

MR3673049 76A05 35Q35

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Circumventing the lack of dissipation in certain Oldroyd models. (English, French summaries)

C. R. Math. Acad. Sci. Paris **355** (2017), no. 7, 753–759.

Summary: “We modify an argument of Renardy proving existence and regularity for a subset of a class of models of non-Newtonian fluids suggested by Oldroyd, including the upper-convected and lower-convected Maxwellian models. We suggest an effective method for solving these models, which can provide a variational formulation suitable for finite element computation.”

Following [M. Renardy, *Z. Angew. Math. Mech.* **65** (1985), no. 9, 449–451; MR0814684; *Z. Angew. Math. Mech.* **68** (1988), no. 4, T40–T44; MR0944503], the authors offer a Sobolev-space analysis of the existence and regularity of solutions to the equations of motion (linear momentum balance) for the well-known “3-parameter” Oldroyd model of non-linear viscoelasticity:

$$(1) \quad \mathbf{T} + \lambda \mathfrak{D}_t \mathbf{T} = \mu(\mathbf{E}\mathbf{T} + \mathbf{T}\mathbf{E}) + 2\eta\mathbf{E},$$

where \mathbf{T} is Cauchy stress, $\mathfrak{D}_t \mathbf{T} = \partial_t \mathbf{T} + \mathbf{u} \cdot \nabla \mathbf{T} + \mathbf{T}\mathbf{W} - \mathbf{W}\mathbf{T}$ its Jaumann or “corotational” rate, with $\mathbf{E} = (\nabla \mathbf{u} + \nabla \mathbf{u}^T)/2$ and $\mathbf{W} = (\nabla \mathbf{u} - \nabla \mathbf{u}^T)/2$ denoting, respectively, the deformation rate and vorticity of the velocity field $\mathbf{u}(t, \mathbf{x})$. The three parameters in question are λ, μ, η , where inessential subscripts have, here, been discarded. The authors offer a presumably improved iterative method which they claim could lead to improved numerical simulations, although they provide no illustrative calculations.

As a minor terminological quibble, it should be pointed out that (1) generally does not serve to define a “deviatoric” (i.e. traceless) stress, which \mathbf{T} is declared to be by the authors. However, for the incompressible fluids assumed in the present work, the stress is in any event defined rheologically only up to an additive isotropic pressure.

In the course of their analysis, the authors introduce a fictitious velocity field $\tilde{\mathbf{u}} = \lambda \mathbf{u}$ (which they denote by \mathbf{v}) that is reminiscent of but quite distinct from the classical Johnson-Segalman [M. W. Johnson, Jr and D. Segalman, *J. Non-Newton. Fluid Mech.* **2** (1977), no. 3, 255–270, doi10.1016/0377-0257(77)80003-7] “non-affine” deformation rate $\tilde{\mathbf{E}} = \mu \mathbf{E}/\lambda$. The latter serves to define a local but globally incompatible deformation gradient given by the Lagrangian ODEs

$$(2) \quad \dot{\tilde{\mathbf{F}}} = d_t \tilde{\mathbf{F}} = \partial_t \tilde{\mathbf{F}} + \mathbf{u} \cdot \nabla \tilde{\mathbf{F}} = \tilde{\mathbf{L}} \tilde{\mathbf{F}}, \quad \text{where } \tilde{\mathbf{L}} = \tilde{\mathbf{E}} + \mathbf{W},$$

with $\tilde{\mathbf{L}}$ denoting a fictitious velocity gradient. This serves to define the counterparts of the Cauchy-Green strain and its work-conjugate (second Piola-Kirchhoff) stress, respectively, by

$$(3) \quad \tilde{\mathbf{C}} = \tilde{\mathbf{F}}^T \tilde{\mathbf{F}} \quad \text{and} \quad \tilde{\mathbf{S}} = \tilde{\mathbf{F}}^{-1} \mathbf{T} \tilde{\mathbf{F}}^{-T},$$

where superscript $\pm T$ define transpose and inverse transpose, respectively. It follows that (1) can be reduced to the Lagrangian ODE

$$d_t \tilde{\mathbf{S}} + \frac{1}{\lambda} \tilde{\mathbf{S}} = -G d_t \tilde{\mathbf{C}}^{-1},$$

where $G = \eta/\lambda$ represents an elastic modulus. This ODE can be formally integrated to

give a Maxwell-type integral representation of stress in terms of fictitious strain history determined by (2). This establishes a crucial connection between the “rate-type” ODE model and the integral model. Should this prove useful, it is worth noting that a larger subset of Oldroyd’s 8-parameter model can be treated by adopting a more general form for $\tilde{\mathbf{E}}$, of the type proposed elsewhere [J. D. Goddard, *Adv. Appl. Mech.* **19** (1979), 143–219 (pp. 151ff), doi10.16/S0065-2156(08)70310-7].

Note that (3) can also be rewritten in terms of a nominal elastic potential and a dissipation potential given respectively by

$$\varphi_e(\tilde{\mathbf{S}}) = \tilde{\mathbf{S}} \cdot \tilde{\mathbf{S}}/2G \quad \text{and} \quad \varphi_d(\tilde{\mathbf{S}}) = \tilde{\mathbf{S}} \cdot \tilde{\mathbf{S}}/2\eta,$$

with nominal elastic and dissipative deformation rates

$$d_t \tilde{\mathbf{C}}_e = d_t(\partial_{\tilde{\mathbf{S}}} \varphi_e) \quad \text{and} \quad d_t \tilde{\mathbf{C}}_d = \partial_{\tilde{\mathbf{S}}} \varphi_d.$$

In this respect, the present model represents a variant of the “Generalized Standard Material” of B. Halphen and Nguyen Quoc Son [*J. Mécanique* **14** (1975), 39–63; [MR0416177](#)], whose relevance to the rheology of complex fluids has been discussed in the treatise of P. Saramito [*Complex fluids*, Math. Appl. (Berlin), 79, Springer, Cham, 2016 (Section 5.3); [MR3560883](#)]. Because of this, the reviewer has some difficulty understanding the lack of dissipation attributed to the Oldroyd model by the work at hand. *Joe D. Goddard*

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thesis, University of Lisbon, Portugal, 1997.

Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.

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Citations

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From Reviews: 0

MR3624977 74A30 74Q15

Placidi, Luca; **Andreaus, Ugo** [**Andreaus, Ugo A.**] (I-ROME-NDM);
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Identification of two-dimensional pantographic structure via a linear D4 orthotropic second gradient elastic model. (English summary)

J. Engrg. Math. **103** (2017), 1–21.

Summary: “A linear elastic second gradient orthotropic two-dimensional solid that is invariant under 90° rotation and for [*sic*] mirror transformation is considered. Such anisotropy is the most general for pantographic structures that are composed of two identical orthogonal families of fibers. It is well known in the literature that the corresponding strain energy depends on nine constitutive parameters: three parameters related to the first gradient part of the strain energy and six parameters related to the second gradient part of the strain energy. In this paper, analytical solutions for simple problems, which are here referred to the heavy sheet, to the nonconventional bending, and to the trapezoidal cases, are developed and presented. On the basis of such analytical solutions, gedanken experiments were developed in such a way that the whole set of the nine constitutive parameters is completely characterized in terms of the materials that the fibers are made of (i.e., of the Young’s modulus of the fiber materials), of their cross sections (i.e., of the area and of the moment of inertia of the fiber cross sections), and of the distance between the nearest pivots. On the basis of these considerations, a remarkable form of the strain energy is derived in terms of the displacement fields that closely resembles the strain energy of simple Euler beams. Numerical simulations confirm the validity of the presented results. Classic bone-shaped deformations are derived in standard bias numerical tests and the presence of a floppy mode is also made numerically evident in the present continuum model. Finally, we also show that the largeness [*sic*] of the boundary layer depends on the moment of inertia of the fibers.”

This work provides an interesting extension of previous applications cited by the authors of second-gradient elasticity to the continuum descriptions of orthotropic fiber lattices or “fabrics”. This provides improvements on the classical treatments cited below in the present review. The authors employ a somewhat unusual terminology, “pantographic structure” and “pivots” for “lattice” or “truss” and “joints”. They include inertial effects arising in lattice dynamics, effects which have also been treated recently in a similar analysis [S. C. Pradhan and A. Kumar, *Compos. Struct.* **93** (2011), no. 2, 774–779, doi:10.1016/j.compstruct.2010.08.004]. They also identify static material instabilities in the form of “floppy modes” associated with the vanishing of certain shear moduli, which appear to represent a well-known linear-elastic instability of cubic lattices

in any space dimension, identified in a previous study [J. Christoffersen, *J. Appl. Mech.* **47** (1980), no. 1, 71–74, doi:10.1115/1.3153640].

Joe D. Goddard

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Citations	From References: 0	From Reviews: 0
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MR3605103 74A25 70F10 82C05 82C70

Yang, Zidong (1-GWU-MAE); **Lee, James D.** (1-GWU-MAE);

Liu, I-Shih (BR-FRJ-IM); **Eskandarian, Azim** (1-VAPI-ME)

On non-equilibrium molecular dynamics with Euclidean objectivity. (English summary)

Acta Mech. **228** (2017), no. 2, 693–710.

Summary: “In continuum mechanics, the concept of objectivity requires that the qualitative and quantitative description of physical phenomena remains unchanged under a change in reference frame. It means that the observations in different reference frames are coherent and thus the observed motions can be regarded as objectively equivalent. On the other hand, concerning the material constitution, the principle of material objectivity (also often referred as principle of material frame-indifference, or simply the principle of objectivity) requires that constitutive equations of a material body must be independent of the observer (reference frame). Both objectivity and principle of objectivity have been widely used in modern continuum mechanics studies. However, in molecular dynamics (MD) simulation, which is a prevalent numerical method in nanoscience, consideration is rarely given to the concept of objectivity or principle of objectivity since most of the MD simulations have been performed in inertial systems, where Galilean-invariance is assumed. This research aims to investigate the conditions for Euclidean objectivity in non-equilibrium molecular dynamics (NEMD), where reference frames are non-inertial and multi-physics effects are present in the atomistic material system. By supplementing fictitious acceleration to the governing equation and requiring the principle of objectivity on the constitutive equation, this research arrives at a special solution for NEMD that is Euclidean-invariant. Several sets of simulations demonstrate that equivalent motions can be achieved in NEMD. This study may provide new directions for future MD applications.”

This is yet another addition to the voluminous literature on the so-called *principle of material frame-indifference* (MFI) or *principle of material objectivity*, enunciated in the celebrated encyclopedia article by C. A. Truesdell III and W. Noll [in *Handbuch der Physik, Band III/3*, 1–602, Springer, Berlin, 1965; MR0193816] and adopted thereafter in countless textbooks and research papers on continuum mechanics (e.g., G. A. Maugin [*Continuum mechanics through the twentieth century*, Solid Mech. Appl., 196, Springer, Dordrecht, 2013 (p. 65); MR3057677] offers an authoritative historical perspective), as indicated in the above abstract. As implied by the above abstract, MFI asserts that constitutive equations for various tensorial fluxes must be invariant under time-dependent affine transformations of material or observer. In particular, if two histories of material deformation differ only by a time-dependent affine transformation, consisting of a time-dependent translation plus a rigid body rotation, then all tensorial fluxes at the present time must, according to MFI, transform as if the rotation and translation had always been given by their present value. This static transformation is of course mathematically equivalent to a static change of Cartesian coordinates in Euclidean

space, which the present authors ostensibly designate as “Euclidean-invariant”. Fluxes which transform this way are said to be *objective*.

Insofar as this principle applies to continuum-level constitutive equations for real materials composed of molecules with collective motion governed by Newtonian mechanics, there are legitimate concerns as to the validity of MFI. Such concerns are most readily grounded in the observation that Newton’s Second Law (in its simplest form) holds only in mechanically privileged frames of reference, namely inertial (or Galilean) frames, whereas other frames involve extraneous body forces arising from frame acceleration. Thus, the landmark paper of I. Müller [Arch. Rational Mech. Anal. **45** (1972), no. 4, 241–250; [MR1553565](#)] concludes that the stress and heat flux given by the kinetic theory of gases do not satisfy MFI. According to this analysis, the MFI breaks down on the same (collisional) time scales as the Newtonian approximation, such that *there can exist no frame-indifferent Newtonian gas*.

Müller’s analysis was promptly challenged by the preeminent advocate of MFI [C. Truesdell, Meccanica **11** (1976), no. 4, 196–199, [doi:10.1007/BF02128292](#)], and the ensuing controversy is reflected in numerous papers and reviews, notably [A. I. Murdoch, Proc. R. Soc. Lond. Ser. A **380** (1982), no. 1779, 417–426, [doi:10.1098/rspa.1982.0050](#); A. I. Murdoch, Arch. Rational Mech. Anal. **83** (1983), no. 2, 185–194; [MR0697958](#); M. Heckl and I. Müller, Acta Mech. **50** (1983), no. 1-2, 71–95, [doi:10.1007/BF01170442](#); C. G. Speziale, Appl. Mech. Rev. **51** (1998), no. 8, 489–504, [doi:10.1115/1.3099017](#)] as well as more recent papers [I.-S. Liu, Contin. Mech. Thermodyn. **17** (2005), no. 2, 125–133; [MR2145456](#); I.-S. Liu and R. Sampaio, Acta Mech. **225** (2014), no. 2, 331–348; [MR3160656](#)] co-authored by one author of the paper reviewed here. It is curious that the present paper cites none of this background literature, *not even the papers of one of the co-authors* that contain some of this background, including a debate with Murdoch over the issue at hand.

As for technical content, the present paper may be viewed as the numerical (NEMD) counterpart of Müller’s kinetic theory and, as such, is clearly capable of simulating much denser and more complicated molecular systems.

The authors’ somewhat elusive terminology makes for a certain difficulty of interpretation. Thus, “objectivity” apparently morphs into “Euclidean objectivity”, whose connection to the “Euclidean-invariance” introduced later in the paper is not immediately evident. At any rate, it seems that, as one of the stated contributions of the present work, the authors recast the NEMD momentum balances in terms of a “Euclidean-invariant” form arising from a non-inertial observer frame. An appeal is made to a previous publication that appears in the *International Journal of Terraspace Science and Engineering* [Z. Yang, J. D. Lee, A. Eskandarian, Int. J. Terraspace Sci. Eng. **8** (2016), 79–92; per bibl.], which does not seem to be widely available in academic libraries. In any event, this reviewer does not see why this approach offers any advantage over choosing an inertial observer frame with superposition of an arbitrary time-dependent affine transformation on a given motion of the material relative to this frame, as is done routinely, e.g. in geophysical fluid dynamics. After all, this simply modifies the apparent body force and the global velocity gradient imposed on the material, and most homogenization schemes require that one specify this velocity gradient in terms of average molecular motion. The paper could then be more aptly characterized by a somewhat less lofty title such as, “The effects of global rotation on NEMD simulations”. In any event, it seems that the paper is focused mainly on the effects of rotation

on heat flux, and the reviewer could not sort out the implications for constitutive modeling of heat flux and stress.

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Citations

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From Reviews: 1

MR3560883 76-02 35Q35 76A10

Saramito, Pierre (F-GREN-LJK)

★**Complex fluids.**

Modeling and algorithms.

Mathématiques & Applications (Berlin) [Mathematics & Applications], 79.

Springer, Cham, 2016. *xvi*+276 pp. ISBN 978-3-319-44361-4; 978-3-319-44362-1

From the preface: “The object of this book is twofold: modeling and algorithms. The first goal of this book is to present in a comprehensive text the modeling of complex fluids. Complex fluid models are introduced by increasing the level of complexity, and the relations between all the models are addressed using hierarchical diagrams. The second goal is to present an up-to-date mathematical and numerical analysis of the corresponding equations and to propose several practical numerical algorithms for the approximation of the solutions. The various numerical methods presented here are then suitable for implementation on computers, using some finite element libraries. These numerical methods are able to compute velocities, pressures, and stresses at each position and at each time when explicit computations are no more possible for complex geometries and flow conditions. Numerous examples of practical flow computations are presented along with this book. Software implementations are based on the Rheolef finite element library [283–285] developed by the author. Rheolef is a free software available as a standard package under the Debian and Ubuntu GNU/Linux systems and that can be installed from source code on others systems.”

The book is largely focused on numerical simulation of the flow of fairly standard models of complex fluids in simple geometries. Hence, the terminology “modeling” should be interpreted as the modeling of flow, to the extent this can be viewed as independent of the evaluation of rheological models.

As indicated in the author’s prefatory outline, the first three chapters of the book are devoted to viscoplastic fluids, proceeding from Newtonian fluids and the Navier-Stokes equations, to introduce concepts, notation and numerical methods employed in the subsequent treatment, through “quasi-Newtonian” (“generalized Newtonian” in other literature), and thence to more general viscoplastic fluids. All the above rheological models are history-independent and strictly dissipative, so that the relation between local stress and deformation rate is determined by a dissipation potential, referred to by the author as the “energy of dissipation function”. As unfortunately is the case with much contemporary literature, the author borrows this phenomenological construct from past studies that overlook the landmark work of D. G. B. Edelen [Arch. Rational Mech. Anal. **51** (1973), 218–227; [MR0337117](#); J. D. Goddard, Acta Mech. **225** (2014), no. 8, 2239–2259; [MR3237898](#)], which, incidentally, is touched on and denoted by “pseudo-potential” in the treatise by G. A. Maugin [*The thermomechanics of plasticity and fracture*, Cambridge Texts Appl. Math., Cambridge Univ. Press, Cambridge, 1992; [MR1173212](#)]. Also, while the present author introduces the associated variational principles for quasi-static flows, he does not cite other important papers on the subject [R.

Hill, *J. Mech. Phys. Solids* **5** (1956), 66–74; [MR0081645](#); A. I. Leonov, *J. Non-Newton. Fluid Mech.* **28** (1988), no. 1, 1–28, [doi:10.1016/0377-0257\(88\)80007-7](#)].

The final two chapters of the book deal with history-dependent viscoelastic and elastoviscoplastic models, of the type described by Lagrangian ODEs for the evolution of stress in terms of deformation rate. Such models represent multi-potential variants of the bi-potential model of B. Halphen and Nguyen Quoc Son [*J. Mécanique* **14** (1975), 39–63; [MR0416177](#)] referred to by them, and by much of the subsequent French literature, as the “generalized standard model”. In the most general form, these models involve networks of elastic and dissipative elements with associated potentials. In contrast to the extremes of ideal elasticity and ideal viscoplasticity, such models generally do not admit a variational principle.

The book provides a historical overview of various rheological models, embellished with portraits of pioneers in the field, together with a hierarchical reduction of models. While this may appear a bit perfunctory to the sophisticated reader, it may be attractive to the novice. As a potentially much more useful contribution, the author offers a comprehensive survey of recent and past work on numerical algorithms, such as operator splitting for Lagrangian ODEs. The graphics are exemplary, with many attractive images of flow fields, illustrations of computational meshes, and mathematical graphs.

The bibliography is perforce selective and the terminology a bit unorthodox, with various laws of continuum thermodynamics enunciated as “principles”, and without reference to the celebrated methodology of B. D. Coleman et al. based on the Clausius-Duhem inequality. Also, there is no direct citation of certain classic works on non-Newtonian fluid mechanics [B. D. Coleman, H. Markovitz and W. Noll, *Viscometric flows of non-Newtonian fluids. Theory and experiment*, Springer Tracts in Natural Philosophy, Vol. 5, Springer-Verlag New York, Inc., New York, 1966; [MR0210369](#); W. R. Schowalter, *Mechanics of non-Newtonian fluids*, Pergamon Press, Oxford, 1978], works which offer analytical insights on some of the flows considered in the present work. As something of a quibble, I note that the author’s terminology “frame-invariant” for “objective” tensor represents a conventional but (to this reviewer) dubious borrowing from the modern continuum-mechanics terminology “frame-indifferent”. Unfortunately, “frame-invariant” may blur the distinction between truly invariant quantities and quantities that transform tensorially under changes of observer frame. The written English is generally satisfactory although occasionally unconventional.

The author’s preface declares the book to be primarily intended for undergraduate students and researchers in applied mathematics, engineering sciences, computational mechanics, and physics; and the reader is assumed to be familiar with computational methods such as finite differences and finite elements, together with the corresponding variational formulations of partial differential equations. This required background of knowledge would probably exclude most undergraduates in U.S. universities, but some of the topics might be accessible to their counterparts in elite European institutions. On the other hand, the reviewer does not hesitate to recommend the book to graduate students and more senior investigators, as a readable and largely self-contained introduction to

the numerical simulation of the flow of complex fluids, an introduction that also contains a useful compendium of past works on the subject. Joe D. Goddard

Citations	From References: 0	From Reviews: 0
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MR3448812 74Q05 74A25

Berdichevsky, Victor L. (1-WYNS-ME)

Homogenization in probabilistic terms: the variational principle and some approximate solutions. (English summary)

J. Mech. Phys. Solids **87** (2016), 86–114.

Summary: “Studying of materials with evolving random microstructures requires the knowledge of probabilistic characteristics of local fields because the path of the microstructure evolution is controlled by the local fields. The probabilistic characteristics of local fields are determined by the probabilistic characteristics of material properties. In this paper it [*sic*] is considered the problem of finding the probabilistic characteristic of local fields, if the probabilistic characteristics of material properties are given. The probabilistic characteristics of local fields are sought from the variational principle for probabilistic measure. Minimizers of this variational problem provide all statistical information of local fields as well as the effective coefficients. Approximate solutions are obtained for electric current in composites for two cases: multi-phase isotropic composites with lognormal distribution of conductivities and two-phase isotropic composites. The solutions contain a lot of statistical information that has not been available previously by analytical treatments.”

Much of the background theory and essential literature references for this article are contained in a treatise by the same author [*Variational principles of continuum mechanics. I*, Interact. Mech. Math., Springer, Berlin, 2009; MR2555074; *II*; MR2561362] which, based on a partial reading, is highly recommended by this reviewer. Although the treatise under review contains a wealth of citations of important literature, in particular Russian literature, I found no references to other, possibly relevant works on probabilistic field theories such as the (latest edition of the) treatise by D. R. Axelrad [*Foundations of the probabilistic mechanics of discrete media*, Elsevier, 2016; per revr.; first edition, Found. Philos. Sci. Tech. Ser., Pergamon, Oxford, 1984; MR0738970], the many research papers by Axelrad’s former colleague M. Ostoja-Starzewski [e.g. *Int. J. Solids Struct.* **35** (1998), no. 19, 2429–2455, doi:10.1016/s0020-7683(97)00144-3], nor the well-known treatise by M. J. Beran [*Statistical continuum theories*, Monogr. Stat. Phys. Thermodyn., 9, Interscience, New York, 1968], none of which, I should hasten to add, deals extensively with variational principles.

The present paper exhibits many earmarks of the pedagogical approach found in the author’s earlier treatise [op. cit.], emphasizing and elucidating the underlying mathematics by means of numerous illustrative examples and applications. While especially useful for newcomers to the subject, it may be worthwhile to offer here a mathematically economical overview.

The probabilistic description of scalar or tensor fields $u(x)$, $\mathbb{R}^n \mapsto \mathbb{R}^m$ (with $n = 3$ in Berdichevsky’s physical applications), involves a normalized positive (probability) measure $d[u]$ on the function space U containing $u(x)$ with “expectations” or “averages”

of functionals $L[u]$

$$\langle L \rangle = \int_U L[u] d[u], \quad \text{with} \quad \int_U d[u] = 1,$$

representing a convex linear combination. Hence, variational (or minimax) principles for L carry over to $\langle L \rangle$ whenever variation and averaging commute. (In cases where $u(x)$ can be represented by $u(x, \omega)$, with ω in an abstract event space Ω with probability measure $\mu(d\omega)$ and $L[u]$ given by an integral over x , this commutativity follows from an appropriate form of Fubini's theorem.)

Berdichevsky considers problems where

$$L[u] = \int_V L(x, u, \nabla u, \dots) dV(x),$$

$$\text{with } \delta L = \int_V [\partial_u L \cdot \delta u(x) + \partial_{\nabla u} L \cdot \nabla \delta u \dots] dV(x),$$

involving u and a number of its spatial derivatives (representing, e.g., elements of a Banach space), and he restricts attention to measures based on the probability density on a denumerable set of spatially discrete points:

$$d[u] = f(x_1, x_2, \dots, x_p; u_1, u_2, \dots, u_p) dV(u_1) dV(u_2) \dots dV(u_p),$$

where $u_i = u(x_i)$, dV denotes the Euclidean volume element and p may be infinite. In the case of homogeneous (translation invariant) f considered by Berdichevsky, dependence on x_i can be reduced to dependence on $y_i = x_i - x_1$, $i = 2, \dots, p$.

Certain relations given by the author can be expressed concisely in terms of the *characteristic functional* [M. S. Bartlett and D. G. Kendall, Proc. Cambridge Philos. Soc. **47** (1951), 65–76; [MR0039947](#); V. V. Sazonov, Teor. Veroyatnost. i Primenen. **3** (1958), 201–205; [MR0098423](#)]

$$\mathcal{P}[v] = \langle \exp \iota(v, u) \rangle, \quad \text{where } (v, u) = \int_V v(x) \cdot u(x) dV(x),$$

and $v(x)$ is a deterministic (dual) vector field. It follows that the *autocorrelations* $B^{(q)}$ considered by the author are defined generally by Fréchet derivatives:

$$B^{(q)}(x_1, x_2, \dots, x_q) = \langle u_1 \otimes u_2 \otimes \dots \otimes u_q \rangle = (-\iota)^q \delta_v^q \mathcal{P}[v]|_{v=0}$$

$$= (-\iota)^q \prod_{i=1}^q \delta_{v(x_i)} \mathcal{P}[v]|_{v=0}, \quad \text{for } m = 1, 2, \dots$$

In the special case of fields $u = \nabla \varphi = \partial_x \varphi$ derivable from a potential, referred to as “potentiality” by the author, one has the standard relation

$$(u, v) = - \int_V \varphi \nabla \cdot v dV + \int_{\partial V} \varphi v_n dS,$$

in which a solenoidal field v , such that $\nabla \cdot v = 0$, may be regarded as conserved “flow” dual to “force” u derivable from a potential. In the highly restricted case where the solenoidal field has vanishing normal component v_n on ∂V , the preceding equation gives the result $(u, v) = 0$ indicated by the author, and the characteristic functional reduces to the trivial form $\mathcal{P}[v] \equiv 1$.

As a special case, one can generate the characteristic functional for the above probability density f by taking

$$v = \xi_1 \delta(x - x_1) + \xi_2 \delta(x - x_2) + \dots + \xi_p \delta(x - x_p), \quad \text{with } (v, u) = \sum_{i=1}^p \xi_i \cdot x_i,$$

where δ denotes the Dirac measure [cf. M. S. Bartlett and D. G. Kendall, op. cit.], reducing the characteristic functional to the Fourier transform, say $\hat{f}(x_1, x_2, \dots, x_p; \xi_1, \xi_2, \dots, \xi_p)$, of $f(x_1, x_2, \dots, x_p; u_1, u_2, \dots, u_p)$ depending on “wave” vectors $\xi_1, \xi_2, \dots, \xi_p$. The moments $B^{(q)}$, $q \leq p$, are then given by partial derivatives

$$(-i)^q \partial_{\xi_1} \partial_{\xi_2} \cdots \partial_{\xi_q} \hat{f}|_{\{\xi_1, \dots, \xi_p\}=0}.$$

In the further special case of potentiality, one has

$$B^{(q)}(x_1, x_2, \dots, x_q) = \partial_1 \partial_2 \cdots \partial_q B(x_1, x_2, \dots, x_q),$$

where $B(x_1, x_2, \dots, x_q) = \langle \varphi_1 \varphi_2 \cdots \varphi_q \rangle$,

with $\partial_i = \partial_{x_i}$, $\varphi_i = \varphi(x_i)$, which appears to generalize a result given by Berdichevsky for $q = 2$.

The above ideas and techniques also apply *mutatis mutandi* to higher-order tensor fields u of the kind that arise in continuum mechanics, where potentiality represents “compatibility” or, as the author calls it, “gradient compatibility” [V. L. Berdichevsky, op. cit. (Section 16.8)].

As pointed out by the author, the potentials may represent potential energies associated with reversible processes or dissipation potentials for strictly dissipative processes. As signaled in the author’s abstract, he applies the latter idea to the scalar (electrical) conductivity of random media. In particular, focusing mainly on linear laws and the associated quadratic forms for dissipation rate or dissipation potential, he illustrates the application of variational principles and their duals to the well-known problem of deriving bounds for effective conductivity, for which he considers some special statistics.

Joe D. Goddard



Citations	From References: 1	From Reviews: 0
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MR3381465 74C15 26D10

Müller, Stefan [[Müller, Stefan¹](#)] (D-BONN-CM); [Scardia, Lucia](#) (4-BATH); [Zeppieri, Caterina Ida](#) (D-MUNS-AMM)

★**Gradient theory for geometrically nonlinear plasticity via the homogenization of dislocations.** (English summary)

Analysis and computation of microstructure in finite plasticity, 175–204, *Lect. Notes Appl. Comput. Mech.*, 78, Springer, Cham, 2015.

Summary: “This article gives a short description and a slight refinement of recent work [MSZ15] [[MR3283554](#)] [SZ12] [[MR3023380](#)] on the derivation of gradient plasticity models from discrete dislocations models. We focus on an array of parallel edge dislocations. This reduces the problem to a two-dimensional setting. As in the work Garroni, Leoni & Ponsiglione [GLP10] [[MR2677615](#)] we show that in the regime where the number of dislocation N_ϵ is of the order $\log \frac{1}{\epsilon}$ (where ϵ is the ratio of the lattice spacing to the macroscopic dimensions of the body) the contributions of the self-energy of the dislocations and their interaction energy balance. Upon suitable rescaling one obtains a continuum limit which contains an elastic energy term and a term which depends on the homogenized dislocation density. The main novelty is that our model allows for microscopic energies which are not quadratic and reflect the invariance under rotations. A key mathematical ingredient is a rigidity estimate in the presence of dislocations

which combines the nonlinear Korn inequality of Friesecke, James & Müller [FJM02] [MR1916989] and the linear Bourgain & Brezis estimate [BB07] [MR2293957] for vector fields with controlled divergence. The main technical improvement of this article compared to [MSZ15] is the removal of the upper bound $W(F) \leq C \text{dist}^2(F, \text{SO}(2))$ on the stored energy function.”

This paper represents an ongoing effort to construct mathematically rigorous models, based on microscopic models of dislocation distributions, in which the elastic energy is composed of a contribution from the usual strain energy plus an additional energy arising from strain incompatibility associated with dislocations.

Readers interested in the physical underpinnings are encouraged to peruse the authors’ above-cited previous paper and references therein, particularly the 2010 paper by Garroni, Leoni and Ponsiglione mentioned above. While this class of models addresses an important issue of elastic energy, it does not deal with the dissipative plastic flow arising from dislocation movement, as the uninitiated might be led to infer from the titles of various papers in the field.

{For the collection containing this paper see [MR3380564](#)}

Joe D. Goddard

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Citations	From References: 0	From Reviews: 0
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[MR3335165](#) [76A20](#) [74F10](#) [76S05](#)

[Knox, D. J.](#) (4-STRA-MS); [Wilson, S. K.](#) [[Wilson, Stephen K.](#)] (4-STRA-MS);

[Duffy, B. R.](#) [[Duffy, Brian R.](#)] (4-STRA-MS);

[McKee, S.](#) [[McKee, Sean](#)] (4-STRA-MS)

Porous squeeze-film flow. (English summary)

IMA J. Appl. Math. **80** (2015), *no. 2*, 376–409.

Summary: “The squeeze-film flow of a thin layer of Newtonian fluid filling the gap between a flat impermeable surface moving under a prescribed constant load and a flat thin porous bed coating a stationary flat impermeable surface is considered. Unlike in the classical case of an impermeable bed, in which an infinite time is required for the two surfaces to touch, for a porous bed contact occurs in a finite contact time. Using a lubrication approximation, an implicit expression for the fluid layer thickness and an explicit expression for the contact time are obtained and analysed. In addition, the fluid particle paths are calculated, and the penetration depths of fluid particles into the porous bed are determined. In particular, the behaviour in the asymptotic limit of small permeability, in which the contact time is large but finite, is investigated. Finally, the results are interpreted in the context of lubrication in the human knee joint, and some conclusions are drawn about the contact time of the cartilage-coated femoral condyles and tibial plateau and the penetration of nutrients into the cartilage.”

This paper is a straight-forward and competently executed treatment of a well-known problem of Stokes flow in a clear fluid with Darcy flow of the same fluid in an adjacent porous medium. Owing to the pioneering 1967 work of G. S. Beavers and D. D. Joseph [J. Fluid Mech. **30** (1967), no. 1, 197–207, [doi:10.1017/S0022112067001375](#)], it is now understood that a difficulty arises in the correct matching of PDEs of different order at the nominal boundary between fluid and porous media, in essence the intersection of biharmonic and harmonic velocity fields in the case of incompressible flu-

ids. The 2009 paper by D. A. Nield [Transp. Porous Media **78** (2009), no. 3, 537–540, [doi:10.1007/s11242-009-9344-y](https://doi.org/10.1007/s11242-009-9344-y)] in the present work discusses various resolutions of the problem, including the simple Beavers-Joseph interfacial slip condition adopted in the present work:

$$[[\mathbf{v}_t]] = \frac{\sqrt{k} \partial \mathbf{v}_t}{\alpha \partial n}$$

for the jump $[[\mathbf{v}_t]]$ of the tangential component $\mathbf{v}_t = (\mathbf{I} - \mathbf{n} \otimes \mathbf{n})\mathbf{v}$ of the fluid-velocity field \mathbf{v} , where \mathbf{n} is the unit normal to the interface, k (with units of length squared) is the Darcy permeability of a presumably isotropic porous medium, and α is a non-dimensional material constant of order unity. We recall that boundary conditions similar to the above slip condition can be justified for flows nearly parallel to the interface by adopting an empirical modification of Darcy’s law, such as a generalized Brinkman-Darcy equation for incompressible fluids with negligible inertia:

$$\mu' \nabla^2 \mathbf{v} = \nabla p + \mu k^{-1} \mathbf{v}, \quad \text{with } \nabla \cdot \mathbf{v} = 0,$$

where μ denotes fluid viscosity and μ' is an effective viscosity for shearing of the fluid within the porous medium. The latter viscosity should depend on k and other microstructural parameters defining an isotropic medium.

Given the generally singular perturbation for $k = 0$ and the past controversy [K. Vafai and S. J. Kim, *Int. J. Heat Fluid Flow* **16** (1995), no. 1, 11–15, [doi:10.1016/0142-727X\(94\)00002-T](https://doi.org/10.1016/0142-727X(94)00002-T)] surrounding the modeling of such flows, it might be worthwhile to consider the effect of alternative boundary conditions on the results presented in the present paper. This may be all the more desirable for poro-elastohydrodynamic problems associated with the lubrication of the cartilage in skeletal joints. *Joe D. Goddard*

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Note: This list reflects references listed in the original paper as accurately as possible with no attempt to correct errors.

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MR3319781 92E20 80A30 92C45

Knight, Daniel (1-OHS-KBM); **Shinar, Guy** (IL-JMED);

Feinberg, Martin (1-OHS-KBM)

Sharper graph-theoretical conditions for the stabilization of complex reaction networks. (English summary)

Math. Biosci. **262** (2015), 10–27.

Summary: “Across the landscape of all possible chemical reaction networks there is a surprising degree of stable behavior, despite what might be substantial complexity and nonlinearity in the governing differential equations. At the same time there are reaction networks, in particular those that arise in biology, for which richer behavior is exhibited. Thus, it is of interest to understand network-structural features whose presence enforces dull, stable behavior and whose absence permits the dynamical richness that might be necessary for life. We present conditions on a network’s *Species-Reaction Graph* that ensure a high degree of stable behavior, so long as the kinetic rate functions satisfy certain weak and natural constraints. These graph-theoretical conditions are considerably more incisive than those reported earlier.”

The present paper contributes to a voluminous and long-standing body of work on the mathematical analysis of chemical and biochemic kinetics, a field in which one of the authors has made early and sustained contributions [M. Feinberg, *Arch. Rational Mech. Anal.* **46** (1972), 1–41; [MR0378591](#)]. The kinetic equations typically involve multinomial forms of the “mass-action” variety in the various chemical composition variables and, as recognized in the present work, these taken together with mass balances on the chemical species determine a network structure with an associated graph. The latter is in fact a *hypergraph* associating species and reactions, with (König) representation as a bipartite graph whose “hyperedges” connect one set of nodes, representing species, to a second distinct set, representing reactions [O. N. Temkin, A. V. Zeigarnik and D. Bonchev, *Chemical reaction networks: a graph-theoretical approach*, CRC Press, Boca Raton, FL, 1996 (p. 56)]. The kinetic equations define currents on edges constrained by reaction stoichiometry which contribute to mass accumulation at the species-nodes in unsteady-state situations.

In keeping with previous works by the present group, the present paper attempts to develop certain purely mathematical criteria which serve *inter alia* to distinguish what are declared to be a “dull” stable behavior of non-biological systems from a possibly “richer” behavior of biochemical reaction networks. The previously developed, somewhat abstract concept of *concordance*, based on the structure of the reaction network and certain properties of the kinetics, is applied in the present paper to various biochemical reaction networks.

In this and previous works, the authors seem unconcerned by the possible connections to a venerable body of literature on the thermodynamics of chemical networks and graphs [D. G. B. Edelen, *Int. J. Eng. Sci.* **11** (1973), no. 8, 819–839, [doi:10.1016/0020-7225\(73\)90032-3](#); A. S. Perelson and G. F. Oster, *Arch. Rational Mech. Anal.* **57**

(1974), 31–98; [MR0363178](#); D. G. B. Edelen, *Int. J. Eng. Sci.* **13** (1975), 763–784; [MR0446115](#); J. Bataille, D. G. B. Edelen and J. Kestin, *Int. J. Eng. Sci.* **17** (1979), no. 5, 563–572; [MR0659355](#); S. Schuster et al., *J. Math. Biol.* **45** (2002), no. 2, 153–181; [MR1920585](#); D. A. Beard et al., *J. Theoret. Biol.* **228** (2004), no. 3, 327–333; [MR2079958](#); H. Qian and D. A. Beard, *Biophys. Chem.* **114** (2005), no. 2-3, 213–220, [doi:10.1016/j.bpc.2004.12.001](#); F. Yang, H. Qian and D. A. Beard, *Metab. Eng.* **7** (2005), no. 4, 251–259, [doi:10.1016/j.ymben.2005.03.002](#); R. Datta et al., *Phys. A* **387** (2008), no. 13, 3348–3372, [doi:10.1016/j.physa.2008.01.070](#)] (as a minuscule sample), some of which is touched on in a recent article by the reviewer [*Ind. Eng. Chem. Res.* **54** (2015), no. 16, 4078–4083, [doi:10.1021/ie503661b](#)]. This literature suggests that much of the “dull” stability and lack of multiple equilibria of non-biological reactions can be attributed in part to their dissipative nature. While one can argue that this property may not be shared by “active” biochemical systems, it is hard to see how such systems could be globally non-dissipative, when all biochemical or biochemomechanical processes are accounted for. Of course, this kind of stability may not rule out the multiplicity of equilibrium states in systems with complex multi-well energy landscapes. Although more physical than chemical, the kinetics of protein folding come to mind, where one can have a multiplicity of folded states that, for all intents and purposes, can be considered stable.

Joe D. Goddard

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[MR3270200](#) [74D10](#) [74A40](#) [74A45](#) [74R05](#) [80A10](#) [80A17](#)

Keller, Arne [[Keller, Arne²](#)] ([CH-ETHZ-GL](#)); **Hutter, Kolumban** ([CH-ETHZ-GL](#))

A viscoelastic damage model for polycrystalline ice, inspired by Weibull-distributed fiber bundle models. Part II: Thermodynamics of a rank-4 damage model. (English summary)

Contin. Mech. Thermodyn. **26** (2014), no. 6, 895–906.

{This review is also provided for Part I [A. Keller and K. Hutter, *Contin. Mech. Thermodyn.* **26** (2014), no. 6, 879–894; [MR3270199](#)].}

Summary of Part I: “We consider a constitutive model for polycrystalline ice, which contains delayed-elastic and viscous deformations, and a damage variable. The damage variable is coupled to the delayed-elastic deformation by a fiber bundle ansatz. We construct an isotropic theory, which can be calibrated with experimental data. Furthermore, we generalize the theory to a damage model in terms of rank-four tensors. This general model allows the evolution of anisotropic damage.”

Summary of Part II: “We consider a viscoelastic-viscoplastic continuum damage model for polycrystalline ice. The focus lies on the thermodynamics particularities of such a constitutive model and restrictions on the constitutive theory which are implied by the entropy principle. We use Müller’s formulation of the entropy principle, together

with Liu’s method of exploiting it with the aid of Lagrange multipliers.”

This effort to model the failure of ice represents an interesting addition to the literature on ice mechanics and fracture mechanics, offering certain thermodynamic restrictions on the assumed continuum-level constitutive equations.

It is not clear to the reviewer whether and how the fracture of ice is related to its plastic-flow behavior, a subject which is discussed in a previous comprehensive review coauthored by one of the present authors [L. Placidi, K. Hutter and S. H. Faria, *GAMM-Mitt.* **29** (2006), no. 1, 80–117; [MR2224584](#)] which, curiously, is not cited in the present work. Ice plasticity has a venerable history that goes back at least to James Thompson [Proc. Roy. Soc. London **8** (1856–1857), 455–458] (brother of Lord Kelvin) and is treated in several more recent works [J. F. Nye, Proc. Roy. Soc. London A **207** (1951), no. 1091, 554–572, [doi:10.1098/rspa.1951.0140](#); D. J. Goodman, H. J. Frost and M. F. Ashby, *Philos. Mag. A* **43** (1981), no. 3, 665–695, [doi:10.1080/01418618108240401](#); F. Louchet, *Comptes Rendus Phys.* **5** (2004), no. 7, 687–698, [doi:10.1016/j.crhy.2004.09.001](#)]. This leads one to wonder, as non-mathematical musing, if the conjectured “fracture” of the present work may be regarded as an asymptotic rate-dependent quasi-brittle failure arising from unstable rate-independent elastoplasticity.

The authors employ a standard additive decomposition of strain into viscous and visco-elastic or “delayed elastic” deformations, involving a tensorial internal variable describing damage, thereby providing a tensorial generalization of a one-dimensional “spring-dashpot” model.

The upshot of the elaborate thermodynamic analysis seems to be the requirement that the internal variable describing damage be derivable from an elastic potential, an idea that is already well known in other continuum models endowed with internal variables. It would seem that a further generalization would involve positive-definite fourth-rank viscosity and elasticity tensors, instead of the scalar forms assumed in the present model. In other words, is it obvious why damage is anisotropic while the associated viscosity and elasticity are assumed to remain isotropic? To turn the question around, if viscosity and elasticity are isotropic, why is the damage considered to be anisotropic? At any rate, there seems to be no assessment of the degree of anisotropy.

As pointed out by the authors, the specification of the associated thermodynamic potential is problematical, which may suggest that its existence is not essential to their phenomenological constitutive model.

As another matter, scant theoretical justification is offered for their interpretation of the failure of presumably polycrystalline ice in terms of a generalized Weibull “fiber-bundle” (or “weakest-link”) model. As a counterpoint, one can cite other works indicating that the Weibull model may not provide an accurate description of micro-mechanical damage, e.g. [L. Afferrante, M. Ciavarella and E. Valenza, *Int. J. Solids Structures* **43** (2006), no. 17, 5147–5157, [doi:10.1016/j.ijsolstr.2005.08.002](#); R. Danzer et al., *Eng. Fract. Mech.* **74** (2007), no. 18, 2919–2932, [doi:10.1016/j.engfracmech.2006.05.028](#); P. M. Duxbury and P. L. Leath, *J. Phys. A* **20** (1987), no. 6, L411, [doi:10.1088/0305-4470/20/6/013](#); P. M. Duxbury, S. G. Kim and P. L. Leath, *Size effect and statistics of fracture in random materials*, *Mater. Sci. Eng. A* **176** (1994), no. 1-2, 25–31, [doi:10.1016/0921-5093\(94\)90955-5](#)]. That the one-dimensional version of the present

model achieves a reasonable fit to certain experimental data may suggest that it should stand on its own as an empiricism, without appeal to Weibull. *Joe D. Goddard*

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MR3270199 [74D10](#) [74A40](#) [74A45](#) [74R05](#) [80A10](#) [80A17](#)
Keller, Arne [[Keller, Arne²](#)] ([CH-ETHZ-GL](#)); **Hutter, Kolumban** ([CH-ETHZ-GL](#))
A viscoelastic damage model for polycrystalline ice, inspired by Weibull-distributed fiber bundle models. Part I: Constitutive models. (English summary)
Contin. Mech. Thermodyn. **26** (2014), no. 6, 879–894.

{This review is also provided for Part II [A. Keller and K. Hutter, *Contin. Mech. Thermodyn.* **26** (2014), no. 6, 895–906; [MR3270200](#)].}

Summary of Part I: “We consider a constitutive model for polycrystalline ice, which contains delayed-elastic and viscous deformations, and a damage variable. The damage variable is coupled to the delayed-elastic deformation by a fiber bundle ansatz. We construct an isotropic theory, which can be calibrated with experimental data. Furthermore, we generalize the theory to a damage model in terms of rank-four tensors. This general model allows the evolution of anisotropic damage.”

Summary of Part II: “We consider a viscoelastic-viscoplastic continuum damage model for polycrystalline ice. The focus lies on the thermodynamics particularities of such a constitutive model and restrictions on the constitutive theory which are implied by the entropy principle. We use Müller’s formulation of the entropy principle, together with Liu’s method of exploiting it with the aid of Lagrange multipliers.”

This effort to model the failure of ice represents an interesting addition to the literature on ice mechanics and fracture mechanics, offering certain thermodynamic restrictions on the assumed continuum-level constitutive equations.

It is not clear to the reviewer whether and how the fracture of ice is related to its plastic-flow behavior, a subject which is discussed in a previous comprehensive review coauthored by one of the present authors [L. Placidi, K. Hutter and S. H. Faria, *GAMM-Mitt.* **29** (2006), no. 1, 80–117; [MR2224584](#)] which, curiously, is not cited in the present work. Ice plasticity has a venerable history that goes back at least to James Thompson [*Proc. Roy. Soc. London* **8** (1856–1857), 455–458] (brother of Lord Kelvin) and is treated in several more recent works [J. F. Nye, *Proc. Roy. Soc. London A* **207** (1951), no. 1091, 554–572, [doi:10.1098/rspa.1951.0140](#); D. J. Goodman, H. J. Frost and M. F. Ashby, *Philos. Mag. A* **43** (1981), no. 3, 665–695, [doi:10.1080/01418618108240401](#); F. Louchet, *Comptes Rendus Phys.* **5** (2004), no. 7, 687–698, [doi:10.1016/j.crhy.2004.09.001](#)]. This leads one to wonder, as non-mathematical musing, if the conjectured “fracture” of the present work may be regarded as an asymptotic rate-dependent quasi-brittle failure arising from unstable rate-independent elastoplasticity.

The authors employ a standard additive decomposition of strain into viscous and visco-elastic or “delayed elastic” deformations, involving a tensorial internal variable describing damage, thereby providing a tensorial generalization of a one-dimensional “spring-dashpot” model.

The upshot of the elaborate thermodynamic analysis seems to be the requirement that the internal variable describing damage be derivable from an elastic potential, an idea

that is already well known in other continuum models endowed with internal variables. It would seem that a further generalization would involve positive-definite fourth-rank viscosity and elasticity tensors, instead of the scalar forms assumed in the present model. In other words, is it obvious why damage is anisotropic while the associated viscosity and elasticity are assumed to remain isotropic? To turn the question around, if viscosity and elasticity are isotropic, why is the damage considered to be anisotropic? At any rate, there seems to be no assessment of the degree of anisotropy.

As pointed out by the authors, the specification of the associated thermodynamic potential is problematical, which may suggest that its existence is not essential to their phenomenological constitutive model.

As another matter, scant theoretical justification is offered for their interpretation of the failure of presumably polycrystalline ice in terms of a generalized Weibull “fiber-bundle” (or “weakest-link”) model. As a counterpoint, one can cite other works indicating that the Weibull model may not provide an accurate description of micro-mechanical damage, e.g. [L. Afferrante, M. Ciavarella and E. Valenza, *Int. J. Solids Structures* **43** (2006), no. 17, 5147–5157, doi:10.1016/j.ijsolstr.2005.08.002; R. Danzer et al., *Eng. Fract. Mech.* **74** (2007), no. 18, 2919–2932, doi:10.1016/j.engfracmech.2006.05.028; P. M. Duxbury and P. L. Leath, *J. Phys. A* **20** (1987), no. 6, L411, doi:10.1088/0305-4470/20/6/013; P. M. Duxbury, S. G. Kim and P. L. Leath, *Size effect and statistics of fracture in random materials*, *Mater. Sci. Eng. A* **176** (1994), no. 1-2, 25–31, doi:10.1016/0921-5093(94)90955-5]. That the one-dimensional version of the present model achieves a reasonable fit to certain experimental data may suggest that it should stand on its own as an empiricism, without appeal to Weibull. *Joe D. Goddard*

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Citations	From References: 3	From Reviews: 0
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MR3240290 74D05 35A15 35Q74 74A15

Golden, J. M. [[Golden, John Murrrough](#)] (IRL-DIT-SM)

Free energies for materials with memory in terms of state functionals. (English summary)

Meccanica **49** (2014), no. 9, 2207–2235.

Summary: “The aim of this work is to determine what free energy functionals are expressible as quadratic forms of the state functional I^t which is discussed in earlier papers. The single integral form is shown to include the functional ψ_F proposed a few years ago, and also a further category of functionals which are easily described but more complicated to construct. These latter examples exist only for certain types of materials. The double integral case is examined in detail, against the background of a new systematic approach developed recently for double integral quadratic forms in terms of strain history, which was used to uncover new free energy functionals. However, while, in principle, the same method should apply to free energies which can be given by quadratic forms in terms of I^t , it emerges that this requirement is very restrictive; indeed, only the minimum free energy can be expressed in such a manner.”

This work draws heavily on previous work, including the monograph by G. Amendola, M. Fabrizio and J. M. Golden [*Thermodynamics of materials with memory*, Springer, New York, 2012; [MR2856615](#)], reviewed by I. Nistor, and a score of papers by the author and coworkers that are also cited in Mathematical Reviews. This body of work,

referred to in the following by “A&c”, appears to a large extent to be an elaboration, restricted to linear viscoelasticity, on the works of B. D. Coleman [Arch. Ration. Mech. Anal. **17** (1964), 1–46; [MR0171419](#); Arch. Ration. Mech. Anal. **17** (1964), 230–254; [MR0171420](#)] and Coleman and D. R. Owen [Arch. Ration. Mech. Anal. **36** (1970), 245–269; [MR0269165](#); Arch. Ration. Mech. Anal. **54** (1974), 1–104; [MR0395502](#)]. Here and in A&c, the authors attribute to an Italian paper by D. Graffi [Rend. Sem. Mat. Univ. Padova **68** (1982), 17–29 (1983); [MR0702143](#)] several conditions that appear tantamount to those given by Coleman and Coleman and Owen, but the reviewer has not taken pains to translate the former. As a commentary on style, the reviewer notes that the present paper, like the other papers in this body of work, involves an often rambling presentation, dense with algebra and multiple citations, without precise pagination, of results presented elsewhere. This not only makes for difficult reading but conveys the impression of minor incremental progression in the field.

A main goal of the present paper and much of A&c is the investigation of various *free energy* functionals represented as quadratic forms in the variables defining the history of certain “state” variables. The prototypical example is thermo-viscoelastic free energy depending on the history of (infinitesimal) mechanical strain and temperature. A&c provide interesting extensions to free energies that may depend on the temperature gradient, taking the theory beyond the standard “simple material” to higher-gradient theories of the van der Waals–Korteweg–Cahn–Hilliard variety.

As indicated below, the exact motivation behind this quest for free energies is less evident to the reviewer than it perhaps should be. In particular, it is worth recalling that in equilibrium thermo-mechanics, various partial derivatives of the (*unique*) free energy function deliver up constitutive equations along with criteria (“Maxwell relations”) for their thermodynamic consistency. Also, the associated extremum principles occupy a central place in various field theories and numerical methods. However, knowledge of the derivatives of free energy, i.e. the constitutive equations themselves, is essential for most applications, as well as for the actual construction of the free energy function. Moreover, the knowledge of derivatives is generally of a finer variety than knowledge of integrals.

In principle, *free energy functionals* occupy a similar position in the non-equilibrium thermo-mechanics of materials with memory. However, rarely in the reviewer’s experience does one rely on *a priori* knowledge of free energy to deliver up constitutive equations (e.g. for stress and heat flux), or even to assess the thermodynamic consistency of given constitutive equations. Moreover, the associated extremum principles appear to have a much more restricted applicability to field theories and boundary value problems. Finally, and as established in the classic work of Coleman and Owen [op. cit.], the non-equilibrium free energy in the standard theory of simple materials with memory does not enjoy the property of uniqueness. Rather, it consists of a convex set of functionals which contains a maximal and a minimal member, which is one focus of the present work. Setting aside certain meta-mathematical concerns about the foundations of the subject, the reviewer will venture a few comments on the more mathematical aspects of the present paper and related works of A&c.

The present paper is one of several in which A&c explore free energies depending on a state variable that differs from the standard strain and temperature variables. The current paper is restricted to the special case of a scalar stress $T(t)$ at present time t in an isothermal simple material given by a functional $T(t) = T[E^t(s)](t)$ of the history of a scalar strain $E^t(s) = E(t - s)$, $s \in \mathbb{R}^+$. (Here, as below, square brackets are used to denote functionals.) In a strictly linear theory, it seems evident that invertible linear transformations between independent variables should be allowed, and A&c adopt a particular version based on W. Noll’s work. Noll indicated in the introduction to [Arch.

Ration. Mech. Anal. **48** (1972), 1–50; [MR0445985](#)] that his new definition of state is motivated by theories of plasticity and hysteresis, presumably rate-independent and not included in existing definitions of fading memory nor representative of standard theories of viscoelasticity. However, in much later writings [“Five contributions to natural philosophy”, Dept. Math. Sci., Carnegie Mellon Univ., 2004 (Chapter 3, p. 2)], he included a “materials of the rate type” definition of state and equivalent histories [W. Noll, op. cit., 1972]. In the present paper this is reduced to a scalar form $I^t(s)$ discussed below.

It should be recalled that the crucial connection between stress and free energy rests on a classic result of Coleman [op. cit., 1964] for materials exhibiting instantaneous elastic response to strain jumps $[[E^t]]$. In this case, the functional for stress $T(t) = T[[E^t(s)]](t)$ is given in terms of a free energy functional $\psi[[E^t(s)]](t)$ by

$$(1) \quad T(t) = \partial_{E_0} \psi[[E^t(s)]](t), \text{ where } E_0 = -[[E^t(0)]] = E^t(0) - E^t(0^+) = E(t) - E(t^-),$$

where the partial derivative ∂_{E_0} , taken at fixed past history $E^t(s)$, $s \in \mathbb{R}^{++}$, can obviously be replaced by $\partial_{E(t)}$. Analogous reasoning is employed by A&c, although it is not always evident. Thus, given the quadratic functional considered by the author:

$$(2) \quad \psi[[E^t(s)]](t) = \psi_e(E(t)) + \frac{1}{2} \int_0^\infty \int_0^\infty G(s_1, s_2) \dot{E}^t(s_1) \dot{E}^t(s_2) ds_1 ds_2, \text{ with } G(s_1, s_2) = G(|s_1 - s_2|),$$

where ψ_e denotes a quadratic rest-state free energy, formulae presented below give the stress as

$$(3) \quad T(t) = T_e(E(t)) + \int_0^\infty G(s) \dot{E}^t(s) ds, \text{ with } T_e = \partial_{E(t)} \psi_e,$$

which are special cases of more general linear tensorial forms treated by Coleman, Coleman and Owen, and in A&c.

As in other works in A&c, the author proposes related quadratic forms for *work* and *dissipation* based on the Clausius-Duhem inequality, with a restriction to processes that involve finite values for these quantities. As a minor concern, it is not clear why the prototypical free-energy balance in the author’s Equation 2.9 is declared to be “the first law”, since the definition of free energy involves the entropy, which properly speaking is the subject of “the second law”. Indeed, since the author ostensibly treats isothermal processes, the first law, i.e. the energy balance, must also generally involve heat transfer that is not explicitly identified in the present work.

Focusing here on the quadratic form for free energy, it is worth noting that, subject to minor restriction on the *kernel* G , (2)-(3) admit a (denumerable) set of strain jumps

$$[[E]]_* = E^t(s_*^-) - E^t(s_*^+),$$

and one may presumably express $E^t(s)$ as a continuous, differentiable function $E_c^t(s) \in C^1$ plus a sequence of (Heaviside) step functions. This leads formally to Dirac distributions generated by differentiation, $\dot{E}^t(s) = \partial_t E^t(s) = -\partial_s E^t(s)$. In line with the preferences of the author, one can avoid the explicit appearance of distributions by employing the equivalent representation

$$(4) \quad \int_{s_* - \epsilon}^{s_* + \epsilon} f(s) \dot{E}^t(s) ds = \int_{s_* - \epsilon}^{s_* + \epsilon} E^t(s) \dot{f}(s) ds + [[E]]_* f(s_*),$$

in which $f \in C^1$ and $\dot{f}(x) = df/ds$, for any interval $(s_* - \epsilon, s_* + \epsilon)$, with $\epsilon > 0$, containing a single jump.

One obvious merit of the double integral representation (2) is its applicability to

products of Dirac distributions in the independent variables s_1 and s_2 , with results equivalent to the quadratic form in $E^t(s)$ obtained from (2) and (4). The same cannot be said of the single-integral form obtained formally from the singular kernel, $G(s_1, s_2) = \delta(s_1 - s_2)G_0(s_1, s_2)$, where δ denotes the Dirac distribution. The author considers various examples of the associated single-integral forms, and A&c cite nonlinear models involving single integrals for stress and free energy, models which, the reviewer notes, enjoy a long-standing popularity in the literature on the nonlinear viscoelasticity of polymers [R. I. Tanner, *J. Rheol.* **32** (1988), no. 7, 673–702, doi:10.1122/1.549986].

The above relations can be cast into a somewhat simpler form in terms of Fourier transforms (denoted here by carets):

$$\widehat{f}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} f(t) dt,$$

and a major part of A&c and related works is devoted to the properties of the transform $\widehat{G}(\omega)$ and related kernels. Although this is admittedly a matter of taste, the reviewer wonders if it might not have been easier to proceed at the outset in terms of Fourier transforms and distributions (generalized functions), particularly in an applied mathematics setting where one finds prominent expositions *cum* asymptotic analysis [M. J. Lighthill, *Introduction to Fourier analysis and generalised functions*, Cambridge Monographs on Mechanics and Applied Mathematics, Cambridge Univ. Press, New York, 1958; MR0092119], not to mention a large literature on transfer functions for linear systems. Beyond this observation, the present review will finish with a couple of comments on the alternative to (2) explored in the related works by A&c based on quadratic forms in the “minimal-state” variable:

$$(5) \quad I^t(\tau) = \int_0^{\infty} G(s + \tau) \dot{E}^t(s) ds = \int_{\tau}^{\infty} G(s) \dot{E}^t(s - \tau) ds,$$

whose significance is discussed in A&c [L. Deseri, M. Fabrizio and M. Golden, *Arch. Ration. Mech. Anal.* **181** (2006), no. 1, 43–96; MR2221203; G. Amendola, M. Fabrizio and J. M. Golden, *op. cit.*]. Roughly speaking, (5) represents the non-equilibrium stress arising from a backward shifted strain history followed by a static continuation to the present. Hence, one is now adopting non-equilibrium stress itself as the relevant state variable, in the manner of a complementary (Gibbs-type) free energy. When this is done, the quadratic functional in I^t leads generally to a nonlinear form in G , as a kind of generalization of the inverse elastic moduli defining complementary free energy in elasto-statics.

For initial and boundary value problems in linear viscoelasticity, it is stated somewhat abstractly in related work (e.g. in Section 9 of [L. Deseri, M. Fabrizio and M. Golden, *op. cit.*]) that this kind of variable offers advantages over the usual functional for stress in terms of strain history. However, even if confirmed by specific applications unfamiliar to the reviewer, he still does not understand whether and how a knowledge of a free energy functional is crucial to those applications.

Joe D. Goddard

Citations

From References: 18

From Reviews: 0

MR3524024 80A22 74Nxx 76Txx

Frémond, Michel (I-ROME2-CE)

★Phase change in mechanics.

Lecture Notes of the Unione Matematica Italiana, 13.

Springer, Heidelberg, 2012. *xiii*+303 pp. \$69.95.

ISBN 978-3-642-24608-1; 978-3-642-24609-8

From the preface: “A model is a theory which predicts the evolution of a structure. The basic elements of a mechanical predictive theory are described. They involve the choice of the state quantities which characterize the investigated physical phenomenon, the basic equations of mechanics: the equations of motion, the laws of thermodynamics and the constitutive laws. The theory is applied to phase change. Phase change involves microscopic motions which have macroscopic effects. These motions are taken into account in the macroscopic predictive theories. Numerous examples which are used or may be used in engineering are given for different phase change and damage problems. Moreover, when phase change occurs, temperatures may be discontinuous, for instance when warm rain falls on frozen soil. This situation is also investigated.

“These lecture notes are based on a course given at the XXX Scuola Estiva di Fisica Matematica at Ravello in September 2005 and on lectures given at the Università di Roma ‘Tor Vergata’.”

The present treatise is concerned with the rather special case of fairly standard thermo-mechanical field theory in physical space x and time t , with the local x - t state defined by $E(x, t) = \{T(t, x), \varepsilon(x, t), \beta(x, t), \text{grad } \beta(x, t)\}$, involving temperature T , infinitesimal strain tensor $\varepsilon = [\varepsilon_{ij}]$, and a single internal variable β supposed to represent the volume fraction β in a one-phase or a constituent in a two-phase material. “Phase” is used in a loose sense, e.g. to designate damaged vs. undamaged material in the applications to damage mechanics. The effects of mass density variation are

explicitly neglected, with the exception of one example involving cloud formation. As discussed below, the constitutive modeling appears to be focused on solid-like behavior, with little consequence for the applications involving fluids, where there appears to be a minimum of mechanics content.

The author adopts the standard assumption of a (Coleman-Noll) *simple material*, which rules out dependence of the state on $\text{grad}T$, but at the same time he allows for a dependence on $\text{grad}\beta$. Setting aside the question of thermodynamic consistency addressed by others [Nguyen Quoc Son and S. Andrieux, *C. R. Méc.* **333** (2005), no. 2, 139–145, [doi:10.1016/j.crme.2004.09.010](https://doi.org/10.1016/j.crme.2004.09.010)], the inclusion of $\text{grad}\beta$ in E allows for composition gradients in steady “equilibrium” states without the occurrence of processes such as mass diffusion. Hence, the author’s thermodynamic potential must be interpreted as that of Helmholtz rather than that of Gibbs, and this modification of the standard thermodynamics of phase change (e.g. involving Clapeyron relations, etc.) will restrict the applicability of the present treatment. While the term “mixtures” is frequently employed, scant connection is made to the standard *theory of mixtures* [K. R. Rajagopal and L. Tao, *Mechanics of mixtures*, Ser. Adv. Math. Appl. Sci., 35, World Sci. Publ., River Edge, NJ, 1995; [MR1370661](https://doi.org/10.1016/j.crme.2004.09.010)].

The structure of the author’s constitutive model constitutes a special case of a general theory in which his state space E represents a material configuration space as a manifold of material points $\xi \in \mathbb{R}^n$, with tangent space of generalized velocities $\dot{\xi} \in \mathbb{R}^n$, dual (cotangent) space of generalized forces $f \in \mathbb{R}^n$, and power or virtual power by a pairing $f \cdot \dot{\xi}$. In the author’s model $n = 11$ and $f = \{0, \sigma, B, \mathbf{H}\} \in \mathbb{R}^{10}$, where $\sigma = [\sigma_{ij}]$ is Cauchy stress, and B and $\mathbf{H} = [H_i]$ are “phase forces”. Except for one bibliographic citation [M. E. Gurtin, *Phys. D* **92** (1996), no. 3–4, 178–192; [MR1387065](https://doi.org/10.1016/0167-2789(96)00097-8)], I found no discussion of the relation of \mathbf{H} to the classical van der Waals–Cahn–Hilliard or Korteweg forces [J. W. Cahn and J. E. Hilliard, *J. Chem. Phys.* **28** (1958), no. 2, 258–267, [doi:10.1063/1.1744102](https://doi.org/10.1063/1.1744102); D. D. Joseph, A. Huang and H. Hu, *Phys. D* **97** (1996), no. 1–3, 104–125, [doi:10.1016/0167-2789\(96\)00097-8](https://doi.org/10.1016/0167-2789(96)00097-8); J. S. Rowlinson, *J. Statist. Phys.* **20** (1979), no. 2, 197–244; [MR0523642](https://doi.org/10.1016/0167-2789(96)00097-8)].

Following the classic paper of B. Halphen and Nguyen Quoc Son [*J. Méc.* **14** (1975), 39–63; [MR0416177](https://doi.org/10.1016/0167-2789(96)00097-8)], the author adopts a “bipotential” model involving non-dissipative rate-independent forces and dissipative rate-dependent forces given, respectively, by the “normality” conditions:

$$(1) \quad f^{nd}(\xi) = \partial_{\xi} \Psi^{nd}(\xi), \quad \text{and} \quad f^d(\xi, \dot{\xi}) = \partial_{\dot{\xi}} \Psi^d(\xi, \dot{\xi}),$$

where Ψ^{nd} is a standard thermodynamic (Helmholtz) potential and Ψ^d is a dissipation potential or “pseudopotential” (denoted by Φ by the author). The latter is adopted as a phenomenological Ansatz, following J.-J. Moreau and others, reflecting the usual oversight of the rigorous mathematical treatment of D. G. B. Edelen [*Arch. Rational Mech. Anal.* **51** (1973), 218–227; [MR0337117](https://doi.org/10.1016/0167-2789(96)00097-8); J. D. Goddard, *Acta Mech.* **225** (2014), no. 8, 2239–2259; [MR3237898](https://doi.org/10.1016/0167-2789(96)00097-8); erratum, *Acta Mech.* **226** (2015), no. 3, 975; [MR3317827](https://doi.org/10.1016/0167-2789(96)00097-8)] (which, *inter alia*, allows for additive powerless force in the expression for f^d with breakdown of normality and generalized Onsager symmetry).

Assuming convexity of the potentials in (1), one has convex conjugates $\Phi^{nd}(\xi)$, $\Phi^d(\xi, \dot{\xi})$ with

$$(2) \quad \xi^{nd}(f) = \partial_f \Phi^{nd}(f) \quad \text{and} \quad \dot{\xi}^d(f) = \partial_f \Phi^d(f),$$

with, as the most primitive constitutive models,

$$\text{iso-velocity (Kelvin-Voigt): } \dot{\xi} = \dot{\xi}^d = \dot{\xi}^{nd}, \quad f = f^{nd} + f^d,$$

or

$$\text{iso-force (Maxwell-Reuss): } f = f^{nd} = f^d, \quad \dot{\xi} = \dot{\xi}^{nd} + \dot{\xi}^d.$$

These correspond, respectively, to parallel or serial arrangement of non-dissipative and dissipative elements, the first representing solid-like and the second fluid-like behavior. The author appears early on in his treatise (Equation 3.9, p. 10) to adopt the first model, although, as mentioned above, this seems not to be important for his subsequent applications to fluids.

After the initial statement of principles involving the above constitutive theory, virtual work principles and the associated balances, the author presents a bevy of special applications involving both continuum and discrete “lumped-parameter” models, with frequent restatement or reformulation of balances. Advanced numerical methods are employed for some examples. The thermomechanical models employed must be regarded as highly idealized and mainly pedagogical, as there is little or no comparison with experiment or with other literature on the modeling of phase-change processes, e.g. [S. H. Davis, *Theory of solidification*, Cambridge Monogr. Mech., Cambridge Univ. Press, Cambridge, 2001; [MR1868285](#); W. J. Boettinger et al., *Ann. Rev. Mater. Res.* **32** (2002), 163–194, [doi:10.1146/annurev.matsci.32.101901.155803](#); M. Militzer, *Current Opinion Solid State Mater. Sci.* **15** (2011), no. 3, 106–115, [doi:10.1016/j.cossms.2010.10.001](#)] and others too numerous to cite.

Although the author is well versed in modern continuum mechanics and the book is based on lectures notes in a presumably advanced school, my casual perusal suggests that it would need extensive revision for use in a typical North American graduate-level course in thermo-mechanics. It might, however, provide a useful reference to certain carefully selected applications.

Joe D. Goddard