SOME OPEN PROBLEMS IN ELASTICITY

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ABSTRACT. Some outstanding open problems of nonlinear elasticity are described. The problems range from questions of existence, uniqueness, regularity and stability of solutions in statics and dynamics to issues such as the modelling of fracture and self-contact, the status of elasticity with respect to atomistic models, the understanding of microstructure induced by phase transformations, and the passage from three-dimensional elasticity to models of rods and shells. Refinements are presented of the author's earlier work [25] on showing that local minimizers of the elastic energy satisfy certain weak forms of the equilibrium equations.

Dedicated to Jerry Marsden on the occasion of his 60th birthday

1. INTRODUCTION.

In this paper I highlight some outstanding open problems in nonlinear (sometimes called finite) elasticity theory. While many of these will be well known to experts on analytic aspects of elasticity, I hope that the compilation will be of use both to those new to the field and to researchers in solid mechanics having different perspectives. Of course the selection of problems is a personal one, and indeed represents a list of those problems I would like most to be able to solve but cannot. In particular it concentrates on *general* open problems, or ones that illustrate general difficulties, rather than those related to very specific experimental situations, which is not to imply that the latter are not important or instructive. I have not included any open problems connected with the numerical computation of solutions, since I recently discussed some of these in [32].

The only new results of the paper are in connection with the problem of showing that local minimizers of the total elastic energy satisfy the weak form of the equilibrium equations. As I pointed out in [25], there are hypotheses under which some forms of the equilibrium equations can be proved to hold, and in Section 2.4 I take the opportunity to present some refinements of this old work.

The paper is essentially self-contained, and can be read by those having no knowledge of elasticity theory. For those seeking further background on the subject I have written a short introduction [29] to some of the issues, intended for research students, which I hope is a quick and easy read. For more serious study in the spirit of this paper, the reader is referred to the books of Antman [14], Ciarlet [81, 82, 83], Marsden & Hughes [182] and Šilhavý [255]. Other excellent but older books and survey articles are Antman [13], Ericksen [113], Gurtin [139], and Truesdell & Noll [252]. Valuable additional perspectives can be found in the books of Green & Zerna [136], Green & Adkins [135] and Ogden [200].

It is an honour to dedicate this article to Jerry Marsden, both as a friend and in recognition of his important contributions to elasticity, and thus to help celebrate his many talents as a mathematician, thinker and writer.

2. Elastostatics

2.1. The stored-energy function and equilibrium solutions. Consider an elastic body occupying in a reference configuration the bounded domain $\Omega \subset \mathbf{R}^3$. We suppose that Ω has a Lipschitz boundary $\partial \Omega = \partial \Omega_1 \cup \partial \Omega_2 \cup N$, where $\partial \Omega_1, \partial \Omega_2$ are disjoint relatively open subsets of $\partial \Omega$ and N has two-dimensional Hausdorff measure $\mathcal{H}^2(N) = 0$ (i.e. N has zero area). Deformations of the body are described by mappings

$$\mathbf{y}: \Omega \rightarrow \mathbf{R}^3$$
,

where $\mathbf{y}(\mathbf{x}) = (y_1(\mathbf{x}), y_2(\mathbf{x}), y_3(\mathbf{x}))$ denotes the deformed position of the material point $\mathbf{x} = (x_1, x_2, x_3)$. We assume that \mathbf{y} belongs to the Sobolev space $W^{1,1}(\Omega; \mathbf{R}^3)$, so that in particular the *deformation gradient* $D\mathbf{y}(\mathbf{x})$ is well defined for a.e. $\mathbf{x} \in \Omega$. For each such \mathbf{x} we can identify $D\mathbf{y}(\mathbf{x})$ with the 3×3 matrix $(\partial y_i/\partial x_j)$.

We require the deformation \mathbf{y} to satisfy the boundary condition

(2.1)
$$\mathbf{y}|_{\partial\Omega_1} = \bar{\mathbf{y}}(\cdot),$$

where $\bar{\mathbf{y}}: \partial \Omega_1 \to \mathbf{R}^3$ is a given boundary displacement.

We suppose for simplicity that the body is homogeneous, i.e. the material response is the same at each point. In this case the total elastic energy corresponding to the deformation \mathbf{y} is given by

(2.2)
$$I(\mathbf{y}) = \int_{\Omega} W(D\mathbf{y}(\mathbf{x})) \, d\mathbf{x},$$

where $W = W(\mathbf{A})$ is the stored-energy function of the material. We suppose that $W: M_+^{3\times 3} \to \mathbf{R}$ is C^1 and bounded below, so that without loss of generality $W \ge 0$. (Here and below, $M^{m\times n}$ denotes the space of real $m \times n$ matrices, and $M_+^{n\times n}$ denotes the space of those $\mathbf{A} \in M^{n\times n}$ with det $\mathbf{A} > 0$.) The *Piola-Kirchhoff* stress tensor is given by

(2.3)
$$\mathbf{T}_R(\mathbf{A}) = D_{\mathbf{A}} W(\mathbf{A}).$$

By formally computing

$$\frac{d}{d\tau}I(\mathbf{y}+\tau\varphi)|_{\tau=0}=0,$$

we obtain the weak form of the Euler-Lagrange equation for I, that is

(2.4)
$$\int_{\Omega} D_{\mathbf{A}} W(D\mathbf{y}) \cdot D\varphi \, d\mathbf{x} = 0$$

for all smooth φ with $\varphi|_{\partial\Omega_1} = 0$. This can be shown (cf. Antman & Osborn [16]) to be equivalent to the balance of forces on arbitrary subbodies. If \mathbf{y} , $\partial\Omega_1$ and $\partial\Omega_2$ are sufficiently regular then (2.4) is equivalent to the pointwise form of the equilibrium equations

(2.5)
$$\operatorname{div} D_{\mathbf{A}} W(D\mathbf{y}) = 0 \quad \text{in } \Omega,$$

together with the natural boundary condition of zero applied traction

(2.6)
$$D_{\mathbf{A}}W(D\mathbf{y})\mathbf{n} = 0 \quad \text{on } \partial\Omega_2,$$

where $\mathbf{n} = \mathbf{n}(\mathbf{x})$ denotes the unit outward normal to $\partial \Omega$ at \mathbf{x} . (More generally, we could have prescribed nonzero tractions of various types on $\partial \Omega_2$, as well as including the potential energy of body forces such as gravity in the expression for

the energy (2.2), but for simplicity we have not done this, since the main difficulties we address are already present without these additions.)

To avoid interpenetration of matter, it is natural to require that $\mathbf{y}: \Omega \to \mathbf{R}^3$ be invertible. To try to ensure that deformations have this property, we suppose that

(2.7)
$$W(\mathbf{A}) \to \infty \text{ as } \det \mathbf{A} \to 0 + .$$

So as to also prevent orientation reversal we define $W(\mathbf{A}) = \infty$ if det $\mathbf{A} \leq 0$. Then $W: M^{3\times 3} \to [0,\infty]$ is continuous. Clearly if $I(\mathbf{y}) < \infty$ then

(2.8)
$$\det D\mathbf{y}(\mathbf{x}) > 0 \text{ for a.e. } \mathbf{x} \in \Omega.$$

Since **y** is not assumed to be C^1 , (2.8) does not imply even local invertibility. For studies of local and global invertibility in the context of elasticity, or relevant to it, see Ball [21], Bauman & Phillips [48], Ciarlet & Nečas [84], Fonseca & Gangbo [121], Giaquinta, Modica & Souček [131], Meisters & Olech [183], Weinstein [259] and Šverák [237].

For any elastic material, the stored-energy function W is *frame-indifferent*, i.e.

(2.9)
$$W(\mathbf{RA}) = W(\mathbf{A}) \text{ for all } \mathbf{R} \in \mathrm{SO}(3), \mathbf{A} \in M^{3 \times 3}.$$

In addition, if the material has a nontrivial isotropy group \mathcal{S} , W satisfies the material symmetry condition

 $W(\mathbf{AQ}) = W(\mathbf{A})$ for all $\mathbf{Q} \in \mathcal{S}, \mathbf{A} \in M^{3 \times 3}$.

The case S = SO(3) corresponds to an *isotropic* material.

For *incompressible* materials the deformation \mathbf{y} is required to satisfy the constraint

det
$$D\mathbf{y}(\mathbf{x}) = 1$$
 a.e. $\mathbf{x} \in \Omega$.

All of the problems and results contained in this article have corresponding incompressible versions, some of which we cite in the references. However, in general we do not state these explicitly.

2.2. Existence of equilibrium solutions. There are two traditional routes to proving the existence of equilibrium solutions. The first, pioneered by Stoppelli [232], [233] and described in the book of Valent [253], is to use the implicit function theorem in a suitable Banach space X to prove the existence of an equilibrium solution close to a given one, when the data of the problem are slightly perturbed. In order to make this work, it is necessary to use spaces X of sufficiently smooth mappings, for example subspaces of $W^{2,p}(\Omega; \mathbf{R}^3)$ for p > 3 or $C^{2+\alpha}(\Omega; \mathbf{R}^3)$, so as to control the nonlinear dependence on Dy. In addition, the linearized elasticity operator at the given solution should be invertible as a map from X to a suitable target space Y. While this method automatically delivers smooth solutions, it is by its nature restricted to small perturbations (for example, small boundary displacements from a stress-free state), and because of the regularity properties required for the linearized operator it in general only applies to situations when $\overline{\partial \Omega_1}$ and $\overline{\partial \Omega_2}$ do not meet, for example when one of them is empty. In particular, mixed boundary conditions typically encountered in applications, for example (2.1)with $\partial \Omega_1$ comprising the two end-faces of a cylindrical rod, are in general not allowed, at least with the techniques as currently developed (see Section 2.7).

The second route is to prove the existence of a global minimizer of I via the direct method of the calculus of variations. In principle such a minimizer should satisfy the equilibrium equations, at least in weak form, but this turns out to be

a subtle matter (see Sections 2.3, 2.4). More generally we could ask for conditions ensuring that there exist some kind of local minimizer.

Let

$$\mathcal{A} = \{ \mathbf{y} \in W^{1,1}(\Omega; \mathbf{R}^3) : I(\mathbf{y}) < \infty, \mathbf{y}|_{\partial \Omega_1} = \bar{\mathbf{y}} \},\$$

where the boundary condition is understood in the sense of trace. In the definition of \mathcal{A} we could include the requirement that y be invertible; this can be done in various ways, one of which is discussed in Section 2.5.

Definition 2.1. Let $1 \le p \le \infty$. The deformation $\mathbf{y} \in \mathcal{A}$ is a $W^{1,p}$ local minimizer of I if there exists $\varepsilon > 0$ such that $I(\mathbf{z}) \ge I(\mathbf{y})$ for any $\mathbf{z} \in \mathcal{A}$ with $\|\mathbf{z} - \mathbf{y}\|_{W^{1,p}} \le \varepsilon$.

The problem of proving the existence of local, but not global, minimizers is discussed later (see Problem 9). A typical result on global minimization is the following.

Theorem 2.1. Suppose that W satisfies the hypotheses

(H1) W is polyconvex, i.e. $W(\mathbf{A}) = g(\mathbf{A}, \operatorname{cof} \mathbf{A}, \det \mathbf{A})$ for all $\mathbf{A} \in M^{3\times 3}$ for some convex g,

(H2) $W(\mathbf{A}) \ge c_0(|\mathbf{A}|^2 + |\text{cof } \mathbf{A}|^{3/2}) - c_1 \text{ for all } \mathbf{A} \in M^{3 \times 3},$ where $c_0 > 0$.

Then if \mathcal{A} is nonempty, there exists a global minimizer \mathbf{y}^* of I in \mathcal{A} .

Here and below we take $|\cdot|$ to be the Euclidean norm on $M^{3\times 3}$ with corresponding inner product $\mathbf{A} \cdot \mathbf{B} = \text{tr} (\mathbf{A}^T \mathbf{B})$. Theorem 2.1 is a refinement by Müller, Qi & Yan [190] of the result in Ball [19]. For the problem to be nontrivial we need that $\mathcal{H}^2(\partial \Omega_1) > 0$.

The hypothesis (H1) is known to be too strong for the following reason. Let $f: M^{m \times n} \to \mathbf{R} \cup \{+\infty\}$ be Borel measurable and bounded below. We recall f is said to be *quasiconvex at* $\mathbf{A} \in M^{m \times n}$ if the inequality

(2.10)
$$\int_{\Omega} f(\mathbf{A} + D\varphi(\mathbf{x})) \, d\mathbf{x} \ge \int_{\Omega} f(\mathbf{A}) \, d\mathbf{x}$$

holds for any $\varphi \in C_0^{\infty}(\Omega; \mathbf{R}^m)$, and is *quasiconvex* if it is quasiconvex at every $\mathbf{A} \in M^{m \times n}$. Here $\Omega \subset \mathbf{R}^n$ is any bounded open set whose boundary $\partial\Omega$ has zero *n*-dimensional Lebesgue measure. A standard scaling argument (see, for example, Ball & Murat [44]) shows that contrary to appearances these definitions do not depend on Ω . Results of Morrey [187] and Acerbi & Fusco [3] imply that if $f: M^{m \times n} \to \mathbf{R}$ is quasiconvex and satisfies the growth condition

(2.11)
$$C_1 |\mathbf{A}|^p - C_0 \le f(\mathbf{A}) \le C_2(|\mathbf{A}|^p + 1) \text{ for all } \mathbf{A} \in M^{m \times n}$$

where p > 1 and where C_0 and $C_1 > 0, C_2 > 0$ are constants, then

(2.12)
$$\mathcal{F}(\mathbf{y}) = \int_{\Omega} f(D\mathbf{y}) \, d\mathbf{x}$$

attains a global minimum on

$$\mathcal{A} = \{ \mathbf{y} \in W^{1,1}(\Omega; \mathbf{R}^m) : \mathbf{y}|_{\partial \Omega_1} = \bar{\mathbf{y}} \}.$$

Here we assume that Ω has Lipschitz boundary $\partial \Omega$, that $\partial \Omega_1 \subset \partial \Omega$ is \mathcal{H}^{n-1} measurable and that $\bar{\mathbf{y}} : \partial \Omega_1 \to \mathbf{R}^m$ is given such that \mathcal{A} is nonempty. As shown by

Ball & Murat [44], quasiconvexity of f is necessary for the existence of a global minimizer for all perturbed functionals of the form

$$\mathcal{F}_1(\mathbf{y}) = \int_{\Omega} [f(D\mathbf{y}(\mathbf{x})) + h(\mathbf{x}, \mathbf{y}(\mathbf{x}))] d\mathbf{x}$$

with $h(\cdot, \cdot) \geq 0$ continuous. These results strongly suggest that (H1) should be replaced by the requirement that W be quasiconvex, a weaker condition than polyconvexity. For example, it is easily seen that a larger class of W for which Theorem 2.1 holds consists of those of the form $W = W_1 + f$, where W_1 satisfies (H1) and (H2), and where $f: M^{3\times3} \to \mathbf{R}$ is quasiconvex and satisfies (2.11). That this really is a larger class can be seen by taking f = KF for a large K > 0, where F is quasiconvex but not polyconvex. Such F exist satisfying $F(\mathbf{RAQ}) = F(\mathbf{A})$ for all $\mathbf{R}, \mathbf{Q} \in \mathrm{SO}(3), \mathbf{A} \in M^{3\times3}$, and can be constructed by the method of Šverák [238]¹. More generally we could take f to satisfy

(2.13)
$$f(\mathbf{A}) \ge C_1 |\mathbf{A}|^p - C_0$$

for some $p > 1, C_1 > 0, C_0$ and to be the supremum of a nondecreasing sequence of continuous quasiconvex functions $f^k : M^{3 \times 3} \to [0, \infty)$, each satisfying a growth condition

$$0 \le \mathbf{f}^k(\mathbf{A}) \le \alpha_k |\mathbf{A}|^p - \beta_k$$

for constants $\alpha_k > 0, \beta_k$. (Kristensen [163] has shown that a function f satisfying (2.13) is the supremum of such a sequence if and only if f is closed $W^{1,p}$ quasiconvex in the sense of Pedregal [205], namely that Jensen's inequality $\langle \nu, f \rangle \geq f(\bar{\nu})$ holds for all homogeneous $W^{1,p}$ gradient Young measures² ν .)

However, as they stand none of the existence theorems for minimizers of integrals of general quasiconvex functions apply to elasticity, since they all assume growth conditions such as (2.11) which are not consistent with the condition (2.7). (The same applies to other results, such as the relaxation theorem of Dacorogna [88].) In particular, it is not clear whether or not a quasiconvex W satisfying our hypotheses can be written as the supremum of everywhere finite continuous quasiconvex functions. This is not true in general for quasiconvex functions $f: M^{m \times n} \to [0, \infty]$; for example we can take m = n = 2, $f(\mathbf{A}) = 0$ if $\mathbf{A} \in {\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4}$ and $f(\mathbf{A}) = \infty$ otherwise, where the \mathbf{A}_i are diagonal matrices in a Tartar configuration (see Tartar [250]), for example $\mathbf{A}_1 = \text{diag}(-2, 1)$, $\mathbf{A}_2 = \text{diag}(1, 2)$, $\mathbf{A}_3 = \text{diag}(2, -1)$ and $\mathbf{A}_4 =$ diag (-1, -2). Then f is quasiconvex, since any \mathbf{y} with $D\mathbf{y} \in {\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3, \mathbf{A}_4}$ a.e. has constant gradient (this following, for example, from the general result of Chlebík

$$H(\mathbf{A}) = \min(|\mathbf{U}(\mathbf{A}) - \mathbf{1}|^p, |\mathbf{U}(\mathbf{A}) - \lambda \mathbf{1}|^p),$$

¹For example we can take $F = H^{qc}$ to be the quasiconvexification of

where $\lambda > 1$ and $\mathbf{U}(\mathbf{A}) = (\mathbf{A}^T \mathbf{A})^{1/2}$. The quasiconvexification H^{qc} of H is defined to be the supremum of all quasiconvex functions $\psi \leq H$.

²See Young [262], Tartar [248], Ball [27] for the definition and properties of the Young measure $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ corresponding to a sequence of mappings $\mathbf{z}^{(j)}: \Omega \to \mathbf{R}^s$ satisfying a suitable bound, say $\|\mathbf{z}^{(j)}\|_{L^1} \leq M < \infty$, where $\Omega \subset \mathbf{R}^n$ is open (or measurable). For each $\mathbf{x} \in \Omega$, ν_x is a probability measure on \mathbf{R}^s giving the limiting distribution of values of $\mathbf{z}^{(j)}(\mathbf{p})$ as $j \to \infty$ and $\mathbf{p} \to \mathbf{x}$. If $f: \mathbf{R}^s \to \mathbf{R}$ is continuous, then the weak limit of $f(z^{(j)})$ in $L^1(E)$, where $E \subset \Omega$ is measurable, is given by the function $x \mapsto \langle \nu_{\mathbf{x}}, f \rangle$, whenever the weak limit exists. In particular, if $\mathbf{z}^{(j)} \to \mathbf{z}$ in $L^1(E)$, then $\mathbf{z}(\mathbf{x}) = \bar{\nu}_{\mathbf{x}}$ for $\mathbf{x} \in E$, where $\bar{\mu}$ denotes the centre of mass of a measure μ . Such a Young measure is homogeneous if $\nu = \nu_{\mathbf{x}}$ is independent of \mathbf{x} . If $1 , a <math>W^{1,p}$ gradient Young measure is a Young measure $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ corresponding to a sequence $z^{(j)} = D\mathbf{y}^{(j)}$ of gradients bounded in $L^p(\Omega; M^{m \times n})$, where we identify $M^{m \times n}$ with \mathbf{R}^{mn} .

& Kirchheim [77]). But the argument of Tartar shows that if f were the supremum of continuous quasiconvex functions $f^k: M^{2\times 2} \to [0,\infty)$ we would have f(0) = 0, a contradiction.

A further reason for preferring quasiconvexity to polyconvexity is that, unlike quasiconvexity, polyconvexity is not closed with respect to periodic homogenization (Braides [55]).

Problem 1. Prove the existence of energy minimizers for elastostatics for quasiconvex stored-energy functions satisfying (2.7).

A principal difficulty here is that there is no known useful characterization of quasiconvexity. If W is quasiconvex then W is rank-one convex, that is the map $t \mapsto W(\mathbf{A} + t\mathbf{a} \otimes \mathbf{n})$ is convex for each $\mathbf{A} \in M^{m \times n}$ and $\mathbf{a} \in \mathbf{R}^m, \mathbf{n} \in \mathbf{R}^n$. For 40 years it seemed possible that in fact rank-one convexity was equivalent to quasiconvexity, until Šverák [239] found his well-known counterexample for the dimensions $n \geq 2, m \geq 3$. Then Kristensen [164] used Šverák's example to show that for the same dimensions there is no local characterization of quasiconvexity. In the absence of a characterization leading to a new proof technique, one is forced to make direct use of the definition (2.10), which leads to serious problems of approximation by piecewise affine functions when (2.7) holds.

In Ball [19] it was shown how the hypotheses (H1), (H2) can be satisfied for a class of isotropic materials including models of natural rubbers, via theorems exploiting the representation

(2.14)
$$W(\mathbf{A}) = \Phi(v_1, v_2, v_3)$$

of the stored-energy function W of an isotropic material, where Φ is a symmetric function of the singular values $v_i = v_i(\mathbf{A})$, that is of the eigenvalues of $(\mathbf{A}^T \mathbf{A})^{1/2}$ (for a different proof of such theorems see Le Dret [103]). However it is not obvious how to verify (H1) when the material is not isotropic, for example when it has cubic symmetry.

Problem 2. Are there ways of verifying polyconvexity and quasiconvexity for a useful class of anisotropic stored-energy functions?

To illustrate the difficulty in verifying (H1), in the isotropic case it is much more convenient to use the representation (2.14) rather than the equivalent representation $W(\mathbf{A}) = h(I_1, I_2, I_3)$ in terms of the principal invariants $I_j = I_j(\mathbf{A})$. Perhaps it is significant that the function Φ in (2.14) has the same regularity as W, while his less regular (see Ball [24], Sylvester [244], Šilhavý [256]). At any rate the more symmetric form (2.14) lends itself more easily to discussing convexity properties. For non-isotropic materials suitable representations do not seem to be available; for example, in the case of cubic symmetry it does not seem to be convenient to use the usual integrity basis (given, for example, in Green & Adkins [135]).

2.3. Regularity and the classification of singularities. The main open question concerning regularity is to decide when global, or local, minimizers of I are smooth. A special case is

Problem 3. When is the minimizer \mathbf{y}^* in Theorem 2.1 smooth?

Here smooth means C^{∞} in Ω , and C^{∞} up to the boundary (except in the neighbourhood of points $\mathbf{x}_0 \in \overline{\partial \Omega_1} \cap \overline{\partial \Omega_2}$ where singularities can be expected). Clearly

additional hypotheses on W are needed for this to be true. One might assume, for example, that $W: M_+^{3\times 3} \to \mathbf{R}$ is C^{∞} , and that (H1) is strengthened by assuming W to be strictly polyconvex (i.e. that g is strictly convex). Also for regularity up to the boundary we would need to assume both smoothness of the boundary (except perhaps at $\partial \Omega_1 \cap \partial \Omega_2$) and that $\bar{\mathbf{y}}$ is smooth. The precise nature of these extra hypotheses is to be determined. Problem 3 is unsolved even in the simplest special cases. In fact the only situation in which smoothness of \mathbf{y}^* seems to have been proved is for the pure displacement problem ($\partial \Omega_2$ empty) with small boundary displacements from a stress-free state. For this case Zhang [263], following work of Sivaloganathan [225], gave hypotheses under which the smooth solution to the equilibrium equations delivered by the implicit function theorem was in fact the unique global minimizer \mathbf{y}^* of I given by Theorem 2.1.

An even more ambitious target would be to somehow classify possible singularities in minimizers of I given by (2.2) for generic stored-energy functions W. If at the same time one could associate with each such singularity a condition on W that prevented it, one would also, by imposing all such conditions simultaneously, possess a set of hypotheses implying regularity. In fact it is possible to go a little way down this road. Consider first the kind of singularity frequently observed at phase boundaries in elastic crystals, in which the deformation gradient $D\mathbf{y}$ is piecewise constant, with values \mathbf{A}, \mathbf{B} on either side of a plane $\{\mathbf{x} \cdot \mathbf{n} = k\}$. It was shown in Ball [20] that, under the natural assumption that there is some matrix \mathbf{A}_0 that is a local minimizer of $W(\cdot)$, every such deformation \mathbf{y} that is locally a weak solution of the Euler-Lagrange equation is trivial, that is $\mathbf{A} = \mathbf{B}$, if and only if W is strictly rank-one convex (i.e. the map $t \mapsto W(\mathbf{A} + t\mathbf{a} \otimes \mathbf{n})$ is strictly convex for every \mathbf{A} and all nonzero \mathbf{a}, \mathbf{n}). Thus strict rank-one convexity is exactly what is needed to eliminate this particular kind of singularity.

Another physically occuring singularity is that of *cavitation*. For radial cavitation the deformation has the form $\mathbf{y} : B(0,1) \to \mathbf{R}^3$, where B(0,1) is the unit ball in \mathbf{R}^3 , and

$$\mathbf{y}(\mathbf{x}) = r(|\mathbf{x}|) \frac{\mathbf{x}}{|\mathbf{x}|}.$$

Thus if r(0) > 0, **y** is discontinuous at $\mathbf{x} = 0$, where a hole of radius r(0) is formed. If (H1) holds, then since polyconvexity implies quasiconvexity, the minimizer of I among smooth ($W^{1,3}$ is enough, see below) **y** satisfying $\mathbf{y}(\mathbf{x}) = \lambda \mathbf{x}$ for $|\mathbf{x}| = 1$ (i.e. $r(1) = \lambda$) is given by the homogeneous deformation

$$\tilde{\mathbf{y}}_{\lambda}(\mathbf{x}) \equiv \lambda \mathbf{x}.$$

However, it was shown in Ball [23] that for a class of stored-energy functions W satisfying (H1) and the growth condition in (H2) but with $2 \le p < 3$, $q < \frac{3}{2}$, I attains a minimum among radial deformations satisfying the boundary condition $\mathbf{y}(\mathbf{x}) = \lambda \mathbf{x}$ for $|\mathbf{x}| = 1$, and that for $\lambda > 0$ sufficiently large the minimizer $\bar{\mathbf{y}}$ satisfies r(0) > 0. Furthermore $\bar{\mathbf{y}}$ satisfies the weak form of the Euler-Lagrange equation (2.4). As a specific example we can take

(2.15)
$$W(\mathbf{A}) = |\mathbf{A}|^2 + h(\det \mathbf{A}),$$

for $h: (0, \infty) \to \mathbf{R}$ smooth with h'' > 0, $\lim_{\delta \to \infty} \frac{h(\delta)}{\delta} = \lim_{\delta \to 0+} h(\delta) = \infty$. Cavitation is a common failure mechanism in polymers; for interesting pictures of almost radial cavitation of roughly spherical rubber particles imbedded in a matrix of

Nylon-6 see Lazzeri & Bucknall [166]. In [190] Müller, Qi & Yan show that if (H2) holds then no deformation with finite energy can exhibit cavitation. A somewhat stronger condition, which by the Sobolev embedding theorem obviously prevents not only cavitation but any other discontinuity in \mathbf{y} , is that $W(\mathbf{A}) \geq c_0 |\mathbf{A}|^p - c_1$ for all \mathbf{A} , where $c_0 > 0$ and p > 3. In fact even if p = 3 any finite-energy deformation is continuous on account of (2.8) and the result of Vodop'yanov, Gol'dshtein and Reshetnyak [254].

There is an extensive literature on cavitation in elasticity; a sample of the more mathematical developments can be found in the papers of Antman & Negrón-Marrero [15], James & Spector [147], Müller & Spector [191], Polignone & Horgan [212, 213], Sivaloganathan [224, 226, 227], Sivaloganathan & Spector [230, 229, 228], Pericack-Spector & Spector [209], Stringfellow & Abeyaratne [234], and Stuart [235, 236].

An interesting feature of cavitation is that it provides a realistic example of the *Lavrentiev phenomenon*, whereby the infimum of the energy is different in different function spaces. Here it takes the form

$$\inf_{\mathcal{A}_1} I < \inf_{\mathcal{A}_3} I = I(\tilde{\mathbf{y}}_{\lambda}),$$

where $\mathcal{A}_p = \{\mathbf{y} \in W^{1,p}(B(0,1); \mathbf{R}^3) : \mathbf{y}|_{\partial B(0,1)} = \lambda \mathbf{x}\}$. More generally, there is a theory of minimization for elasticity with W polyconvex in function spaces not allowing cavitation due to Giaquinta, Modica & Souček [133, 131, 132] (see also the less technically demanding approach of Müller [188]). Thus the same W can have different minimizers in different function spaces; if we enlarge the space to allow not only cavitation but crack formation (see Section 2.8), then we can have different minimizers in at least three different spaces.

In the case of cavitation there is a change of topology of the deformed configuration associated with the Lavrentiev phenomenon, but one-dimensional examples in Ball & Mizel [43] for integrals of the form

$$I(y) = \int_{a}^{b} f(x, y(x), y_x(x)) \, dx$$

show that the phenomenon can occur when the minimizer y is continuous with unbounded gradient. This leads to the question:

Problem 4. Can the Lavrentiev phenomenon occur for elastostatics under growth conditions on the stored-energy function ensuring that all finite-energy deformations are continuous?

Of course if \mathbf{y}^* is smooth then the Lavrentiev phenomenon cannot hold under the hypotheses of Theorem 2.1. Some interesting recent progress on Problem 4 is due to Foss, Hrusa & Mizel [122, 181], who provide examples of the Lavrentiev phenomenon in two dimensions for a homogeneous isotropic polyconvex stored-energy function Wsatisfying the corresponding growth condition $W(\mathbf{A}) \geq c_0 |\mathbf{A}|^p - c_1$ for all $\mathbf{A} \in M_+^{2\times 2}$ for some p > 2 and (2.7). In these examples the reference configuration is given by a sector of a disk described in polar coordinates by $\Omega_{\alpha} = \{(r, \theta) : 0 < r < 1, 0 < \theta < \alpha\}$, and the boundary conditions are of the 'container' type that the origin is fixed, that $\mathbf{y}(\Omega_{\alpha}) \subset \Omega_{\beta}$, and that $\mathbf{y}(1, \theta) = (1, \frac{\beta}{\alpha}\theta)$, where $0 < \beta < \frac{3}{4}\alpha$. Whether such examples can be constructed for mixed boundary conditions of the type (2.1), even in two dimensions, or be associated with singularities in the interior of Ω , remains

open. The Lavrentiev phenomenon has important implications for the numerical computation of minimizers (see Ball [32] and the references therein).

There are striking examples of variational problems of the form (2.12) for which the global minimizer is not smooth. The first such example was found by Nečas [197], who showed that if $m = n^2$ with n sufficiently large then there exists a strictly convex $f = f(D\mathbf{y})$ whose corresponding integral

(2.16)
$$\mathcal{F}(\mathbf{y}) = \int_{B(0,1)} f(D\mathbf{y}) \, d\mathbf{x}$$

has as global minimizer

$$y_{ij}^*(\mathbf{x}) = \frac{x_i x_j}{|\mathbf{x}|}, \qquad \mathbf{x} \in B(0,1)$$

subject to its own (smooth) boundary values on $\partial B(0, 1)$. Here \mathbf{y}^* is Lipschitz but not C^1 . Then Hao, Leonardi & Nečas, [141] modified the example to work for $n \geq 5$ with minimizer

(2.17)
$$y_{ij}^* = \frac{x_i x_j}{|\mathbf{x}|} - \frac{1}{n} |\mathbf{x}| \delta_{ij}.$$

By a more sophisticated method, Šverák & Yan [241] showed that there exists a convex f such that (2.17) gives a minimizer for n = 3. In fact, working in the five-dimensional space of 3×3 traceless symmetric matrices we thus obtain an example with n = 3, m = 5. Šverák & Yan also obtained a similar example for the case n = 4, m = 3. Note that the above maps \mathbf{y}^* are *one-homogeneous*, i.e. $\mathbf{y}^*(s\mathbf{x}) = s\mathbf{y}^*(\mathbf{x})$ for all $s \ge 0$. In contrast Phillips [210] has shown that when n = 2 any one-homogeneous weak solution \mathbf{y} to a strongly elliptic system of the form div $\mathbf{A}(D\mathbf{y}) = 0$ is linear.

Even if \mathbf{y}^* is not smooth everywhere, we can ask for smoothness outside a closed set of Lebesgue measure zero. That such a result is true is strongly suggested by the classical partial regularity theorem of Evans [116], which (with the incorporation of a weakening of the growth condition due to Acerbi & Fusco [4]) states that any global minimizer has this property for a class of integrals of the form (2.16) with fsatisfying (2.11) and the strong quasiconvexity condition that for some $p \geq 2$

$$\int_{\Omega} [f(\mathbf{A} + D\varphi) - f(\mathbf{A})] \, d\mathbf{x} \ge \gamma \int_{\Omega} [|D\varphi|^2 + |D\varphi|^p] \, d\mathbf{x},$$

for all $\mathbf{A} \in M^{m \times n}$, all $\varphi \in C_0^{\infty}(\Omega; \mathbf{R}^m)$. Recently, Kristensen & Taheri [165] have proved the same result but for $W^{1,p}$ local minimizers. However, it is not known how to extend these theorems to the case of elasticity when (2.7) holds (see Ball [31] for a brief discussion).

In proving regularity or partial regularity, it is not sufficient to just use the fact (if it is a fact, see below) that \mathbf{y}^* satisfies the weak form of the Euler-Lagrange equation. This follows from the example of Müller & Šverák [193] of a Lipschitz mapping $\mathbf{y}: \Omega \to \mathbf{R}^2$, with $\Omega \subset \mathbf{R}^2$ a bounded domain, that is nowhere C^1 and solves the weak form of the Euler-Lagrange equation for an integral

$$I(\mathbf{y}) = \int_{\Omega} F(D\mathbf{y}) \, d\mathbf{x}$$

with F strictly quasiconvex. As shown by Kristensen & Taheri [165] y can even be a $W^{1,\infty}$ local minimizer.

There seems to be little indication from experiment that natural rubbers have equilibrium solutions with singularities other than those involving cavitation or other forms of fracture. Thus it seems a reasonable conjecture that minimizers are smooth for models of natural rubber for which the stored-energy function satisfies growth conditions prohibiting discontinuities for deformations of finite energy. In view of the above and other counterexamples for elliptic systems, if minimizers are smooth it must be for special reasons applying to elasticity. Three plausible such reasons are: (a) the fact that the integrand $W(D\mathbf{y})$ does not depend explicitly on \mathbf{y} (though dependence on \mathbf{x} is allowed), (b) the fact that the dimensions m = n = 3 are low, (c) the frame-indifference of W (see (2.9)). A fourth possible reason is (d) invertibility of \mathbf{y} , which we discuss now.

That invertibility could have an effect on regularity was first shown by Bauman, Owen & Phillips [45], who gave an example of an essentially two-to-one equilibrium solution in a ball for two-dimensional elasticity, with stored-energy function of the form (2.15), that is C^1 but not smooth, and is such that det $D\mathbf{y}$ vanishes at the centre of the ball. An instructive example (resulting from discussions with X. Yan and J. Bevan) is that of minimizing the two-dimensional energy for an incompressible material

$$I(\mathbf{y}) = \int_B |D\mathbf{y}|^2 \, d\mathbf{x},$$

where B = B(0, 1) is the unit disc in \mathbf{R}^2 , and $\mathbf{y} : B \to \mathbf{R}^2$, in the set of admissible mappings

(2.18)
$$\mathcal{A} = \{ \mathbf{y} \in W^{1,2}(B; \mathbf{R}^2) : \det D\mathbf{y} = 1 \text{ a.e. }, \mathbf{y}|_{\partial B} = \bar{\mathbf{y}} \},$$

where in polar coordinates $\bar{\mathbf{y}} : (r, \theta) \mapsto (\frac{1}{\sqrt{2}}r, 2\theta)$. Then there exists a global minimizer y^* of I in \mathcal{A} . (Note that \mathcal{A} is nonempty since $\bar{\mathbf{y}} \in \mathcal{A}$.) But since by degree theory there are no C^1 maps \mathbf{y} satisfying the boundary condition (2.18), it is immediate that y^* is not C^1 .

For interesting maximum principles satisfied by smooth equilibrium solutions in two-dimensional elasticity, with stored-energy function of the form (2.15), see Bauman, Owen & Phillips [46, 47].

2.4. Satisfaction of the Euler-Lagrange equation and uniform positivity of the Jacobian. Here we return to the computation formally leading to the weak form (2.4) of the Euler-Lagrange equation, under the assumption (2.7). If $\mathbf{y}^* \in W^{1,\infty}(\Omega; \mathbf{R}^3)$ is a $W^{1,\infty}$ local minimizer of I in

$$\mathcal{A} = \{ \mathbf{y} \in W^{1,1}(\Omega; \mathbf{R}^3) : \mathbf{y}|_{\partial \Omega_1} = \bar{\mathbf{y}} \},\$$

and if (2.8) holds in the stronger form that for some $\varepsilon > 0$

(2.19)
$$\det D\mathbf{y}^*(\mathbf{x}) \ge \varepsilon \text{ for a.e. } \mathbf{x} \in \Omega,$$

then it is easily seen that \mathbf{y}^* satisfies (2.4). In fact we can then pass to the limit $\tau \to 0$ using bounded convergence in the difference quotient

(2.20)
$$\int_{\Omega} \frac{1}{\tau} [W(D\mathbf{y}^* + \tau D\varphi) - W(D\mathbf{y}^*)] \, dx,$$

since by (2.19) we have $\det(D\mathbf{y}^*(\mathbf{x}) + \tau D\varphi(\mathbf{x})) \geq \varepsilon/2$ for a.e. $\mathbf{x} \in \Omega$. However, if only (2.7) is assumed, or if \mathbf{y}^* is not assumed in advance to be in $W^{1,\infty}(\Omega; \mathbf{R}^3)$, then it is not obvious how to pass to the limit.

Problem 5. Prove or disprove that, under reasonable growth conditions on W, global or suitably defined local minimizers of I satisfy the weak form (2.4) of the Euler-Lagrange equation.

Problem 6. Prove or disprove that, under reasonable growth conditions on W, global or suitably defined local minimizers of I satisfy (2.19).

If $W(\mathbf{A}) \to \infty$ as $|\mathbf{A}| \to \infty$ and if $\mathbf{y}^* \notin W^{1,\infty}$, or if (2.19) does not hold, then $W(D\mathbf{y}^*)$ is essentially unbounded. This is at first sight inconsistent with \mathbf{y}^* being a minimizer, but we know from the one-dimensional examples in Ball & Mizel [43] and from the example of cavitation that *it can pay to have the integrand infinite somewhere so that it is smaller somewhere else.* In general, it is not possible to estimate the integrand in the difference quotient (2.20) in terms of $W(D\mathbf{y}^*)$, the only relevant quantity that is obviously integrable. This difficulty was pointed out by Antman [12], who was the first to address the issue of satisfaction of the Euler-Lagrange equation holds (see also Ball [22]) without any supplementary growth conditions on W.

It is perhaps worth making the simple observation that a smooth deformation **y** may satisfy $I(\mathbf{y}) < \infty$ and det $D\mathbf{y}(\mathbf{x}) > 0$ a.e. without (2.19) holding. As an example we may take $\Omega = B(0, 1)$ and

$$\mathbf{y}(\mathbf{x}) = |\mathbf{x}|^2 \mathbf{x},$$

with $W(\mathbf{A}) = -\log \det \mathbf{A} + g(\mathbf{A})$, where $g: M^{3 \times 3} \to \mathbf{R}$ is smooth.

For a class of strongly elliptic stored-energy functions of the form $W(\mathbf{A}) = g(\mathbf{A}) + h(\det \mathbf{A})$, where $g: M^{3\times3} \to \mathbf{R}$ and $h: (0, \infty) \to [0, \infty)$ are smooth with $h(\delta) \to \infty$ as $\delta \to 0+$ at a polynomial rate, Bauman, Owen & Phillips [45] show that if $\mathbf{y} \in C^{1,\beta}$ satisfies the energy-momentum weak form of the Euler-Lagrange equation in (2.22) below, then in fact \mathbf{y} is a smooth solution of the Euler-Lagrange equation (2.5) and the strict positivity condition (2.19) holds.

As was pointed out in Ball [25], it is possible to derive different first-order necessary conditions for a minimizer when (2.7) holds. (Later Giaquinta, Modica & Souček [133] derived the same first-order conditions in their framework of Cartesian currents, under somewhat stronger hypotheses.) We give here improved versions of these results.

We consider the following conditions that may be satisfied by W:

(C1) $|D_{\mathbf{A}}W(\mathbf{A})\mathbf{A}^T| \le K(W(\mathbf{A})+1)$ for all $\mathbf{A} \in M^{3\times 3}_+$,

where K > 0 is a constant, and

(C2)
$$|\mathbf{A}^T D_{\mathbf{A}} W(\mathbf{A})| \le K(W(\mathbf{A}) + 1)$$
 for all $\mathbf{A} \in M^{3 \times 3}_+$,

where K > 0 is a constant.

As usual, $|\cdot|$ denotes the Euclidean norm on $M^{3\times 3}$, for which the inequalities $|\mathbf{A} \cdot \mathbf{B}| \leq |\mathbf{A}| \cdot |\mathbf{B}|$ and $|\mathbf{AB}| \leq |\mathbf{A}| \cdot |\mathbf{B}|$ hold. But of course the conditions are independent of the norm used up to a possible change in the constant K.

Proposition 2.2. Let W satisfy (C2). Then W satisfies (C1).

Proof. Since W is frame-indifferent the matrix $D_{\mathbf{A}}W(\mathbf{A})\mathbf{A}^{T}$ is symmetric (this is equivalent to the symmetry of the Cauchy stress tensor – see (2.27) below). Hence

$$D_{\mathbf{A}}W(\mathbf{A})\mathbf{A}^{T}|^{2} = [D_{\mathbf{A}}W(\mathbf{A})\mathbf{A}^{T}] \cdot [\mathbf{A}(D_{\mathbf{A}}W(\mathbf{A}))^{T}]$$

$$= [\mathbf{A}^{T}D_{\mathbf{A}}W(\mathbf{A})] \cdot [\mathbf{A}^{T}D_{\mathbf{A}}W(\mathbf{A})]^{T}$$

$$\leq |\mathbf{A}^{T}D_{\mathbf{A}}W(\mathbf{A})|^{2},$$

from which the result follows.

Example 2.1. Let

$$W(\mathbf{A}) = (\mathbf{A}^T \mathbf{A})_{11} + \frac{1}{\det \mathbf{A}}.$$

Then W satisfies (C1) and (2.9), but not (C2).

Theorem 2.3. For some $1 \leq p < \infty$ let $\mathbf{y} \in \mathcal{A} \cap W^{1,p}(\Omega; \mathbf{R}^3)$ be a $W^{1,p}$ local minimizer of I in \mathcal{A} . (i) Let W satisfy (C1). Then

(2.21)
$$\int_{\Omega} [D_{\mathbf{A}} W(D\mathbf{y}) D\mathbf{y}^T] \cdot D\varphi(\mathbf{y}) \, d\mathbf{x} = 0$$

for all $\varphi \in C^1(\mathbf{R}^3; \mathbf{R}^3)$ such that φ and $D\varphi$ are uniformly bounded and satisfy $\varphi(\mathbf{y})|_{\partial\Omega_1} = 0$ in the sense of trace.

(ii) Let W satisfy (C2). Then

(2.22)
$$\int_{\Omega} [W(D\mathbf{y})\mathbf{1} - D\mathbf{y}^T D_{\mathbf{A}} W(D\mathbf{y})] \cdot D\varphi \, d\mathbf{x} = 0$$

for all $\varphi \in C_0^1(\Omega; \mathbf{R}^3)$.

We use the following simple lemma.

Lemma 2.4. (a) If W satisfies (C1) then there exists $\gamma > 0$ such that if $\mathbf{C} \in M^{3\times 3}_+$ and $|\mathbf{C} - \mathbf{1}| < \gamma$ then

$$|D_{\mathbf{A}}W(\mathbf{CA})\mathbf{A}^T| \leq 3K(W(\mathbf{A})+1)$$
 for all $\mathbf{A} \in M^{3\times 3}_+$

(b) If W satisfies (C2) then there exists $\gamma > 0$ such that if $\mathbf{C} \in M^{3 \times 3}_+$ and $|\mathbf{C}-\mathbf{1}| < \gamma$ then

(2.23)
$$|\mathbf{A}^T D_{\mathbf{A}} W(\mathbf{AC})| \leq 3K(W(\mathbf{A}) + 1) \text{ for all } \mathbf{A} \in M_+^{3 \times 3}$$

Proof. We prove (a); the proof of (b) is similar. We first show that there exists $\gamma > 0$ such that if $|\mathbf{C} - \mathbf{1}| < \gamma$ then

(2.24)
$$W(\mathbf{CA}) + 1 \le \frac{3}{2}(W(\mathbf{A}) + 1) \text{ for all } \mathbf{A} \in M_+^{3 \times 3}.$$

For $t \in [0,1]$ let $\mathbf{C}(t) = t\mathbf{C} + (1-t)\mathbf{1}$. Choose $\gamma \in (0, \frac{1}{6K})$ sufficiently small so that $|\mathbf{C} - \mathbf{1}| < \gamma$ implies that $|\mathbf{C}(t)^{-1}| \leq 2$ for all $t \in [0,1]$. This is possible since

$$\begin{aligned} | &= \sqrt{3} < 2. \text{ For } |\mathbf{C} - \mathbf{1}| < \gamma \text{ we have that} \\ W(\mathbf{CA}) - W(\mathbf{A}) &= \int_0^1 \frac{d}{dt} W(\mathbf{C}(t)\mathbf{A}) \, dt \\ &= \int_0^1 D_{\mathbf{A}} W(\mathbf{C}(t)\mathbf{A}) \cdot [(\mathbf{C} - \mathbf{1})\mathbf{A}] \, dt \\ &= \int_0^1 D_{\mathbf{A}} W(\mathbf{C}(t)\mathbf{A}) (\mathbf{C}(t)\mathbf{A})^T \cdot ((\mathbf{C} - \mathbf{1})\mathbf{C}(t)^{-1}) \, dt \\ &\leq K \int_0^1 [W(\mathbf{C}(t)\mathbf{A}) + 1] \cdot |\mathbf{C} - \mathbf{1}| \cdot |\mathbf{C}(t)^{-1}| \, dt \\ &\leq 2K\gamma \int_0^1 (W(\mathbf{C}(t)\mathbf{A}) + 1) \, dt. \end{aligned}$$

Let $\theta(\mathbf{A}) = \sup_{|\mathbf{C}-\mathbf{1}| < \gamma} W(\mathbf{C}\mathbf{A})$. Then

$$W(\mathbf{CA}) - W(\mathbf{A}) \le \theta(\mathbf{A}) - W(\mathbf{A}) \le 2K\gamma(\theta(\mathbf{A}) + 1),$$

from which (2.24) follows.

Finally, if $|\mathbf{C} - \mathbf{1}| < \gamma$ we have from (C1) and (2.24) that

$$\begin{aligned} |D_{\mathbf{A}}W(\mathbf{C}\mathbf{A})\mathbf{A}^{T}| &= |D_{\mathbf{A}}W(\mathbf{C}\mathbf{A})(\mathbf{C}\mathbf{A})^{T}\mathbf{C}^{-T}| \\ &\leq K(W(\mathbf{C}\mathbf{A})+\mathbf{1})|\mathbf{C}^{-T}| \\ &\leq 3K(W(\mathbf{A})+\mathbf{1}), \end{aligned}$$

as required.

1

Proof of Theorem 2.3. (i) Given φ as in the theorem, define for $|\tau|$ sufficiently small

$$\mathbf{y}_{\tau}(\mathbf{x}) := \mathbf{y}(\mathbf{x}) + \tau \varphi(\mathbf{y}(\mathbf{x})).$$

Then $\mathbf{y}_{\tau} \in \mathcal{A}$ and

$$D\mathbf{y}_{\tau}(\mathbf{x}) = (\mathbf{1} + \tau D\varphi(\mathbf{y}(\mathbf{x})))D\mathbf{y}(\mathbf{x}) \text{ a.e. } \mathbf{x} \in \Omega.$$

In particular det $D\mathbf{y}_{\tau}(\mathbf{x}) > 0$ for a.e. $\mathbf{x} \in \Omega$ and $\lim_{\tau \to 0} \|\mathbf{y}_{\tau} - \mathbf{y}\|_{W^{1,p}} = 0$. Hence $I(\mathbf{y}_{\tau}) \geq I(\mathbf{y})$ for $|\tau|$ sufficiently small. But

$$\frac{1}{\tau}(I(\mathbf{y}_{\tau}) - I(\mathbf{y})) = \frac{1}{\tau} \int_{\Omega} \int_{0}^{1} \frac{d}{ds} W((\mathbf{1} + s\tau D\varphi(\mathbf{y}(\mathbf{x})))D\mathbf{y}(\mathbf{x})) \, ds \, d\mathbf{x}$$
$$= \int_{\Omega} \int_{0}^{1} DW((\mathbf{1} + s\tau D\varphi(\mathbf{y}(\mathbf{x})))D\mathbf{y}(\mathbf{x})) \cdot [D\varphi(\mathbf{y}(\mathbf{x}))D\mathbf{y}(\mathbf{x})] \, ds \, d\mathbf{x}.$$

Since by Lemma 2.4(a) the integrand is bounded by the integrable function

$$3K(W(D\mathbf{y}(\mathbf{x}))+1) \sup_{\mathbf{z}\in\mathbf{R}^3} |D\varphi(\mathbf{z})|,$$

we may pass to the limit $\tau \to 0$ using dominated convergence to obtain (2.21).

(ii) This follows in a similar way to (i) from Lemma 2.4 (b). Since most of the details have already been written down in Bauman, Owen & Phillips [46] we just sketch the idea. Let $\varphi \in C_0^1(\Omega; \mathbf{R}^3)$. For sufficiently small $\tau > 0$ the mapping θ_{τ} defined by

$$\theta_{\tau}(\mathbf{z}) := \mathbf{z} + \tau \varphi(\mathbf{z})$$

belongs to $C^1(\Omega; \mathbf{R}^3)$, satisfies det $D\theta_{\tau}(\mathbf{z}) > 0$, and coincides with the identity on $\partial \Omega$. Standard arguments from degree theory imply that θ_{τ} is a diffeomorphism of Ω to itself. Thus the 'inner variation'

$$\mathbf{y}_{\tau}(\mathbf{x}) := \mathbf{y}(\mathbf{z}_{\tau}), \quad \mathbf{x} = \mathbf{z}_{\tau} + \tau \varphi(\mathbf{z}_{\tau})$$

defines a mapping $\mathbf{y}_{\tau} \in \mathcal{A}$, and

$$D\mathbf{y}_{\tau}(x) = D\mathbf{y}(\mathbf{z}_{\tau})[\mathbf{1} + \tau D\varphi(\mathbf{z}_{\tau})]^{-1}$$
 a.e. $\mathbf{x} \in \Omega$.

Since $\mathbf{y} \in W^{1,p}$ it follows easily that $\|\mathbf{y}_{\tau} - \mathbf{y}\|_{W^{1,p}} \to 0$ as $\tau \to 0$. Changing variables we obtain

$$I(\mathbf{y}_{\tau}) = \int_{\Omega} W(D\mathbf{y}(\mathbf{z})[\mathbf{1} + \tau D\varphi(\mathbf{z})]^{-1}) \det(\mathbf{1} + \tau D\varphi(\mathbf{z})) d\mathbf{z},$$

from which (2.22) follows using (2.23) and dominated convergence.

In order to give an interpretation of Theorem 2.3 (i), let us make the following

Invertibility Hypothesis. \mathbf{y} is a homeomorphism of Ω onto $\Omega' := \mathbf{y}(\Omega), \ \Omega'$ is a bounded domain, and the change of variables formula

(2.25)
$$\int_{\Omega} f(\mathbf{y}(\mathbf{x})) \det D\mathbf{y}(\mathbf{x}) \, d\mathbf{x} = \int_{\Omega'} f(\mathbf{z}) \, d\mathbf{z}$$

holds whenever $f : \mathbf{R}^3 \to \mathbf{R}$ is measurable, provided that one of the integrals in (2.25) exists.

Sufficient conditions for this hypothesis to hold are given in [21] and Šverák [237].

Theorem 2.5. Assume that the hypotheses of Theorem 2.3 (i) and the Invertibility Hypothesis hold. Then

(2.26)
$$\int_{\Omega'} \sigma(\mathbf{z}) \cdot D\varphi(\mathbf{z}) \, d\mathbf{z} = 0$$

for all $\varphi \in C^1(\mathbf{R}^3; \mathbf{R}^3)$ such that $\varphi|_{\mathbf{y}(\partial \Omega_1)} = 0$, where the Cauchy stress tensor σ is defined by

$$\sigma(\mathbf{z}) := \mathbf{T}(\mathbf{y}^{-1}(\mathbf{z})), \quad z \in \Omega'$$

and

(2.27)
$$\mathbf{T}(\mathbf{x}) = (\det D\mathbf{y}(\mathbf{x}))^{-1} D_{\mathbf{A}} W(D\mathbf{y}(\mathbf{x})) D\mathbf{y}(\mathbf{x})^{T}.$$

Proof. Since by assumption $\mathbf{y}(\bar{\Omega})$ is bounded, we can assume that φ and $D\varphi$ are uniformly bounded. Thus (2.26) follows immediately from (2.21), (2.25) and (2.27).

Thus Theorem 2.3 (i) asserts that **y** satisfies the spatial (Eulerian) form of the equilibrium equations. Theorem 2.3 (ii), on the other hand, involves the so-called energy-momentum tensor $W(\mathbf{A})\mathbf{1} - \mathbf{A}^T D_{\mathbf{A}}W(\mathbf{A})$, and is a multi-dimensional version of the Du Bois Reymond or Erdmann equation of the one-dimensional calculus of variations.

The hypotheses (C1) and (C2) imply that W has polynomial growth. More precisely, we have

Proposition 2.6. Suppose W satisfies (C1) or (C2). Then for some s > 0 $W(\mathbf{A}) \leq M(|\mathbf{A}|^s + |\mathbf{A}^{-1}|^s) \text{ for all } \mathbf{A} \in M_+^{3 \times 3}.$ *Proof.* Let $\mathbf{V} \in M^{3 \times 3}$ be symmetric. For $t \ge 0$

$$\left| \frac{d}{dt} W(e^{t\mathbf{V}}) \right| = \left| (D_{\mathbf{A}} W(e^{t\mathbf{V}}) e^{t\mathbf{V}}) \cdot \mathbf{V} \right|$$
$$= \left| (e^{t\mathbf{V}} D_{\mathbf{A}} W(e^{t\mathbf{V}})) \cdot \mathbf{V} \right|$$
$$\leq K(W(e^{t\mathbf{V}}) + 1) |\mathbf{V}|.$$

From this it follows that

(2.29)
$$W(e^{\mathbf{V}}) + 1 \le (W(\mathbf{1}) + 1)e^{K|\mathbf{V}|}.$$

Now set $\mathbf{V} = \ln \mathbf{U}$, where $\mathbf{U} = \mathbf{U}^T > 0$, and denote by v_i the eigenvalues of \mathbf{U} . Since

$$|\ln \mathbf{U}| = \left(\sum_{i=1}^{3} (\ln v_i)^2\right)^{1/2}$$

 $\leq \sum_{i=1}^{3} |\ln v_i|,$

it follows that

$$\begin{split} e^{K|\ln \mathbf{U}|} &\leq (v_1^K + v_1^{-K})(v_2^K + v_2^{-K})(v_3^K + v_3^{-K}) \\ &\leq 3^{-3} \Big(\sum_{i=1}^3 v_i^K + \sum_{i=1}^3 v_i^{-K}\Big)^{1/3} \\ &\leq C \Big(\sum_{i=1}^3 v_i^{3K} + \sum_{i=1}^3 v_i^{-3K}\Big)^3 \\ &\leq C_1[|\mathbf{U}|^{3K} + |\mathbf{U}^{-1}|^{3K}], \end{split}$$

where C > 0, $C_1 > 0$ are constants. From (2.29) we thus obtain

$$W(\mathbf{U}) \le M(|\mathbf{U}|^{3K} + |\mathbf{U}^{-1}|^{3K}),$$

where $M = C_1(W(1) + 1)$. The result now follows from the polar decomposition $\mathbf{A} = \mathbf{R}\mathbf{U}$ of an arbitrary $\mathbf{A} \in M^{3\times 3}_+$, where $\mathbf{R} \in \mathrm{SO}(3)$, $\mathbf{U} = \mathbf{U}^T > 0$.

It is easily seen that if W is isotropic then both (C1) and (C2) are equivalent to the condition that

$$|(v_1\Phi_{,1}, v_2\Phi_{,2}, v_3\Phi_{,3})| \le K(\Phi(v_1, v_2, v_3) + 1)$$

for all $v_i > 0$ and some K > 0, where Φ is given by (2.14) and $\Phi_{,i} = \partial \Phi / \partial v_i$. In particular, both (C1) and (C2) hold for the class of *Ogden materials* ([198, 199]), for which Φ has the form

$$\Phi(v_1, v_2, v_3) = \sum_{i=1}^{M} a_i \varphi(\alpha_i) + \sum_{i=1}^{N} b_i \psi(\beta_i) + h(v_1 v_2 v_3)$$

where $\varphi(\alpha) = v_1^{\alpha} + v_2^{\alpha} + v_3^{\alpha}$, $\psi(\beta) = (v_2v_3)^{\beta} + (v_3v_1)^{\beta} + (v_1v_2)^{\beta}$, $a_i > 0, b_i > 0, \alpha_i \neq 0$, $\beta_i \neq 0$, and where $h : (0, \infty) \to [0, \infty)$ is convex, with $h(\delta) \to \infty$ as $\delta \to 0$, provided that $|\delta h'(\delta)| \leq K_1(h(\delta) + 1)$ for all $\delta > 0$.

2.5. **Regularity and self-contact.** An interesting approach to the problem of invertibility (i.e. non-interpenetration of matter) in mixed boundary-value problems is due to Ciarlet & Nečas [84]. They proposed minimizing

$$I(\mathbf{y}) = \int_{\Omega} W(D\mathbf{y}) \, d\mathbf{x}$$

subject to the boundary condition (2.1) and the global constraint

$$\int_{\Omega} \det D\mathbf{y}(\mathbf{x}) \, d\mathbf{x} \le \text{volume}\left(\mathbf{y}(\Omega)\right)$$

and they gave hypotheses under which the minimum was attained, these hypotheses being weakened by Qi [217]. They further showed that any minimizer is one-to-one almost everywhere, and that assuming sufficient regularity of the free boundary $\mathbf{y}(\partial \Omega_2)$ the tangential components of the normal stress vector vanish there. Consequently they identified the above constrained boundary-value problem as corresponding to the case of smooth (i.e. frictionless) self-contact. A related but somwhat different formulation has recently been proposed by Pantz [202]; see also Giaquinta, Modica & Souček [131].

Problem 7. Justify the Ciarlet-Nečas minimization problem, or an appropriate modification of it, as a model of smooth self-contact.

The problem here is to construct suitable variations in the neighbourhood of a region of self-contact of a minimizer to establish that in some sense the tangential stress components vanish there. This is non-trivial because in principle the two parts of the boundary in contact with one another could be wildly deformed and interlocked in a very complex configuration. If such a result could be obtained, a more ambitious target would be to establish the regularity properties of the free boundary in both the self-contacting and non self-contacting regions.

2.6. Uniqueness of solutions. For mixed boundary-value problems of elasticity nonuniqueness of equilibrium solutions is common-place, the most familiar examples being those associated with buckling of rods, plates and shells. Buckling can occur even for pure zero-traction boundary conditions, such as in the eversion of part of a spherical shell. For the pure zero-traction problem one can even have nonuniqueness among homogeneous dilatations (see Ball [23]). Nonuniqueness of these types is expected to hold, and to some extent can be proved rigorously, when the stored-energy function satisfies favourable hypotheses such as strict polyconvexity (though see Section 2.7). For stored-energy functions corresponding to elastic crystals, for which there are many minimum energy configurations with a continuum of different sets of phase boundaries, the extent of non-uniqueness is of course much greater.

For pure displacement boundary conditions, with a strictly polyconvex (or strictly quasiconvex) stored-energy function satisfying favourable growth conditions, the situation as regards uniqueness is less clear. In the paper [153] Fritz John proved uniqueness for smooth deformations with uniformly small strains (but possibly large rotations). In the same paper he gave a heuristic counter-example to uniqueness for the case of an annular two-dimensional body, and this has been made rigorous by Post & Sivaloganathan [214] (see Section 2.7), who also proved nonuniquenesss for an analogous three-dimensional problem with Ω a torus. But what if Ω is homeomorphic to a ball? In this case we have already seen that cavitation provides one counterexample to uniqueness, though the cavitating solution is discontinuous.

Problem 8. Prove or disprove the uniqueness of sufficiently smooth equilibrium solutions to pure displacement boundary-value problems for homogeneous bodies when the stored-energy function W is strictly polyconvex and Ω is homeomorphic to a ball.

The answer to this problem probably depends on both the geometry of Ω and the boundary conditions. For example, suppose that Ω is a ball, and that the boundary conditions correspond to severely squeezing the ball until it has a dumb-bell shape consisting of two roughly ball-shaped regions connected by a narrow passage. In this case one might expect, though it is not obvious how to prove it, that there might be equilibrium solutions in which material from one half of Ω is pulled through into the other half, but prevented from returning by the constriction. On the other hand, an elegant result of Knops & Stuart [159] implies uniqueness for the case when the boundary displacements are linear and Ω is star-shaped (see also Taheri [247]).

2.7. Structure of the solution set.

Problem 9. Devise general methods for proving the existence of local minimizers of I that are not global minimizers, and of other weak solutions of the equilibrium equations.

For the existence of local minimizers there are two natural approaches. First we could try to use the direct method of the calculus of variations in a suitable subset of \mathcal{A} . For example, under the hypotheses of Theorem 2.1 suppose that we want to prove the existence of a local minimizer with respect to some metric don \mathcal{A} . Assume that d is such that if $z^{(j)} \in \mathcal{A}$ with $z^{(j)} \rightharpoonup z$ in $W^{1,1}(\Omega; \mathbf{R}^3)$ and $\sup I(z^{(j)}) < \infty$ then $d(z^{(j)}, z) \rightarrow 0$.

Let $U \subset \mathcal{A}$ be open with respect to d, with closure \overline{U} and boundary ∂U . By the direct method, I attains a minimum \hat{y} on \overline{U} . Suppose now that we can prove that

$$\inf_{\partial U} I > \inf_{U} I > \inf_{\mathcal{A}} I.$$

Then $\hat{y} \in U$ and is a local, but not global, minimizer with respect to d. I believe that it should be possible to implement this method in some realistic examples, but have not seen it done. The only results on local minimizers in nonlinear elasticity using the direct method that I am aware of are due to Post & Sivaloganathan [214], who prove the existence of local but not global minimizers for certain two-dimensional problems (see Section 2.6) for which the domain Ω has nontrivial topology by global minimization in a weakly closed homotopy class, and to Taheri [246], who generalizes the results in [214] to a wider class of domains.

The second approach is to find by some method a sufficiently smooth solution \hat{y} to the equilibrium equations and attempt to show directly that it is a local minimizer. For local minimizers in $W^{1,\infty}(\Omega; \mathbf{R}^3)$ (weak local minimizers) this can be done in principle by checking positivity of the second variation. However for local minimizers in $W^{1,p}(\Omega; \mathbf{R}^3)$ with $1 \leq p < \infty$, or in $L^q(\Omega; \mathbf{R}^3)$, $1 \leq q \leq \infty$, the task is made much more difficult by the absence of a known generalization to higher dimensions of the Weierstrass fundamental sufficiency theorem of the one-dimensional calculus of variations (for a discussion see [31]). Sometimes it is possible to circumvent the lack of such a theory. For example, in a dead-load traction problem arising from the bi-axial load experiments of Chu & James [78, 79] on CuAlNi single crystals, it is proved in Ball & James [38], Ball, Chu & James [34] (see also Ball, Chu & James [35]) that certain $\hat{\mathbf{y}}$ with $D\hat{\mathbf{y}} = \mathbf{A} = \text{constant}$ are local

(but not global) minimizers in $L^1(\Omega; \mathbf{R}^3)$, by an argument exploiting the geometric incompatibility of **A** with deformation gradients having lower energy.

How can one prove the existence of equilibrium solutions that are not local minimizers? In exceptional cases one may know an equilibrium solution explicitly (for example a trivial solution) and be able to show that it does not satisfy some necessary condition for a local minimizer. If we can also prove the existence of a global minimizer then we have at least two equilibrium solutions. This can be done, for example, for the case of some mixed boundary-value problems when the stored-energy function is polyconvex but not quasiconvex at the boundary (see Ball & Marsden [42]). Another approach would be to try to use Morse theory or mountain-pass methods, but it is not clear how to do this so that, for example, appropriate conditions of Palais-Smale type can be verified; for results in an interesting model problem see Zhang [264].

More generally, one can ask for a description of how the set of equilibrium solutions varies as a function of relevant parameters such as boundary displacements or loads. For the pure traction problem near a stress-free state an interesting study of this type is that of Chillingworth, Marsden & Wan [75, 76] and Wan & Marsden [257].

Problem 10. Develop local and global bifurcation theories for nonlinear elastostatics that apply to mixed displacement-traction boundary conditions.

As an illustration, the most well-known bifurcation problem in elasticity is that of buckling of a thin rod. Although this problem has been treated from the perspective of rod theory in hundreds of papers since the time of Euler [115], there is no rigorous three-dimensional theory that justifies the usual picture of buckling, for example the existence of critical buckling loads or displacements, with corresponding branches of bifurcating buckled solutions. There are at least two difficulties in providing such a theory. The first is that unless the problem is formulated in a somewhat unrealistic way, there is no sufficiently explicit trivial compressed solution about which to linearize the equilibrium equations. For example, suppose that in a stressfree reference configuration a homogeneous isotropic elastic rod occupies the region $\Omega = (0, L) \times D$, where $D \subset \mathbf{R}^2$ is the cross-section. A natural boundary-value problem to consider, corresponding to clamped ends, consists of the equilibrium equations (2.4) and the boundary conditions (2.1), (2.6), with the choices $\partial\Omega_1 =$ $\{0, L\} \times D, \partial\Omega_2 = (0, L) \times \partial D$, and

(2.30)
$$\bar{\mathbf{y}}(0,\mathbf{x}') = (0,\mathbf{x}'), \quad \bar{\mathbf{y}}(L,\mathbf{x}') = (\lambda L,\mathbf{x}'), \quad x' \in D,$$

where $\lambda > 0$. For $\lambda \neq 1$ the homogeneous deformation $\mathbf{y}(x_1, \mathbf{x}') = (\lambda x_1, \mathbf{x}')$ does not in general satisfy the zero traction condition (2.6). For example, for the compressive case $\lambda < 1$ the rod will typically want to bulge, leading to boundary layers near $x_1 = 0$ and $x_1 = L$. In order to have a homogeneously deformed trivial solution

$$\mathbf{y}(\mathbf{x}) = (\lambda x_1, \mu x_2, \mu x_3),$$

one can replace (2.30) by the conditions

$$y_1(0, \mathbf{x}') = 0, \quad y_1(L, \mathbf{x}') = \lambda L, \quad \mathbf{x}' \in D,$$

corresponding to the less realistic case of frictionless end-faces constrained to lie in the planes $\{0\} \times \mathbf{R}^2$ and $\{\lambda L\} \times \mathbf{R}^2$. To prevent sliding of the end-faces one could

add the further constraint that

$$\int_D y_2 \, d\mathbf{x}' = \int_D y_3 \, d\mathbf{x}' = 0 \quad \text{at } x_1 = 0, L.$$

In this case the natural boundary conditions at $x_1 = 0, L$ for the variational problem are that the stress vector **t** across the end-faces has constant transverse components t_2, t_3 which are equal at $x_1 = 0, L$. If we try to prescribe compressive loads at $x_1 = 0, L$ rather than displacements we encounter other difficulties (see [30] for a discussion of one of these).

The second more serious difficulty has already been mentioned, namely the lack of regularity of solutions to the linearized equilibrium equations as one approaches points of $\overline{\partial\Omega_1} \cap \overline{\partial\Omega_2}$, or points of discontinuity of the applied traction in a pure traction formulation of the problem, which prohibits use of the implicit function theorem in natural spaces. Perhaps it might be possible to work in spaces with suitable weights in the neighbourhood of $\overline{\partial\Omega_1} \cap \overline{\partial\Omega_2}$. But it seems odd that fine details of what goes on near $\overline{\partial\Omega_1} \cap \overline{\partial\Omega_2}$ should have a significant bearing on the buckling phenomenon, so perhaps there is a different approach to be discovered that circumvents this difficulty.

Once a local bifurcation picture has been established, the next thing to understand is what happens to bifurcating solutions for large parameter values. For the case when $\partial\Omega_1 \cap \partial\Omega_2$ is empty global results have recently been obtained by Healey & Rosakis [143], Healey & Simpson [144] and Healey [142].

2.8. Energy minimization and fracture. Many of the problems described above have generalizations to *variational models of fracture*. Since typical fracture problems are described by deformations that have jump discontinuities across twodimensional crack surfaces, fracture cannot in general be modelled in the context of Sobolev spaces. A generalization of the energy functional (2.2) to deformations allowing for fracture is

(2.31)
$$I(y) = \int_{\Omega} W(D\mathbf{y}) \, d\mathbf{x} + \int_{S_{\mathbf{y}}} g(\mathbf{y}^+ - \mathbf{y}^-, \nu_{\mathbf{y}}) \, d\mathcal{H}^2,$$

where \mathbf{y} belongs to the class SBV(Ω) of mappings of special bounded variation, i.e. those whose gradient is a bounded measure having no Cantor part. In (2.31) $S_{\mathbf{y}}$ denotes the set of jump points of \mathbf{y} , $\nu_{\mathbf{y}}$ the measure theoretic normal to $S_{\mathbf{y}}$, and \mathbf{y}^{\pm} the traces of \mathbf{y} on either side of $S_{\mathbf{y}}$. The second integral represents the surface energy of cracks, as postulated in the Griffith theory of fracture (see, for example, [74]), the simplest case $g = \text{constant corresponding to a contribution to the energy$ $proportional to the total crack surface area <math>\mathcal{H}(S_{\mathbf{y}})$. Despite much deep work on such models (see, for example, Acerbi, Fonseca & Fusco [2], Ambrosio [5, 6], Ambrosio & Braides [7], Ambrosio, Fusco & Pallara [8, 9], Ambrosio & Pallara [10], Braides [56], Braides & Coscia [57, 58], Braides, Dal Maso & Garroni [62], Buttazzo [72]), and their apparent potential for making an impact on understanding fracture, there have been only isolated attempts to discover their implications for practical problems of fracture mechanics (see, for example, Francfort & Marigo [123], Bourdin, Francfort & Marigo [54]).

Problem 11. Clarify the status of models based on the energy functional (2.31) with respect to classical fracture mechanics and to nonlinear elastostatics.

Two key issues are fracture initiation and stability, which are both related to the study of local minimizers for the functional (2.31). A technical obstacle in such a study is the lack of a general method of calculating a general variation of I about a given \mathbf{y} in the direction of nearby deformations having possibly very different sets of jump points. An understanding of local minimizers would also clarify the status of the nonlinear elastostatics model based on (2.2) with respect to that based on (2.31), and thereby demystify the apparent sensitivity of the elastostatics model to growth behaviour for very large strains.

3. Dynamics

3.1. Continuum thermomechanics. We recall briefly the elements of continuum thermomechanics. The basic balance laws are the *balance of linear momentum*

(3.1)
$$\frac{d}{dt} \int_{E} \rho_{R} \mathbf{y}_{t} \, d\mathbf{x} = \int_{\partial E} \mathbf{t}_{R} \, dS + \int_{E} \mathbf{b} \, d\mathbf{x},$$

the balance of angular momentum

(3.2)
$$\frac{d}{dt} \int_{E} \rho_{R} \mathbf{x} \wedge \mathbf{y}_{t} \, d\mathbf{x} = \int_{\partial E} \mathbf{x} \wedge \mathbf{t}_{R} \, dS + \int_{E} \mathbf{x} \wedge \mathbf{b} \, d\mathbf{x},$$

and the balance of energy

(3.3)
$$\frac{d}{dt} \int_{E} \left(\frac{1}{2} \rho_{R} |\mathbf{y}_{t}|^{2} + U \right) d\mathbf{x} = \int_{E} \mathbf{b} \cdot \mathbf{y}_{t} d\mathbf{x} + \int_{\partial E} \mathbf{t}_{R} \cdot \mathbf{y}_{t} dS + \int_{E} r \, d\mathbf{x} - \int_{\partial E} \mathbf{q}_{R} \cdot \mathbf{n} \, dS.$$

Here $\mathbf{y} = \mathbf{y}(\mathbf{x}, t)$ denotes the deformation, \mathbf{t}_R the Piola-Kirchhoff stress vector, $\rho_R > 0$ the (constant) density in the reference configuration, \mathbf{b} the body force, U the internal energy, \mathbf{q}_R the heat flux vector and r the heat supply. The balance laws are assumed to hold for all Lipschitz domains $E \subset \Omega$, and the unit outward normal to ∂E is denoted by \mathbf{n} . In addition to the balance laws, thermomechanical processes are required to obey the Second Law of Thermodynamics, which we assume to hold in the form of the *Clausius-Duhem inequality*

(3.4)
$$\frac{d}{dt} \int_{E} \eta \, d\mathbf{x} \ge -\int_{\partial E} \frac{\mathbf{q}_{R} \cdot \mathbf{n}}{\theta} \, dS + \int_{E} \frac{r}{\theta} \, d\mathbf{x}$$

for all E, where η is the entropy and θ the temperature. Standard arguments now show that $\mathbf{t}_R = \mathbf{T}_R \mathbf{n}$, where \mathbf{T}_R is the Piola-Kirchhoff stress tensor, and that for sufficiently smooth processes (3.1), (3.3), (3.4) reduce to the pointwise forms

(3.5)
$$\rho_R \mathbf{y}_{tt} - \operatorname{div} \mathbf{T}_R - \mathbf{b} = 0$$

(3.6)
$$\frac{d}{dt}\left(\frac{1}{2}|\mathbf{y}_t|^2 + U\right) - \mathbf{b} \cdot \mathbf{y}_t - \operatorname{div}\left(\mathbf{y}_t\mathbf{T}_R\right) + \operatorname{div}\mathbf{q}_R - r = 0$$

(3.7)
$$\eta_t + \operatorname{div}\left(\frac{\mathbf{q}_R}{\theta}\right) - \frac{r}{\theta} \geq 0,$$

and that (3.2) is equivalent to the symmetry of the Cauchy stress tensor

$$\mathbf{T} = (\det D\mathbf{y})^{-1} \mathbf{T}_R (D\mathbf{y})^T$$

Eliminating r from (3.6), (3.7), using (3.5) and denoting by

(3.8)
$$\psi = U - \theta \eta$$

the *Helmholtz free energy*, we obtain that for sufficiently smooth processes

(3.9)
$$-\psi_t - \theta_t \eta + \mathbf{T}_R \cdot D\mathbf{y}_t - \frac{\mathbf{q}_R \cdot \operatorname{grad} \theta}{\theta} \ge 0.$$

Adopting the prescription of Coleman & Noll [87], we assume that given an arbitrary deformation $\mathbf{y} = \mathbf{y}(\mathbf{x}, t)$ and temperature field $\theta = \theta(\mathbf{x}, t)$ we can choose a body force $\mathbf{b} = \mathbf{b}(\mathbf{x}, t)$ and heat supply $r = r(\mathbf{x}, t)$ to balance (3.5), (3.6), so that (3.9) becomes an identity to be satisfied by the constitutive equations. For the case of a *thermoelastic material*, for which $T_R, \eta, \psi, \mathbf{q}_R$ are assumed to be functions of $D\mathbf{y}, \theta, \operatorname{grad} \theta$, this leads to the relations

(3.10)
$$\psi = \psi(D\mathbf{y}, \theta), \quad \mathbf{T}_R = D_\mathbf{A}\psi, \quad \eta = -D_\theta\psi,$$

and then (3.9) reduces to the inequality

(3.11)
$$-\frac{\mathbf{q}_R \cdot \operatorname{grad} \theta}{\theta} \ge 0.$$

(Note that, although this inequality must be satisfied by the constitutive equation for \mathbf{q}_R , for processes involving shocks (3.11) is not equivalent to (3.7), since the cancellations in the argument used to obtain (3.9) are no longer valid.) For thermoelastic materials the balance of angular momentum is satisfied identically as a consequence of the requirement that \mathbf{T}_R is frame-indifferent, i.e.

$$\mathbf{T}_R(\mathbf{RA}, \theta) = \mathbf{RT}_R(\mathbf{A}, \theta)$$
 for all $\mathbf{R} \in \mathrm{SO}(3)$,

which is equivalent to the condition that

(3.12)
$$\psi(\mathbf{RA}, \theta) = \psi(\mathbf{A}, \theta) \text{ for all } \mathbf{R} \in \mathrm{SO}(3).$$

The condition of material symmetry becomes

(3.13)
$$\psi(\mathbf{AQ}, \theta) = \psi(\mathbf{A}, \theta) \text{ for all } \mathbf{Q} \in \mathcal{S}$$

where S is the isotropy group. The equations of *isothermal* thermoelasticity are obtained from (3.5), (3.10) by assuming that $\theta(\mathbf{x}, t) = \theta_0 = \text{constant}$. Thus the balance of linear momentum becomes

(3.14)
$$\rho_R \mathbf{y}_{tt} - \operatorname{div} D_\mathbf{A} W(D\mathbf{y}) - \mathbf{b} = 0,$$

where $W(\mathbf{A}) = \psi(\mathbf{A}, \theta_0)$. As regards the entropy inequality, we again adopt the Coleman & Noll point of view, choosing r to balance (3.6). (Here we follow Dafermos [93], who gives a similar reduction for isentropic thermoelasticity.) Since, from (3.11), $\mathbf{q}_R = 0$ when grad $\theta = 0$, (3.7) becomes

(3.15)
$$(\frac{1}{2}\rho_R |\mathbf{y}_t|^2 + \psi)_t - \mathbf{b} \cdot \mathbf{y}_t - \operatorname{div}\left(\mathbf{y}_t \mathbf{T}_R\right) \le 0$$

For the more general case of a thermoviscoelastic material (of strain-rate type), $T_R, \eta, \psi, \mathbf{q}_R$ are assumed to be functions of $D\mathbf{y}, D\mathbf{y}_t, \theta$, grad θ . By the same method we find that

$$\psi = \psi(D\mathbf{y}, \theta), \ \eta = -D_{\theta}\psi,$$

and that

$$\mathbf{S} \cdot D\mathbf{y}_t - \frac{\mathbf{q}_R \cdot \operatorname{grad} \theta}{\theta} \ge 0,$$

where

$$\mathbf{T}_R = D_{\mathbf{A}}\psi + \mathbf{S}(D\mathbf{y}, D\mathbf{y}_t, \theta, \operatorname{grad} \theta).$$

In the isothermal case we obtain the equation of motion

(3.16)
$$\rho_R \mathbf{y}_{tt} - \operatorname{div} D_\mathbf{A} W(D\mathbf{y}) - \operatorname{div} \mathbf{S}(D\mathbf{y}, D\mathbf{y}_t) - \mathbf{b} = 0,$$

where $W = \psi(D\mathbf{y}, \theta_0)$, $\mathbf{S}(D\mathbf{y}, D\mathbf{y}_t) = \mathbf{S}(D\mathbf{y}, D\mathbf{y}_t, \theta_0, 0)$, together with the energy inequality (3.15). The frame-indifference of **S** takes the form

(3.17)
$$\mathbf{S}(D\mathbf{y}, D\mathbf{y}_t) = D\mathbf{y}\,\Sigma(\mathbf{U}, \mathbf{U}_t),$$

for some matrix-valued function Σ , where $\mathbf{U} = (D\mathbf{y}^T D\mathbf{y})^{1/2}$.

3.2. Existence of solutions.

Problem 12. Prove the global existence and uniqueness of solutions to initialboundary value problems for properly formulated dynamic theories of nonlinear elasticity.

To discuss this problem let us begin with isothermal thermoelasticity. The governing equations are (3.14). These equations need to be supplemented by boundary conditions such as (2.1), (2.6) and by the initial conditions

(3.18)
$$\mathbf{y}(\mathbf{x},0) = \mathbf{y}_0(\mathbf{x}), \quad \mathbf{y}_t(\mathbf{x},0) = \mathbf{y}_1(\mathbf{x}).$$

If the body force is conservative, so that

$$\mathbf{b} = -\operatorname{grad}_{\mathbf{y}} h(\mathbf{x}, \mathbf{y}),$$

then (3.14) formally comprises a Hamiltonian system, and could be alternatively obtained by applying Hamilton's principle to the functional

$$\int_0^T \int_\Omega \left(\frac{1}{2} \rho_R |\mathbf{y}_t|^2 - W(D\mathbf{y}) - h(\mathbf{x}, \mathbf{y}) \right) \, d\mathbf{x} \, dt.$$

In particular, solutions formally satisfy the balance of energy

$$(3.20) E(\mathbf{y}, \mathbf{y}_t) = E(\mathbf{y}_0, \mathbf{y}_1), \quad t \ge 0$$

where

$$E(\mathbf{y}, \mathbf{v}) = \int_{\Omega} \left(\frac{1}{2} \rho_R |\mathbf{v}|^2 + W(D\mathbf{y}) + h(\mathbf{x}, \mathbf{y}) \right) \, d\mathbf{x}.$$

However, weak solutions of the quasilinear wave equation (3.14) do not in general satisfy (3.20), since singularities such as shock waves can dissipate energy. Correspondingly, although equality holds in the dissipation inequality (3.15) for smooth solutions, in general it does not do so for weak solutions. Interpreted in the sense of distributions or measures, (3.15) acts as an admissibility criterion for weak solutions.

In one dimension (3.14) takes the form

(3.21)
$$\rho_R y_{tt} - \sigma(y_x)_x - b = 0,$$

where $\sigma(y_x) = W'(y_x)$, which setting $u_1 = \rho_R y_t$, $u_2 = y_x$ is equivalent to the system of two conservation laws

$$\mathbf{u}_t - \mathbf{f}(\mathbf{u})_x = \mathbf{g},$$

where

$$\mathbf{f}(\mathbf{u}) = \left(\begin{array}{c} \sigma(u_2) \\ \rho_R^{-1} u_1 \end{array} \right), \qquad \mathbf{g} = \left(\begin{array}{c} b \\ 0 \end{array} \right).$$

This system is strictly hyperbolic if $\sigma' = W'' > 0$, so that W is strictly convex.

Two approaches have been employed to study (3.22), the Glimm scheme [134] and variants of it such as front-tracking (introduced by Dafermos [91]), and the method of compensated compactness as pioneered by Tartar [248], [249] and DiPerna [101], [102].

The Glimm scheme and variants apply to strictly hyperbolic systems of the form (3.22) with $\mathbf{u} \in \mathbf{R}^n, \mathbf{f} : \mathbf{R}^n \to \mathbf{R}^n, \mathbf{g} \in \mathbf{R}^n$. They involve a semi-explicit construction of the solutions in terms of approximation of the initial data by piecewise constant functions, together with an analysis of wave interactions. They are restricted to initial data having small total variation, and thus, via total variation estimates on the solution, to solutions of small total variation. Glimm's original work assumed that the system was 'genuinely nonlinear', but this restriction was removed by Liu [175]. Thanks to work of Bressan [63, 64], Bressan & Colombo [66], Bressan, Crasta & Piccoli [67], Bressan & Goatin [69], Bressan & Le Floch [68], Bressan & Lewicka [70], Bressan, Liu & Yang [71] and Liu & Yang [177, 176, 178], the solutions obtained in these ways are now known to be unique in appropriate function classes. For genuinely nonlinear systems of two conservation laws, such as (3.21) with $W'' > 0, W''' \neq 0$, more is known (see Dafermos [93, Chapter XI]). Most of this work is for solutions on the whole real line; for a treatment of (3.21) with displacement boundary conditions see Liu [174].

The method of compensated compactness, on the other hand, has up to now been restricted to systems of at most two conservation laws, such as (3.21). Starting from a sequence of approximate solutions obtained from the method of vanishing viscosity (or by a variational time-discretization scheme, see Demoulini, Stuart & Tsavaras [99]), it uses information coming from the existence of a suitable family of 'entropies' (quantities for which there is a corresponding conservation law satisfied by smooth solutions) to pass to the limit using weak convergence. However, there is no corresponding uniqueness theorem. These results are described in the books of Bressan [65], Dafermos [93], and Serre [222]. In a recent development, Bianchini & Bressan [52] have made a breakthrough by obtaining for the first time total variation estimates directly from the vanishing viscosity method.

For the three-dimensional equations (3.14) very little is known. Hughes, Kato & Marsden [146] proved that if W satisfies the strong ellipticity condition

(3.23)
$$D^2W(\mathbf{A})(\mathbf{a} \otimes \mathbf{n}, \mathbf{a} \otimes \mathbf{n}) \ge \mu |\mathbf{a}|^2 |\mathbf{n}|^2$$
 for all $\mathbf{A} \in M^{3 \times 3}_+, \mathbf{a}, \mathbf{n} \in \mathbf{R}^3$,

where $\mu > 0$, then for smooth initial data (3.18) defined on the whole of \mathbf{R}^3 with det $D\mathbf{y}_0 > 0$, there exists a unique smooth solution on a small time interval [0, T), T > 0. This result was extended to pure displacement boundary conditions by Kato [155]. For related results see Dafermos & Hrusa [94], and Dafermos [93, Chapter V]. There seem to be no short-time existence results known for mixed displacement-traction boundary conditions. Interesting results concerning large time existence for sufficiently smooth and small initial data on the whole of R^3 have been obtained by John [154]. For corresponding results for incompressible elasticity see Hrusa & Renardy [145], Ebin & Saxton [107], Ebin & Simanca [108, 109] and Ebin [105, 106].

In the variables $\mathbf{A} = D\mathbf{y}, \mathbf{p} = \rho_R \mathbf{y}_t$, (3.14) becomes the system

(3.24)
$$\mathbf{A}_t = \mathbf{D}, \quad D_{ij} = \rho_R^{-1} v_{i,j},$$

(3.25)
$$\mathbf{p}_t = \operatorname{div} D_{\mathbf{A}} W(D\mathbf{y}) + \mathbf{b},$$

which is hyperbolic if

 $D^2W(\mathbf{A})(\mathbf{a} \otimes \mathbf{n}, \mathbf{a} \otimes \mathbf{n}) > 0$ for all $\mathbf{A} \in M^{3 \times 3}_+$ and nonzero $\mathbf{a}, \mathbf{n} \in \mathbf{R}^3$.

There is no theory of weak solutions for such multi-dimensional systems. In particular, it is unclear what conditions on W are natural for existence, and whether these conditions will be the same as those guaranteeing existence for elastostatics, namely quasiconvexity or polyconvexity. The system (3.24), (3.25) is special in the sense that there is an involution

$$A_{ij,k} - A_{ik,j} = 0$$

which is satisfied by all weak solutions. Exploiting this in the context of a general system having involutions, Dafermos [92], [93] proves a theorem implying that if W is quasiconvex and satisfies (3.23) then any Lipschitz solution A, p of (3.24), (3.25) on $\mathbb{R}^3 \times [0,T]$, T > 0, is unique within the class of weak solutions admissible with respect to the entropy W, of uniformly small local oscillation, and satisfying the same initial data as \mathbf{A}, \mathbf{p} . An unpublished idea of LeFloch, found independently by Qin [218], leads to the observation that for polyconvex W the hypothesis of uniformly small oscillation can be removed. These results are interesting because they so far represent the only use of quasiconvexity and polyconvexity in the context of dynamics. See Sverák [240] for an idea of how quasiconvexity (in an augmented space) might be used to prove existence by passage to the limit using weak convergence, in the spirit of compensated compactness. For the full system of three-dimensional nonlinear thermoelasticity (3.5)-(3.7), which has the additional conservation law (3.6), the state of knowledge (or rather lack of it) is similar. For these systems an additional difficulty is that of ensuring invertibility of solutions, and in particular the condition det $D\mathbf{y}(\mathbf{x}, t) > 0$.

For a thermoviscoelastic material, one can hope that a sufficiently well-behaved viscous part \mathbf{S} of the stress will guarantee existence without any convexity conditions on W. Indeed, in the one-dimensional isothermal case, for which the equation of motion takes the form

(3.26)
$$\rho_R y_{tt} - \sigma(y_x, y_{xt})_x - b = 0,$$

for which Dafermos [90] and Antman & Seidman [17] have proved existence and uniqueness for a general class of σ . The special case of the equation

(3.27)
$$\rho_R y_{tt} - \sigma(y_x)_x - y_{xxt} = 0$$

has been treated in numerous papers (see, for example, Greenberg, MacCamy & Mizel [137], Andrews [11], Pego [207]). For corresponding results for thermoviscoelasticity see Racke & Zheng [219].

For the isothermal case in three dimensions it is natural to consider in place of (3.27) the equation

$$\rho_R \mathbf{y}_{tt} - \operatorname{div} D_\mathbf{A} W(D\mathbf{y}) - \Delta \mathbf{y}_t = 0,$$

for which a theory of existence is available (see Rybka [221], Friesecke & Dolzmann [125]). However the corresponding viscous stress $\mathbf{S} = D\mathbf{y}_t$ is not of the form (3.17), and so is not frame-indifferent. The only existence theory for weak or strong solutions of (3.16) with \mathbf{S} frame-indifferent appears to be that of Potier-Ferry [215, 216], who, for pure displacement boundary conditions, established global existence and uniqueness of solutions for initial data close to a smooth equilibrium having strictly positive second variation. Potier-Ferry assumed that the linearized

elasticity operator at the equilibrium is strongly elliptic, and that a corresponding positivity condition holds for the linearized viscous stress. He uses methods of Sobolevskii [231] (for an alternative treatment also based on Sobolevskii's work see Xu & Marsden [261] and Xu [260]).

A recent monograph covering various aspects of the analysis of thermoelasticity is that of Jiang & Racke [148].

A different approach to the existence of solutions in elasticity is to weaken the concept of solution to that of a measure-valued solution, in which the unknown is a Young measure $\nu_{\mathbf{x},t}$ in appropriate variables satisfying an integral identity obtained by formally passing to the weak limit in a sequence of approximate solutions. Using a variational time-discretization method, the global existence of such solutions has been proved by Demoulini [98] for the viscoelastic equation (3.16) with **S** frame-indifferent, and by Demoulini, Stuart & Tsavaras [100] for the equations (3.14) of elastodynamics with W polyconvex (exploiting the idea of Le Floch and Qin [218]). However they are unable to handle the constraint det $D\mathbf{y} > 0$. Of course the significance of such results would be greatly enhanced if there were examples known of cases in which there was no corresponding weak solution.

3.3. The relation between statics and dynamics. For suitable boundary conditions, the Second Law of Thermodynamics endows the equations of motion of continuum thermodynamics with a *Lyapunov function*, that is a function of the state variables that is nonincreasing along solutions. For example, suppose that the the mechanical boundary conditions are that $\mathbf{y} = \mathbf{y}(\mathbf{x}, t)$ satisfies

$$\mathbf{y}(\cdot,t)|_{\partial\Omega_1} = \bar{\mathbf{y}}(\cdot)$$

and the condition that the applied traction on $\partial \Omega_2$ is zero, and that the thermal boundary condition is

$$\theta(\cdot, t)|_{\partial\Omega} = \theta_0,$$

where $\theta_0 > 0$ is a constant. Assume that the heat supply r is zero, and that the body force is given by (3.19). Then from (3.1), (3.3) and (3.4) with $E = \Omega$ we find that the *ballistic free energy*

(3.28)
$$\mathcal{E} = \int_{\Omega} \left[\frac{1}{2} \rho_R |\mathbf{y}_t|^2 + U - \theta_0 \eta + h \right] d\mathbf{x}$$

is nonincreasing along solutions. (This is a result of Duhem [104] for the case of thermoelasticity. See Coleman & Dill [86], Ericksen [111] and Ball [26, 28] for further discussion and references.) For a thermoviscoelastic material, if $\mathbf{v}(\cdot, t) \to 0$, $\mathbf{y}(\cdot, t) \to \mathbf{y}(\cdot)$ and $\theta(\cdot, t) \to \theta_0$ as $t \to \infty$ the integrand in (3.28) formally tends to $W(D\mathbf{y}) + h(\mathbf{x}, \mathbf{y})$, where $W(D\mathbf{y}) = \psi(D\mathbf{y}, \theta_0)$ and ψ is the Helmholtz free energy

$$\psi(D\mathbf{y},\theta_0) = U(D\mathbf{y},\theta_0) - \theta_0 \eta(D\mathbf{y},\theta_0).$$

This motivates minimization of

$$I(\mathbf{y}) = \int_{\Omega} \left[W(D\mathbf{y}) + h(\mathbf{x}, \mathbf{y}) \right] \, d\mathbf{x}.$$

(For pure zero traction boundary conditions, when uniformly rotating equilibria are to be expected, we do not expect that $\mathbf{y}_t \to 0$, and the corresponding entropy maximization problem is studied by Lin [173]). As applied to such problems, the calculus of variations can be viewed as representing a crude version of dynamics in which true dynamic orbits are replaced by all paths in a phase space of mappings $\{\mathbf{y}, \mathbf{y}_t, \theta\}$ along which \mathcal{E} is nonincreasing.

Problem 13. Develop a qualitative dynamics for dynamic theories of elasticity.

Of course a prerequisite for such a qualitative dynamics is a global existence theory for solutions. Given such a theory, the points at issue are the usual ones for dissipative dynamical systems, namely whether solutions converge to equilibrium states as $t \to \infty$, the structure of regions of attraction, the existence of stable and unstable manifolds of equilibria, the existence of a global attractor, and so on. In particular one can ask whether dynamic orbits generically realize suitably defined local minimizing sequences for the ballistic free energy. This is especially interesting in the case when the ballistic free energy does not attain a minimum (as in models of elastic crystals – see Section 4.2). In fact for the one-dimensional viscoelastic model of this type studied by Ball, Holmes, James, Pego & Swart [36] and Friesecke & McLeod [128], it is known that no dynamic solutions realize global minimizing sequences; it is unclear whether or not this is a one-dimensional phenomenon.

Problem 14. Develop criteria for the dynamic stability and instability of equilibria.

Koiter [162] is among those who have drawn attention to the problem of justifying the *energy criterion for stability*, that an equilibrium solution is stable if it is a local minimizer of the corresponding elastic energy (for example, of the ballistic free energy for a thermoviscoelastic material). To keep the discussion simple, consider the case of isothermal motion of a thermoviscoelastic material, for which the equation of motion is given by (3.16), and assume that the body force is zero. The corresponding Lyapunov function is

$$E(\mathbf{y}, \mathbf{v}) = \int_{\Omega} \left[\frac{1}{2} \rho_R |\mathbf{v}|^2 + W(D\mathbf{y}) \right] \, d\mathbf{x},$$

for which $\mathbf{y} = \mathbf{y}^*, \mathbf{v} = 0$ is a local minimizer provided \mathbf{y}^* is a local minimizer of

$$E(\mathbf{y}) = \int_{\Omega} W(D\mathbf{y}) \, d\mathbf{x}.$$

Since there are different types of local minimizer corresponding to different metrics d on different spaces X of deformations \mathbf{y} , in particular $W^{1,\infty}$ local minimizers and $W^{1,p}$ local minimizers for $1 \leq p < \infty$, it is not clear which kinds of local minimizers are needed to ensure dynamical stability. As emphasised, for example, by Knops & Wilkes [160], the standard argument for establishing Lyapunov stability with respect to a metric d requires more than just that \mathbf{y}^* is a strict local minimizer with respect to d (that is $I(\mathbf{y}) > I(\mathbf{y}^*)$ whenever $\mathbf{y} \neq \mathbf{y}^*$ and $d(\mathbf{y}, \mathbf{y}^*)$ is sufficiently small). What is needed, in addition to the continuity of I with respect to d and the continuity in time of dynamic orbits with respect to d, is that \mathbf{y}^* lies in a *potential well*, namely that for some $\varepsilon > 0$

$$\inf_{d(\mathbf{y},\mathbf{y}^*)=\varepsilon} I(\mathbf{y}) > I(\mathbf{y}^*).$$

For a way of verifying that a strict local minimizer in a space based on $W^{1,p}$ for 1 satisfies this requirement when <math>W is strictly polyconvex see Ball & Marsden [42], and for the case when W is strictly quasiconvex see Evans & Gariepy [117] and Sychev [242]. However, we do not know in general how to prove that a given \mathbf{y}^* is a strict $W^{1,p}$ local minimizer. Further, for W that are not

quasiconvex almost nothing is known. These questions are related to the open problem, already mentioned in Section 2.7, of generalizing to higher dimensions the Weierstrass fundamental sufficiency theorem.

The only rigorous result justifying the energy criterion in any generality (in particular, in three dimensions) seems to be that of Potier-Ferry [216], who for pure displacement boundary conditions establishes asymptotic stability, with respect to the norm of $W^{2,p} \times W^{2,p}$, p > 3, of smooth equilibria having strictly positive second variation, under the hypotheses described in Section 3.2.

Finally, little is known about criteria justifying instability of an equilibrium solution. An instructive example is that of Friesecke & McLeod [129], who for a problem of one-dimensional viscoelasticity exhibit an equilibrium solution \bar{u} which, with respect to a topology in which the dynamics is well-posed, (a) is dynamically stable, but (b) is such that there is a continuous path in the phase space (not a dynamical solution) leaving \bar{u} along which the energy strictly decreases, so that in particular \bar{u} is not a local minimizer.

4. Multiscale problems

4.1. From atomic to continuum.

Problem 15. Establish the status of elasticity theory with respect to atomistic models.

Is it possible to derive elasticity theory from atomistic models? Such models range from full quantum many-body theory to approximations such as density-functional theory, Thomas-Fermi theory, and models in which electronic effects are not explicitly considered but incorporated into interatomic potentials. There is an extensive physics and materials literature on such models and on methods for bridging the atomistic and continuum length-scales (see Phillips [211] for an introduction). Here I will concentrate on what little is known rigorously for the the case of elastic crystals. However, another important class of materials is that of cross-linked polymers, which involves some different issues that are considered from the point of view of statistical mechanics in Deam & Edwards [97], Edwards & Vilgis [110].

For crystals, the first question to answer is why they occur in the first place, that is why at low temperature the minimum energy configuration of a very large number of atoms is spatially periodic. This is the famous unsolved 'crystal problem', nicely reviewed by Radin [220]. Likewise, there is no fundamental understanding of the statistical mechanics of crystals, which would explain their stability and instabilities. Given this impasse, in attempts to pass from atomistic to continuum models of crystals some initial atomic order is always assumed. In the context of free-energy minimization, one can draw a distinction between two kinds of approach. In the first, an appropriate limit of a discrete energy functional is sought along sequences of explicit atomic configurations. For example the atoms may be assumed to occupy a periodic lattice in a reference configuration, and to be displaced according to a given sufficiently smooth continuum deformation \mathbf{y} (the *Cauchy-Born hypothesis*), the number of atoms being sent to infinity with a suitable scaling for the energy. In this approach there is no attempt to explain why the atoms adopt the assumed configurations. A recent example is the work of Blanc, Le Bris & Lions [53], who obtain in a suitable scaling a limiting energy of the form

$$I(\mathbf{y}) = \int_{\Omega} W(D\mathbf{y}) \, dx$$

in the cases of (a) a two-body interaction, (b) Thomas-Fermi theory. As is well-known the case of two-body interactions leads to a W satisfying the *Cauchy relations*, namely that the linearized elasticity coefficients at a natural state (say $D\mathbf{y} = \mathbf{1}$)

$$c_{ijkl} = \frac{\partial^2 W(\mathbf{1})}{\partial A_{ij} \partial A_{kl}}$$

possess the symmetries

$$c_{ijkl} = c_{jikl} = c_{klij} = c_{ikjl}.$$

These symmetries are known not to hold in general (see Love [179], Weiner [258]). Blanc, LeBris & Lions also obtain second-order terms in the expansion of the energy with respect to the scaling parameter, identifying these with surface energies. For fundamental results on linear deformations with the Cauchy-Born hypothesis see Lieb & Simon [172] and Fefferman [118]; in these papers the dependence on the deformation gradient enters implicitly through the given Bravais lattice. For more recent extensions of the results of [172] see Catto, Le Bris & Lions [73].

The second approach is to consider the true minimizers of the discrete problems, and to try to understand what functional their limit minimizes. One example of this approach is the interesting study by Friesecke & Theil [130] of a model two-dimensional problem of a lattice of particles linked by harmonic springs between their nearest and next nearest neighbours. They determine open regions of atomic parameters in which the Cauchy-Born hypothesis holds in the appropriate limit, and open regions in which it does not. Another interesting recent study in this spirit is that of Penrose [208], who considers a two-dimensional model problem of a lattice of rotatable disks with one-body wall interactions and angledependent two-body interactions. By suitably restricting the statistical ensemble, so that, for example, certain angles between atoms in the deformed configuration are constrained to lie in certain intervals (these constraints being designed to deter dislocations), he proves the existence of an elastic free energy W corresponding to taking the thermodynamic limit with prescribed linear boundary data. He also deduces a convexity property of W weaker than rank-one convexity, and suggests that W might in fact be quasiconvex. Other work in this spirit is that of Braides, Dal Maso & Garroni [62], Braides & Gelli [60, 61] and Foccardi & Gelli [119], who calculate the Γ -limits of certain discrete functionals with nearest-neighbour or pairwise interactions, obtaining a limiting functional allowing fracture of the general form (2.31) together with a corresponding function space on which to minimize it (namely SBV(Ω) or GSBV(Ω)). This acts as a reminder that, since the predictions of minimization problems can depend on the function space, as we have seen in Section 2.3 in connection with the Lavrentiev phenomenon, a proper atomistic to continuum derivation should deliver not only the limiting governing equations or energy, but the appropriate function space as well.

For a proposed scheme for the passage from atomistic to continuum models for thin films, rods or tubes see Friesecke & James [126]. There seems to be no work on atomistic derivations of dynamic theories of elasticity, or even of elastostatics in the context of deformations that are not global energy minimizers. In some situations it is desirable to simultaneously use a continuum and a discrete model. For example, one may wish to study the interaction of a defect or other localized region (such as the vicinity of a crack tip), in which atomistic effects may be important, with the surrounding bulk material, where a continuum theory is appropriate. One way of handling the resulting matching problem is the *quasicontinuum method* (see Tadmor, Ortiz & Phillips [245]). A rigorous understanding of such methods is lacking.

4.2. From microscales to macroscales. Materials undergoing phase transformations involving a change of shape at a critical temperature typically develop characteristic patterns of *microstructure*, in which the deformation gradient has large variations on a fine length-scale that varies from material to material but can be as small as a few atomic spacings. Such microstructures often contain twinned regions consisting of many parallel layers separated by sharp interfaces, the deformation gradient alternating between two distinct values in adjacent layers.

Why does fine microstructure form? To what extent can we predict its morphology? What are the properties of the material at a macroscale much larger than the microscale of the microstructure? Whereas it would be desirable to answer such questions in the context of a suitably formulated dynamical theory, it is neither clear what such a theory should be (especially as regards the kinetics of interfaces), nor do we currently have the techniques to give answers corresponding to any such theory. Hence we will discuss some more specific open problems that arise in static models of such phase transformations.

Consider a single crystal of thermoelastic material that undergoes a diffusionless phase transformation involving a change of shape at the temperature θ_c . For definiteness, suppose that there is an interval E of temperatures, containing θ_c , such that for $\theta \in E$, $\theta > \theta_c$, the minimum energy configuration (called *austenite*) of the crystal is cubic. Taking the reference configuration to be undistorted austenite at $\theta = \theta_c$, we suppose that for $\theta \in E$, $\theta \leq \theta_c$, a minimum energy configuration (called *martensite*) is given by the transformation strain $U(\theta)$. We suppose that the Helmholtz free-energy function $\psi(\mathbf{A}, \theta)$ attains a finite minimum with respect to $\mathbf{A} \in M_+^{3\times 3}$ for each $\theta \in E$, so that by adding to it a suitable function of θ we may assume for the purposes of free-energy minimization that

$$\min_{\mathbf{A}\in M_+^{3\times 3}}\psi(\mathbf{A},\theta)=0$$

Let

$$K(\theta) = \{ \mathbf{A} \in M^{3 \times 3}_+ : \psi(\mathbf{A}, \theta) = 0 \}$$

be the set of energy-minimizing deformation gradients. Note that by (3.12), (3.13)

$$SO(3)K(\theta)S = K(\theta),$$

where we take S to be the subgroup P^{24} of SO(3) consisting of the 24 rotations mapping a cube into itself. It is thus reasonable to suppose that for $\theta \in E$,

(4.1)
$$K(\theta) = \begin{cases} \alpha(\theta) \mathrm{SO}(3), & \theta > \theta_c, \\ \mathrm{SO}(3) \cup \bigcup_{i=1}^N \mathrm{SO}(3) U_i(\theta_c), & \theta = \theta_c, \\ \bigcup_{i=1}^N \mathrm{SO}(3) U_i(\theta), & \theta < \theta_c, \end{cases}$$

where $\alpha(\cdot)$ describes the thermal expansion, with $\alpha(\theta_c) = 1$, and where the $U_i(\theta)$, $1 \leq i \leq N$, are the distinct positive definite symmetric matrices of the form

 $Q^T U(\theta)Q, Q \in P^{24}$. We assume that N is independent of $\theta \in E$. If $U_i(\theta_c) \neq \mathbf{1}$ the transformation is *first-order*, while if $U_i(\theta_c) = \mathbf{1}$ it is *second-order*. We say that each U_i describes a different *variant* of martensite. For example, in the case of a cubic-to-tetragonal transformation we may take

$$U(\theta) = U_1(\theta) = \operatorname{diag}(\eta_3, \eta_1, \eta_1),$$

where $\eta_1(\theta) > 0, \eta_3(\theta) > 0$, and then we find that N = 3, and that

$$U_2(\theta) = \text{diag}(\eta_1, \eta_3, \eta_1), \quad U_3(\theta) = \text{diag}(\eta_1, \eta_1, \eta_3).$$

For other transformations we get different numbers of variants; for example, for cubic-to-orthorhombic transformations N = 6, and for cubic to monoclinic transformations N = 12.

Note that in adopting (4.1) we exclude large shears leaving the crystal lattice invariant (see Ericksen [113]), the inclusion of which would lead to $K(\theta)$ consisting of an infinite number of energy wells for each θ , and to an energy-minimization problem of a different character to that based on (4.1) (see Fonseca [120]).

The total free energy corresponding to the deformation $\mathbf{y}: \Omega \to \mathbf{R}^3$ is given by

$$I_{\theta}(\mathbf{y}) = \int_{\Omega} \psi(D\mathbf{y}, \theta) \, d\mathbf{x}$$

Zero-energy microstructures (at the temperature θ) correspond to sequences of deformations $\mathbf{y}^{(j)}$ such that

(4.2)
$$\lim_{i \to \infty} I_{\theta}(\mathbf{y}^{(j)}) = 0.$$

If we assume a mild growth condition on ψ , such as

$$\psi(\mathbf{A}, \theta) \ge c_0 |\mathbf{A}|^p - c_1 \text{ for all } \mathbf{A} \in M_+^{3 \times 3},$$

where $c_0 > 0, c_1$ and p > 1 are constants, then (4.2) is equivalent to the statement that $D\mathbf{y}^{(j)} \to K(\theta)$ in measure, or that the Young measure $(\nu_{\mathbf{x}})_{\mathbf{x}\in\Omega}$ corresponding to (a subsequence of) $D\mathbf{y}^{(j)}$ satisfies

$$\operatorname{supp} \nu_x \subset K(\theta) \quad \text{a.e. } \mathbf{x} \in \Omega.$$

The set of macroscopic deformation gradients corresponding to zero-energy microstructures is the set of gradients $D\mathbf{y}: \Omega \to M_+^{3\times 3}$ such that $D\mathbf{y}^{(j)} \to D\mathbf{y}$ in L^p for some sequence $y^{(j)}$ satisfying (4.2). Equivalently, following the results of Kinderlehrer & Pedregal [156, 157], this is the set of gradients $D\mathbf{y}$ such that

$$D\mathbf{y}(\mathbf{x}) \in K(\theta)^{\mathrm{qc}}$$
 a.e. $\mathbf{x} \in \Omega$.

where for a compact set $K \subset M^{3\times 3}$, K^{qc} denotes the quasiconvexification of K. Equivalent definitions of K^{qc} are

$$\begin{split} K^{\rm qc} &= \{\bar{\nu} : \nu \text{ is a homogeneous } W^{1,\infty} \text{ Young measure with supp } \nu \subset K \} \\ &= \{\mathbf{A} \in M^{3 \times 3} : \varphi(\mathbf{A}) \leq \max_{\mathbf{B} \in K} \varphi(\mathbf{B}) \text{ for all quasiconvex } \varphi \} \\ &= \bigcap \{E \supset K : E \text{ quasiconvex} \}. \end{split}$$

Here $\mathcal{A}_{\mathbf{A}} = \{ \mathbf{y} \in W^{1,1}(\Omega; \mathbf{R}^3) : \mathbf{y}|_{\partial\Omega} = \mathbf{A}\mathbf{x} \}$, and a set E is quasiconvex if it is the zero set $\varphi^{-1}(0)$ of a nonnegative quasiconvex function φ . We also have that

$$K^{\mathrm{qc}} = \{ \mathbf{A} \in M^{3\times 3}_+ : \inf_{\mathcal{A}_{\mathbf{A}}} I_{\theta}(\mathbf{y}) = 0 \}.$$

We can similarly define the *polyconvexification* K^{pc} and the *rank-one convexification* K^{rc} of a compact set $K \subset M_+^{3\times 3}$ by

$$K^{pc} = \{ \mathbf{A} \in M^{3 \times 3} : \varphi(\mathbf{A}) \le \max_{\mathbf{B} \in M^{3 \times 3}} \varphi(\mathbf{B}) \text{ for all polyconvex } \varphi \},$$
$$K^{rc} = \{ \mathbf{A} \in M^{3 \times 3} : \varphi(\mathbf{A}) \le \max_{\mathbf{B} \in M^{3 \times 3}} \varphi(\mathbf{B}) \text{ for all rank-one convex } \varphi \}.$$

Clearly

Problem 16. Determine $K(\theta)^{\text{qc}}$ for $\theta \leq \theta_c$.

For $\theta > \theta_c$ we have that $K(\theta)^{\rm qc} = K(\theta)$ (cf. Ball & James [41]). For $\theta \leq \theta_c$ the problem is open. In particular, $K(\theta)^{\rm qc}$ is not known for the cubic-to-tetragonal case either when $\theta < \theta_c$ or $\theta = \theta_c$. In [41] Ball & James computed $K^{\rm qc}$ for the case of two wells

$$K = \mathrm{SO}(3)\mathbf{U} \cup \mathrm{SO}(3)\mathbf{V},$$

with $\mathbf{U} = \mathbf{U}^T > 0$, $\mathbf{V} = \mathbf{V}^T > 0$, det $\mathbf{U} = \det \mathbf{V}$ and with SO(3)U rank-one connected to SO(3)V, which occurs for orthorhombic-to-monoclinic transformations. In this case by linear changes of variables we can assume that

(4.4)
$$\mathbf{U} = \text{diag}(\eta_1, \eta_2, \eta_3), \ \mathbf{V} = \text{diag}(\eta_2, \eta_1, \eta_3),$$

where $\eta_1 > 0, \eta_2 > 0, \eta_3 > 0$ and $\eta_1 \neq \eta_2$. (This includes the case $\mathbf{U} = \mathbf{U}_1(\theta), \mathbf{V} = \mathbf{U}_2(\theta)$ of two tetragonal wells.) The answer in this case is (see Ball & James [37]) that K^{qc} consists of those $\mathbf{A} \in M_+^{3\times 3}$ such that

$$\mathbf{A}^T \mathbf{A} = \left(\begin{array}{ccc} a & c & 0 \\ c & b & 0 \\ 0 & 0 & \eta_3^2 \end{array}\right).$$

where $ab - c^2 = \eta_1^2 \eta_2^2$, $a + b + 2|c| \leq \eta_1^2 + \eta_2^2$. The proof is by calculating K^{pc} , showing that $K^{pc} \subset K^{rc}$, and using (4.3). Friesecke [124] has announced that he can calculate $K(\theta)^{pc}, \theta < \theta_c$, in the cubic-to-tetragonal case. However, whether in general $K(\theta)^{pc} = K(\theta)^{qc}$ is unknown. (Despite this, in their study of nonclassical austenite-martensite interfaces Ball & Carstensen [33] were able to show that for $\theta < \theta_c$ the identity matrix is rank-one connected to $K(\theta)^{qc}$ if and only if it is rank-one connected to $K(\theta)^{pc}$.)

Problem 17. For free-energy functions $\psi(\mathbf{A}, \theta)$ of elastic crystals, determine for which $\partial \Omega_1 \subset \partial \Omega$ and $\mathbf{g} : \partial \Omega_1 \to \mathbf{R}^3$ the minimum of

$$I_{\theta}(\mathbf{y}) = \int_{\Omega} \psi(D\mathbf{y}, \theta) \, d\mathbf{x}$$

in $\mathcal{A} = \{ \mathbf{y} \in W^{1,1}(\Omega; \mathbf{R}^3) : \mathbf{y}|_{\partial \Omega_1} = \mathbf{g} \}$ is attained, and for which it is not.

A solution to this problem (also to the corresponding problem including applied loads on $\partial \Omega_2$) would help clarify the validity of the hypothesis of Ball & James [39] that the formation of microstructure is associated with non-attainment of minimum energy. For example, is non-attainment generic or exceptional?

It is probably overly optimistic to expect a general answer to Problem 17. A simpler special case for which the answer is in general unknown is when $\partial \Omega_1 = \partial \Omega$,

 $\mathbf{g}(\mathbf{x}) = \mathbf{A}\mathbf{x}$, and $\mathbf{A} \in K(\theta)^{\mathrm{qc}} \setminus K(\theta)$. In this case the problem is equivalent to asking whether for such \mathbf{A} there exists a deformation \mathbf{y} satisfying $\mathbf{y}|_{\partial\Omega} = \mathbf{A}\mathbf{x}$ and

$$D\mathbf{y}(\mathbf{x}) \in K(\theta)$$
 a.e.

For the corresponding two-well problem in which $K(\theta)$ is replaced by $K = \mathrm{SO}(3)\mathbf{U} \cup \mathrm{SO}(3)\mathbf{V}$ with \mathbf{U}, \mathbf{V} given by (4.4), there is no \mathbf{y} with $\mathbf{y}|_{\partial\Omega} = \mathbf{A}\mathbf{x}$ and $D\mathbf{y}(\mathbf{x}) \in K$ a.e.. This non-attainment result was proved by Ball & Carstensen [33] using the result of Ball & James [40] that any \mathbf{y} with $D\mathbf{y}(\mathbf{x}) \in K^{\mathrm{qc}}$ a.e. is a plane strain, the point being that a plane strain \mathbf{y} cannot coincide with a linear mapping $\mathbf{A}\mathbf{x}$ on the boundary of a three-dimensional region Ω unless $D\mathbf{y}(\mathbf{x}) = \mathbf{A}$ a.e. . In the corresponding two-dimensional problem the answer is different. In fact, if $\Omega \subset \mathbf{R}^2$ and $K = SO(2)\mathbf{U} \cup SO(2)\mathbf{V}$, where

$$\mathbf{U} = \operatorname{diag}(\eta_1, \eta_2), \ \mathbf{V} = \operatorname{diag}(\eta_2, \eta_1),$$

and $\eta_1 > 0, \eta_2 > 0$ then Müller & Šverák [194] modified the theory of convex integration due to Gromov [138] to show that there exists \mathbf{y} with $\mathbf{y}|_{\partial\Omega} = \mathbf{A}\mathbf{x}, D\mathbf{y}(\mathbf{x}) \in K$ a.e. for any $\mathbf{A} \in K^{\text{qc}}$. (For variations on the method see Dacorogna & Marcellini [89], Müller & Sychev [192], Sychev [243] and Kirchheim [158].) Whether these exotic minimizers exist in three dimensions, and if so whether they are physically relevant, is unclear. If, as seems likely, they do exist, then it is natural to ask whether they are admissible, in the sense that they can be obtained as limits of minimizers for a corresponding functional incorporating interfacial energy, for example

$$I_{\theta}^{\varepsilon}(\mathbf{y}) = \int_{\Omega} [\psi(D\mathbf{y}(\mathbf{x}), \theta) + \varepsilon^2 |D^2 \mathbf{y}(\mathbf{x})|^2] \, d\mathbf{x}$$

in the limit $\varepsilon \to 0$.

For general information on the models and techniques described in this section see Ball & James [37], Bhattacharya [50], Hane [140], Müller [189], Luskin [180] and Pedregal [204], [206].

4.3. From three-dimensional elasticity to theories of rods and shells. A rod is a three-dimensional body whose form is close to that of a curve in \mathbb{R}^3 . We can describe a reasonably wide class of such bodies as those which occupy in a reference configuration the bounded domain

$$\Omega_h = \{ \mathbf{r}(s) + \mathbf{Q}(s)(0, \mathbf{x}') : s \in (0, L), \mathbf{x}' \in hD \},\$$

where $\mathbf{r} : (0, L) \to \mathbf{R}^3$ is a smooth embedded curve parametrized by arc-length, so that $|\mathbf{r}'(s)| = 1$, where the cross-section $D \subset \mathbf{R}^2$ is a bounded domain with $0 \in D$, and where $\mathbf{Q} : (0, L) \to \mathrm{SO}(3)$ is a smooth mapping with $\mathbf{Q}(s)\mathbf{e}_1 = \mathbf{r}'(s)$ for each $s \in (0, L)$, which describes how the cross-section is rotated. The parameter h > 0 measures the thickness of the rod. The simple case of an initially straight rod of circular cross-section corresponds to the choice $\mathbf{r}(s) = s\mathbf{e}_1$, $D = B(0, 1) \subset$ \mathbf{R}^2 , $\mathbf{Q}(s) = \mathbf{1}$, so that $\Omega_h = (0, L)\mathbf{e}_1 \times hD$.

A *shell* is a three-dimensional body whose form is close to that of a two-dimensional surface. A class of such bodies consists of those occupying in a reference configuration the bounded domain

$$\Omega_h = \{ \mathbf{r}(s_1, s_2) + \tau \mathbf{n}(s_1, s_2) : (s_1, s_2) \in S, |\tau| \le h \},\$$

where $S \subset \mathbf{R}^2$ is a bounded domain, and $\mathbf{r} : S \to \mathbf{R}^3$ is a smooth embedded oriented surface with unit normal $\mathbf{n}(s_1, s_2)$. Here h > 0 is the thickness of the shell. A *plate* is a flat shell, corresponding to

(4.5)
$$\Omega_h = S \times (-h, h)$$

When h is small, such thin rods and shells are traditionally described respectively by one-dimensional rod and two-dimensional shell models, in which the independent variables are respectively (s, t) and (s_1, s_2, t) , where t is time. There is an immense literature on the many such theories, well surveyed in the books of Antman [14], and Ciarlet [82, 83]. However there are only the beginnings of a rigorous theory justifying such models with respect to three-dimensional elasticity.

Problem 18. Give a rigorous derivation of models of rods, plates and shells, showing that their solutions well approximate appropriate solutions to three-dimensional elasticity for small values of the thickness parameter h.

There seem to be no results of this type for dynamical theories of elasticity, so we concentrate on what is known for elastostatics. Here one would ideally like results showing that the solution sets for boundary-value value problems of threedimensional elasticity converge as $h \to 0$ to corresponding sets for an appropriate rod or shell theory, together with appropriate error estimates. In passing to the limit $h \to 0$ other parameters such as loads may need to be scaled with h. Taking into account such scaling, one would like the convergence and error estimates to be uniform with respect to parameters such as loads entering the boundary conditions, so that in particular the description of buckling according to the three-dimensional theory could be correlated with that for the rod or shell theory identified. One of the many difficulties to be overcome in order to achieve such results is to understand how boundary-layers behave in the limit $h \to 0$. Such boundary layers will occur, for example, at the ends of a rod, where, according to Saint-Venant's principle one expects the limiting rod theory to see only resultant loads and moments applied to the ends. Higher-order corrections in h can be expected to yield more sophisticated theories, for example involving numbers of *directors* (vectors depending on the independent variables giving a better description of the three-dimensional deformation).

An isolated theory that addresses some of these difficulties is Mielke's treatment [184], [185] of Saint-Venant's problem for an initially straight rod of uniform crosssection and prescribed resultant loads and moments at its two ends, in which via a six-dimensional centre manifold he identifies a Cosserat theory of rods whose solutions attract for long rods those of three-dimensional elasticity having uniformly small strains and the same resultant loads and moments. In this connection, for three-dimensional nonlinear elasticity Ericksen [113], [112], [114] has derived equations describing beautiful semi-inverse solutions for helical deformations of a rod. For developments see Muncaster [195], [196], and for an existence theory for the corresponding problem defined on cross-sections see [18].

For plates with a St. Venant-Kirchhoff stored-energy function Monneau [186] has devised a scheme which shows that for periodic boundary conditions and sufficiently small external forces, there is a solution of the three-dimensional equilibrium equations which converges as $h \to 0$ to the solution of the corresponding Kirchhoff-Love plate theory, together with error estimates.

However, the principal method that has so far produced rigorous results of the desired type is Γ -convergence (see De Giorgi & Franzoni [96], Dal Maso [95]). The first application of Γ -convergence to nonlinear elasticity was that of Acerbi, Buttazzo & Percivale [1], who used it to derive a one-dimensional model for an elastic string. Then Le Dret & Raoult [167, 168, 169, 170] and Ben Belgacem [49] used it to derive a corresponding two-dimensional membrane theory (see also Bradies, Fonseca & Francfort [59]). Le Dret & Raoult have also [171] investigated which Cosserat theories of plates Γ -converge to the membrane theory limit as the thickness goes to zero. Bhattacharya & James [51] used Γ -convergence to derive equations for thin films of martensitic material, an interesting conclusion being that in the two-dimensional theory there can be exact austenite-martensite interfaces (for developments see Shu [223]).

In interesting recent work Friesecke, James & Müller [127] have derived a theory of nonlinear bending of plates starting from the nonlinear elastic energy

$$I^{h}(\mathbf{y}) = \int_{\Omega_{h}} W(D\mathbf{y}(\mathbf{x})) \, d\mathbf{x},$$

where Ω_h is given by (4.5). This is a more delicate problem than for the membrane theory since for the boundary conditions for which the bending theory is expected to be valid, $I^h(\mathbf{y}_h)$ is expected to be of order h^3 for minimizers \mathbf{y}_h , whereas for boundary conditions leading to the membrane theory we expect that $I^h(\mathbf{y}_h)$ is of order h. Hence the limit $h \to 0$ corresponds to a singular perturbation. The corresponding bending theory has energy functional

$$\frac{1}{24}\int_S Q_2(II)\,ds_1ds_2,$$

where II denotes the second fundamental form $II_{ij} = \mathbf{n}_{,i} \cdot \mathbf{y}_{,j}$, $\mathbf{n} = \mathbf{y}_{,1} \wedge \mathbf{y}_{,2}$ and where

$$Q_2(\mathbf{A}) = \min_{\mathbf{a} \in \mathbf{R}^3} Q_3(\mathbf{A} + \mathbf{a} \otimes \mathbf{e}_3 + \mathbf{e}_3 \otimes \mathbf{a}),$$

$$Q_3(\mathbf{A}) = D^2 W(\mathbf{1})(\mathbf{A}, \mathbf{A}).$$

The proof is via a refinement of a rigidity result for SO(3) of John [149], [152] (see also Kohn [161]). John [150], [151] also rigorously obtains equations for shells of isotropic material, assuming that the radius of curvature of the shell is large and the maximum strain is uniformly small, providing interior estimates for the validity of the approximation. For other related work see Pantz [201], [203]. For plates satisfying general boundary conditions one expects some theory incorporating both the membrane and bending cases, but the form this should take is unclear. For work in this direction see Ciarlet [80] and Ciarlet & Roquefort [85].

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