of determining equations for the unknown symmetry generator components $\xi^i(x, u, p), \eta^v(x, u, p), \theta^\lambda(x, u, p)$.
3. If the arbitrary elements p of the original model (2.12) contained arbitrary functions, introduce restrictions of the form

$$\frac{\partial \xi^i(x, u, p)}{\partial p_\gamma} = 0, \quad \frac{\partial \eta^v(x, u, p)}{\partial p_\delta} = 0, \quad \frac{\partial \theta^\lambda(x, u, p)}{\partial x_j} = 0, \tag{2.22}$$

etc., as appropriate, to exclude the dependence of transformation components of the arbitrary elements on variables they do not depend on, as well as the dependence of transformation components of the variables of the system on inappropriate arbitrary elements. For example, for the DE family (2.16), the infinitesimal generator of the generalized equivalence transformations has the form

$$v = \xi(x, t, u, c) \frac{\partial}{\partial x} + \tau(x, t, u, c) \frac{\partial}{\partial t} + \eta(x, t, u, c) \frac{\partial}{\partial u} + \theta(x, t, u, c) \frac{\partial}{\partial c}, \tag{2.23}$$

and since $c = \text{const}$, the transformation for c must not explicitly depend on the variables x, t, u . Therefore the restrictions on the component θ are given by

$$\frac{\partial \theta(x, t, u, c)}{\partial x} = \frac{\partial \theta(x, t, u, c)}{\partial t} = 0 = \frac{\partial \theta(x, t, u, c)}{\partial u} = 0. \tag{2.24}$$

4. In order to simplify computations, additional restrictions can be introduced at this stage, for example,

$$\frac{\partial \xi^i(x, u, K)}{\partial p_\gamma} = 0, \quad i = 1, \dots, s, \quad \gamma = 1, \dots, m, \tag{2.25}$$

if the transformations for the independent variables are assumed to be independent of the arbitrary elements.

5. Append all restrictions, in the form of linear PDEs, to the split system of determining equations.
6. Simplify and solve the augmented split system of determining equations, to find the infinitesimal generators \mathbf{v} (2.15) of the generalized equivalence transformations.
7. Integrate to obtain the global group (2.14) of generalized equivalence transformations

$$\begin{aligned}\tilde{x}_i &= f_i(\mathbf{x}, \mathbf{u}, \mathbf{p}; \mu), \quad i = 1, \dots, s, \\ \tilde{u}_\mu &= g_\mu(\mathbf{x}, \mathbf{u}, \mathbf{p}; \mu), \quad \mu = 1, \dots, n, \\ \tilde{p}_\ell &= G_\ell(\mathbf{x}, \mathbf{u}, \mathbf{p}; \mu), \quad \ell = 1, \dots, m.\end{aligned}\tag{2.26}$$

Specifically, for each infinitesimal generator (2.15), the corresponding one-parameter Lie group of equivalence transformations is found through the solution of the initial-value problem

$$\begin{aligned}\frac{d}{d\mu}\tilde{x}_i &= \xi^i(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{p}}), \quad \tilde{x}_i|_{\mu=0} = x_i, \quad i = 1, \dots, s, \\ \frac{d}{d\mu}\tilde{u}_\nu &= \eta^\nu(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{p}}), \quad \tilde{u}_\nu|_{\mu=0} = u_\nu, \quad \nu = 1, \dots, n, \\ \frac{d}{d\mu}\tilde{p}_\lambda &= \theta^\lambda(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}, \tilde{\mathbf{p}}), \quad \tilde{p}_\lambda|_{\mu=0} = p_\lambda, \quad \lambda = 1, \dots, m.\end{aligned}\tag{2.27}$$

where μ is the group parameter.

After the equivalence transformation (2.26) have been found, they can be used to observe which forms of the arbitrary elements (constitutive functions and/or parameters) \mathbf{p} can be related to other sets of arbitrary elements $\tilde{\mathbf{p}}$; such sets of related arbitrary elements can be treated as one for all solution and classification purposes. In particular, the set $\tilde{\mathbf{p}}$ can be chosen to eliminate or simplify the arbitrary element set \mathbf{p} ; as a result, one may need to deal with a simpler model (e.g., a simpler PDE boundary value problem) than the originally posed one.

The above procedure is readily generalized to the cases when the given model involves arbitrary functions and their derivatives, and/or arbitrary functions that depend on more complex combinations of independent and dependent variables and/or derivatives of dependent variables of the model. The latter, for example, is a common case for the stored mechanical energy density function in hyperelasticity theory.

The construction of invariance relations is illustrated in the next section to construct constitutive models for the creep and rupture behavior of metallic alloys. An example of a computation of equivalence transformations for a family of nonlinear wave equations, and the resulting significant simplification of the model using parameter reduction, is presented in Section 5 below.

Invariance relations for the creep and rupture behavior of metallic alloys

One important field in which invariant relations are used is the high temperature creep of metallic alloys, devoted to industrial applications. Landmarks in this context are the Larson-Miller and the Dorn models (see e.g. [36] and the references therein). Those relations intrinsically have the meaning of invariants, and further allow to extrapolate experimental data at different temperatures, assuming that the microstructure of the material remains stable during the creep test. The two main objectives of this kind of

investigation are either the determination of the time needed to reach a given strain for fixed stress and temperature, or the estimation of the time leading to rupture, in the same controlled conditions. In principle, both problems, although interrelated (viscoplasticity is coupled to damage), are treated separately, namely a creep problem, and damage leading to rupture. We consider in the present study the creep behaviour of the 9Cr1Mo martensitic stainless steel, which is also known for its good thermal-fatigue strength and oxydation resistance ([37]).

According to experts in the field, one of the most crucial problem in determining the integrity of structural components is the creep behaviour of ferritic-martensitic steels used in supercritical plants at high temperature due to their reduced cost, lower thermal expansion coefficient, and better radiation stability combined with adequate corrosion resistance (see [38] and the references therein) [39]. We approach the creep and rupture behavior from a phenomenological standpoint, with the objective to construct constitutive laws for the creep and rupture of metallic alloys, relying on a combination of experimental data and symmetry analysis. We shall rely on experimental data of [40], obtained for the 9Cr1Mo alloy, when submitted to creep tests carried out at different constant temperatures and different constant stress levels.

In the present case, the observable variables are the strain rate $u_1 = \dot{\epsilon}$ and the time to rupture $u_2 = t_R$, while the control variables are the applied stress $p_1 = \sigma$, the absolute temperature $p_2 = T$, and the time $p_3 = t$.

Rupture behavior: master curves

Isothermal rupture curves at different temperatures are first considered, and represented in the logarithmic plane (see Fig. 4). If we consider only “simple” geometrical mappings such as translations or homothetic mappings, it can be seen that a master curve can be obtained by shifting the curves along the $\log t_R$ and $\log \sigma$ axis, as shown in Fig. 5. From a mathematical point of view, one then looks for the following geometrical mapping:

$$\begin{cases} \tilde{T} = T + \mu \\ \log \tilde{t}_R = a_1(\mu) + \log t_R \\ \log \tilde{\sigma} = b_1(\mu) + \log \sigma \end{cases} \quad (3.1)$$

with $a_1(\mu)$ and $b_1(\mu)$ the shift factors along the $\log t_R$ and $\log \sigma$ axis respectively. If the (arbitrary) chosen value of \tilde{T} is 748 K, then $a_1(\mu)$ and $b_1(\mu)$ correspond to the shift required to move the curve at T to make it coincide with those at \tilde{T} , if μ is defined by $\tilde{T} = T + \mu$. If we assume that Eqs. (3.1) define a Lie group, then the standard Lie group axioms have to be fulfilled (cf. [5]). It can be readily shown that they yield the following conditions to be satisfied by functions $a_1(\mu)$ and $b_1(\mu)$:

$$\begin{cases} a_1(0) = 0 \\ a_1(-\mu) = -a_1(\mu) \\ a_1(\mu_1 + \mu_2) = a_1(\mu_1) + a_1(\mu_2) \end{cases}, \quad \begin{cases} b_1(0) = 0 \\ b_1(-\mu) = -b_1(\mu) \\ b_1(\mu_1 + \mu_2) = b_1(\mu_1) + b_1(\mu_2) \end{cases} \quad (3.2)$$

for all μ, μ_1, μ_2 in \mathbb{R} . From Eqs. (3.2), one can infer the linearity of $a_1(\mu)$ and $b_1(\mu)$ with respect to μ :

$$a_1(\mu) = \alpha\mu, \quad b_1(\mu) = \beta\mu, \quad (3.3)$$

where α and β are true constants. Those last relations are in great accordance with the experimental values of the shift factors. The two fits give the following values of the

coefficients:

$$\alpha = -0.0403636, \quad \beta = -0.00584727, \tag{3.4}$$

that will be used here and in all subsequent developments. Hence, if one inserts (3.3) into (3.1), the following observed Lie group is obtained:

$$G_1^{obs} : \begin{cases} \tilde{T} = T + \mu \\ \tilde{t}_R = e^{\alpha\mu} t_R \\ \tilde{\sigma} = e^{\beta\mu} \sigma \end{cases} \tag{3.5}$$

and maps an experimental curve into another one. Of course, this Lie group is only valid for the explored values of T , but its validity is presently assumed for all T between the extremal values 748 K and 923 K. The components of the generator \mathbf{v}_1^{obs} associated with G_1^{obs} are given by the derivation of Eqs. (3.5) with respect to μ at $\mu = 0$, viz:

$$\mathbf{v}_1^{obs} = \alpha t_R \frac{\partial}{\partial t_R} + \beta \sigma \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial T}. \tag{3.6}$$

The Lie group generated by this vector field allows to shift all rupture responses in the same plane to the response obtained for a chosen reference temperature; the curve associated with this response is designated as the master curve. A similar strategy may be applied to the curves presented in Fig. 6, picturing the “isostrain” creep curves in the logarithmic plane $\log \sigma$ vs. $\log t$. As previously, one shall search the transformation rules:

$$\begin{cases} \tilde{\varepsilon} = e^{\mu} \varepsilon \\ \log \tilde{t} = a_2(\mu) + \log t \\ \log \tilde{\sigma} = b_2(\mu) + \log \sigma \end{cases} \tag{3.7}$$

mapping a curve at ε to a reference curve at $\tilde{\varepsilon} = 5\%$ (observe that the chosen value of the reference strain is arbitrary). The obtained master curve is shown in Fig. 7. The axioms of Lie symmetries lead as in section 3.1 to the linearity of $a_2(\mu)$ and $b_2(\mu)$ with respect to μ :

$$a_2(\mu) = \gamma\mu, \quad b_2(\mu) = \delta\mu, \tag{3.8}$$

with γ and δ new constants given by:

$$\gamma = 1.57167, \quad \delta = -0.0172415. \tag{3.9}$$

The calculated linear fit of $a_2(\mu)$ and $b_2(\mu)$ is validated in Fig. 8, and a second Lie group G_2^{obs} is obtained by inserting (3.8) into (3.7):

$$G_2^{obs} : \begin{cases} \tilde{\varepsilon} = e^{\mu} \varepsilon \\ \tilde{t} = e^{\gamma\mu} t \\ \tilde{\sigma} = e^{\delta\mu} \sigma \end{cases}. \tag{3.10}$$

The generator \mathbf{v}_2^{obs} of G_2^{obs} is given by:

$$\mathbf{v}_2^{obs} = \gamma t \frac{\partial}{\partial t} + \delta \sigma \frac{\partial}{\partial \sigma} + \varepsilon \frac{\partial}{\partial \varepsilon}. \tag{3.11}$$

The prolongations of the vector fields \mathbf{v}_1^{obs} and \mathbf{v}_2^{obs} account for the component with respect to $\dot{\varepsilon}$ and shall prove useful in the sequel. They can be computed with the prolongation formulae ([5]):

$$\begin{aligned} \text{pr}^{(1)}\mathbf{v}_1^{obs} &= \alpha t_R \frac{\partial}{\partial t_R} + \beta \sigma \frac{\partial}{\partial \sigma} + \frac{\partial}{\partial T}, \\ \text{pr}^{(1)}\mathbf{v}_2^{obs} &= \gamma t \frac{\partial}{\partial t} + \delta \sigma \frac{\partial}{\partial \sigma} + \varepsilon \frac{\partial}{\partial \varepsilon} + \dot{\varepsilon}(1 - \gamma) \frac{\partial}{\partial \dot{\varepsilon}}. \end{aligned} \tag{3.12}$$

At this stage, recall that two generators (ν_1^{obs} and ν_2^{obs}) have been identified from the experimental data set. We now look for a set of constitutive equations that can capture the creep behaviour of the material. The first constitutive relation expresses the rupture time t_R versus the loading parameters (T and σ in the present case) while the second one gives the evolution of the strain rate $\dot{\epsilon}$ as a function of $t, \sigma, \epsilon,$ and T :

$$\Delta_1 = t_R - f(\sigma, T) = 0, \tag{3.13}$$

$$\Delta_2 = \dot{\epsilon} - h(t, \sigma, \epsilon, T) = 0. \tag{3.14}$$

In those two equations, h and f are unknown functions that will be further determined. As concerns the classification of symmetries, it seems reasonable to apply the symmetry condition ν_1^{obs} to Δ_1 and ν_2^{obs} to Δ_2 . Indeed, the generator ν_1^{obs} (ν_2^{obs} respectively) has been built by only considering rupture curves (creep curves respectively). The satisfaction of those symmetry conditions means that each constitutive law (creep and rupture) keeps the same form and remains valid when the considered parameter changes. Finally, the complete set of symmetry conditions writes:

$$\text{pr}^{(1)}\nu_1^{obs} \Delta_1 = 0, \quad \text{whenever } \Delta_1 = 0, \tag{3.15}$$

$$\text{pr}^{(1)}\nu_2^{obs} \Delta_2 = 0, \quad \text{whenever } \Delta_2 = 0, \tag{3.16}$$

and it is associated with the sets $K_1 = \{1\}$ and $K_2 = \{2\}$. The next step consists in writing the constitutive models in terms of invariants.

Formulation of the constitutive equations for creep and rupture

As $m_1 = 1$ and $m_2 = 1$, the methodologies described in section 2 can be applied. The first methodology (direct solving of the symmetry conditions) has already been applied in [11]; we shall here consider the strategy involving a combination of invariants, in the spirit of the extrapolation methods of the literature, see the review article [36] and references therein. Thus, one looks for two new functions $\Sigma_1(I_1, I_2)$ and $\Sigma_2(J_1, J_2, J_3)$ such that

$$\Sigma_1(I_1, I_2) = 0 \Leftrightarrow \Delta_1 = 0, \tag{3.17}$$

$$\Sigma_2(J_1, J_2, J_3) = 0 \Leftrightarrow \Delta_2 = 0, \tag{3.18}$$

with I_1, I_2 the invariants of ν_1^{obs} given by the solution of the system

$$\frac{dt_R}{\alpha t_R} = \frac{d\sigma}{\beta \sigma} = dT, \tag{3.19}$$

and J_1, J_2, J_3 the invariants of ν_2^{obs} given by the solution of the same characteristic system:

$$\frac{dt}{\gamma t} = \frac{d\sigma}{\delta \sigma} = \frac{d\epsilon}{\epsilon} = \frac{d\dot{\epsilon}}{(1 - \gamma)\dot{\epsilon}}. \tag{3.20}$$

Solving (3.19) and (3.20) gives the following invariants for rupture

$$I_1 = \log t_R - \alpha T, \quad I_2 = \log \sigma - \beta T, \tag{3.21}$$

and creep

$$J_1 = \log t - \gamma \log \epsilon, \quad J_2 = \log \sigma - \delta \log \epsilon, \quad J_3 = \log \dot{\epsilon} - (1 - \gamma) \log \epsilon. \tag{3.22}$$

Considering rupture, the experimental representation of $\log(t_R)$ vs. $1/T$ pictured in Fig. 9 suggests a relation of the form:

$$\log t_R \approx \frac{F_1(\sigma)}{T} + F_2(\sigma). \tag{3.23}$$

We here decide to keep the dependence of the slope F_1 with respect to σ , since the very low number of experimental points in Fig. 9 does not allow to assume a constant slope. To follow as closely as possible the mathematical structure of (3.23), the following expression is proposed:

$$\Sigma_1(I_1, I_2) = \frac{K_1}{I_2} + K_2 I_1 + K_3 I_2 = 0, \tag{3.24}$$

in which K_1, K_2, K_3 are constants, which warrants a hyperbolic dependence with respect to T . Eq. (3.24) leads to:

$$\log t_R = \frac{a}{\log \sigma - \beta T} + b \log \sigma + (\alpha - b\beta)T \tag{3.25}$$

with $a = -K_1/K_2$ and $b = -K_3/K_2$ new constants. Eq. (3.25) shows that a linear term in T appears by combining the invariants I_1 and I_2 , giving a relation which slightly differs from the Larson-Miller or Dorn relationships. However, this linear term is necessary to fullfill the symmetry condition (3.15) that follows from the experimental data set. The validation of Eq. (3.25) is given in Fig. 10, in which a good agreement with the experimental data presented in [40] is observed (the coefficients a and b are adjusted). As to the creep strain rate, we introduce in accordance with the “convenient creep laws” of [40] the power function:

$$\Sigma_2(J_1, J_2, J_3) = e^{J_3} - A e^{cJ_1} e^{dJ_2} = \dot{\epsilon} \epsilon^{-(1-\gamma)} - A t^c \epsilon^{-c\gamma} \sigma^d \epsilon^{-d\delta} = 0 \tag{3.26}$$

with A, c and d some constants, which leads in turn to:

$$\dot{\epsilon} = A t^c \sigma^d \epsilon^{1-\gamma-c\gamma-d\delta}. \tag{3.27}$$

It can be easily shown that the symmetry conditions (3.15) and (3.16) are fulfilled. If we denote by (i) $\epsilon(t = 0, \sigma, T) = \epsilon_0(\sigma, T)$ the initial value of the strain ϵ and (ii) the exponent $\nu = \gamma + c\gamma + d\delta$, then the resolution of Eq. (3.27) allows to write:

$$\epsilon(t) = (1 + c)^{-1/\nu} \left[(1 + c)\epsilon_0(\sigma, T)^\nu + A\nu t^{c+1} \sigma^d \right]^{1/\nu}. \tag{3.28}$$

If the temperature T and the strain ϵ are assigned fixed values, and if we assume that the initial strain can be written in terms of a Hookean relation:

$$\epsilon_0(\sigma, T) = \frac{\sigma}{E(T)} \tag{3.29}$$

with $E(T)$ the Young modulus at T , then the “isostrain” curves may be obtained by expressing the time $t(\sigma)$ from Eq. (3.28), viz:

$$t(\sigma) = \left[\frac{(c + 1)(\epsilon^\nu - \sigma^\nu E(T)^{-\nu})}{A\nu\sigma^d} \right]^{1/(1+c)}. \tag{3.30}$$

The inverse functional dependence $\sigma(t)$ can be numerically calculated. The validation of the model $\log \sigma$ vs. $\log t$ can then be carried out through Eq. (3.30), and is pictured in Fig. 11; the model and the experimental data are seen to be in good agreement (the coefficients $E(T), A$ and c, d are here adjusted). Figure. 12 pictures the creep curves at different stress levels as predicted by the present model.

Computation of the Lie algebra for creep and rupture

To summarize the previous sections, the following constitutive equations have been obtained as representative of the creep and rupture behaviours of the considered 9Cr1Mo stainless steel:

$$\dot{\epsilon} = A t^c \sigma^d \epsilon^{1-\gamma-c\gamma-d\delta} \quad \text{if } t \leq t_R, \tag{3.31}$$

Table 1 Some creep invariants encountered in the literature (see, e.g., Ref. [61])

Authors	Invariant(s)
Larson & Miller	$T(\log t + \log B_2)$
Dorn	$\frac{B_1}{T} - \log t$
Monkman-Grant	$\log t_R + m \log \dot{\epsilon}_{min}$
Modified Monkman-Grant	$\log \left(\frac{t_R}{\dot{\epsilon}_R} \right) + m' \log \dot{\epsilon}_{min}$

Table 2 Commutator table of the Lie algebra of Eq. (3.31)

	\mathbf{v}_2^1	\mathbf{v}_2^2	\mathbf{v}_2^3	\mathbf{v}_2^4
\mathbf{v}_2^1	0	0	$(c + 1)\mathbf{v}_2^1$	$2(c + 1)\mathbf{v}_2^1$
\mathbf{v}_2^2	0	0	$(c + 1)\mathbf{v}_2^2$	$(c + 1)\mathbf{v}_2^2$
\mathbf{v}_2^3	$-(c + 1)\mathbf{v}_2^1$	$-(c + 1)\mathbf{v}_2^2$	0	0
\mathbf{v}_2^4	$-2(c + 1)\mathbf{v}_2^1$	$-(c + 1)\mathbf{v}_2^2$	0	0

$$t_R = \sigma^b e^{\frac{a}{\log \sigma - \beta T} + (\alpha - b\beta)T}. \tag{3.32}$$

Those formulations of the constitutive laws are compatible with the observed master curves. We can now proceed to the Lie analysis of these constitutive equations.

The Lie algebra of the creep model is computed following the methodology described by [5]. It contains 4 generators $\mathbf{v}_2^i, i = 1, \dots, 4$ with prolongations given by:

$$\text{pr}^{(1)}\mathbf{v}_2^1 = \sigma^d t^{-c} \frac{\partial}{\partial t} + c\dot{\epsilon} \sigma^d t^{-c-1} \frac{\partial}{\partial \dot{\epsilon}}, \tag{3.33}$$

$$\text{pr}^{(1)}\mathbf{v}_2^2 = \sigma^d \epsilon^{1-\nu} \frac{\partial}{\partial \epsilon} + (1 - \nu)\sigma^d \epsilon^{-\nu} \dot{\epsilon} \frac{\partial}{\partial \dot{\epsilon}}, \tag{3.34}$$

$$\text{pr}^{(1)}\mathbf{v}_2^3 = t \frac{\partial}{\partial t} + \left(\frac{c + 1}{\nu} \right) \epsilon \frac{\partial}{\partial \epsilon} + \left(\frac{c + 1 - \nu}{\nu} \right) \dot{\epsilon} \frac{\partial}{\partial \dot{\epsilon}}, \tag{3.35}$$

$$\text{pr}^{(1)}\mathbf{v}_2^4 = t \frac{\partial}{\partial t} - \left(\frac{c + 1}{d} \right) \sigma \frac{\partial}{\partial \sigma} - \dot{\epsilon} \frac{\partial}{\partial \dot{\epsilon}}, \tag{3.36}$$

in which we recall that $\nu = \gamma + c\gamma + d\delta$. The commutation table of this Lie algebra is given in Table 2. In order to show the practical interest of this table, let us consider the particular combination of the calculated generators:

$$\frac{\nu}{c + 1} \left(\text{pr}^{(1)}\mathbf{v}_2^3 + \left(\frac{c + 1 - \nu}{\nu} \right) \text{pr}^{(1)}\mathbf{v}_2^4 \right) = t \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial \epsilon} - \left(\frac{c + 1 - \nu}{d} \right) \sigma \frac{\partial}{\partial \sigma} \tag{3.37}$$

which has no component with respect to $\dot{\epsilon}$ and which is obviously a Lie symmetry of (3.31). The flow of this generator is given in logarithmic double axes by:

$$\begin{cases} \log \bar{t} = \mu + \log t \\ \log \bar{\sigma} = - \left(\frac{c+1-\nu}{d} \right) \mu + \log \sigma \\ \log \bar{\epsilon} = \mu + \log \epsilon. \end{cases} \tag{3.38}$$

This last set of relations is of great interest since it describes a master curve in the $\log \epsilon$ vs. $\log t$ representation. More precisely, the curve $\log \bar{\epsilon}$ vs. $\log \bar{t}$ obtained for a stress level $\bar{\sigma}$ is linked to the curve obtained for σ by a translation of vector (μ, μ) , the shift being defined by $\mu = \frac{d}{c+1-\nu} \log(\sigma/\bar{\sigma})$.

The Lie algebra of the rupture model has two generators $\mathbf{v}_1^i, i = 1, 2$, given by:

$$\mathbf{v}_1^1 = t_R \left(\frac{b(\log \sigma - \beta T)^2 - a}{\log \sigma - \beta T} \right) \frac{\partial}{\partial t_R} + \sigma(\log \sigma - \beta T) \frac{\partial}{\partial \sigma}, \tag{3.39}$$

$$\mathbf{v}_1^2 = t_R \left(\frac{(\alpha - b\beta)(\log \sigma - \beta T)^2 + a\beta}{\log \sigma - \beta T} \right) \frac{\partial}{\partial t_R} + (\log \sigma - \beta T) \frac{\partial}{\partial T}, \tag{3.40}$$

Table 3 Commutator table of the Lie algebra of Eq. (3.32)

	v_1^1	v_1^2
v_1^1	0	$\beta v_1^1 + v_1^2$
v_1^2	$-\beta v_1^1 - v_1^2$	0

Table 4 Some creep laws encountered in the literature (see, e.g., Ref. [61])

References	Relationship
[71, 72]	$\epsilon = f_1(\sigma)f_2(t)f_3(T)$
[73–76]	$\dot{\epsilon} = f_1(\sigma)f_2(t)f_3(T)$
[73, 74, 77, 78]	$\dot{\epsilon} = g_1(\sigma)g_2(\epsilon_c)g_3(T)$
[74]	$E(t)\Phi[\epsilon(t)] = \sigma(t) + \int_0^t K(t, \tau)\sigma(\tau)d\tau$

and its commutator table is given in Table 3. If we denote by ϕ^{1,t_R} and ϕ^{2,t_R} the component in t_R of v_1^1 and v_1^2 respectively, then the following local combination:

$$\begin{aligned}
 \mathbf{v} = \frac{\phi^{2,t_R}v_1^1 - \phi^{1,t_R}v_1^2}{t_R} &= \sigma [a\beta + (\alpha - b\beta)(\log \sigma - \beta T)^2] \frac{\partial}{\partial \sigma} \\
 &+ (a - b(\log \sigma - \beta T)^2) \frac{\partial}{\partial T}
 \end{aligned}
 \tag{3.41}$$

is a symmetry of Eq. (3.32) having no component in t_R and whose components in σ and T do not depend on t_R . Consequently, \mathbf{v} has the form of Eq. (2.4), and the flow of this vector field is given by the solution of the system of differential equations (2.6):

$$\frac{d\bar{\sigma}}{d\mu} = \bar{\sigma} [a\beta + (\alpha - b\beta)(\log \bar{\sigma} - \beta\bar{T})^2]
 \tag{3.42}$$

$$\frac{d\bar{T}}{d\mu} = a - b(\log \bar{\sigma} - \beta\bar{T})^2
 \tag{3.43}$$

with the initial conditions

$$\bar{\sigma}(0) = \sigma, \quad \bar{T}(0) = T
 \tag{3.44}$$

and the equality $\bar{t}_R = t_R$. Consequently, the numerical solution of (3.42) and (3.43) provides a parametric representation $(T(\mu), \sigma(\mu))$ of the “iso- t_R ” curves in the (T, σ) plane, see Fig. 13. This kind of theoretical chart is of high practical interest, as it allows to extrapolate the rupture time of a specimen at any stress level or any temperature, provided that the rupture time is known for a given value of σ and T .

Summarizing this section, material data have been given the structure of experimental Lie groups, using as a subsequent step the Lie group structure to construct a material constitutive law in terms of initially unknown constitutive functions. The Lie symmetries can accordingly be considered as an interpolation method enabling to link in a continuous manner experimental data, but relying on a well-chosen limited set of experimental measurements.

Invariance relations and master responses associated to a rheological model

The formulation of the constitutive model including a set of parameters is here followed by the symmetry analysis, leading to invariance relations and master responses inherent to the model. In the context of rheology, this approach proves quite promising for dissipative material with a complex nonlinear constitutive law, including the state laws satisfied by the observable variables and the kinetics of internal variables traducing the evolution

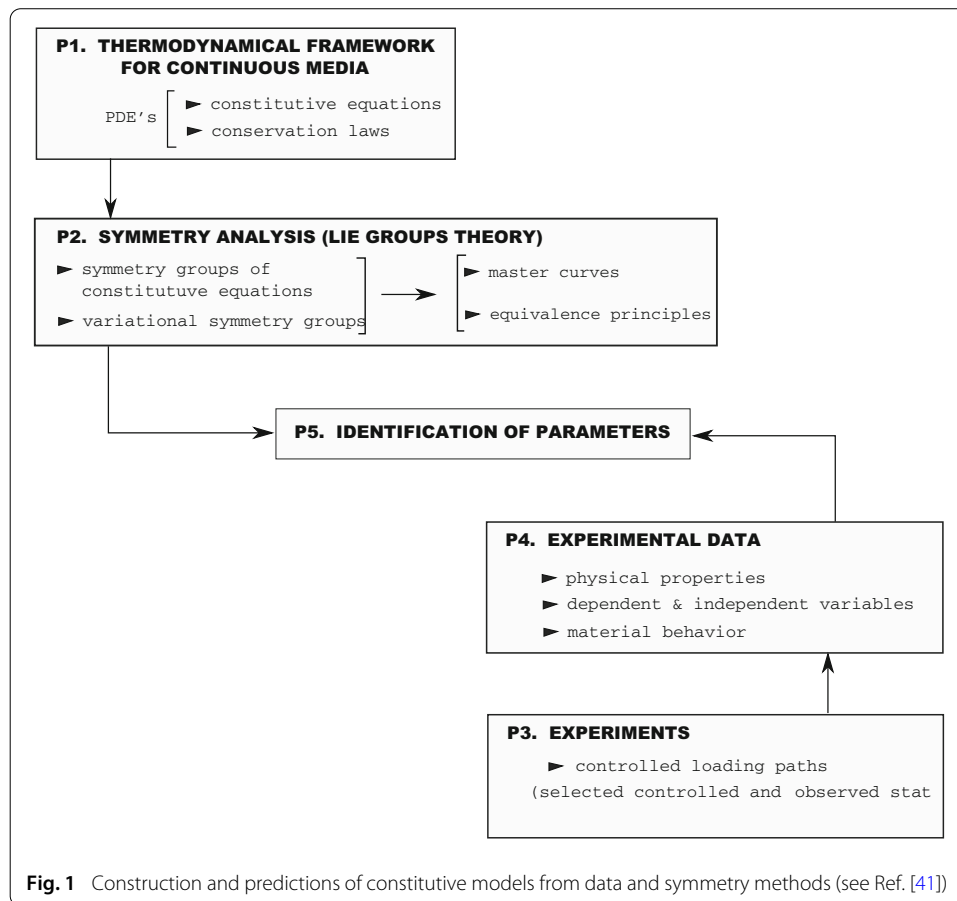


Fig. 1 Construction and predictions of constitutive models from data and symmetry methods (see Ref. [41])

laws of the internal variables. The invariants associated to those symmetries can then be calculated and used to synthesize the material’s response into master responses reflecting the material’s response when the control parameters change. The proposed algorithm reflecting the entire methodology is summarized in the diagram of Fig. 1. The formulation of rheological models can be guided by the framework of the thermodynamics of irreversible processes, as explained in the sequel.

Construction of the constitutive laws in the framework of TIP

In mechanics or rheology, constitutive laws for dissipative materials are generally written under the umbrella of the thermodynamics of irreversible processes (TIP) [42], relying on the energy density to describe the energetic part of the constitutive law and the dissipation potential for its dissipative part. Relying on Callen’s axiomatic, [43], and a generalization of De Donder’s thermodynamics, let the total internal energy $E(\mathbf{y}, \mathbf{z})$ characterizing the medium depend on a set of extensive variables $\mathbf{y} = (S, V\varepsilon, N_k, \dots)$, where S , $V\varepsilon$, and N_k are respectively the entropy, the volume weighted deformation, the number of moles of the k^{th} species, further identified to a set of internal variables \mathbf{z} describing the irreversible evolution of the microstructure (such as plasticity, viscoplasticity, and damage). The thermodynamical system is a finite volume V with boundary ∂V of a solid continuum body. The extensity property of E expresses as

$$E(\lambda\mathbf{y}, \lambda\mathbf{z}) = \lambda E(\mathbf{y}, \mathbf{z}). \tag{4.1}$$

Taking the derivative of previous equation with respect to λ at $\lambda = 1$, the Euler relation is obtained in the form of the Gibbs relation

$$E(\mathbf{y}, \mathbf{z}) = \mathbf{Y}(\mathbf{y}, \mathbf{z}) \cdot \mathbf{y} - \mathbf{A}(\mathbf{y}, \mathbf{z}) \cdot \mathbf{z} \tag{4.2}$$

satisfied by the internal energy $E(\mathbf{y}, \mathbf{z})$, with $\mathbf{Y} = E_{,y}$ the intensive variables (vector) and $\mathbf{A} = -E_{,z}$ the generalized non equilibrium forces respectively. The intensive variables are dual of the extensive ones in a thermodynamical sense. For example, the second order Cauchy stress tensor σ , is conjugated to the second order strain tensor ε . The extensive variables are called control variables, since they are the arguments of an appropriate thermodynamical potential. Accounting for the Gibbs relation:

$$\frac{dE}{dt}(\mathbf{y}, \mathbf{z}) = \mathbf{Y}(\mathbf{y}, \mathbf{z}) \cdot \frac{d\mathbf{y}}{dt} - \mathbf{A}(\mathbf{y}, \mathbf{z}) \cdot \frac{d\mathbf{z}}{dt}, \tag{4.3}$$

the Gibbs-Duhem relation results from the differentiation of Eq. (4.2), viz

$$\mathbf{y} \cdot \frac{d\mathbf{Y}}{dt} - \mathbf{z} \cdot \frac{d\mathbf{A}}{dt} = 0. \tag{4.4}$$

The constitutive law is specified in rate form from the total time derivation of the intensive variables \mathbf{Y} and \mathbf{A} as

$$\begin{aligned} \dot{\mathbf{Y}}(\mathbf{y}, \mathbf{z}) &= \mathbf{a}^u(\mathbf{y}, \mathbf{z}) \cdot \dot{\mathbf{y}} + \mathbf{b}(\mathbf{y}, \mathbf{z}) \cdot \dot{\mathbf{z}} \\ -\dot{\mathbf{A}}(\mathbf{y}, \mathbf{z}) &= \mathbf{b}^T(\mathbf{y}, \mathbf{z}) \cdot \dot{\mathbf{y}} + \mathbf{g}(\mathbf{y}, \mathbf{z}) \cdot \dot{\mathbf{z}} \end{aligned} \tag{4.5}$$

with $\mathbf{a}^u(\mathbf{y}, \mathbf{z}) = E_{,yy}$ the Tisza matrix, $\mathbf{b}(\mathbf{y}, \mathbf{z}) = E_{,zy}$, $\mathbf{g}(\mathbf{y}, \mathbf{z}) = E_{,zz}$ the coupling and the dissipation matrices respectively, [44].

In the more general setting of the theory of irreversible process (abbreviated T.I.P.) or the thermodynamics with internal variables (abbreviated T.I.V.), the kinetic laws of the internal variables are written based on the setting up of the dissipation potential D , a positive and homogeneous function of degree n in the rate of the internal variables, [42], allowing to express the thermodynamic forces or affinities reflecting all dissipative variables \mathbf{A} versus the dual internal variable \mathbf{z} as

$$\mathbf{A}(\mathbf{z}) = \frac{\partial D}{\partial \dot{\mathbf{z}}}. \tag{4.6}$$

Using previous relation results in a dissipation expressing as

$$\Phi = \mathbf{A} \cdot \dot{\mathbf{z}} = \frac{\partial D(\mathbf{z})}{\partial \dot{\mathbf{z}}} = nD \geq 0 \tag{4.7}$$

due to Euler's identity for homogeneous functions of degree n (in classical T.I.P., D is taken as homogeneous of degree two). The previous relation can be inverted to give the rate of the internal variable versus the affinity, using the Legendre-Fenchel transform, involving the pseudo-potential of dissipation, defined as

$$D^*(\mathbf{A}) = \sup_{\mathbf{A}} (\mathbf{A} \cdot \dot{\mathbf{z}} - D(\dot{\mathbf{z}})) \tag{4.8}$$

where \mathbf{A} is restricted to a convex set K , [42]. When $D^*(\mathbf{A})$ is differentiable, the evolution law of the internal variable \mathbf{z} is given by

$$\dot{\mathbf{z}} = \frac{\partial D^*(\mathbf{A})}{\partial \mathbf{A}}. \tag{4.9}$$

Choosing as a specific model a quadratic and convex pseudo potential of dissipation D^* , one obtains the following set of independent non linear kinetic relations (for a number of N processes)

$$\dot{z}_k = -\frac{z_k - z_k^r}{\tau_k}, \quad k = 1..N, \tag{4.10}$$

considering a spectral decomposition of dissipative phenomena modelled by internal variables z_k . The variables z_k^r represent the value of the internal variable z at its relaxed equilibrium state, for the dissipation mode k , defined as the state for which the thermodynamic affinity A^r vanishes. The distribution of the relaxation times therein τ_k is described from Prigogine's fluctuation theorem, the contribution of each mode being proportional to the square root of the corresponding relaxation time [44].

A Lagrangian formulation of the previous dissipative constitutive laws is further constructed by the homotopy formula from the self-adjoint system of PDE's (4.5), accounting for the Gibbs relation Gibbs-Duhem relations (4.4), see [45,46]:

$$L = E_{,y} \cdot \dot{y} + E_{,z} \cdot \dot{z} = \frac{dE(y, z)}{dt}. \quad (4.11)$$

This thermodynamic Lagrangian incorporates the thermodynamic information related to the material, in terms of relations between the extensive control variables and the dual intensive thermodynamic forces, where the generalized coordinates $\{y, z, \dot{y}, \dot{z}\}$ correspond to the Lagrange variables of the considered spatially uniform system. The set of internal variables completes the set of control variables, ensuring the self-adjointness of the constitutive equations [45]. The kinetic information, viz the set of equations (4.10) is then incorporated into the previous thermodynamic Lagrangian via Lagrange multipliers $\lambda = \{\lambda_k, k = 1..N\}$, hence the augmented Lagrangian, L_{aug} , accounting for both the thermodynamic and the kinetic information inherent to the material's constitutive law, writes

$$l_{aug} = \dot{e} + \sum_{k=1}^N \lambda_k \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k} \right), \quad (4.12)$$

where the internal energy E has been replaced by the internal energy density e , which also satisfies the Maxwell conditions. The Lagrangian density l_{aug} in Eq. (4.12) is the volumetric density of a Lagrangian L_{aug} , such that

$$L_{aug} = \int_V l_{aug} dV. \quad (4.13)$$

The Lagrange multipliers in l_{aug} resemble thermodynamic affinities dual to the rate of internal variables, hence the kinetic part of the total Lagrangian thereabove resembles a dissipation potential. Observe that the incorporation of the kinetic laws Eq. (4.10) clearly breaks the symmetry (discrete symmetry) under time reversal $t \rightarrow -t$, since the new Lagrangian contains an irreversible information. The set of Lagrange equations obtained from the stationarity condition of the action functional built from l_{aug} is completely equivalent to the constitutive equations (4.5) and the kinetic laws (4.10). The kinetic evolution equations Eq. (4.9) have symmetry properties depending on the specific form taken by the relaxation time therein.

Symmetry analysis of the augmented Lagrangian

Relying on the formulated least action principle of the dissipative constitutive laws, we next exploit the associated variational symmetries to determine invariance properties of the set of constitutive equations (thermodynamic and kinetic informations), relying on the methodology presented in [45–48]. We focus in the sequel (but without loss of generality) on the specific energy $e(\varepsilon, s, z_k)$, depending on the strain ε , the specific entropy s , and some specific internal variables z_k , $k = 1..N$, accounting for internal dissipative phenomena (related to the microstructure).

The search for the variational symmetries of the Jacobi action built from the augmented Lagrangian amounts to find the infinitesimal generators on the (first order) jet space sustained by the control variables $\{t, \varepsilon, s, z_k\}$. As a concrete illustration, and without loss of generality, considering the time t as the sole independent variable and as the dependent variables the vector $\mathbf{y} = \varepsilon, s, z_k$, a generator of a symmetry group expresses as

$$\mathbf{v}_{cont} = \xi \frac{\partial}{\partial t} + \phi^\varepsilon \frac{\partial}{\partial \varepsilon} + \phi^s \frac{\partial}{\partial s} + \phi^{z_k} \frac{\partial}{\partial z_k} \tag{4.14}$$

with the variations of the dependent variables given by

$$\delta \varepsilon = \mu \phi^\varepsilon ; \delta s = \mu \phi^s ; \delta z_k = \mu \phi^{z_k}, \tag{4.15}$$

with μ the group parameter, [5]. In Eq. (4.14), the subscript “cont” means that only components with respect to control variables are at first introduced. The variations given in Eq. (4.15) are responsible for the variations of intensive observable variables $\delta \sigma$, δT , and δA_k , obtained from the second partial derivatives of the potential e . The symmetry group acting on the set of variables $\{t, \varepsilon, s, z_k\}$ is automatically extended to the enlarged set of variables $\{t, \varepsilon, s, z_k, \sigma, T, A_k\}$: thereby, the total vector field, generator of the symmetries of the constitutive laws, is decomposed into the sum of the “control” vector field and the “observable” vector field:

$$\mathbf{v} = \mathbf{v}_{cont} + \mathbf{v}_{obs} \quad \text{with} \quad \mathbf{v}_{obs} = \phi^\sigma \frac{\partial}{\partial \sigma} + \phi^T \frac{\partial}{\partial T} + \phi^{A_k} \frac{\partial}{\partial A_k}. \tag{4.16}$$

The components of the intensive variables of the observable and internal vector fields are given by the structure of the constitutive law (Eq. 4.5) for the elementary representative volume element (RVE):

$$\phi^\sigma = e_{,\varepsilon\varepsilon} \phi^\varepsilon + e_{,s\varepsilon} \phi^s + e_{,z_k\varepsilon} \phi^{z_k} \tag{4.17}$$

$$\phi^T = e_{,\varepsilon s} \phi^\varepsilon + e_{,ss} \phi^s + e_{,z_k s} \phi^{z_k} \tag{4.18}$$

$$\phi^{A_i} = e_{,\varepsilon z_i} \phi^\varepsilon + e_{,s z_i} \phi^s + e_{,z_k z_i} \phi^{z_k}. \tag{4.19}$$

The components of the vector field \mathbf{v}_{obs} are thus completely determined by those of the vector field \mathbf{v}_{cont} . Let return now to a general situation, and decompose the Lagrangian of Eq. (4.12) into a thermodynamic and a kinetic contribution, as

$$l_{aug} = l_{thermo} + l_{kine} \tag{4.20}$$

with

$$l_{thermo} = \dot{e} \quad \text{and} \quad l_{kine} = \sum_{k=1}^N \lambda_k \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k} \right). \tag{4.21}$$

As shown previously, the invariance condition associated with the sole contribution l_{thermo} is automatically verified, see also [45]. The satisfaction of the Euler-Lagrange equations for \dot{e} as a Lagrangian is fully equivalent to the Maxwell conditions for the second order partial derivatives of the potential function e . Thus, the invariance condition of the action integral simplifies to the differential condition involving the sole kinetic information (and kinetic Lagrangian)

$$\text{pr}^{(1)} \mathbf{v} l_{kine} + l_{kine} \text{Div} \boldsymbol{\xi} = 0, \tag{4.22}$$

accounting for the relation $\text{Div} \boldsymbol{\xi} = D_t \boldsymbol{\xi} = \dot{\boldsymbol{\xi}}$.

The connection between the variational symmetry condition and the local symmetry of the field equations is next established. If ν is a variational symmetry for some functional $S = \int_t \int_V l dV dt$, it is also a symmetry of the corresponding Lagrange equations:

$$\text{pr}^{(1)}\nu l + l\text{Div}\xi = 0 \quad \Rightarrow \quad \text{pr}^{(1)}\nu(E(l)) = 0, \quad (4.23)$$

but the converse is generally not true: the set of all variational symmetries denoted by G_S is always included into the set of local symmetries, G_Δ , i.e. $G_S \subset G_\Delta$. In the present case, we consider only variational symmetries along the optimal path where the constitutive laws are satisfied. Accounting for the expression of l_{kine} , viz

$$l_{kine} = \sum_{k=1}^N \lambda_k \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k} \right), \quad (4.24)$$

the condition $l_{kine} = 0$ is satisfied along the optimal path, hence the variational symmetry condition resumes to

$$\text{pr}^{(1)}\nu l_{kine} = 0 \text{ whenever } l_{kine} = 0. \quad (4.25)$$

Thanks to the linearity of the prolongation and doing a spectral decomposition of the dissipative mechanisms, the evolution of the internal variables are mutually independent, hence the symmetry conditions (4.25) may be decoupled, resulting in the new set of N independent symmetry conditions:

$$\text{pr}^{(1)}\nu \left(\dot{z}_k + \frac{z_k - z_k^r}{\tau_k} \right) = 0 \text{ whenever } \dot{z}_k + \frac{z_k - z_k^r}{\tau_k} = 0, \quad (4.26)$$

which is equivalent to the local symmetry condition.

The same condition holds for the more general evolution equation (4.9), thus allowing to extend the symmetry analysis to more complex dissipative phenomena. A classification of symmetries according to the form of the pseudo-potential of dissipation can also be done. Previous considerations entail that variational symmetries along the optimal path are fully equivalent to local symmetries directly computed from the constitutive laws.

The symmetries of the formulated augmented lagrangian formulation are those of the pseudo-potential of dissipation $D^*(A)$. The infinitesimal generator of the general invariance condition (4.25) is also split into the sum of a control and an observable vector field, with the components of the last contribution completely expressed from the components of the control vector; this implies searching for symmetries in a subset of the total jet space, since the state laws for the observable variables are automatically satisfied.

The presented general thermodynamically based material framework originates in pioneering works [49–52], and it covers a broad spectrum of rheological models in viscoelasticity, viscoplasticity, plasticity and also continuum damage mechanics.

In the next section, the invariance properties of the constitutive equations are exploited to set up a predictive methodology allowing to condense the materials response into equivalence principles. This has consequences on the experimental side, since the later enable to define equivalent experimental set up allowing a gain of time by selecting an optimal set of control variables (e.g. temperature, strain rate).

Invariance properties of the constitutive equations

Considering for instance a general internal variable formulation of inelasticity for generalized standard materials, the symmetries of the constitutive laws are implicitly reflected

by the form taken by the thermodynamic potential (or the pseudo potential of dissipation introduced in Eq. (4.8)) and the dissipation function. The search for the Lie groups of constitutive laws is further used as a systematic tool for the construction of the so-called master curves, that condense the information related to the behavior of a material under varying experimental conditions. The experimental conditions are defined by the values taken by a set of control parameters such as temperature, strain rate. Hence, the knowledge of symmetry groups allows a prediction regarding the modification of the material's response when these parameters vary. Thus, starting from a known set of constitutive equations, i.e. a known expression for e , z_k^r and τ_k , it is a priori possible to compute some symmetries of the behavior by applying the symmetry condition (4.26). Due to the equivalence of the local and variational symmetry conditions, a conservation law may be obtained using Noether's theorem, viz $\text{Div} \mathbf{P} = 0$, with

$$P_i = \sum_{k=1}^q \sum_{j=1}^4 \xi_j u_{k,j} \frac{\partial l_{kine}}{\partial u_{k,i}} - \sum_{j=1}^q \phi_j \frac{\partial l_{kine}}{\partial u_{j,i}} - \xi_i l_{kine} \tag{4.27}$$

see e.g. [5], with l_{kine} the kinetic Lagrangian density, defined in the general thermodynamic setting exposed in the previous section as

$$l_{kine} = \sum_k \lambda_k \left(\dot{z}_k - \frac{\partial D^*(A)}{\partial A_k} \right) \equiv 0. \tag{4.28}$$

Recall that the dependent variables arguments of the kinetic Lagrangian, viz the variables u_k , are internal variables. For a uniform elementary representative volume element, only the time derivative appears in previous conservation law expression; BVPs accounting for the spatial variation of the fields over spatial domains will be considered later on in this contribution.

Application: construction of the master curve of a dry polyamid (PA66) and time temperature equivalence

The invariants build from the Lie symmetry analysis of the constitutive law will further be translated into master curves, as explained below. The constitutive model set up presently for the purpose of uniaxial tests involves the strain ϵ as control variable, and the stress σ as the corresponding observable variable. The temperature T , dual of the entropy s , plays the role of a parameter. The internal variables z_k and the thermodynamic affinities A_k are not controlled; their values at the relaxed state are governed by the strain history. The exploitation of the general constitutive Eq. (4.5) and (4.10) delivers the following state law (see [53]):

$$\begin{cases} \dot{\sigma} - E_u \dot{\epsilon} + \sum_{k=1}^n b_k^1 \frac{z_k - z_k^r}{\tau_k} = 0 \\ -\dot{s} + \alpha_u E_u \dot{\epsilon} + \sum_{k=1}^n b_k^2 \frac{z_k - z_k^r}{\tau_k} = 0 \\ -\dot{A}_i - b_i^1 \dot{\epsilon} + \sum_{k=1}^n g_{ik} \frac{z_k - z_k^r}{\tau_k} = 0 \quad i = 1..n \end{cases} \tag{4.29}$$

with E_u the constant instantaneous Young's modulus, b_k^1 , α_u (dilatation coefficients), b_k^2 , and g_{ik} being defined from the second order partial derivatives of the Helmholtz free energy, see [54]. The simplest model for the evolution of the internal variables is

$$z_k^r = c_k \epsilon. \tag{4.30}$$

If one starts from a particular expression of the kinetic laws, involving a temperature dependence of the relaxation times of Arrhenius kind, the following kinetic model may be written

$$\dot{z}_k + \frac{z_k - c_k \varepsilon}{\frac{h}{kT} \exp\left(\frac{\Delta H - T \Delta S_k}{RT}\right)} = 0, \tag{4.31}$$

where h is the Planck constant, k the Boltzmann constant, R the gas constant, c_k , ΔH , ΔS_k some material constants. The required symmetry condition expresses accordingly

$$\text{pr}^{(1)}\nu \left(\dot{z}_k + \frac{z_k - c_k \varepsilon}{\frac{h}{kT} \exp\left(\frac{\Delta H - T \Delta S_k}{RT}\right)} \right) = 0. \tag{4.32}$$

The particular solution is obtained

$$\nu_0 = \xi \frac{\partial}{\partial t} + \phi^T \frac{\partial}{\partial T} + \phi^\sigma \frac{\partial}{\partial \sigma} + \phi^s \frac{\partial}{\partial s} + \phi^{A_k} \frac{\partial}{\partial A_k} \tag{4.33}$$

with:

$$\begin{aligned} \xi = t; \quad \phi^T = -\frac{RT^2}{RT + \Delta H}; \quad \phi^\sigma = -\alpha_u E_u \phi^T; \\ \phi^{A_k} = -b_k^2; \quad \phi^T; \quad \phi^\varepsilon = 0; \quad \phi^{z_k} = 0. \end{aligned} \tag{4.34}$$

This solution is further interpreted as a mathematical formulation of the so-called time-temperature equivalence principle for polymers. The integration of the induced first order differential system leads to a one-parameter group of transformations, where the temperature is transformed as

$$\begin{aligned} \bar{T} = \exp \left(L_W \left(\frac{\Delta H}{R} \exp \left(\frac{\mu T - T \ln(T^*) + \frac{\Delta H}{R}}{T} \right) \right) \right. \\ \left. - \mu + \ln T^* - \frac{\Delta H}{RT} \right) \end{aligned} \tag{4.35}$$

with $L_W(x)$ the Lambert function, and $T^* = T/T_0$ with $T_0 = 1$ K. The theoretical shift factor is obtained by inverting the previous implicit relation:

$$\frac{\mu(T, \bar{T})}{\ln 10} = \frac{\Delta H(T - \bar{T})}{RT\bar{T} \ln 10} + \frac{1}{\ln 10} \ln \frac{T}{\bar{T}}. \tag{4.36}$$

This explicit expression of the group parameter $\mu(T, \bar{T})$ highlights an invariance property satisfied by the secant modulus $E_s(t, T)$, defined as the ratio of stress to strain:

$$E_s(t, T) = \frac{\sigma(t, T)}{\varepsilon(t, T)} = \frac{\bar{\sigma}(\bar{t}, \bar{T})}{\bar{\varepsilon}(\bar{t}, \bar{T})} = E_s(\bar{t}, \bar{T}) = E_s(e^\mu t, \bar{T}) \tag{4.37}$$

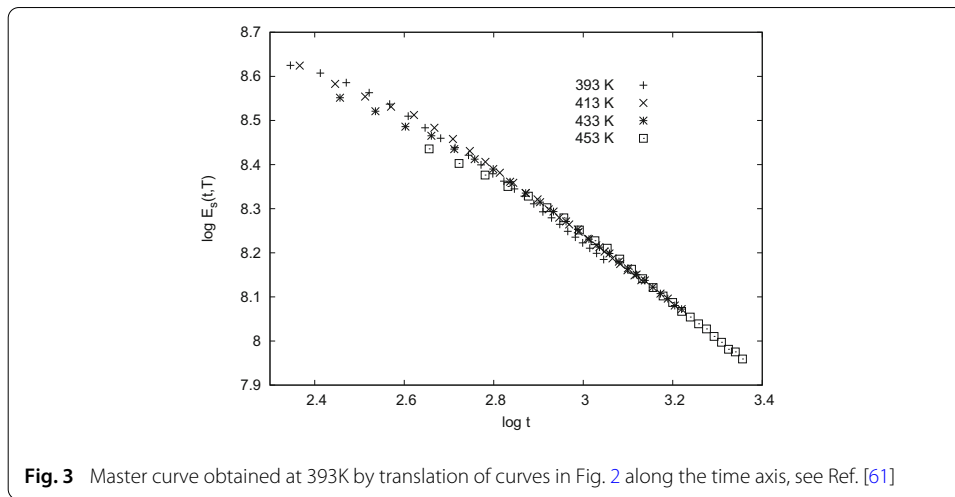
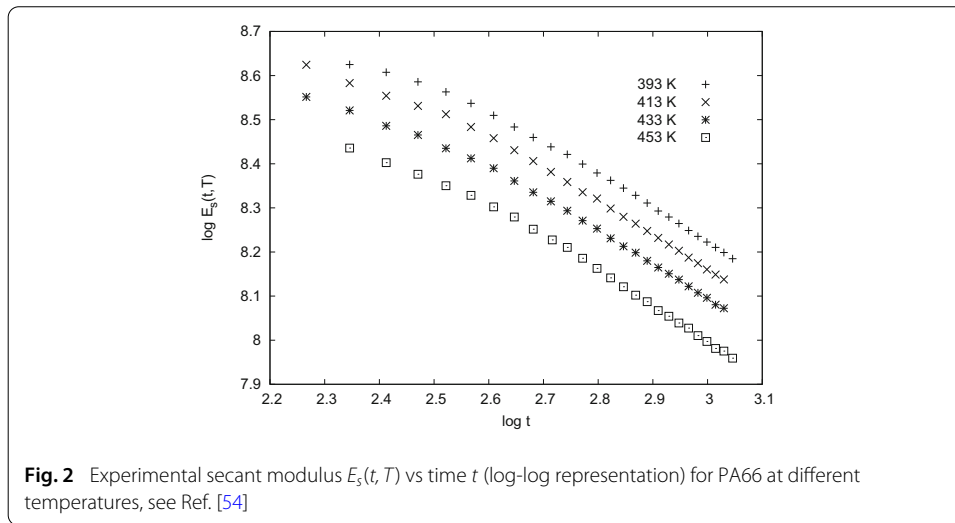
leading to the logarithmic relation between times:

$$\log \bar{t} = \log t + \frac{\mu}{\ln 10} \tag{4.38}$$

This allows rewriting Eq. (4.37) under the form:

$$E_s(\log t, T) = E_s(\log t + \frac{\mu}{\ln 10}, \bar{T}). \tag{4.39}$$

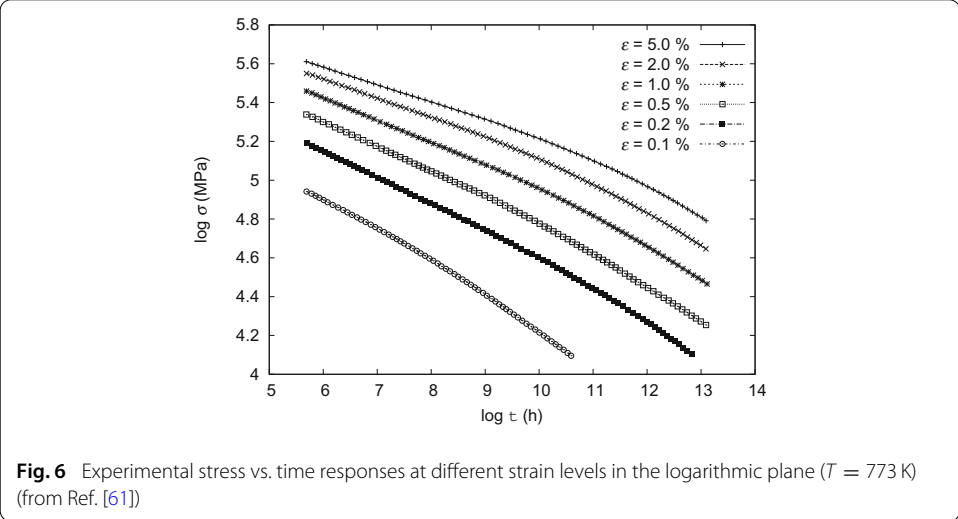
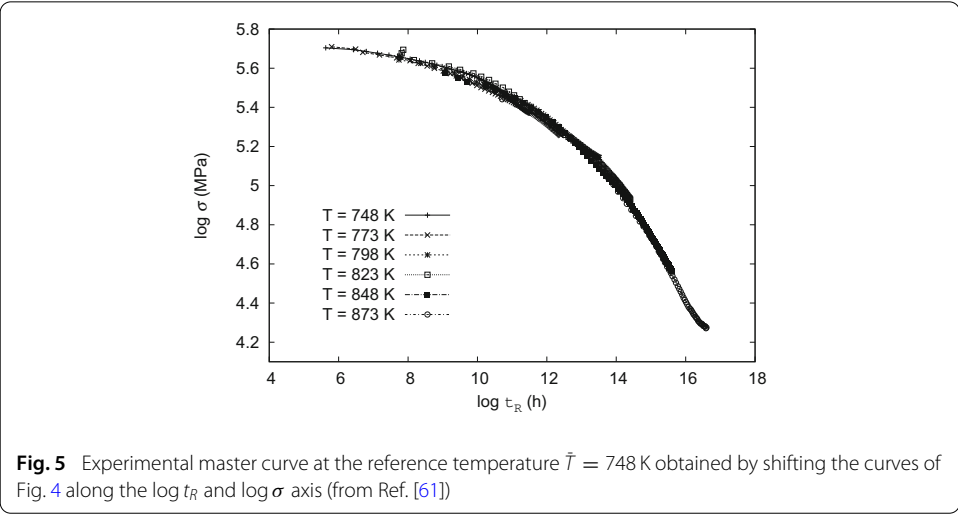
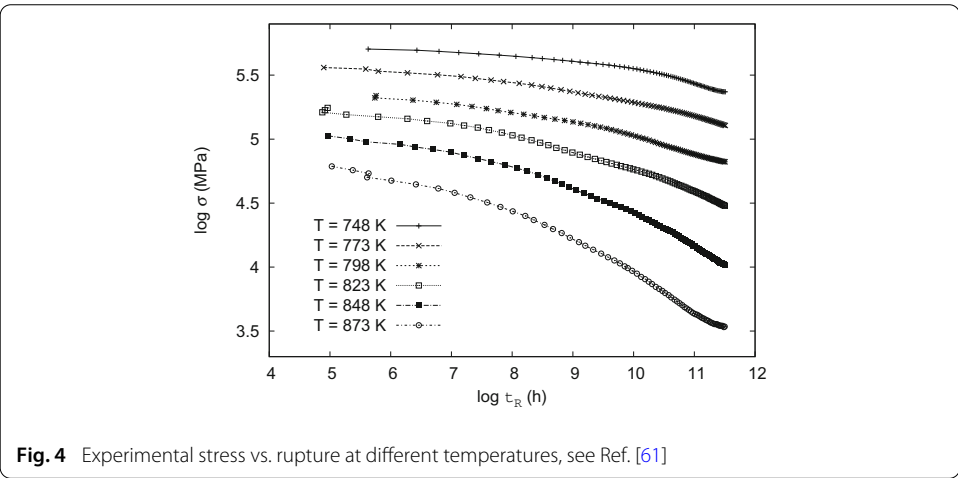
This relation links the two secant moduli $E_s(\log \bar{t}, \bar{T})$ and $E_s(\log t, T)$ obtained at \bar{T} and T by a translation by $\frac{\mu}{\ln 10}$ on the time logarithmic scale, given explicitly in Eq. (4.36). The obtained invariance property is a theoretical formulation of the time-temperature equivalence principle. The latter was successfully confirmed by experimental data on

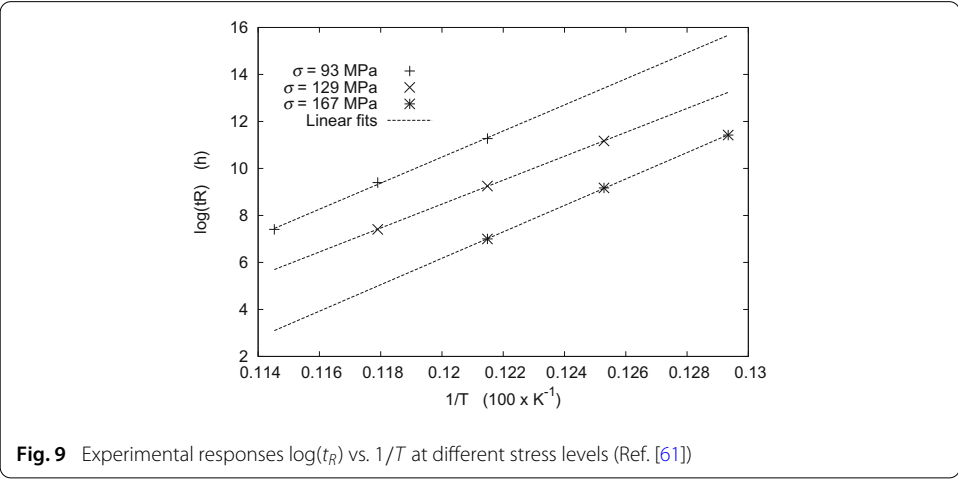
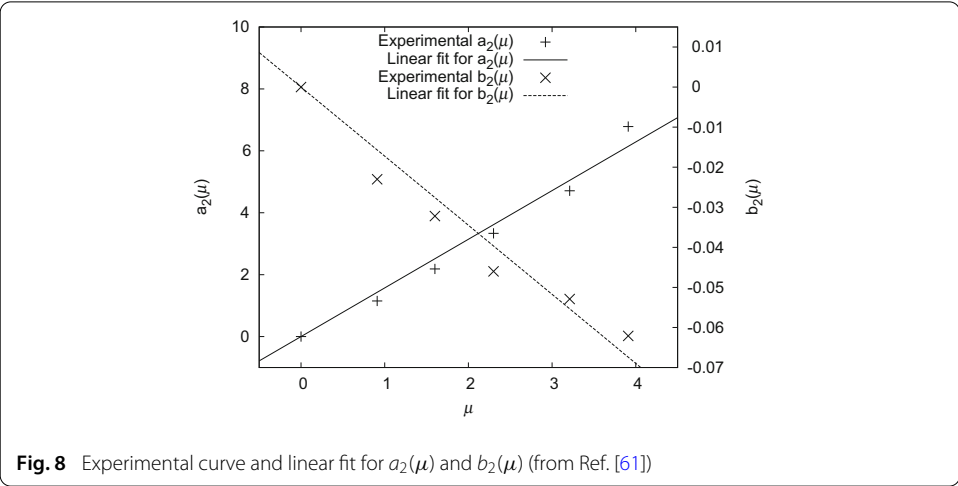
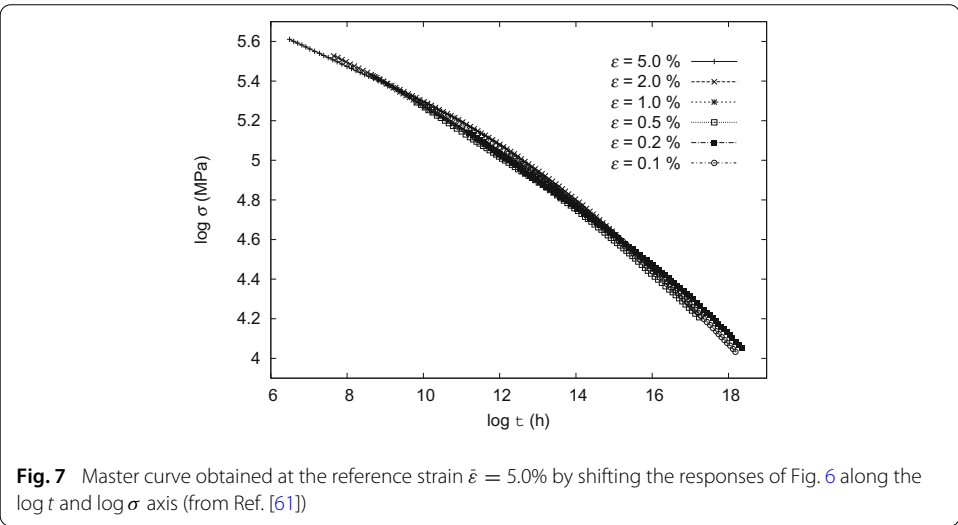


various materials, and fitted with the empirical Williams-Landel-Ferry (WLF) expression (see e.g. [55–57]) or the Kohlrausch relation ([58–60]).

As an illustration of the time-temperature equivalence principle, and referring to the experimental validation of the predicted shift factor (DM-P5), let consider the data summarized in Fig. 2. The evolution of the secant modulus $E_s(t, T)$ for isothermal tests on a polymer (polyamid 66, PA66) is plotted at different constant temperatures and for a given strain rate ($\dot{\epsilon} = 1.8 \times 10^{-4} \text{ s}^{-1}$). Every curve is parameterized by the temperature \bar{T} (in the range 413K – 453K) and can be translated along the $\log t$ axis with a horizontal shift factor $a_{\bar{T} \rightarrow T}$ to coincide with a unique curve. This unique curve is called “master curve” at the reference temperature $T = 393\text{K}$, see Fig. 3.

The notion of equivalence transformation is exemplified below for the case of nonlinear wave propagation in fiber-reinforced materials, showing that the initial model including several parameters can be reduced to a model with no arbitrary parameters.





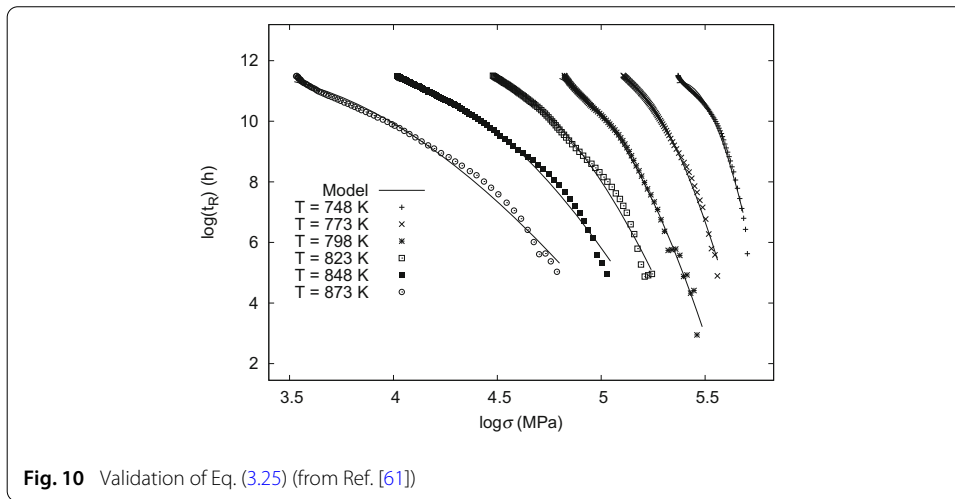


Fig. 10 Validation of Eq. (3.25) (from Ref. [61])

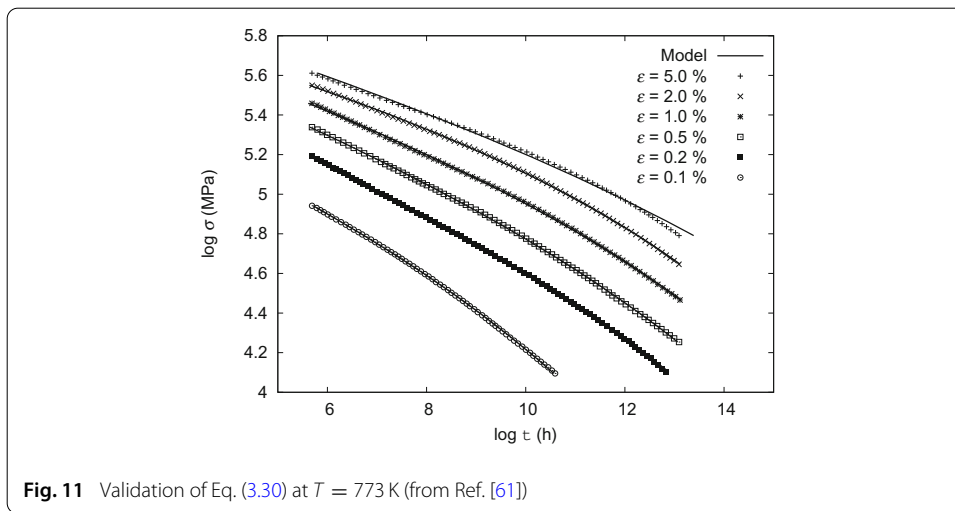


Fig. 11 Validation of Eq. (3.30) at $T = 773$ K (from Ref. [61])

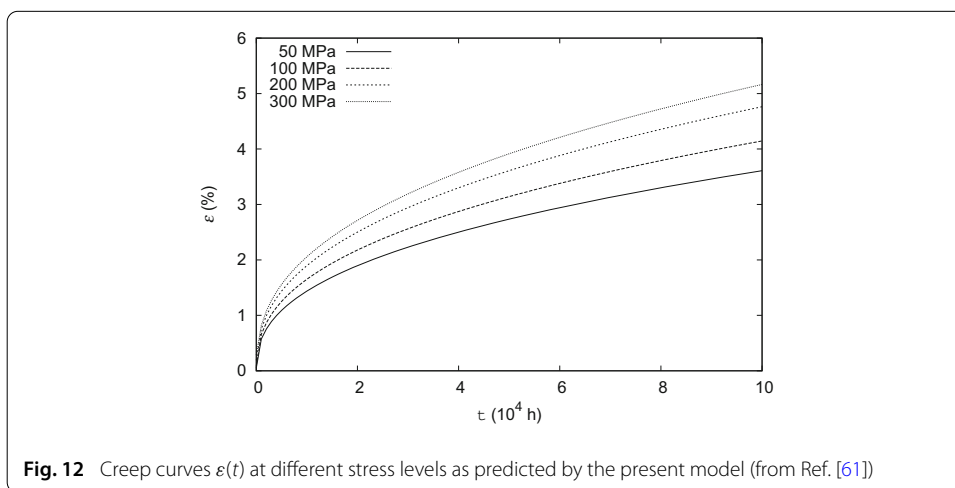
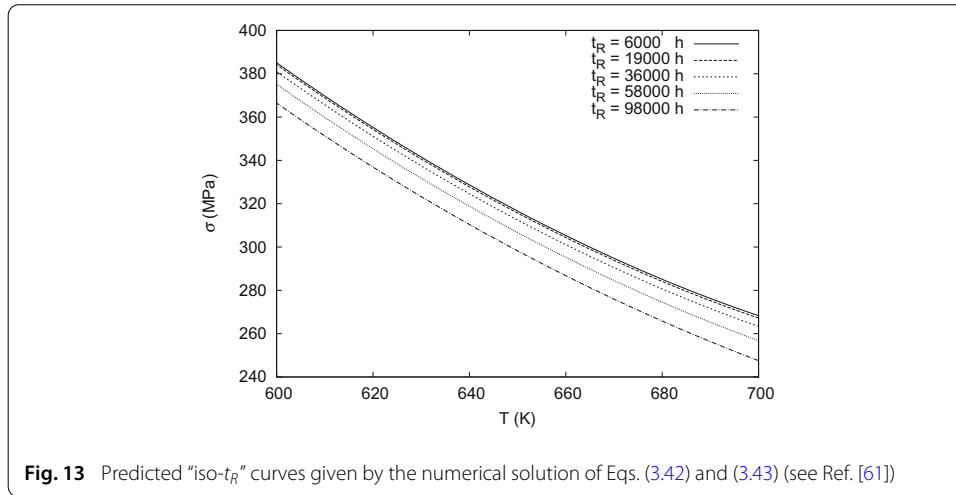


Fig. 12 Creep curves $\epsilon(t)$ at different stress levels as predicted by the present model (from Ref. [61])



Nonlinear anti-plane shear wave models for fiber-reinforced materials: equivalence transformations and constitutive model simplification

Multiple mechanical models of elastic structures such as biological and cell membranes, textiles, and rubbers, are modeled using the framework of incompressible hyperelasticity, which may include anisotropy effects such as a presence of elastic fibers [62]. In a solid body in three dimensions, the actual position $\mathbf{x} = (x_1, x_2, x_3)$ of a material point depends on its Lagrange coordinates $\mathbf{X} = (X_1, X_2, X_3)$ and time t :

$$\mathbf{x} = \boldsymbol{\phi}(\mathbf{X}, t).$$

The deformation gradient is given by

$$\mathbf{F}(\mathbf{X}, t) = \nabla \boldsymbol{\phi}, \quad F_{ij} = \frac{\partial \phi_i}{\partial X_j}; \tag{5.1}$$

for the incompressible case, the Jacobian $J = \det \mathbf{F} = 1$. The full system of equations of motion of an incompressible hyperelastic material in three dimensions is given by the Newton’s second law (momentum balance equation) and the incompressibility condition:

$$\rho_0 \mathbf{x}_{tt} = \text{div}_{(\mathbf{X})} \mathbf{P} + \rho_0 \mathbf{R}, \quad J = \det \mathbf{F} = 1. \tag{5.2}$$

In (5.2), ρ_0 is the Lagrangian mass density, \mathbf{P} is the first Piola-Kirchhoff tensor computed from the strain energy density W , and $\mathbf{R} = \mathbf{R}(\mathbf{X}, t)$ is the total body force per unit mass. The arbitrary element present in this class of models is the functional form of the strain energy density function W :

$$W = W_{iso}(I_1, I_2) + W_{aniso}(I_4, \dots, I_9),$$

where W_{iso} and W_{aniso} are isotropic and anisotropic contributions, respectively; I_1, I_2 are invariants of the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, and I_4, \dots, I_9 are pseudo-invariants involving fiber direction vectors (for details, see, e.g., [62,63], and references therein). A wide class of materials is described using Mooney-Rivlin isotropic energy part and the standard reinforcement anisotropic model [63]:

$$W = a(I_1 - 3) + b(I_2 - 3) + q(I_4 - 1)^2, \tag{5.3}$$

where $a, b, q > 0$ are constant material parameters.

In [63], it has been shown that for a shear wave propagating in X_1 -direction, i.e., with finite displacements $G(X_1, t)$ arising from the incompressibility-compatible ansatz

$$\mathbf{x} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 + G(X_1, t) \end{bmatrix},$$

in a medium with a single fiber family making an angle γ with the X_1 -direction, the displacement $G(X_1, t)$ satisfies

$$G_{tt} = (\alpha + \beta \cos^2 \gamma (3 \cos^2 \gamma (G_x)^2 + 6 \sin \gamma \cos \gamma G_x + 2 \sin^2 \gamma)) G_{xx} \tag{5.4}$$

(here for simplicity of notation, we have renamed X_1 by x in $G(X_1, t) \equiv G(x, t)$). The model involves three arbitrary elements, the material parameters $\alpha = 2(a + b) > 0$, $\beta = 4q > 0$, and the material fiber angle $\gamma \in [0, \pi/2]$.

When $\gamma = \pm\pi/2$, i.e., the fibers are aligned along the material z -direction, and the PDEs (5.4) reduce to the classical linear wave equations $G_{tt} = \alpha G_{xx}$, in particular, fiber effects vanish. When the fiber angle is $\gamma = 0$, i.e., when the wave propagates along the fibers, the equation (5.4) assumes a particularly simple form

$$G_t = (\alpha + 3\beta G_x^2) G_{xx}. \tag{5.5}$$

We now use the algorithm of Section 2.2 to compute equivalence transformations of the PDEs (5.4). For the sake of simplicity, we denote

$$k = \tan \gamma \in \mathbb{R}.$$

The PDE family (5.4) thus involves three arbitrary elements: α, β, k . The corresponding infinitesimal generators of point equivalence transformations (2.21) take the form

$$\mathbf{v} = \xi \frac{\partial}{\partial x} + \tau \frac{\partial}{\partial t} + \eta \frac{\partial}{\partial G} + \zeta^1 \frac{\partial}{\partial \alpha} + \zeta^2 \frac{\partial}{\partial \beta} + \zeta^3 \frac{\partial}{\partial k}. \tag{5.6}$$

For the current application, it is sufficient to consider regular equivalence transformations (2.14), so the dependencies of the infinitesimal components are chosen as follows:

$$\begin{aligned} \xi &= \xi(x, t, G), & \tau &= \tau(x, t, G), & \eta &= \eta(x, t, G), \\ \zeta^\nu &= \zeta^\nu(\alpha, \beta, k), & \nu &= 1, 2, 3. \end{aligned}$$

After the solution of determining equations, one obtains eight linearly independent basis generators of equivalence transformations, given by

$$\begin{aligned} \mathbf{v}_1 &= \frac{\partial}{\partial G}, & \mathbf{v}_2 &= \frac{\partial}{\partial x}, & \mathbf{v}_3 &= \frac{\partial}{\partial t}, & \mathbf{v}_4 &= t \frac{\partial}{\partial G}, \\ \mathbf{v}_5 &= t \frac{\partial}{\partial t} + x \frac{\partial}{\partial x} + G \frac{\partial}{\partial G}, & \mathbf{v}_6 &= -\frac{1}{2} t \frac{\partial}{\partial t} + \alpha \frac{\partial}{\partial \alpha} + \beta \frac{\partial}{\partial \beta}, \\ \mathbf{v}_7 &= -x \frac{\partial}{\partial x} - 2\alpha \frac{\partial}{\partial \alpha} - \frac{4\beta}{k^2 + 1} \frac{\partial}{\partial \beta} + k \frac{\partial}{\partial k}, \\ \mathbf{v}_8 &= -x \frac{\partial}{\partial G} + \frac{2\beta k}{(k^2 + 1)^2} \frac{\partial}{\partial \alpha} + \frac{4\beta k}{k^2 + 1} \frac{\partial}{\partial \beta} + \frac{\partial}{\partial k}. \end{aligned} \tag{5.7}$$

The transformation generator \mathbf{v}_8 in (5.7) corresponds to shifts in $k \equiv \tan \gamma$. The global group (2.26) is found by integration, and has the form

$$\begin{aligned} \bar{x} &= x, & \bar{t} &= t, & \bar{G} &= G - Sx, & \tan \bar{\gamma} &= \tan \gamma + \mu, \\ \bar{\alpha} &= \alpha + 2\beta \cos^4 \gamma \left(\frac{s^2}{2} + \mu \tan \gamma \right), & \bar{\beta} &= \beta \cos^4 \gamma \left(\tan^2 \gamma + 2\mu \tan \gamma + \mu^2 + 1 \right)^2, \end{aligned}$$

with a group parameter $\mu \in \mathbb{R}$. Choosing $\mu = -k = -\tan \gamma$, one invertibly maps the PDE (5.4) into the form (5.5) with $\tilde{\gamma} = 0$. This equivalence transformation is given by

$$x = \tilde{x}, \quad t = \tilde{t}, \quad G = \tilde{G} - x \tan \gamma, \quad \alpha = \tilde{\alpha} + \tilde{\beta} \tan^2 \gamma, \quad \beta = \tilde{\beta} \cos^{-4} \gamma. \tag{5.8}$$

The substitution of (5.8) into the full PDE (5.4) yields

$$\tilde{G}_{\tilde{t}\tilde{t}} = (\tilde{\alpha} + 3\tilde{\beta}(\tilde{G}_{\tilde{x}})^2) \tilde{G}_{\tilde{x}\tilde{x}} \tag{5.9}$$

with

$$\tilde{\alpha} = \alpha + \frac{\beta}{4} \sin^2 2\gamma, \quad \tilde{\beta} = \beta \cos^4 \gamma,$$

which is the “simpler” equation (5.5).

Note that the equation (5.9) has the parameter $\tilde{\alpha}^*$ that may not be positive. In particular, loss of hyperbolicity may occur when the coefficient of G_{xx} becomes negative [62]. A sufficient condition for the loss of hyperbolicity not to happen under the indicated transformation is given by

$$\sin^2(2\gamma) < \frac{4\alpha}{\beta}. \tag{5.10}$$

The condition (5.10) is satisfied for all fiber orientations γ , for example, in the common situation of relatively weak fiber contributions, $\beta < 4\alpha$. In this case, obvious non-dimensionalizing scaling transformations

$$\hat{x} = \frac{\tilde{x}}{L}, \quad \hat{t} = \frac{\sqrt{\tilde{\alpha}}\tilde{t}}{L}, \quad \hat{G} = \sqrt{\frac{3\tilde{\beta}}{\tilde{\alpha}}}\frac{\tilde{G}}{L}, \quad L \in \mathbb{R}^+ \tag{5.11}$$

of the PDE family (5.9) can be used to further map all these equations into a single nonlinear wave equation

$$\hat{G}_{\hat{t}\hat{t}} = (1 + (\hat{G}_{\hat{x}})^2) \hat{G}_{\hat{x}\hat{x}}. \tag{5.12}$$

Thus through systematically computed equivalence transformations, the PDE family (5.4) with three constitutive parameters is invertibly reduced to a wave equation (5.12) with *no arbitrary elements*. For properties of the PDE (5.12), sample numerical solutions of boundary value problems, and the extended versions of the model, see [62].

Discussion and concluding remarks

Lie symmetries and related ideas provide a set of powerful tools in the realm of mechanics of materials. While the Lie theory and related methods and ideas applicable to ODE/PDE models have been significantly extended to include nonlocal and approximate symmetries, methods of moving frames and co-frames, and various approaches to produce invariant (in some sense) numerical methods (e.g., [5,6,64–70]), it is usually the most basic and fundamental ideas and simplest Lie symmetry-based computations that yield most useful results for complex PDE models in nonlinear mechanics. In particular, symmetry ideas prove useful in many different ways to construct a constitutive law of a given material from experimental results, in terms of a functional relation between control variables and additional parameters. Thereby, symmetries are used to solve an inverse problem, assuming the measured data have a structure akin to a Lie group, when considering a continuous range of variation of the adopted parameters.

Once a set of constitutive equations (in other words, constitutive parameters and/or functions) is determined, equivalence transformations can be systematically sought and applied to relate and simplify the forms of constitutive dependencies, thereby leading to model reduction. Lie groups of symmetries, equivalence transformations, and related structures can be computed algorithmically using symbolic softwares, such as the GeM package for Maple [16–19] and other packages.

The knowledge of the Lie symmetries of the constructed constitutive model allows as a next step to extrapolate the material response for a continuous variation of the inherent parameters. This powerful and systematic methodology is especially interesting to predict the material's response for values of the parameters that are not easily accessible in experiments. In the context of model reduction, Lie symmetries constitute a powerful tool revealing the intrinsic invariance properties of boundary value problems formulated in the framework of TIP (thermodynamics of irreversible processes), and using these invariance properties to exhibit relations between the constitutive model variables and parameters having a physical meaning reflected by the free energy density and the dissipation potential. The present methodology exploiting Lie symmetries in a combined direct and inverse manner can potentially be applied to a wide class of materials with a complex rheology, including polymers, metals, ceramics, metallic and polymeric foams and constitutive laws, such as nonlinear elasticity, viscoelasticity and viscoplasticity, with or without damage.

For the above-discussed applications, work on the applications of symmetry-based methods will continue in various directions:

- Development of constitutive models synthesizing data issued from measurements, thereby using symmetry methods as an interpolation method, allowing to rely on a minimum amount of data.
- Applications in material modelling, since a natural framework for building constitutive models (including multiphysical couplings, material nonlinearities) is the thermodynamics of irreversible processes relying on energetic and dissipative potentials, the proposed Lagrangian formulation of dissipative constitutive laws proves convenient to articulate symmetries, conservation laws (invariance relations) and master responses giving a graphical representation of those invariance relations amongst variables and parameters.
- Extrapolation of existing models to enable predictions of the variation of parameters in a range where measurements can not easily be done.
- Reduction of the number of parameters in models to the minimum using equivalence transformations.
- Development of specialized symmetry-preserving numerical schemes for complex boundary value problems in continuum mechanics and thermodynamics.

Abbreviations

A_i : Lie algebra $\{\mathbf{v}_i^1, \dots, \mathbf{v}_i^{m_i}\}$ of the equation $\Delta_i = 0$; $\mathbf{A} = 0$: set of constitutive equations $\{\Delta_1 = 0, \dots, \Delta_n = 0\}$; ϵ : strain; $\dot{\epsilon}$: strain rate; G_i^{obs} : i^{th} Lie group formulated from experimental data; $\Phi_i^{p_k}$: transformation function of the parameter p_k for the i^{th} experimental group; $\Phi_i^{u_k}$: transformation function of the observable variable u_k for the i^{th} experimental group; K_i : set of indexes k such that $\mathbf{v}_i^{obs_k}$ is a symmetry of $\Delta_i = 0$; $\log x$: natural logarithm of x ; m : number of parameters (range of \mathbf{p}); m_i : range of K_i ; μ : parameter of a Lie group; n : number of observables (range of \mathbf{u}); n_i : number of generators in the Lie algebra A_i ; ϕ^x : x -component of a symmetry generator; \mathbf{p} : set of parameters $\{p_1, \dots, p_m\}$; P_j : domain of p_j (interval of variation); \mathcal{P} : Cartesian product $P_1 \times P_2 \dots \times P_m$, domain of \mathbf{p} ; $\text{pr}^0 \mathbf{v}$: prolongation of the vector field \mathbf{v} (no order specified); $\text{pr}^{(k)} \mathbf{v}$: k -order prolongation of the vector field \mathbf{v} ; Q : activation energy; q : number of "observed" symmetries; R : perfect gas constant; σ : Cauchy stress; t : time; t_R : time at rupture; T : absolute temperature; \mathbf{u} : set of observables

$\{u_1, \dots, u_n\}$; \mathbf{u}^{-j} : set of observables $\{u_1, \dots, u_{j-1}, u_{j+1}, \dots, u_n\}$; \mathcal{U}_i : domain of u_i ; \mathcal{U} : Cartesian product $\mathcal{U}_1 \times \mathcal{U}_2 \cdots \times \mathcal{U}_n$, domain of \mathbf{u} ; \mathcal{U}^{-j} : Cartesian product $\mathcal{U}_1 \times \cdots \times \mathcal{U}_{j-1} \times \mathcal{U}_{j+1} \cdots \times \mathcal{U}_n$, domain of \mathbf{u}^{-j} ; \mathbf{v}_i^{obs} : generator of the Lie group G_i^{obs} ; \mathbf{v}_i^j : j^{th} generator of the Lie algebra A_i ; $\tilde{\mathbf{x}}$: transformed value of the quantity \mathbf{x} by a Lie group.

Acknowledgements

The authors thank Vincent Magnenet for his contribution to parts of the theoretical developments and results presented in this paper.

Authors' contributions

Authors' contributions: all authors contributed approximately equally to 964 this manuscript.

Funding

A. C. is grateful to NSERC of Canada for research support through a Discovery grant RGPIN-2019-05570. Other funding: no funding.

Availability of data and material

Availability of data and materials: data used in graphs and tables is available in previous publications: see Refs. [41, 54, 61].

Competing interests

Not applicable

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Received: 18 December 2019 Accepted: 29 November 2020

Published online: 05 January 2021

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