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Part III
Research

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Virtual Production of Filaments and Fleeces

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1 Consistency out of Chaos—A Challenge for Production

Production processes for manufacturing continuous filaments and fleeces are on-line processes in which the individual process steps are highly coordinated with each other and integrated into a tightly linked chain. The process chain for fleeces formed from filaments consists of the operations melting, spinning, swirling, and deposition. Here, molten polymer exits an extruder via a tube and is distributed on a spinning plate, where it is pressed through capillary jets and spun to filaments by means of aerodynamic forces. The filaments are swirled in an open air jet, decelerated, and deposited on a moving conveyor belt. The overlapping of thousands of filaments produces a fleece, with its typically irregular and cloud-like structure. The application spectrum for fleeces is extremely broad and ranges from everyday products like diapers and vacuum cleaner bags to high-tech goods like battery separators and medical products. Naturally, filament spinning is also used in conjunction with further processing steps, in the production of technical yarn products or synthetic short-fibers, for example. Moreover, we include the production of fiber-like insulation materials, such as glass wool and mineral wool, in the category of filament production, since these processes are based on similar physical, albeit technically different, principles.

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The fluctuating characteristics of filaments and fleeces—a consequence of the stochastic, and often turbulence-induced, impacts on production processes—can lead to problems in product quality. In the spinning processes, for example, such problems might come in the form of fluctuations in filament diameter and strength, due to an unsteady temperature history during cooling. These problems can frequently be traced back to the economic necessity of high machine throughput rates and tight filament bundling. Above and beyond the problems of the individual filaments, fleeces also exhibit problems with fluctuations in the weight and strength of the material. These latter arise on a sufficiently small scale from the production principle itself, since a chaotic, turbulence-driven overlapping of the filaments takes the place of an expensive weaving procedure. The bold challenge faced by production is therefore to create *consistency out of chaos*, a challenge that has already resulted in the development of astonishing installations and processes through decades of technical advances in machine engineering. The currently available and continuously improving instruments for simulating such complex processes, however, represent a qualitatively new opportunity for the simulation-supported design and control of these installations and processes. With their help, it is now possible to take the next step toward creating even *more consistency out of chaos*.

2 Simulatable, but only in Principle—A Challenge for Mathematics

Fundamentally, almost all the steps in the process chain outlined above—melting and spinning, for filaments, plus swirling and deposition, for fleeces—can be viewed as continuum-mechanical, multi-phase problems. Depending on the degree of cooling and the stage in the process, one is treating a viscous, viscoelastic, or elastic filament phase, coupled with turbulent airflow, in a complex machine geometry. Classical continuum mechanics offers the models for such multi-phase problems. There is an abundance of numerical discretization ideas, solution algorithms, and even ready-made software tools in the arsenal of applied mathematicians and engineers. In other words, the problems can indeed be simulated, in principle. Unfortunately, however, *only in principle*.

A closer look reveals, in fact, the hopelessness of such a monolithic approach: as our examples of fleece production (Sect. 6) and glass wool production (Sect. 7) show, the actual production processes demand the coupled filament flow simulation of thousands of filaments having diameters as small as 10 microns in highly turbulent flows across macroscopic scales on the order of meters. The mathematical challenge is therefore to use modeling strategies such as homogenization and asymptotics, along with the generation of surrogate models having a grey box character, to prepare adequate models for all the partial aspects and then to couple these aspects together. After a thoroughgoing analysis of these models, numerical algorithms must then be developed and adapted to the problem. Only in this way can one portray the processes so as to allow realistic application scenarios to be computed in an acceptable time and, thus, made accessible to optimization. The procedure

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requires, in particular, the compatibility between the various modeling approaches, the derivation of coupling conditions, and the identification of model parameters. Using this procedure, we want to avoid the trap of *simulatable in principle*, and achieve instead the state of *simulatable in practice*, which will allow us to contribute significantly to the design and optimization of production processes. By concentrating diverse approaches from various mathematical areas in a single application domain, the Fraunhofer ITWM has an outstanding opportunity to substantiate its claim to be a problem-solver, to make innovative contributions to existing research into applied mathematics, and to initiate the exploration of brand new thematic areas. Our contribution to this book is designed to document the current state of our work, but we hope that it also generates a host of new questions.

3 Studies in Filament Dynamics and Fleece Production at the Fraunhofer ITWM

The work in filament dynamics at the Fraunhofer ITWM has its origins in a project that has absolutely nothing to do with filaments and their production processes. In 1995, the year the Institute was founded, we began work on simulating the paper flight in a printing press. This was one of the first industrial projects in the Transport Processes Department, and the starting point for at least two thematic areas that are today pursued in force within the Department. The largely two-dimensionally characterized flow of paper in a printing press is a coupled fluid-structure interaction problem. Therefore, particle methods were tested for the flow domains below and above the sheet, which are time variant due to sheet movement. For the sheet dynamics, shell models from continuum mechanics were refurbished, which, in their two-dimensional variant, are mathematically equivalent to rod models for filament dynamics. The work on particle methods led to development of the ITWM software FPM (Finite Pointset Method), which is today one of the best-performing grid-free simulation tools available on the market for a wide and still continuously growing field of continuum mechanical problems. The work on sheet dynamics was the breeding ground for all subsequent research in the area of filament dynamics, which is the subject matter of this chapter. This short story illustrates the enormous power generated by problem-oriented research in industrial projects: the specific questions breed approaches, which then often grow far beyond the original field of investigation and the short-term concerns of daily business.

In 1998, concurrently with the above-mentioned industrial printing press project, our contact with the company Freudenberg, which dates back to before the founding of the ITWM, was revitalized in Kaiserslautern in connection with the topic of fleece production. It took a while, however, before the tender sprout would grow into a large-scale Institute activity, whose salient points we want to selectively outline here. Our work in this area received an initial impulse in 2003, in the form of a large, in-house Fraunhofer project on market-oriented preparatory research. An accompanying dissertation [27] laid the foundation for our turbulent force model in 2005 (Sect. 4.3 and Ref. [9, 16, 17]). The

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following year witnessed the first ideas for stochastic model analogies for deposition simulations (Sect. 4.4 and Ref. [5, 6]). At the same time, again on the basis of a dissertation [29], work commenced on the asymptotic derivation of viscous string models [7, 20]. All three of these thematic areas have been widely pursued and thematically extended up to the present date (see development and status for *turbulent force modeling* [19], for the *stochastic surrogate lay down models* [8, 11–13], and for *asymptotic rod and string models* [1, 4, 14, 18]). Likewise, as a consequence of the above-mentioned Fraunhofer project, there has been an enormous broadening of our industrial customer base. Johns Manville (2003) and Oerlikon Neumag (2004) are examples of a fleece manufacturer and a machine designer in the field of technical textiles. Both remain today steady customers of the Fraunhofer ITWM.

It was then two projects sponsored by the BMBF at the start of this decade that set long-term developments in motion: the project 'Nano-melt-blown fibers for filter media' (NaBlo, 2008–2011) set the stage for our current work on *turbulence reconstruction for filament dynamics* [10]. In the project 'Stochastic production processes for the manufacturing of filaments and fleeces' (ProFil, 2010–2013), a consortium project in the BMBF mathematics program under the leadership of the Fraunhofer ITWM, the complete production chain for filaments and fleeces was simulated for the first time. Several PhD projects resulted either directly from the project [22, 23, 25, 28] or were offshoots from it [26, 30, 31]. These represent an important foundation for further investigations in this thematic area. The project also forms the basis for the current status of the central ITWM software for filament dynamics, the FIDYST suite, with the software tools FIDYST (Fiber Dynamics Simulation Tool, Sect. 5.1) and SURRO (Surrogate Model, Sect. 5.2). On the industrial side, our contact with the company Woltz (2010) and the resulting, on-going cooperation have proven extremely fruitful. Here, we were able to couple the filament and flow dynamics in a complex production process for the first time, in connection with the manufacture of glass wool (Sect. 7 and Ref. [3, 15]). The simulation toolbox VISFID (Viscous Fiber Dynamics, Sect. 5.3) for *coupled flow-filament simulations in spinning processes* was conceived in projects involving this production process.

Although this chapter discusses many of the above-mentioned topics, it makes no attempt to offer a complete historical portrayal. Instead, it attempts to present a cohesive overview from our current perspective. We therefore dedicate some space to the presentation of a consistent and integrated modeling basis (Sect. 4), before we then show the performance status of the software tools available today at the Fraunhofer ITWM (Sect. 5) and demonstrate their capabilities using two typical industrial applications as examples: the production of fleeces in the spunbond process (Sect. 6) and the production of glass wool via rotational spinning (Sect. 7). To promote readability, we offer annotations at various points that summarize more detailed aspects of the work and illustrate how it fits into the framework of current international research. Readers interested primarily in the applications can also begin with Sects. 6 and 7, follow the references to the simulation tools being used (Sect. 5), and consult with the underlying models (found in grey boxes in Sect. 4) as desired.

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In addition to the authors, substantial credit for the modeling ideas, software developments, and industrial projects that serve as the foundations for this chapter must be given to some of our current colleagues from the Transport Processes Department of the Fraunhofer ITWM (Sergey Antonov, Dr. Walter Arne, Dr. Christian Leithäuser, Dr. Robert Feßler, Dr. Simone Gramsch, Dr. Jan Mohring, Johannes Schnebele), as well as to some former colleagues (Dr. Daniel Burkhart, Dr. Marco Günther, Dr. Jalo Liljo, Dr. Ferdinand Olawsky). The past and current PhD projects mentioned here have been or are being supervised by Prof. Nicole Marheineke (FAU Erlangen-Nürnberg), Prof. Andreas Meister (Universität Kassel), and Prof. Hans Hagen, Prof. Axel Klar, Prof. Helmut Neunzert, Prof. Rene Pinnau, and Prof. Klaus Ritter (all from the TU Kaiserslautern).

4 Foundations of the Modeling

The *Cosserat rod theory* serves as the framework for the partial differential equation models considered here for filament dynamics. At their core are 1D balances for linear and angular momentum. These are complemented by *geometric models* for describing angular momentum, *material laws* for the emerging internal stress forces and moments, as well as models for the external forces acting on the system. In view of the target application, the *interaction of the filaments with the surrounding, often turbulent, airflow* is especially significant.

These Cosserat rod models can be used to successfully simulate single filaments in spinning and swirling processes. However, the significant computational effort prevents a virtual mapping of complete fleece deposition processes involving large numbers of filaments. Therefore, *surrogate models based on stochastic differential equations* (SODE) were developed and implemented at the Fraunhofer ITWM, which allow highly efficient simulations of the fleece deposition structure. The parameters of these surrogate models are identified using the Cosserat rod computations for single filaments.

Folklore and Convention We embed our continuum mechanical models in an abstract three-dimensional Euclidean space $\mathbb{E}^3$. In this space, we take $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ to be a fixed orthonormal basis (ONB). Such an ONB induces an isomorphism $i_e : \mathbb{E}^3 \to \mathbb{R}^3$, $\mathbf{a} \mapsto i_e(\mathbf{a}) = \bar{\mathsf{a}} = (\bar{a}_1, \bar{a}_2, \bar{a}_3)$ with $\bar{a}_j = \mathbf{a} \cdot \mathbf{e}_j$, $j = 1, 2, 3$. Because we are operating with different bases, it is important to us to always distinguish between the vectors $\mathbf{a} \in \mathbb{E}^3$ and their component tuples $\bar{\mathsf{a}} \in \mathbb{R}^3$ in the arbitrary, but fixed ONB $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. This is motivated largely by the fact that we also introduce, as a component of the Cosserat rod theory, a temporally and spatially (along the rod) varying director basis $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3\}$. The components of a vector $\mathbf{a}$ in this basis are denoted as $\mathsf{a} = (a_1, a_2, a_3)$. The canonical basis of $\mathbb{R}^3$ (that is, the component tuples of any ONB in relation to itself) is denoted by $\mathsf{e}_1, \mathsf{e}_2, \mathsf{e}_3$.

We use a tensor calculus that is oriented on the calculus of Antman [32]. That is, we consistently use the point $\cdot$ for scalar products and tensor-vector operations; we make no distinction between vectors of $\mathbb{E}^3$ and their adjoints; and, consequently, no distinction

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between row and column vectors of $\mathbb{R}^3$. In contrast to [32], however, we use $\otimes$ in place of a blank space for tensor products. 3×3-matrices are identified with tensors having values in $\mathbb{R}^3 \otimes \mathbb{R}^3$ and are frequently, with respect to a basis, the components of tensors with values in $\mathbb{E}^3 \otimes \mathbb{E}^3$. For all further details of our selected calculus, we refer the reader to [32]. We use a generalized summation convention in which Latin indices run between 1 and 3 and Greek indices, between 1 and 2.

Because we are mainly examining modeling aspects, we generally assume, for the needed manipulations, that there is sufficient differentiability and invertibility—as was just needed—and we do not usually critically reflect upon these points. This does not mean that we consider such reflections superfluous, or that all models we examine have classical solutions. Quantities are always introduced with their SI units, unless this is completely trivial (or forgotten!). Frequently, this clarifies their physical significance better than many words.

4.1 Cosserat Rod Theory

The Cosserat rod theory describes a filament as a spatial curve with oriented cross-sections. This results in a 1D manifold embedded in 3D, to which an element of the rotation group $SO(3)$ is differentiably assigned at each point. The theory is characterized by 1D balances for linear and angular momentum, which result from 3D continuum mechanics by averaging over the cross-sectional areas and restricting degrees of freedom. These restrictions mean that a re-orientation of the cross-sections can indeed be described, but not a genuine deformation that overcomes their planarity. We largely follow [32] in introducing the theory in a material parameterization (Lagrangian description), but we place a general and spatial variant (Eulerian description) on an equal footing alongside it. We take pains to present the theory as self-contained and reflect upon its embedding in 3D continuum mechanics as little as possible. Nevertheless, this embedding can be undertaken in order to thereby identify all elements of the theory in 3D continuum mechanics.

4.1.1 Material Description

Reference State A Cosserat rod or filament is described in its reference state by a curve $\mathbf{r}^\circ : (s_a, s_b) \to \mathbb{E}^3$ and two normalized, orthogonal vectors $\mathbf{d}^\circ_\alpha : (s_a, s_b) \to \mathbb{E}^3$, which are referred to as directors.

One also defines $\mathbf{d}^\circ_3 = \mathbf{d}^\circ_1 \times \mathbf{d}^\circ_2$, so that the directors form a right-handed orthonormal system. The reference state can be assumed for any given point in time, but this is not actually imperative. The interval $(s_a, s_b) \subset \mathbb{R}$ addresses the section of the filament whose dynamic is to be subsequently described. A parameter $s \in (s_a, s_b)$ addresses the materially-determined cross-section of the filament to be modeled. For our applications concerning filament dynamics, we require that $\mathbf{d}^\circ_3 = \partial_s \mathbf{r}^\circ$ and $\partial_s \mathbf{d}^\circ_i = \mathbf{0}$ for the reference state. The geometry and material models formulated in Sect. 4.2 are attuned to this reference state. More precisely, they ensure an absence of tension and torque in the reference state. With

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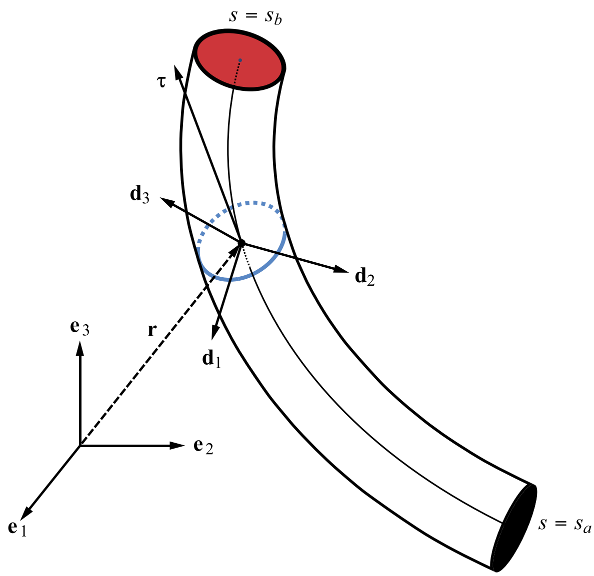

Fig. 1 Cosserat rod, consisting of curve and director triad (Graphic: Steffen Grützner, Fraunhofer ITWM)

these assumptions, we select, in particular, an arc-length parameterization of the reference state, but only of the reference state.

Kinematics At an arbitrary point in time t, the state of the rod is defined by the curve $\mathbf{r}(\cdot, t)$ and the orthonormal directors $\mathbf{d}_\alpha(\cdot, t)$, where $\mathbf{d}_\alpha \cdot \mathbf{d}_\beta = \delta_{\alpha\beta}$. The curve describes the position and the directors describe the orientation of the cross-sections addressed by s (Fig. 1). Using the consistently applied definition $\mathbf{d}_3 = \mathbf{d}_1 \times \mathbf{d}_2$, the directors form a right-handed orthonormal system at all times. Both the referential linking of $\mathbf{d}_3$ with the tangent $\partial_s \mathbf{r}$ and the arc-length parameterization, however, are generally not valid in a moving state.

The velocity and tangent of the rod are characterized by the vector fields

$$\partial_t \mathbf{r} = \mathbf{v}, \qquad \partial_s \mathbf{r} = \boldsymbol{\tau}.$$

Because the directors form a right-handed orthonormal system, there exist also unambiguous vector fields $\boldsymbol{\kappa}$ (1/m) (curvature) and $\boldsymbol{\omega}$ (1/s) (angular velocity), so that the equations

$$\partial_t \mathbf{d}_i = \boldsymbol{\omega} \times \mathbf{d}_i, \qquad \partial_s \mathbf{d}_i = \boldsymbol{\kappa} \times \mathbf{d}_i$$

are valid. These vector fields describe the change in the triad over time, and along the curve. By changing the order of the partial derivatives with respect to t and s, one obtains the following compatibility relations:

$$\partial_t \boldsymbol{\tau} = \partial_s \mathbf{v}, \qquad \partial_t \boldsymbol{\kappa} = \partial_s \boldsymbol{\omega} + \boldsymbol{\omega} \times \boldsymbol{\kappa}.$$

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In order to use the Cosserat rod theory in specific applications, it proves helpful to represent vector fields and model equations partially mixed in two basis systems (external basis and director basis). The change from the invariant formulation to a fixed external basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ is, in this instance, trivial. The transition from the external to the director basis $\{\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3\}$ can always be accomplished technically using the following calculus. As agreed, for an arbitrary vector field $\mathbf{a} \in \mathbb{E}^3$ of the rod, $\bar{\mathsf{a}} \in \mathbb{R}^3$ and $\mathsf{a} \in \mathbb{R}^3$ denote the component tuples relative to the external basis or the director basis. The director basis is transformed with the rotation

$$\mathbf{D} = \mathbf{e}_i \otimes \mathbf{d}_i = D_{ij}\mathbf{e}_i \otimes \mathbf{e}_j \in \mathbb{E}^3 \otimes \mathbb{E}^3 \quad \text{with } D_{ij} = \mathbf{d}_i \cdot \mathbf{e}_j$$

into the external basis. The orthogonal matrix D is assigned to the components D_{ij} of this rotation. If one now considers an arbitrary vector field of the rod, then

$$\mathsf{D} \cdot \bar{\mathsf{a}} = \mathsf{a}, \qquad \mathsf{D} \cdot \partial_t \bar{\mathsf{a}} = \partial_t \mathsf{a} + \omega \times \mathsf{a}, \qquad \mathsf{D} \cdot \partial_s \bar{\mathsf{a}} = \partial_s \mathsf{a} + \kappa \times \mathsf{a}.$$

Moreover, the kinematic base equations for the directors can be transformed into corresponding equations for the rotation matrix:

$$\partial_t \mathsf{D} = -\omega \times \mathsf{D}, \qquad \partial_s \mathsf{D} = -\kappa \times \mathsf{D}.$$

This formulation of the kinematics also serves as the starting point for other representations of the rotation group (Euler angles, unit quaternions, rotation vectors), each of which has its merits, depending on the application.

The fundamental deformation variables for the formulation of objective material laws are the component tuples τ and κ of tangent and curvature in the director basis. More precisely, τ_1 and τ_2 quantify shearing, τ_3, strain, κ_1 and κ_2, bending, and κ_3, torsion. Moreover, with

$$e = \|\boldsymbol{\tau}\|$$

we introduce a further strain measure that refers solely to the curve.

Dynamics Balancing linear and angular momentum (dynamic equations) for a rod leads to the following generalized forms:

$$(\rho A)\partial_t \mathbf{v} = \partial_s \mathbf{n} + \mathbf{k}, \qquad \partial_t \mathbf{h} = \partial_s \mathbf{m} + \boldsymbol{\tau} \times \mathbf{n} + \mathbf{l}.$$

The line density of the rod (ρA) (kg/m) in the reference state is traditionally designated using a slightly confusing symbol that suggests a product. When embedded in 3D continuum mechanics, it results in the integral of the density over the cross-section of the rod in the reference state, and is thus dependent on the filament parameter s, but not on the

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time t. The angular momentum line density $\mathbf{h}$ (kg m/s) is described as a function of the remaining base quantities of our theory, in particular, of the angular velocity (see geometric modeling, Sect. 4.2.1). The internal stress forces $\mathbf{n}$ (N) and torques $\mathbf{m}$ (N m) are modeled via suitable material laws as functions of the internal variables. Section 4.2.2 consists primarily of a discussion of two types of such material laws—elastic and viscous. In the dynamic equations, $\mathbf{k}$ (N/m) and $\mathbf{l}$ (N) denote line force density and line torque density for modeling the external force and torque effects on the rod. Each of these can depend on different internal variables and thus decisively impact the coupling of the dynamic and kinematic equations. In the following discussion, we generally restrict ourselves to models with no external moment effects; that is, $\mathbf{l} = \mathbf{0}$. Ultimately, geometric modeling, material laws, and external forces are the primary determinants of the type of PDE system.

4.1.2 General and Spatial Description

So far, the entire theory has been formulated in a Lagrangian description; that is, the parameter $s \in (s_a, s_b)$ addresses a material point (or cross-section) of the rod. Except for the orientation and a constant, the parameterization is then completely determined by requiring the arc-length parameterization of the reference state. This is not essential, but it simplifies much of the treatment. As we show below, a simple typing concept for the theory's base quantities can be used to formulate the model equations very easily in any other time-dependent parameterization. Without doubt, the most important application case is the spatial description (Eulerian description), in which, for all times, the transformation is made to an arc-length parameterization.

Parametrizations Suitable time-dependent re-parameterizations can be introduced with bijective transformations

$$\phi(\cdot, t) : (s_a, s_b) \to \big(\varphi_a(t), \varphi_b(t)\big), \quad s \mapsto \phi(s, t).$$

In order to define the transformation behavior of the different fields of the Cosserat rod theory, we introduce the term type-n-quantity. A type-n-quantity, $n \in \mathbb{Z}$, is transformed as follows:

$$j^n(s,t)\tilde{f}\big(\phi(s,t), t\big) = f(s,t), \quad j = \partial_s \phi.$$

Here, $f(s,t)$ characterizes a type-n-quantity in the material parameterization (Lagrangian description) and $\tilde{f}(\varphi, t)$ characterizes the associated field in the new parameterization. For the different fields of our theory, we specify that $\mathbf{r}$, $\mathbf{d}_i$, $\mathbf{v}$, $\boldsymbol{\omega}$, $\mathbf{n}$, $\mathbf{m}$ are to be treated as type-0-quantities and $\boldsymbol{\tau}$, $\boldsymbol{\kappa}$, $\mathbf{k}$, $\mathbf{l}$, (ρA), $\mathbf{h}$ as type-1-quantities. This specification allows the various quantities to retain their physical character and defining interrelationships (point-related observables, densities, derivatives, etc.) in the transformation. Time-independent re-parameterizations do not disturb the material character of the parameterization, nor do they change the form of the base equations. In contrast, time-dependent