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Elastostatics in the presence of a temperature distribution or inhomogeneity

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Dedicated to Klaus Kirchgässner on the occasion of his 60th birthday

1. Introduction

We consider the problem of the equilibrium of an elastic body subjected to a temperature gradient. The boundary of the body is free to move, and there are no applied body or surface forces. Suppose the body occupies in a stress-free reference configuration the slab $\Omega = \omega \times (0, \delta)$, where $\omega \subset \boldsymbol{R}^2$ is bounded and $\delta > 0$, and that the temperature gradient is then imposed in the vertical x_3-direction, so that the temperature θ is a given function $\theta = \theta(x_3)$ with $\theta'(x_3) < 0$. Due to thermal expansion the layers $\omega \times \{x_3\}$ will tend to expand with respect to those layers $\omega \times \{x_3'\}$ with $x_3' > x_3$, producing in the case of a thin slab of isotropic material with a small imposed temperature gradient an approximately spherical deformed shape.

If we consider the corresponding two-dimensional problem of the deformation of an elastic strip $\Omega' = (0, l) \times (0, \delta)$ under an imposed temperature gradient in the vertical x_2-direction, an interesting difference emerges. In this two-dimensional problem (which is similar to that of the deformation of a bimetallic strip) an equilibrium solution in which each line $(0, l) \times \{x_2\}$ is uniformly stretched to form a circular arc is possible. However, as observed by Davies [16], no surface $x_3 = \text{constant}$ can be deformed so that its principal stretches are equal and independent of $(x_1, x_2) \in \omega$, while at the same time its principal curvatures k_1, k_2 are equal, positive, and independent of $(x_1, x_2) \in \omega$. Up to a dilation, such a deformation would be an isometry, and thus preserve the Gaussian curvature; but the Gaussian curvature is zero in the reference configuration and equals $k_1 k_2 > 0$ in the deformed configuration. (This is the familiar difficulty encountered when trying to wrap a sphere with paper without forming

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creases.) Thus in the three-dimensional problem some nonuniform deformation must arise. A probable scenario (but one for which we have no hard evidence) is that if ω is a disc or rectangle, say, then a breaking of symmetry occurs as the temperature gradient is increased.

We regard the problem as that of minimizing the total elastic energy

$$I(y) = \int_\Omega W(x, Dy(x))\, dx \tag{1.1}$$

of an elastic body in the absence of any boundary conditions. Here $y\colon \Omega \to \boldsymbol{R}^3$ denotes a typical deformed configuration of the body, and $W = W(x, A)$ is the stored-energy function of the material. Because W depends explicitly on x the material is inhomogeneous. However, as described in Section 3 below, such an inhomogeneity arises naturally from the free-energy function of a homogeneous thermoelastic body when a temperature distribution is imposed. In order for this reduction to a problem for an inhomogeneous elastic body to be appropriate the temperature distribution must be independent of the deformation, one situation in which this is a reasonable assumption being when the material is a poor heat-conductor.

The present study was motivated by an attempt to understand the striking but puzzling phenomenon of *columnar jointing* in basalt, in which columns of polygonal (often hexagonal) cross-section are formed in cooling lava. It is generally agreed that these columns are produced via a fracture process driven by thermal stresses, the cracks which eventually form the surfaces between adjacent columns propagating in an incremental manner into the solidified region in a direction roughly perpendicular to isotherms (see Ryan and Sammis [29], DeGraaf and Aydin [17]). In the initial stages of the cooling process of a lava pond, and ignoring an uppermost layer of material that is separated from the rest of the lava via the action of expanding gases (see Ryan and Sammis [29]), the surface of the pond can be regarded to a first approximation as forming a thin slab of solidified rock subject to a given vertical temperature gradient, as in the present paper.

There is a large engineering literature on the deformation and thermal stresses induced in a plate by a transverse temperature gradient, a problem of wide technological interest. See, for example, [35, 21, 34, 18, 27, 39]. However, this article differs from other work we have encountered on the subject in its use of nonlinear elasticity, its attempt to prove some rigorous results, and the method of linearization employed.

The principal results are as follows. First, under reasonable hypotheses on W we prove rigorously in Proposition 2.1 the intuitively plausible fact that for a genuinely inhomogeneous isotropic material *there are no stress-free configurations*. In particular, for an isotropic body with an imposed temperature gradient in the x_3-direction *the thermal stresses are nonzero*. In Section 3 an isotropic stored-energy function is proposed for the problem of cooling basalt, for which the existence of a minimizer of (1.1) is guaranteed by known existence theorems. The small parameter ε is given by $\varepsilon = \alpha\,\Delta\theta$, where α is the coefficient of thermal expansion and $\Delta\theta$ the temperature difference between the bottom and top of the slab. Then, in Sections 4 and 5 we analyze the case when the inhomogeneity (or variation in temperature) is 'small'. That is, we assume that $W = W(\varepsilon, x, A)$, where ε is a small parameter and $W(0, x, A) \stackrel{\text{def}}{=} W_0(A)$ is independent of x. We formally expand the energy minimizer y^ε of

$$I_\varepsilon(y) = \int_\Omega W(\varepsilon, x, Dy(x))\, dx \tag{1.2}$$

as a power series in ε, i.e.

$$y^\varepsilon = y^{(0)} + \varepsilon u + \varepsilon^2 v + \cdots, \tag{1.3}$$

and show that u minimizes the quadratic functional

$$J(u) = \tfrac{1}{2} \int_\Omega [a(x) + 2G(x) \cdot Du(x) + C(x)Du(x) \cdot Du(x)]\, dx, \tag{1.4}$$

where

$$G(x) \stackrel{\text{def}}{=} D_\varepsilon D_A W(0, x, Dy^{(0)}(x)), \quad C(x) \stackrel{\text{def}}{=} D_A^2 W_0(Dy^{(0)}(x)).$$

The corresponding Euler-Lagrange equation

$$\operatorname{div}(C(x)Du + G(x)) = 0 \tag{1.5}$$

differs from the usual equilibrium equation of linearized elasticity on account of the source term div $G(x)$. If W is isotropic then $G(x) = p(x)\mathbf{1}$ for some scalar function $p = p(x)$. By a piece of good fortune, if $Dy_0(x) = \mathbf{1}$ and $p(x) = rx_3 + s$ then the minimizer u can be determined explicitly by minimizing the *integrand* in (1.4) (see Theorem 4.1). This applies in particular when W has the form proposed in Section 3. The solution shows that to first order in ε the deformed planes $x_3 = \text{const.}$ are approximately spherical of radius $\varrho_\varepsilon = ((3\lambda + 2\mu)/r\varepsilon)$, where λ, μ are the Lamé moduli of W_0 at $\mathbf{1}$.

In Section 5 we justify the expansion (1.3) by means of the implicit function theorem, showing that under suitable hypotheses there is a solution y^ε of the form (1.3) to the Euler-Lagrange equations and natural boundary condition for (1.1), provided ε is sufficiently small. The analysis is a straightforward adaptation of techniques originally due to Stoppelli [30, 31, 32, 33], though our treatment owes much to the book of Valent [36]. In common with previous work the analysis has the unfortunate feature that it assumes $\partial\Omega$ is smooth. An example is presented, having the perhaps undesirable property that W_0 has more than one natural state (modulo rotations), showing that even under favourable growth and polyconvexity conditions y^ε need not necessarily minimize I_ε.

The analyses of Sections 4 and 5 can also be thought of as describing the behaviour of an arbitrary inhomogeneous body of small dimensions. In fact letting $x = \varepsilon z$, $y(x) = \varepsilon \bar{y}(x/\varepsilon)$, we see that

$$\varepsilon^{-3} \int_{\varepsilon\Omega} W(x, Dy(x))\, dx = \int_{\Omega} W(\varepsilon z, D\bar{y}(z))\, dz, \tag{1.6}$$

so that minimizing $\int_{\varepsilon\Omega} W(x, Dy(x))\, dx$ is equivalent to minimizing the functional

$$I_\varepsilon(\bar{y}) = \int_{\Omega} W(\varepsilon x, D\bar{y}(x))\, dx, \tag{1.7}$$

whose integrand has the form studied in Sections 4 and 5.

In Section 6 the minimization problem for (1.1) is studied numerically using a finite-element algorithm and the stored-energy function proposed in Section 3 for the problem of cooling basalt. In the limit $\varepsilon \to 0$ the results agree well with the exact solution to the linearized problem given in Section 4. A typical numerical result showing the deformed configuration of an initially square slab is illustrated in Fig. 1.

One idea for explaining the polygonal columns in basalt, explored in Davies [16], is that a polygonal stress pattern might arise from an elastic instability, perhaps having its origin in the geometrical considerations described at the beginning of the introduction, and that the subsequent

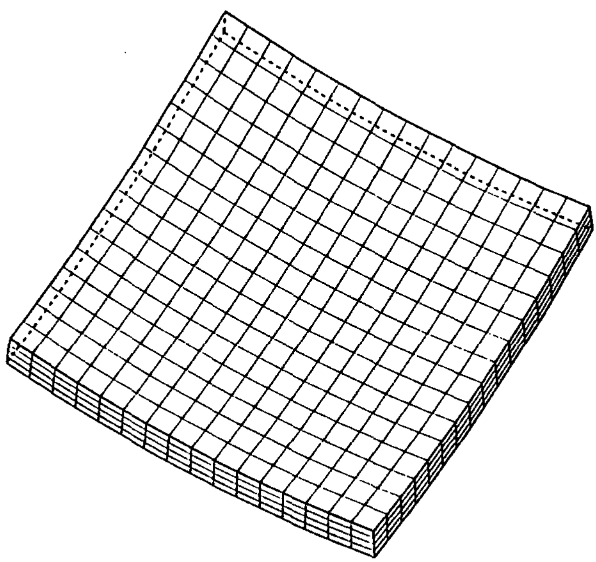

Figure 1
The deformed configuration for a slab $\Omega = (-1, 1)^2 \times (0, \delta)$ under a vertical temperature gradient, calculated by numerical minimization of the total elastic energy. The stored-energy function is given by (3.6)–(3.8) with the constants chosen as in (3.12) and with $\delta = 0.1$, $\varepsilon = 0.016$.

cracking follows this pre-existing pattern. The theoretical analysis in this paper, based as it is on linearization about a natural state, has nothing to say on this matter, while there is no evidence of a polygonal pattern emerging in the numerical results. Nevertheless it seems premature to reject this idea in the absence of a better understanding of what elasticity theory in fact predicts. A more conventional approach to explaining the hexagonal columns might be to consider a model in which the crack geometry is an unknown, and to try and show that a hexagonal crack geometry minimizes the total elastic plus surface energy. Such an approach (which might be attempted either in the context of a plate theory or a three-dimensional model) would still necessitate a calculation of the elastic energy in uncracked regions, as discussed in this paper.

2 Nonexistence of stress-free deformations for inhomogeneous isotropic materials

We consider an elastic body occupying in a reference configuration a bounded open subset $\Omega \subset \boldsymbol{R}^3$, and with bulk energy

$$I(y) = \int_\Omega W(x, Dy(x))\, dx. \tag{2.1}$$

Here $y(x)$ denotes the position in a deformed configuration of the particle at x in the reference configuration, so that $y\colon \Omega \to \boldsymbol{R}^3$. For each x, the deformation gradient $Dy(x)$ can be identified with an element of the subset $M_+^{3\times 3} = \{A \in M^{3\times 3}\colon \det A > 0\}$ of the set $M^{3\times 3}$ of real 3×3 matrices.

In (2.1), $W\colon \Omega \times M_+^{3\times 3} \to \boldsymbol{R}$ denotes the *stored-energy function* of the material. We assume that $W(\cdot, A)$ is measurable for all $A \in M_+^{3\times 3}$, and that $W(x, \cdot)$ is C^1 for a.e. $x \in \Omega$. Since W is assumed to depend explicitly on x, the material is *inhomogeneous*. Of particular interest to the calculations in this paper is the case when the inhomogeneity results from a given temperature distribution; this is explained in Section 3 below. We suppose that $W(x, \cdot)$ is *frame-indifferent*, so that for a.e. $x \in \Omega$

$$W(x, QA) = W(x, A) \quad \text{for all } A \in M_+^{3\times 3},\ Q \in SO(3). \tag{2.2}$$

and *isotropic* with respect to the given reference configuration, so that for a.e. $x \in \Omega$

$$W(x, AR) = W(x, A) \quad \text{for all } A \in M_+^{3\times 3},\ R \in SO(3). \tag{2.3}$$

As is well-known, (2.2) and (2.3) are equivalent to the existence of a function $\Phi\colon \Omega \times (0, \infty)^3 \to \boldsymbol{R}$, symmetric with respect to permutations of its last three arguments, such that

$$W(x, A) = \Phi(x, v_1, v_2, v_3) \tag{2.4}$$

for all $A \in M_+^{3\times 3}$, where $v_i = v_i(A)$, $i = 1, 2, 3$, denote the singular values of A (that is, the eigenvalues of the positive symmetric matrix $\sqrt{A^T A}$).

The Piola-Kirchhoff stress tensor T_R is given by $T_R = D_A W$. Thus a configuration y is *stress-free* if

$$D_A W(x, Dy(x)) = 0 \quad \text{a.e. } x \in \Omega. \tag{2.5}$$

Since any $A \in M_+^{3\times 3}$ can be written in the form

$$A = QDR, \tag{2.6}$$

where $Q,\ R \in SO(3)$ and $D = \operatorname{diag}(v_1, v_2, v_3)$, it follows that

$$D_A W(x, A) = Q \operatorname{diag}\left(\frac{\partial \Phi}{\partial v_1}, \frac{\partial \Phi}{\partial v_2}, \frac{\partial \Phi}{\partial v_3}\right) R. \tag{2.7}$$

Hence (2.5) holds if and only if

$$\frac{\partial \Phi}{\partial v_i}(x, v_1(x), v_2(x), v_3(x)) = 0, \quad \text{a.e. } x \in \Omega \tag{2.8}$$

for $i = 1, 2, 3$, where the $v_i(x)$ are the singular values of $Dy(x)$.

In the following proposition, and the rest of the paper, we denote by $W^{m,p}(\Omega; \boldsymbol{R}^n)$, where $n \geq 1$, $m \geq 1$ are integers, $1 \leq p < \infty$, and $\Omega \subset \boldsymbol{R}^n$ is bounded and open, the Sobolev space of mappings $y: \Omega \to \boldsymbol{R}^n$ which together with their distributional derivatives up to and including order m belong to $L^p(\Omega)$. Thus $y \in W^{1,p}(\Omega; \boldsymbol{R}^n)$ provided $\int_\Omega (|y|^p + |Dy|^p)\, dx < \infty$. By $W^{m,p}_{loc}(\Omega; \boldsymbol{R}^n)$ we mean the space of mappings y which belong to $W^{m,p}(E; \boldsymbol{R}^n)$ for every open E with $\bar{E} \subset \Omega$. In Section 5 we will also use the spaces $W^{s,p}(\partial\Omega; \boldsymbol{R}^n)$ with s not necessarily an integer; we refer to Valent [36, Chapter 2] for the definitions.

Proposition 2.1. Assume that the Baker-Ericksen inequalities

$$\frac{v_i \dfrac{\partial \Phi}{\partial v_i} - v_j \dfrac{\partial \Phi}{\partial v_j}}{v_i - v_j} > 0, \quad v_i \neq v_j \tag{2.9}$$

hold for a.e. $x \in \Omega$. Let $y \in W^{1,3}_{\text{loc}}(\Omega; \boldsymbol{R}^3)$ with $\det Dy(x) > 0$ for a.e. $x \in \Omega$. If y is *stress-free* then y is conformal, i.e.

$$Dy(x) = v(x) R(x), \quad \text{a.e. } x \in \Omega, \tag{2.10}$$

where $v(x) \geq 0$ and $R(x) \in SO(3)$. Hence either $y(x) = c + \lambda R_0 x$, where $c \in \boldsymbol{R}^3$, $\lambda > 0$, $R_0 \in SO(3)$ or

$$y(x) = c - \lambda R_0 \frac{x - a}{|x - a|^2}, \tag{2.11}$$

where $c \in \boldsymbol{R}^3$, $\lambda > 0$, $R_0 \in SO(3)$ and $a \in \boldsymbol{R}^3 - \Omega$.

Remark. As is well-known, the Baker-Ericksen inequalities are a consequence of strong-ellipticity of $W(x, \cdot)$; in fact (*cf.* Ball [2, p. 563]) they follow from the weaker condition of *strict rank-one convexity*, which says that

$$W(x, tA + (1-t)B) < tW(x, A) + (1-t)W(x, B) \tag{2.12}$$

whenever $0 < t < 1$ and $A, B \in M_+^{3\times 3}$ with $A - B = \lambda \otimes \mu$ for some nonzero $\lambda, \mu \in \boldsymbol{R}^3$.

Proof of Proposition 2.1. Let y be stress free. Then by (2.8), (2.9) we have $v_1(x) = v_2(x) = v_3(x) = v(x)$ a.e., where $v \in L^\infty(\Omega)$, $v(x) > 0$ a.e., so that by the decomposition (2.6) y is conformal. The characterization of conformal mappings in $\boldsymbol{R}^3$ given in the theorem is known as *Liouville's theorem*, which was first proved under the assumption that y is of class C^4. Proofs of Liouville's theorem for mappings $y \in W^{1,3}_{\mathrm{loc}}(\Omega; \boldsymbol{R}^3)$ are given by Bojarski and Iwaniec [9] and Reshetnyak [28]. As is suggested by Iwaniec [19], it seems likely that this result holds even if only $y \in W^{1,3/2}_{\mathrm{loc}}(\Omega; \boldsymbol{R}^3)$. □

Now suppose that $\Phi(x, \cdot, \cdot, \cdot)$ has a *unique* critical point given by $v_1(x) = v_2(x) = v_3(x) = v(x)$, and that $v(x)$ is not constant and does not have the form

$$v(x) = \frac{\lambda}{|x-a|^2} \tag{2.13}$$

for any $\lambda > 0$, $a \in \boldsymbol{R}^3 - \Omega$. (Note that (2.13) corresponds to (2.11).) Then by Proposition 2.1 *there is no stress-free deformation* $y \in W^{1,3}_{\mathrm{loc}}(\Omega; \boldsymbol{R}^3)$. In particular this holds for the case when $v(x) = v(x_3)$ and is not constant. A class of stored-energy functions having these properties and appropriate for the problem of cooling basalt is described in Section 3.

In two dimensions (i.e. $y \in W^{1,2}_{\mathrm{loc}}(\Omega; \boldsymbol{R}^2)$ with $\Omega \subset \boldsymbol{R}^2$), the function $v(\cdot)$ in (2.10) must satisfy

$$\Delta(\ln v) = 0, \tag{2.14}$$

since if the conformal mapping y is represented by the analytic function $f(z)$ then $\ln v$ is the real part of the analytic function $\log f'(z)$. Conversely, if $\ln v$ is harmonic then there exists locally a conformal mapping y whose principal stretches both equal $v(x)$; in fact, if w is a harmonic conjugate to $\ln v$ a suitable analytic function f can be obtained from the formula $f'(z) = \exp(\ln v + iW)$. Said differently, (2.14) is equivalent to the vanishing of the Riemann-Christoffel tensor of the metric $g_{ij} = v^2\delta_{ij}$. If now we consider the case, analogous to that in the previous paragraph, when $\Phi(x, \cdot, \cdot)$ has a unique critical point $v_1(x) = v_2(x) = v(x_2)$ with $v(x_2)$ not constant, we find that there exists a stress-free configuration if and only if $v(x_2) = rx_2 + s$ for some constants r and s. Up to a rigid rotation and translation the corresponding stress-free deformation is given by

$$
\begin{aligned}
y_1(x_1, x_2) &= \alpha^{-1} e^{\alpha x_2 + \beta} \sin \alpha x_1, \\
y_2(x_1, x_2) &= \alpha^{-1} e^{\alpha x_2 + \beta} \cos \alpha x_1,
\end{aligned}
\tag{2.15}
$$

which maps each line $x_2 = \text{constant}$ to the circle centre the origin with radius $\alpha^{-1} e^{\alpha x_2 + \beta}$ and lines $x_1 = \text{constant}$ to radial lines.

3. A class of stored-energy functions

In this section we construct a class of stored-energy functions appropriate for the problem of cooling basalt, and having desirable mathematical properties. We model the solidified lava as a homogeneous thermoelastic material with free-energy function $\psi = \psi(\theta, A)$ occupying in a reference configuration the slab $\Omega = \omega \times (0, \delta)$, where $\omega \subset \boldsymbol{R}^2$ is bounded and $\delta > 0$. We suppose that the temperature distribution is linear in the vertical x_3-direction, so that the absolute temperature θ is given by

$$
\theta(x_3) = \theta_0 - \frac{x_3}{\delta} \Delta\theta,
\tag{3.1}
$$

where $\theta_0 > 0$ and $\Delta\theta$ is the temperature difference between the bottom and top of the slab. Regarding the temperature distribution as fixed, we obtain the corresponding inhomogeneous stored-energy function given by[1]

$$
W(x_3, A) = \psi(\theta(x_3), A).
\tag{3.2}
$$

For the minimization problem (2.1) to be relevant in this case the temperature must vary sufficiently slowly with time to be assumed time-independent; in the columnar-jointing problem this is reasonable since basalt is a very poor heat-conductor (a lava pond takes many years to reach thermal equilibrium). For thermoelastic bodies with certain constitutive equations for the heat-flux vector that do not depend on the deformation gradient, a thermodynamic justification of the minimum principle (2.1), (3.2) is given in Ball and Knowles [5].

[1] The assumption that the dependence of W on x_3 is given by (3.2) could be questioned on the grounds that the material may be solidifying under stress, leading to a body which after cooling to a constant temperature is still inhomogeneous. An attempt to take this into account would be to replace (3.2) by a stored-energy function of the form

$$
W(x_3, A) = \psi(\theta(x_3), D(x_3)A),
$$

where $D(x_3) = \operatorname{diag}(\lambda(x_3), \lambda(x_3), \mu(x_3))$ and $\lambda(\cdot)$, $\mu(\cdot)$ are suitable functions. If $\theta(x_3) = \text{const.}$ then a calculation in the spirit of Proposition 2.1 shows that in general there is no stress-free configuration, unlike for (3.2). Note, however, that the body is still *uniform* in the sense of Wang and Truesdell [38] (i.e. it is composed of the same material at each point).

We suppose that $\psi(\theta, \cdot)$ is isotropic, so that

$$\psi(\theta, A) = \Psi(\theta, v_1, v_2, v_3), \tag{3.3}$$

where $v_i = v_i(A)$ are the singular values of A and $\Psi(\theta, \cdot, \cdot, \cdot)$ is symmetric, and choose $\Psi(\theta, \cdot, \cdot, \cdot)$ to have a unique minimizer at $v_1 = v_2 = v_3 = \bar{v}(\theta)$, where $\bar{v}(\theta) = 1 + \alpha(\theta - \theta_0)$, corresponding to a constant coefficient of thermal expansion $\alpha > 0$. A simple way to arrange this, which we adopt, is to suppose that

$$\Psi(\theta, v_1, v_2, v_3) = \bar{v}(\theta^2)\Psi_0\left(\frac{v_1}{\bar{v}(\theta)}, \frac{v_2}{\bar{v}(\theta)}, \frac{v_3}{\bar{v}(\theta)}\right), \tag{3.4}$$

where Ψ_0 has a unique minimizer at $v_1 = v_2 = v_3 = 1$. The reason for the choice for the factor $\bar{v}(\theta)^2$ is explained below. Let $\varepsilon = \alpha\,\Delta\theta$ and

$$v(\varepsilon x_3) = 1 - \varepsilon\frac{x_3}{\delta}. \tag{3.5}$$

Note that if $\varepsilon < 1$ then $v(\varepsilon x_3) > 0$ for all $x \in \Omega$. Combining (3.1)–(3.5) and writing $W(x_3, A) = W(\varepsilon, x_3, A)$, we have that

$$W(\varepsilon, x_3, A) = \Phi(\varepsilon x_3, v_1, v_2, v_3), \tag{3.6}$$

where

$$\Phi(\varepsilon x_3, v_1, v_2, v_3) = v(\varepsilon x_3)^2\Psi_0\left(\frac{v_1}{v(\varepsilon x_3)}, \frac{v_2}{v(\varepsilon x_3)}, \frac{v_3}{v(\varepsilon x_3)}\right). \tag{3.7}$$

Essentially following Ciarlet and Geymonat [15] (see also Ciarlet [14]) we choose Ψ_0 to have the form

$$\begin{aligned}\Psi_0(v_1, v_2, v_3) &= a_1(v_1^2 + v_2^2 + v_3^2) + a_2(v_1^4 + v_2^4 + v_3^4)\\ &\quad + b(v_2^2v_3^2 + v_3^2v_1^2 + v_1^2v_2^2) + c(v_1v_2v_3)^2 - d\ln(v_1v_2v_3),\end{aligned} \tag{3.8}$$

where $a_1 > 0$, $a_2 \geq 0$, $b > 0$, $c \geq 0$, $d > 0$ and

$$d = 2a_1 + 4a_2 + 4b + 2c. \tag{3.9}$$

Let

$$\lambda = 4b + 4c, \quad \mu = 2a_1 + 8a_2 + 2b. \tag{3.10}$$

Let $W_0(A) = \Psi_0(v_1, v_2, v_3)$. Note that $W_0(A) = \psi(\theta_0, A)$. This homogeneous isotropic stored-energy function has the following properties:

1. W_0 is *strictly polyconvex*; i.e. $W_0(A) = g(A, \operatorname{cof} A, \det A)$ for some strictly convex function $g\colon M^{3\times 3} \times M^{3\times 3} \times (0, \infty) \to \boldsymbol{R}$, where $\operatorname{cof} A$ denotes the matrix of cofactors of A.

2. Ψ_0 has a unique critical point at $v_1 = v_2 = v_3 = 1$, which minimizes Ψ_0.

3. The *Lamé moduli* of W_0 at the identity are λ and μ, i.e. (*cf.* Lemma 4.1 below)

$$D^2 W_0(\mathbf{1})(H, H) = \lambda(\operatorname{tr} H)^2 + \frac{\mu}{2}|H + H^T|^2, \quad H \in M^{3\times 3}. \tag{3.11}$$

4. $W_0(A) \to \infty$ as $\det A \to 0+$.

The strict polyconvexity of W_0 follows from Ball [1, Section 5]. Property 2 follows easily from the observation that by the Baker-Ericksen inequalities any critical point of Ψ_0 satisfies $v_1 = v_2 = v_3$. Property 3 is easily verified by choosing H diagonal, while Property 4 is obvious since $\det A = v_1 v_2 v_3$.

The inhomogeneous stored-energy function (3.6) inherits the following properties from those of W_0.

1′. $W(\varepsilon, x_3, \cdot)$ is strictly polyconvex.

2′. $\Phi(\varepsilon x_3, \cdot, \cdot, \cdot)$ has a unique critical point $v_1 = v_2 = v_3 = v(\varepsilon x_3)$, which minimizes $\Phi(\varepsilon x_3, \cdot, \cdot)$.

3′. The Lamé moduli of $W(\varepsilon, x_3, \cdot)$ at the identity are λ and μ, and in particular are independent of x_3.

4′. $W(\varepsilon, x_3, A) \to \infty$ as $\det A \to 0+$.

Note that Property 3′ is a consequence of having chosen the factor $\bar{v}(\theta)^2$ in (3.4).

In the numerical computations in Section 6 the constants were chosen as follows:

$$\begin{aligned} a_1 &= 0.65 \\ a_2 &= 0 \\ b &= 0.45 \\ c &= 0 \\ d &= 2a_1 + 4a_2 + 4b + 2c = 3.1. \end{aligned} \tag{3.12}$$

These values correspond to the Lamé moduli

$$\lambda = 1.8 \quad \text{and} \quad \mu = 2.2,$$

which are, in appropriate units, equivalent to a Young's modulus E of 5.4×10^{11} dynes cm^{-2}, and a Poisson's ratio v of 0.22. These are the values for basalt at a temperature of approximately 700°C, as reported by Ryan and Sammis [29]. The Lamé moduli of basalt are not exactly independent of temperature, as given in Property 3′, but this simplification is probably not important for our purposes. An appropriate value of ε can be estimated from the coefficients of thermal expansion given for basalt at different temperatures in [29]. Taking the representative value $\alpha = 8 \times 10^{-6}\,{}^{\circ}\mathrm{C}^{-1}$, and a temperature difference $\Delta\theta$ of 675°C (corresponding to a temperature $\theta_0 = 700$°C at the bottom of the slab and an air temperature of 25°C), suggests the approximate value $\varepsilon = 5 \times 10^{-3}$. A much smaller value of $\Delta\theta$ might well be appropriate; for example, Ryan and Sammis suggest that cracking will occur if $\Delta\theta$ exceeds 53°C.

We are not aware of proposals for a three-dimensional nonlinear free-energy function for basalt, so that (3.6), (3.7) should be regarded as a guess that is consistent with measured linear moduli and general principles of frame-indifference and isotropy. Our model ignores several other features of the actual situation in cooling basalt as described in [29], such as creep and the glass transition.

In Section 6 it will prove convenient to express $W(\varepsilon, x_3, A)$ in the form

$$\begin{aligned} W(\varepsilon, x_3, A) &= H(\varepsilon, x, I_1, I_2, I_3) \\ &= a_1 I_1 + a_2 I_1^2/v^2(\varepsilon x_3) + (b - 2a_2) I_2/v^2(\varepsilon x_3) + c I_3/v^4(\varepsilon x_3) \\ &\quad - \frac{d}{2} v^2(\varepsilon x_3)[\log I_3 - \log v^6(\varepsilon x_3)], \end{aligned} \tag{3.13}$$

where

$$\begin{aligned} I_1 &= \operatorname{tr}(A^T A) = v_1^2 + v_2^2 + v_3^2, \\ I_2 &= \operatorname{tr}[(\operatorname{cof} A)^T \operatorname{cof} A] = v_1^2 v_2^2 + v_2^2 v_3^2 + v_3^2 v_1^2, \\ I_2 &= \det A = v_1 v_2 v_3. \end{aligned} \tag{3.14}$$

The following result is a consequence of known existence theorems for nonlinear elastostatics (see Ball [1]).

Theorem 3.1. If $W = W(\varepsilon, x_3, A)$ is given by (3.6)–(3.8) and Ω is strongly Lipschitz with $\inf_{x \in \Omega} v(\varepsilon x_3) > 0$ then

$$I_\varepsilon(y) = \int_\Omega W(\varepsilon, x_3, Dy(x))\, dx \tag{3.15}$$

attains an absolute minimum in $\mathscr{A} \stackrel{\text{def}}{=} \{y \in W^{1,1}(\Omega; \boldsymbol{R}^3) \colon \det Dy(x) > 0 \text{ a.e. } x \in \Omega\}$.

4. Linearization with respect to an inhomogeneity

4.1. A formal expansion

Consider a general stored-energy function $W(\varepsilon, x, A)$ such that $W(0, x, A) \stackrel{\text{def}}{=} W(A)$ is independent of x. Thus when $\varepsilon = 0$ the material is homogeneous, while for $\varepsilon > 0$ it is inhomogeneous. Proceeding formally, let $y^{(\varepsilon)}$ be a minimizer of

$$I_\varepsilon(y) = \int_\Omega W(\varepsilon, x, Dy(x))\, dx, \tag{4.1}$$

subject to

$$y|_{\partial\Omega_1} = \bar{y}, \tag{4.2}$$

where $\partial\Omega_1 \subset \partial\Omega$ and $\bar{y}: \partial\Omega_1 \to \boldsymbol{R}^3$ is given. We suppose that y^ε can be expanded as a power series in ε, i.e.

$$y^\varepsilon = y^{(0)} + \varepsilon u + \varepsilon^2 v + \cdots, \tag{4.3}$$

for some mappings $y^{(0)}$, u, v etc. Thus

$$\begin{aligned} I_\varepsilon(y^\varepsilon) &= \int_\Omega W(\varepsilon, x, Dy^\varepsilon)\, dx \\ &= \int_\Omega W_0(Dy^{(0)}(x))\, dx \\ &\quad + \varepsilon \int_\Omega [D_\varepsilon W(0, x, Dy^{(0)}) + D_A W_0(Dy^{(0)}) \cdot Du]\, dx \\ &\quad + \frac{\varepsilon^2}{2} \int_\Omega [D_\varepsilon^2 W(0, x, Dy^{(0)}) + 2D_\varepsilon D_A W(0, x, Dy^{(0)}) \cdot Du \\ &\quad + D_A^2 W_0(Dy^{(0)})Du \cdot Du + 2D_A W_0(Dy^{(0)}) \cdot Dv]\, dx + o(\varepsilon^2). \end{aligned} \tag{4.4}$$

Since $y^{(0)}$ minimizes

$$I(y) = \int_\Omega W_0(Dy(x))\, dx \tag{4.5}$$

subject to (4.2), we have that

$$\int_\Omega D_A W_0(Dy^{(0)}(x)) \cdot D\phi\, dx = 0 \tag{4.6}$$

for all $\phi: \bar{\Omega} \to \boldsymbol{R}^3$ with $\phi|_{\partial\Omega_1} = 0$. Since $u|_{\partial\Omega_1} = 0$ it follows from (4.6) that the coefficient of ε in (4.4) is independent of u. Similarly, the last term in the coefficient of ε^2 vanishes. Hence the coefficient of ε^2 can be written as

$$J(u) = \tfrac{1}{2} \int_\Omega [a(x) + 2G(x) \cdot Du(x) + C(x)Du(x) \cdot Du(x)]\, dx, \tag{4.7}$$

where

$$a(x) \stackrel{\text{def}}{=} D_\varepsilon^2 W(0, x, Dy^{(0)}(x)), \quad G(x) \stackrel{\text{def}}{=} D_\varepsilon D_A W(0, x, Dy^{(0)}(x)),$$

$$C(x) \stackrel{\text{def}}{=} D_A^2 W_0(Dy^{(0)}(x)).$$

A minimizer u of J subject to $u|_{\partial\Omega_1} = 0$ satisfies

$$\begin{aligned} &\operatorname{div}(C(x)Du + G(x)) = 0, \quad x \in \Omega, \\ &(C(x)Du + G(x))\nu|_{\partial\Omega\setminus\partial\Omega_1} = 0, \\ &u|_{\partial\Omega_1} = 0, \end{aligned} \tag{4.8}$$

where $\nu = \nu(x)$ denotes the unit outward normal to $\partial\Omega$ at x.

Note that (4.8) differs from the usual mixed boundary-value problem of linearized elasticity on account of the source term div $G(x)$. Of course (4.8) may be obtained directly as the coefficient of ε in the expansion of the Euler-Lagrange equation

$$\operatorname{div} D_A W(\varepsilon, x, Dy^{\varepsilon}) = 0, \quad x \in \Omega, \tag{4.9}$$

and natural boundary condition

$$D_A W(\varepsilon, x, Dy^{\varepsilon})\nu|_{\partial\Omega\setminus\partial\Omega_1} = 0, \tag{4.10}$$

for I_ε. Similarly we find that v solves the system

$$\begin{aligned} &\operatorname{div}(C(x)Dv + G_1(x)) = 0, \quad x \in \Omega, \\ &(C(x)Dv + G_1(x))\nu|_{\partial\Omega\setminus\partial\Omega_1} = 0, \\ &v|_{\partial\Omega_1} = 0, \end{aligned} \tag{4.11}$$

where

$$\begin{aligned} G_1(x) \stackrel{\text{def}}{=} {}& \tfrac{1}{2}D_\varepsilon^2 D_A W(0, x, Dy^{(0)}(x)) + D_\varepsilon D_A^2 W(0, x, Dy^{(0)}(x))Du(x) \\ & + \tfrac{1}{2}D_A^3 W_0(Dy^{(0)}(x))Du(x) \cdot Du(x), \end{aligned} \tag{4.12}$$

and so on.

4.2. The zero traction problem: an exact solution

We now consider the zero traction problem, for which $\partial\Omega_1$ is empty, and present an exact solution to the linearized problem (4.8) in a special case. We suppose that $W(\varepsilon, x, \cdot)$ is isotropic, and that $Dy^{(0)} = \boldsymbol{1}$. To simplify the expression for $G(x)$ and $C(x)$ we use the following well-known lemma.

Lemma 4.1. (cf. [3, p. 724]) Let $\tilde{W} \in C^2(M_+^{3\times 3})$ be isotropic. Then there exist constants p, λ, μ such that

$$D_A \tilde{W}(\boldsymbol{1}) = p\boldsymbol{1}, \tag{4.13}$$

and

$$D_A^2 \tilde{W}(\boldsymbol{1})H \cdot H = \lambda(\operatorname{tr} H)^2 + \frac{\mu}{2}|H + H^T|^2, \quad H \in M^{3\times 3}. \tag{4.14}$$

Applying Lemma 4.1 to the isotropic function $\tilde{W}(A) = D_\varepsilon W(0, x, A)$, we find that

$$G(x) = p(x)\mathbf{1} \tag{4.15}$$

for some scalar function $p = p(x)$. Applying the lemma with $\tilde{W}(A) = W_0(A)$ we also have that $C(x) = C$ is independent of x, and

$$CH \cdot H = \lambda(\operatorname{tr} H)^2 + \frac{\mu}{2}|H + H^T|^2, \quad H \in M^{3\times 3}, \tag{4.16}$$

for constants λ, μ (the *Lamé moduli*). Setting without loss of generality $a(x) \equiv 0$ in (4.7) we obtain

$$J(u) = \tfrac{1}{2}\int_\Omega Q(x, Du(x))\, dx, \tag{4.17}$$

where

$$Q(x, H) = \lambda(\operatorname{tr} H)^2 + \frac{\mu}{2}|H + H^T|^2 + 2p(x) \operatorname{tr} H. \tag{4.18}$$

We suppose that $Q(x, \cdot)$ is strictly convex on symmetric matrices; equivalently, the Lamé moduli satisfy

$$3\lambda + 2\mu > 0, \quad \mu > 0. \tag{4.19}$$

As a final simplification, motivated by the discussion in Section 3, we suppose that $p = p(x_3)$.

To find an explicit minimizer of $J(\cdot)$ we determine the minimizers $H(\cdot)$ of

$$\bar{J}(H) = \tfrac{1}{2}\int_\Omega Q(x, H(x))\, dx \tag{4.20}$$

in $L^2(\Omega; M^{3\times 3})$, and see if one of them is a gradient, i.e. $H(x) = Du(x)$ for some $u \in H^1(\Omega; \mathbf{R}^3)$. Surprisingly, this strategy works in a useful special case.

Theorem 4.1. Let $W: (-\varepsilon_0, \varepsilon_0) \times \Omega \times M^{3\times 3}_+ \to \mathbf{R}$ be C^2 and isotropic, where $\varepsilon_0 > 0$. Assume that the Lamé moduli λ, μ given by (4.16) satisfy (4.19), and that $p = p(x_3)$. Then there exists a minimizer H of $\bar{J}(\cdot)$ in $L^2(\Omega; M^{3\times 3})$ which is a gradient if and only if

$$p(x_3) = rx_3 + s \tag{4.21}$$

for some $r, s \in \mathbf{R}$. The corresponding $u \in H^1(\Omega; \mathbf{R}^3)$ with $Du = H$ are then given by

$$u(x) = \bar{u}(x) + Kx + c, \tag{4.22}$$

where

$$\begin{aligned}
\bar{u}_1(x) &= -\kappa^{-1}x_1(rx_3+s),\\
\bar{u}_2(x) &= -\kappa^{-1}x_2(rx_3+s),\\
\bar{u}_3(x) &= \tfrac{1}{2}\kappa^{-1}[r(x_1^2+x_2^2-x_3^2)-2sx_3],
\end{aligned} \tag{4.23}$$

$c \in \boldsymbol{R}^3$, K is a skew 3×3 matrix, and $\kappa = 3\lambda + 2\mu$. These are the only weak solutions of the linearized problem (*cf.* (4.8))

$$\begin{aligned}
&\operatorname{div}(CDu + (rx_3+s)\boldsymbol{1}) = 0, \quad x \in \Omega\\
&(CDu + (rx_3+s)\boldsymbol{1})\nu = 0, \quad x \in \partial\Omega.
\end{aligned} \tag{4.24}$$

Proof. The unique minimizer of the integrand $Q(x, H)$ among symmetric matrices H is easily calculated to be

$$\bar{H}(x) = -\kappa^{-1}p(x_3)\boldsymbol{1}. \tag{4.25}$$

Since $Q(x, H + K) = Q(x, H)$ for any skew K it follows that the minimizers of $\bar{J}$ in $L^2(\Omega; M^{3\times 3})$ are of the form

$$H(x) = -\kappa^{-1}p(x_3)\boldsymbol{1} + K(x), \tag{4.26}$$

where $K(x)$ is skew. If $H(x) = Du(x)$ then

$$u_{1,1} = u_{2,2} = u_{3,3} = -\kappa^{-1}p(x_3), \tag{4.27}$$

$$u_{1,2} + u_{2,1} = u_{2,3} + u_{3,2} = u_{3,1} + u_{1,3} = 0. \tag{4.28}$$

Hence $0 = u_{3,311} = u_{3,131} = -u_{1,331} = -u_{1,133} = \kappa^{-1}p_{,33}$ in the sense of distributions, which implies (4.21). If (4.21) holds, then (4.27) implies that $Du(x) - D\bar{u}(x)$ is skew for a.e. x, where $\bar{u}(x)$ is defined in (4.23). As is well known (*cf.* Valent [36, p. 55]) and easily verified, this implies that $Du(x) - D\bar{u}(x)$ is a constant skew matrix, so that u has the form (4.22). It is easily verified that if u is given by (4.22) then $H = Du(x)$ satisfies (4.26), so that u is a minimizer of J. Furthermore

$$CDu + (rx_3+s)\boldsymbol{1} = 0, \tag{4.29}$$

so that (4.24) holds trivially.

By definition, u is a weak solution of (4.24) if $u \in H^1(\Omega; \boldsymbol{R}^3)$ and

$$\int_\Omega (CDu + (rx_3+s)\boldsymbol{1}) \cdot D\phi \, dx = 0 \tag{4.30}$$

for all $\phi \in H^1(\Omega; \boldsymbol{R}^3)$. Thus the difference z between any two weak solutions satisfies

$$\int_\Omega CDz \cdot Dz \, dx = 0, \tag{4.31}$$

so that $Dz(x)$ is skew for a.e. $x \in \Omega$. Thus $z(x) = Kx + c$ for a constant skew matrix K and some $c \in \boldsymbol{R}$. This shows that the only weak solutions of (4.24) are given by (4.22). □

The following lemma verifies that condition (4.21) holds for the stored-energy function $W(\varepsilon, x_3, A)$ given by (3.6)–(3.8).

Lemma 4.2. Let $W(\varepsilon, x_3, A)$ be given by (3.6)–(3.8). Then

$$D_\varepsilon D_A W(0, x_3, \boldsymbol{1}) = p(x_3)\boldsymbol{1} \quad \text{where} \quad p(x_3) = \frac{3\lambda + 2\mu}{\delta} x_3. \tag{4.32}$$

Proof. The first equality follows immediately from (4.13) of Lemma 4.1. Also we have from (3.7) that

$$W(\varepsilon, x_3, A) = v(\varepsilon x_3)^2 W_0(v(\varepsilon x_3)^{-1} A)$$

where, as usual,

$$v(\varepsilon x_3) = 1 - \frac{\varepsilon x_3}{\delta}.$$

So

$$D_A W(\varepsilon, x_3, \boldsymbol{1}) = v(\varepsilon x_3) D_A W_0(v(\varepsilon x_3)^{-1}\boldsymbol{1})\boldsymbol{1}$$

and

$$D_\varepsilon D_A W(0, x_3, \boldsymbol{1}) = \frac{x_3}{\delta} D_A^2 W_0(\boldsymbol{1})\boldsymbol{1}.$$

Hence

$$p(x_3)\boldsymbol{1} \cdot \boldsymbol{1} = \frac{x_3}{\delta} D_A^2 W_0(\boldsymbol{1})\boldsymbol{1} \cdot \boldsymbol{1}$$

and by Lemma 4.1 we have the required result. □

In order to fix the arbitrary translation and linearized rotation in (4.22) we pick a point $\bar{x} \in \Omega$ and require that

$$y^\varepsilon(\bar{x}) = \bar{x}, \quad Dy^\varepsilon(\bar{x}) = Dy^\varepsilon(\bar{x})^T. \tag{4.33}$$

so that there is no local rotation at $\bar{x}$. Since $y^\varepsilon(x) = x + \varepsilon u(x) + \cdots$ this implies that

$$u(\bar{x}) = 0, \quad Du(\bar{x}) = Du(\bar{x})^T. \tag{4.34}$$

Taking without loss of generality $\bar{x} = 0$ we deduce from (4.23) that $K = 0$, $c = 0$, so that $u = \bar{u}$. Hence

$$\begin{aligned} y_1^\varepsilon(x) &= x_1(1 - \varepsilon\kappa^{-1}(rx_3 + s)) + o(\varepsilon), \\ y_2^\varepsilon(x) &= x_2(1 - \varepsilon\kappa^{-1}(rx_3 + s)) + o(\varepsilon), \\ y_3^\varepsilon(x) &= x_3\left(1 - \frac{\varepsilon}{2}\kappa^{-1}(rx_3 + 2s)\right) + \frac{\varepsilon}{2}\kappa^{-1}r(x_1^2 + x_2^2) + o(\varepsilon). \end{aligned} \tag{4.35}$$

Hence to first order in ε, $y = y^\varepsilon$ satisfies

$$2y_3 = g_\varepsilon(x_3) + \varrho_\varepsilon^{-1}(y_1^2 + y_2^2), \tag{4.36}$$

where

$$g_\varepsilon(x_3) = 2x_3\left(1 - \frac{\varepsilon}{2}\kappa^{-1}(rx_3 + 2s)\right), \quad \varrho_\varepsilon = \frac{\kappa}{r\varepsilon}. \tag{4.37}$$

For fixed x_3 the surface (4.36) is a parabolic spheroid which to first order in ε is spherical of radius ϱ_ε.

In the case when $W(\varepsilon, x_3, A)$ is given by (3.6)–(3.8), it follows from Lemma 4.2 that

$$\varrho_\varepsilon = \frac{\delta}{\varepsilon}. \tag{4.38}$$

This is the same result as given for the radius of curvature of a thin elastic plate in a temperature gradient by Timoshenko [35] (see also Johns [21]), who uses an elementary, but approximate, geometric argument. He also points out that to this approximation the corresponding thermal stresses are zero; this corresponds in our calculation to the fact that $D_H Q(x, Du(x)) = 0$ when $p(x) = rx_3 + s$ and u is given by (4.22).

5 Justification of the formal expansion via the implicit function theorem

In this section we use the implicit function theorem to study the problem

$$\operatorname{div} D_A W(\varepsilon, x, Dy) = 0, \quad x \in \Omega, \tag{5.1}$$

$$D_A W(\varepsilon, x, Dy)\nu = 0, \quad x \in \partial\Omega, \tag{5.2}$$

for small ε. In (5.2), $\nu = \nu(x)$ denotes the unit outward normal to $\partial\Omega$. Equations (5.1), (5.2) are respectively the Euler-Lagrange equation and natural boundary condition corresponding to the minimization problem (4.1). They express the balance of forces in Ω and the condition of zero surface traction on $\partial\Omega$ respectively. The analysis uses classical ideas for applying the implicit function theorem to the traction problem of nonlinear elastostatics (see Stoppelli [30, 31, 32, 33], Van Buren [10], Chillingworth, Marsden and Wan [11, 12], Wan and Marsden [37], Marsden and Hughes [22], Valent [36]). We follow Valent's careful treatment quite closely.

Let m be a non-negative integer, and let $\Omega \subset \boldsymbol{R}^3$ be a bounded domain of class C^{m+2}. We make the following hypotheses on $W = W(\varepsilon, x, A)$

(H1) (*domain of definition*) $W: D \to \boldsymbol{R}$ where $D = (-\varepsilon_0, \varepsilon_0) \times \bar{\Omega} \times M^{3\times 3}_+$ and $\varepsilon_0 > 0$.
(H2) (*smoothness*) $W \in C^1(D)$ and $W(\varepsilon, \cdot, \cdot) \in C^{m+3}(\bar{\Omega} \times M^{3\times 3}_+)$ for every $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$.
(H3) (*frame-indifference*) $W(\varepsilon, x, QA) = W(\varepsilon, x, A)$ for all $(\varepsilon, x, A) \in D$ and all $Q \in SO(3)$.
(H4) (*homogeneity at* $\varepsilon = 0$) $W(0, x, A) \stackrel{\text{def}}{=} W_0(A)$ is independent of x.
(H5) (*behaviour of* W_0 *at the identity*)

$$DW_0(\boldsymbol{1}) = 0, \tag{5.3}$$

$$D^2 W_0(\boldsymbol{1})(H, H) \geq c_0 |H|^2 \quad \text{for all symmetric } H \in M^{3\times 3}, \tag{5.4}$$

where $c_0 > 0$.

If W_0 is isotropic then, as is well-known and follows from Lemma 4.1, (5.4) holds if and only if the Lamé moduli of W_0 at $\boldsymbol{1}$ satisfy

$$3\lambda + 2\mu > 0, \quad \mu > 0. \tag{5.5}$$

In Theorem 5.2 below we will also use the stronger smoothness hypothesis

(H2)′ (*analyticity*) $W \in C^\infty(D)$ and $W(\cdot, x, \cdot)$ is analytic at $\varepsilon = 0, A = \boldsymbol{1}$, uniformly in x, i.e. the Taylor expansion of $W(\cdot, x, \cdot)$ at $\varepsilon = 0, A = \boldsymbol{1}$ converges to $W(\cdot, x, \cdot)$ for all $x \in \bar{\Omega}$ and all (ε, A) in some open neighbourhood of $\varepsilon = 0, A = \boldsymbol{1}$ (*cf.* Valent [36, p. 38]).

We denote by $\mathscr{L}$ the finite-dimensional vector space of linearized rigid motions, i.e.

$$\mathscr{L} \stackrel{\text{def}}{=} \{\ell: \boldsymbol{R}^3 \to \boldsymbol{R}^3: \ell(x) = a + Kx \quad \text{for some } a \in \boldsymbol{R}^3, K = -K^T \in M^{3\times 3}\}.$$

Let $H \stackrel{\text{def}}{=} L^2(\Omega: \boldsymbol{R}^3) \times L^2(\partial\Omega; \boldsymbol{R}^3)$, which is a Hilbert space under the natural inner-product. We say that a pair $(f_1, f_2) \in H$ is *equilibrated* if

$$\int_\Omega f_1 \, dx + \int_{\partial\Omega} f_2 \, d\sigma = 0, \tag{5.6}$$

$$\int_\Omega x \wedge f_1 \, dx + \int_{\partial\Omega} x \wedge f_2 \, d\sigma = 0, \tag{5.7}$$

where σ denotes surface measure on $\partial\Omega$, and write

$$E \stackrel{\text{def}}{=} \{(f_1, f_2) \in H: (f_1, f_2) \text{ is equilibrated}\}. \tag{5.8}$$

The following result is easily proved (*cf.* Valent [36, p. 108]).

Lemma 5.1. The orthogonal complement $E^\perp$ of E in H is given by

$$E^\perp = \{(\ell|_\Omega, \ell|_{\partial\Omega}): \ell \in \mathscr{L}\}.$$

Let P denote the orthogonal projection of H onto E. Then (*cf.* Valent [36, p. 108]) we have

Lemma 5.2. $P: H \to E$ is continuous with respect to any topology on H finer than that of $L^2(\Omega; \boldsymbol{R}^3) \times L^2(\partial\Omega; \boldsymbol{R}^3)$.

Proof. This follows from the fact that $E^\perp$ is finite-dimensional. □

We will prove the existence of solutions to (5.1), (5.2) for sufficiently small ε by applying the implicit function theorem to solve the equation

$$F(\varepsilon, y) = 0 \tag{5.9}$$

with

$$F(\varepsilon, y) \stackrel{\text{def}}{=} P(-\operatorname{div} D_A W(\varepsilon, x, Dy), D_A W(\varepsilon, x, Dy)v). \tag{5.10}$$

In order to show that (5.9) is equivalent to (5.1), (5.2) the following lemma will be used.

Lemma 5.3. (*cf.* Valent [36, p. 109]) There exists a neighbourhood N of the identity mapping $id(x) = x$ in $L^1(\Omega; \boldsymbol{R}^3)$ such that if $\phi \in N$ and $\ell \in \mathscr{L}$ with

$$\int_\Omega \ell(x)\,dx + \int_{\partial\Omega} \ell(x)\,d\sigma = 0, \tag{5.11}$$

$$\int_\Omega \phi(x) \wedge \ell(x)\,dx + \int_{\partial\Omega} \phi(x) \wedge \ell(x)\,d\sigma = 0, \tag{5.12}$$

then $\ell = 0$.

Proof. If not there would exist a sequence $\phi^{(j)} \to id$ in $L^1(\Omega; \boldsymbol{R}^3)$ and $\ell^{(k)}(x) = a^{(k)} + K^{(k)}x$ with $|a^{(k)}| + |K^{(k)}| = 1$ and $K^{(k)} + K^{(k)T} = 0$ such that

$$\int_\Omega \ell^{(k)}(x)\,dx + \int_{\partial\Omega} \ell^{(k)}(x)\,d\sigma = 0, \tag{5.13}$$

$$\int_\Omega \phi^{(k)}(x) \wedge \ell^{(k)}(x)\,dx + \int_{\partial\Omega} \phi^{(k)}(x) \wedge \ell^{(k)}(x)\,d\sigma = 0. \tag{5.14}$$

We may without loss of generality suppose that $a^{(k)} \to a$, and $K^{(k)} \to K$, with $(a, K) \neq (0, 0)$. Let $\ell(x) = a + Kx$. Passing to the limit in (5.13), (5.14) we find that $(\ell|_\Omega, \ell|_{\partial\Omega})$ is equilibrated, so that by Lemma 5.1 $\ell = 0$, a contradiction. □

The following version of the implicit function theorem is useful in our context. For a proof see [26] and [40].

Theorem 5.1. Let X, Y, and Z be Banach spaces, U an open subset of $X \times Y$, and $f = f(x, y)$ a C^1 function from U into Z. Let $(x_0, y_0) \in U$ be such that $f(x_0, y_0) = 0$ and $D_y f(x_0, y_0)$ is a bijection of Y onto Z. Then there exists an open neighbourhood U_0 of (x_0, y_0) in $X \times Y$, an open neighbourhood V_0 of x_0 in X, and a C^1 function $g: V_0 \to Y$ such that $\{(x, y) \in U_0: f(x, y) = 0\} = \{(x, y): x \in V_0, y = g(x)\}$. Furthermore, U_0 can be chosen so that $D_y f(x, y)$ is a bijection of Y onto Z for all $(x, y) \in U_0$; in this case, if $x \in V_0$ then

$$Dg(x) = -(D_y f(x, g(x)))^{-1} D_x f(x, g(x)), \tag{5.15}$$

while if f is analytic[2] at $(x, g(x))$ then g is analytic at x.

To apply the implicit function theorem to F given by (5.10) we make the following choice of spaces. Let $p(m+1) > 3$, choose a point $\bar{x} \in \Omega$, and let

$$X = \boldsymbol{R},$$

$$Y = \{y \in W^{m+2,p}(\Omega; \boldsymbol{R}^3): y(\bar{x}) = 0, Dy(\bar{x}) = Dy(\bar{x})^T\},$$

$$Z = (W^{m,p}(\Omega; \boldsymbol{R}^3) \times W^{m+1-(1/p),p}(\partial\Omega; \boldsymbol{R}^3)) \cap E.$$

Since $(m+1)p > 3$, $W^{m+2,p}(\Omega; \boldsymbol{R}^3)$ is continuously embedded in $C^1(\bar{\Omega}; \boldsymbol{R}^3)$. Hence $Dy(\bar{x})$ in the definition of Y is well-defined. By standard embedding theorems Y and Z are closed linear subspaces of $W^{m+2,p}(\Omega; \boldsymbol{R}^3)$ and $W^{m,p}(\Omega; \boldsymbol{R}^3) \times W^{m+1-(1/p),p}(\partial\Omega; \boldsymbol{R}^3)$ respectively, and are thus Banach spaces with the corresponding norms. We define $Y^+ = \{y \in Y: \inf_{x \in \Omega} \det Dy(x) > 0\}$, which is an open subset of Y.

Lemma 5.4. Let (H1), (H2), (H4) hold. Then F defined by (5.10) is a C^1 mapping from $(-\varepsilon_0, \varepsilon_0) \times Y^+$ into Z, and its differential with respect to y at $\varepsilon = 0$, $y = id$ is the mapping

$$Lv = P(-\operatorname{div}(D_A^2 W_0(\boldsymbol{1})Dv), D^2 W_0(\boldsymbol{1})Dv \cdot \nu). \tag{5.16}$$

If further (H2)′ holds, the F is analytic at $\varepsilon = 0$, $y = id$.

[2] i.e. f has a power series expansion about $(x, g(x))$ with nonzero radius of convergence; see [26], [40], [36] for more details.

Proof. We first note that the mapping

$$y \mapsto (-\operatorname{div} D_A W(\varepsilon, x, Dy), D_A W(\varepsilon, x, Dy)v)$$

is C^1 from $(-\varepsilon_0, \varepsilon_0) \times Y^+$ into $W^{m,p}(\Omega; \boldsymbol{R}^3) \times W^{m+1-(1/p),p}(\partial\Omega; \boldsymbol{R}^3)$. This is proved in [36, p. 105] for the case when W is independent of ε, and the addition of the extra variable presents no difficulties. Since, by Lemma 5.2, P is a bounded linear operator from $W^{m,p}(\Omega; \boldsymbol{R}^3) \times W^{m+1-(1/p),p}(\partial\Omega; \boldsymbol{R}^3)$ into Z it follows that F is C^1. That $D_y F(0, id)v = Lv$ follows as in [36, p. 105], as does the analyticity of F at $\varepsilon = 0$, $y = id$ when (H2)′ holds. □

Proposition 5.1. Let (H4), (H5) hold. Then L given by (5.16) is a linear homeomorphism of Y onto Z.

Proof. This is a consequence of the regularity theory for linear elliptic systems, and is proved in [36, p. 38]. (Valent defines Y slightly differently, replacing the conditions $y(\bar{x}) = 0$, $Dy(\bar{x}) = Dy(\bar{x})^T$ by $\int_\Omega y\, dx = 0$, $\int_\Omega Dy(x)\, dx = \int_\Omega Dy(x)^T dx$ respectively, but this does not affect the proof.) □

We can now prove our main result.

Theorem 5.2. Let (H1)–(H5) hold. Then there exist numbers $\varepsilon_1 > 0$ and $\delta > 0$ such that

(a) if $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$ there exists a unique solution $y^\varepsilon \in Y$ of (5.1), (5.2) with $\|y^\varepsilon - id\|_Y < \delta$.
(b) the mapping $\varepsilon \mapsto y^\varepsilon$ is C^1 on $(-\varepsilon, \varepsilon_1)$, and for each $\varepsilon \in (-\varepsilon_1, \varepsilon_1)$ y^ε is a diffeomorphism of $\bar{\Omega}$ onto $y^\varepsilon(\bar{\Omega})$.

If further (H2)′ holds then $\varepsilon \mapsto y^\varepsilon$ is analytic at $\varepsilon = 0$.

Proof. We apply Theorem 5.1 with X, Y, Z as chosen above, $U = (-\varepsilon_0, \varepsilon_0) \times Y^+$, $f = F$ and $(x_0, y_0) = (0, id)$. By Lemma 5.4, F: $U \to Z$ and is C^1. By (H4), (H5) we have $F(0, id) = 0$, while by Proposition 5.1 $D_y F(0, id)$ is a bijection of Y onto Z. Hence by Theorem 5.1 there exist $\varepsilon_0 > 0$, and $\delta > 0$ such that for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ there exists a unique $y^\varepsilon \in Y^+$ with $\|y^\varepsilon - id\|_Y < \delta$ and $F(\varepsilon, y^\varepsilon) = 0$, and such that the mapping $\varepsilon \mapsto y^\varepsilon$ is C^1. Furthermore, if (H2)′ holds then by Lemma 5.4 and Theorem 5.1 the mapping $\varepsilon \mapsto y^\varepsilon$ is analytic at $\varepsilon = 0$.

We can suppose that ε_0 is chosen sufficiently small so that y^ε belongs to the neighbourhood N specified in Lemma 5.3 for all $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$. For any $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$ let $(f_1^\varepsilon, f_2^\varepsilon) = (-\operatorname{div} D_A W(\varepsilon, \cdot, Dy^\varepsilon(\cdot)),\ D_A W(\varepsilon, \cdot, Dy^\varepsilon(\cdot))v)$. By (H3) we have that for any $(\varepsilon, x, A) \in D$ the corresponding Cauchy stress tensor is symmetric, i.e. $D_A W(\varepsilon, x, A)A^T$ is symmetric. Hence (*cf.* Valent [36, p. 107])

$$\int_\Omega f_1^\varepsilon \, dx + \int_{\partial\Omega} f_2^\varepsilon \, d\sigma = 0,$$

$$\int_\Omega y^\varepsilon \wedge f_1^\varepsilon \, dx + \int_{\partial\Omega} y^\varepsilon \wedge f_2^\varepsilon \, d\sigma = 0.$$

Since $P(f_1^\varepsilon, f_2^\varepsilon) = F(\varepsilon, y^\varepsilon) = 0$ we have by Lemma 5.1 that $f_1^\varepsilon = \ell_\varepsilon|_\Omega$, $f_2^\varepsilon = \ell_\varepsilon|_{\partial\Omega}$ for some $\ell_\varepsilon \in \mathscr{L}$. Hence by Lemma 5.3 we have $(f_1^\varepsilon, f_2^\varepsilon) = (0, 0)$. Thus y^ε solves (5.1), (5.2).

It remains to prove that for ε sufficiently small $y^\varepsilon: \bar{\Omega} \to y^\varepsilon(\bar{\Omega})$ is a diffeomorphism. But this follows since $y^\varepsilon \in C^1(\bar{\Omega}; \boldsymbol{R}^3)$, using a remark in [36, p. 18] and the fact that $\det Dy^\varepsilon(x) > 0$ for all $x \in \bar{\Omega}$. □

Remarks. 1. Note that the hypotheses (H1)–(H5), (H2)′ of Theorem 5.2 are satisfied by the stored-energy function $W = W(\varepsilon, x_3, A)$ given by (3.6)–(3.8) provided $v(\varepsilon x_3) > 0$ for all $x \in \bar{\Omega}$.

2. The proof of Theorem 5.2 assumes that Ω is of class C^{m+2}, and thus does not apply when $\Omega = \omega \times (0, \delta)$. In the case $m = 0$ it would be possible to prove the existence of a solution $y^\varepsilon \in W^{2,p}(\Omega; \boldsymbol{R}^3)$ if it were known that an appropriate version of Proposition 5.1 holds in this case. This seems plausible for the case when $\partial\omega$ is smooth or even when ω is a rectangle, but we have been unable to locate such a result in the literature for linear elastostatics. Thus as it stands Theorem 5.2 does not apply to the case when $\Omega = (-1, 1)^2 \times (0, \delta)$ that is treated numerically in Section 6.

3. Note that due to the special form of our problem the fact that the applied loads have maximal symmetry (they are zero) does not cause difficulties as it does for the pure traction problem.

We now turn to the question of whether the solution y^ε to (5.1), (5.2) given by Theorem 5.2 is in fact a minimizer of

$$I_\varepsilon(y) = \int_\Omega W(\varepsilon, x, Dy(x)) \, dx. \tag{5.17}$$

Since the only convexity hypothesis made in Theorem 5.2 is (H5), which is local in nature, there is no reason to suppose that y^ε is a minimizer unless W satisfies additional convexity and growth hypotheses. We therefore suppose that W satisfies the two following conditions:

(H6) $W(\varepsilon, x, \cdot)$ is strictly polyconvex for $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$, $x \in \Omega$.
(H7) There exist constants $p > 3$, $C > 0$, c_0 such that

$$W(\varepsilon, x, A) \geq c_0 + C|A|^p, \quad \text{for all } (\varepsilon, x, A) \in D.$$

It was shown by Zhang [41] that for a large class of smooth stored-energy functions $W = W_0(A)$ satisfying (H5)–(H7) the solution y of the displacement boundary-value problem

$$\operatorname{div} D_A W_0(Dy(x)) = f(x), \quad x \in \Omega, \tag{5.18}$$

$$y|_{\partial\Omega} = id + g, \tag{5.19}$$

given by the implicit function theorem for small smooth f, g is in fact the absolute minimizer of

$$I(y) = \int_\Omega [W_0(Dy) - f \cdot y]\, dx \tag{5.20}$$

subject to (5.19).

By contrast, we show that for an isotropic $W = W(\varepsilon, x, A)$ satisfying (H1)–(H7) it is not true in general that y^ε given by Theorem 5.2 minimizes $I_\varepsilon(\cdot)$ for ε sufficiently small. We choose W to have the form

$$\begin{aligned} W(\varepsilon, x, A) &= \Phi(\varepsilon, x, v_1, v_2, v_3) \\ &= \sum_{i=1}^{3} v_i^2 + \sum_{i=1}^{3} \gamma(v_i) + (v_2 v_3)^{5/4} + (v_3 v_1)^{5/4} + (v_1 v_2)^{5/4} \\ &\quad + h(v_1 v_2 v_3) + \varepsilon |x|^2 H(v_1 v_2 v_3), \end{aligned} \tag{5.21}$$

where as usual the v_i denote the singular values of A. We suppose that $\gamma\colon [0, \infty) \to [0, \infty)$ is convex and smooth with $\gamma(v) = 0$ for $0 \le v \le 4$ and $\gamma(v) \sim v^4$ as $v \to \infty$, and that $H\colon [0, \infty) \to [0, \infty)$ is convex and smooth with $H(\delta) > 0$ for $0 \le \delta \le 2$, $H(\delta) = 0$ for $\delta \ge 3$. Following Ball [2], Ball and Marsden [7], Ball and James [4] we choose $h\colon [0, \infty) \to \boldsymbol{R}$ to be a smooth function satisfying $h'' > 0$, $\lim_{\delta \to 0} h(\delta) = \infty$, h bounded below, and such that $g(\delta) \overset{\text{def}}{=} 3\delta^{2/3} + 3\delta^{5/6} + h(\delta)$ is non-negative with $g(1) = g(8) = 0$, $g(t) > 0$ for $\delta \neq 1, 8$, $g''(1) > 0$. Such a choice of h is possible since $-3\delta^{2/3} - 3\delta^{5/6}$ is a strictly convex function of δ.

We now note that $W\colon D \to \boldsymbol{R}$ is smooth (*cf.* Ball [3]), that $W(\varepsilon, x, \cdot)$ is strictly polyconvex (*cf.* Ball [1]), and that W satisfies (H7) with $p = 4$. Also the only minimizers of $\Phi(0, x, \cdot, \cdot, \cdot)$ are given by $v_1 = v_2 = v_3 = 1$ and $v_1 = v_2 = v_3 = 2$, while if $\varepsilon \neq 0$, $x \neq 0$ then the only minimizer of $\Phi(\varepsilon, x, \cdot, \cdot, \cdot)$ is $v_1 = v_2 = v_3 = 2$.

Next we note that

$$D_A^2 W_0(\boldsymbol{1})(\boldsymbol{1}, \boldsymbol{1}) = \frac{d^2}{dt^2} W_0(t\boldsymbol{1})|_{t=1} = 9g''(\boldsymbol{1}) > 0,$$

while, since each of the terms in (5.21) is rank-one convex,

$$D_A^2 W_0(\boldsymbol{1})(e_1 \otimes e_2, e_1 \otimes e_2) \ge \frac{d^2}{d\tau^2} |\boldsymbol{1} + \tau e_1 \otimes e_2|^2 > 0,$$

where e_1, e_2 denote unit vectors in the x_1, x_2 directions respectively. Hence by Lemma 4.1, $3\lambda + 2\mu > 0$ and $\mu > 0$, which again by Lemma 4.1 gives (H5).

Now let y^ε be the solution of (5.1), (5.2) given by Theorem 5.2. For ε sufficiently small Dy^ε takes values in the neighbourhood of $\boldsymbol{1}$ and therefore $I_\varepsilon(y^\varepsilon) > 0$. But $I(2id) = 0$, and so y^ε is not a minimizer of $\boldsymbol{1}$ and therefore $I_\varepsilon(y^\varepsilon) > 0$.

The above example has the unusual feature that the natural state $v_1 = v_2 = v_3 = 1$ is not unique. It would be interesting to find hypotheses which guarantee that when there is a unique natural state (modulo rotations) then the solution y^ε given by Theorem 5.2 is an absolute minimizer. (A related open problem is to give reasonable hypotheses on the stored-energy function under which at least one of the solutions to the dead-load traction problem found for small loads via the implicit function theorem by Chillingworth, Marsden and Wan [11, 12] and Wan and Marsden [37] is an absolute minimizer of the energy.)

6. Numerical calculations

In Section 4.2 we found an exact solution to the minimization problem (4.1) in the special case where $W(\varepsilon, x, Dy(x))$ is such that $p(x)$ defined by (4.15) is an affine function of x_3 alone. This solution was obtained using the formal expansion of Section 4.1, which was justified via the implicit function theorem in Section 5. In this section we introduce a numerical scheme for solving the minimization problem based on the finite element method. This numerical approach is not restricted to the case of small ε, nor does it require that $p(x)$ be an affine function of x_3. However for the purposes of this paper we restrict our computations to examples of this kind, thus making it possible to make comparisons between the results obtained by the two different methods.

6.1. The numerical method

Let $X = W^{1,1}(\Omega; \boldsymbol{R}^3)$, where $\Omega = (-1, 1) \times (-1, 1) \times (0, \delta)$, and let $y \in X$ solve the minimization problem

$$\min_{y \in X} \int_\Omega W(x, Dy)\, dx, \tag{6.1}$$

where $W: \Omega \times M^{3\times 3}_+ \to \boldsymbol{R}$ is sufficiently smooth. In the actual computations we take $W(x, A) = W(\varepsilon, x_3, A)$ with $W(\varepsilon, x_3, A)$ given by (3.6)–(3.8). We seek to approximate y by $y^h \in S^h \subset X$. To choose an appropriate trial space S^h we divide $\bar{\Omega}$ into $n^2 m$ rectangular bricks, of side-lengths $2/n$ in the x_1 and

x_2 directions and δ/m in the x_3 direction, with a total of $(n+1)^2(m+1)$ vertices or node points. We then let S^h be the space of continuous piecewise trilinear vector functions on the finite element grid; this choice assigns to each node point three linear degrees of freedom, one for each component of the displacement y^h. (See [13] for more details of this space.)

Our numerical approximation now consists in solving the finite dimensional problem:

$$\min_{y^h \in S^h} \int_\Omega W(x, Dy^h)\, dx. \tag{6.2}$$

In practice however we do not numerically solve precisely this problem, since the integral is approximated by numerical quadrature.

The spirit of the method is that as $n, m \to \infty$, the space S^h becomes dense in X, so that we expect that the minimizer y^h in (6.2) converges to y (for example, strongly in X). This would not be hard to prove if it were known that y is sufficiently smooth, but unfortunately there is no suitable regularity result guaranteeing this available in the literature. For minimizers y that are not smooth there is the danger that the *Lavrentiev phenomenon* may occur, according to which the infimum of the total energy among Lipschitz mappings (such as those considered in the finite-element method) is *strictly* greater than the infimum among all mappings in X. In this case one might expect convergence to a minimizer in a smaller space than X. For information on the Lavrentiev phenomenon and its implications for finite-element methods see Ball and Mizel [8], Ball and Knowles [6]. Négron-Marrero [23] has proposed a numerical method for three-dimensional nonlinear elasticity which theoretically circumvents the Lavrentiev phenomenon. We did not employ this or related methods because (a) their numerical implementation in three dimensions is unexplored, and (b) they significantly increase the number of unknowns in an already computationally intensive calculation. Also, as explained at the end of Section 5 it is possible that the result of Zhang [41] could be modified to show that for sufficiently small ε the minimizer y is the same as that given by the implicit function theorem (see Theorem 5.2), and hence is smooth. Furthermore, there is no evidence that the Lavrentiev phenomenon actually occurs for integrands with polyconvexity and growth conditions of the type satisfied by (3.6)–(3.8). Thus for small ε we probably do not go far wrong by assuming convergence, and the numerical results below do indicate that convergence occurs. For larger ε, even in the absence of the Lavrentiev phenomenon there is the danger of getting caught in the local but not global minimum.

In our algorithm we used the conjugate gradient method in the form of [25] (described by [24]) in order to solve (6.2). This is a descent algorithm which requires the computation of the derivatives of $\int_\Omega W\, dx$ with respect to each finite element degree of freedom at every iteration. These derivatives can be computed using the chain rule on the function $H(\varepsilon, x, I_1, I_2, I_3)$ given in (3.13), (3.15) provided the user supplies functions for calculating $\partial H/\partial I_i$ for $i = 1, 2, 3$, as well as for calculating H itself. This leads to the selection of a downhill search direction along which the functional is then minimized (again this happens at each iteration). The computations were performed on a parallel architecture consisting of an array of 16 Inmos T800 transputers. The communications between these processors were handled via Meiko's CStools software. A full description of the implementation of the algorithm is given in [20].

In practice, computational considerations imply that n and m can never be chosen to be particularly large. This is because problem (6.2) is an unconstrained optimization problem with $3(n+1)^2(m+1)$ degrees of freedom, and it is only in recent years that the hardware has become available to solve such problems even for moderate values of n and m. If W were a quadratic form, then, in the absence of rounding errors, we would be guaranteed to find the unique minimizer for this discrete problem in precisely $3(n+1)^2(m+1)$ iterations. Hence if n and m were both doubled, the amount of time required to solve the problem would increase, very roughly, by a factor of about 64. Of course the function that we are minimizing is not quadratic, so that the finite termination criterion does not hold, and in practice the increase in computation time with n and m is not actually as severe as this. Nevertheless it is still apparent that for practical computations we are restricted to choosing only moderate values for n and m.

Despite the above reservations, our numerical method appears to be quite robust even for fairly large values of ε.

6.2. A comparison of results

We now present a comparison between the numerical solution of the non-linear problem given by (6.1) and (3.6)–(3.8) for small ε, and the linearized solution

$$\begin{aligned} y_1^\varepsilon &= x_1 - \varepsilon \frac{x_1 x_3}{\delta} + o(\varepsilon) \\ y_2^\varepsilon &= x_2 - \varepsilon \frac{x_2 x_3}{\delta} + o(\varepsilon) \\ y_3^\varepsilon &= x_3 + \varepsilon \frac{x_1^2 + x_2^2 - x_3^2}{2\delta} + o(\varepsilon) \end{aligned} \tag{6.3}$$

given in (4.35). (Note that by Lemma 4.2 $r = \kappa/\delta$.) Before doing this, however, we give some numerical results which suggest convergence of the numerical scheme to some mapping y as the mesh is refined. In all of the computations which follow, the integration was performed using eight point

Table 1
Convergence of the numerical method as the number of elements, $m-1$, in the vertical direction is increased.

	No. of vertical elements $(m-1)$	No. of degrees of freedom $(3n^2m)$	Largest value of the displacement	Differences in the displacements
$\varepsilon=0.001$	2	5625	0.00786	—
$\delta=0.1$	4	9375	0.00748	0.00038
	8	16875	0.00734	0.00014
$\varepsilon=0.004$	2	5625	0.03492	—
$\delta=0.1$	4	9375	0.03321	0.00171
	8	16875	0.03283	0.00038

Gaussian quadrature on each element. This degree of accuracy appears, from numerical experiment, to be the least one may use with confidence.

In Tables 1 and 2 we show the results of some computations made for an energy density of the form (3.6)–(3.8), with the constants chosen as in (3.12). For the problem of cooling basalt our choice of Ω corresponds in the case $\delta=0.1$ to a slab, say, of thickness 1 metre and lateral dimensions 20 metres square.

Table 1 shows what happens to the maximum displacement,

$$\max_{x\in\Omega}|y^h(x)-x|,$$

in the computed solution as the number of elements in the vertical x_3-direction is increased. In both cases ($\varepsilon=0.001$ and $\varepsilon=0.004$) there is very little difference in the numerical solution when 4 or 8 vertical elements are used.

Table 2 shows the results of similar computations when the number of elements in each horizontal direction is increased. Here there is a noticeable difference in behaviour between the cases of $\varepsilon=0.001$ and $\varepsilon=0.004$. In the first case, convergence seems to begin for quite moderate values of n,

Table 2
Convergence of the numerical method as the number of elements, $(n-1)^2$, in each horizontal plane is increased.

	No. of horizontal elements $(n-1)$	No. of degrees of freedom $(3n^2m)$	Largest value of the displacement	Differences in the displacements
$\varepsilon=0.001$	8	1215	0.00341	—
$\delta=0.1$	12	2535	0.00542	0.00201
	16	4035	0.00678	0.00136
	24	9375	0.00748	0.00070
$\varepsilon=0.004$	8	1215	0.01372	—
$\delta=0.1$	12	2535	0.02168	0.00796
	16	4035	0.02718	0.00550
	24	9375	0.03321	0.00603
	36	20635	0.03683	0.00362

whereas for the larger value of ε convergence appears to be delayed somewhat. Nevertheless, it does show signs of occurring for a sufficiently fine sequence of meshes.

Having demonstrated consistent behaviour of our numerical scheme, we can now compare some computed solutions with the linearized solution (6.3). We recall that the justification of (6.3) in Theorem 5.2 does not strictly speaking apply to our domain Ω (see Remark 2 after the theorem) unless the edges and corners of Ω are smoothed off. In making the comparison we use the fact that in all of the numerical solutions that we obtained for small values of ε the following two symmetries were present, although they were not imposed:

$$\begin{aligned} y_1(x_1, x_2, x_3) &= -y_1(-x_1, x_2, x_3) \\ y_2(x_1, x_2, x_3) &= y_2(-x_1, x_2, x_3) \\ y_3(x_1, x_2, x_3) &= y_3(-x_1, x_2, x_3) \end{aligned}$$

and

$$\begin{aligned} y_1(x_1, x_2, x_3) &= y_1(x_1, -x_2, x_3) \\ y_2(x_1, x_2, x_3) &= -y_2(x_1, -x_2, x_3) \\ y_3(x_1, x_2, x_3) &= y_3(x_1, -x_2, x_3). \end{aligned}$$

Since these symmetries can only be obtained from (4.22) and (4.23) in the case where $K = 0$ and $c = 0$ it is thus reasonable to compare these numerical results with (6.3) which was obtained from (4.22) with $K = 0$ and $c = 0$.

Table 3 shows the difference between numerical solutions and the linearized solution (6.3) as the parameter ε decreases. The computations are made for two different values of δ (the thickness of the plate) and for each of these cases we show how the numerical and linearized solutions differ, and the effect of dividing these differences by ε. The reason for choosing the parameter ε/δ in the table is simply that the linearized solution (6.3) then has the same formula for each of the two values of δ used. The norm that is referred to is the discrete maximum norm over the finite element node points.

Table 3
A comparison between two numerical solutions ($\tilde{y}_1$ when $\delta = 0.1$ and $\tilde{y}_2$ when $\delta = 0.2$) and the linearized solution as $\varepsilon \to 0$.

ε/δ	($\delta = 0.1$) $\lVert\tilde{y}_1 - (y^{(0)} + \varepsilon u)\rVert$	($\delta = 0.1$) $\varepsilon^{-1}\lVert\tilde{y}_1 - (y^{(0)} + \varepsilon u)\rVert$	($\delta = 0.2$) $\lVert\tilde{y}_2 - (y^{(0)} + \varepsilon u)\rVert$	($\delta = 0.2$) $\varepsilon^{-1}\lVert\tilde{y}_2 - (y^{(0)} + \varepsilon u)\rVert$
0.16	0.038733	2.421	0.016433	0.513
0.08	0.015220	1.903	0.004771	0.298
0.04	0.006916	1.729	0.001767	0.221
0.02	0.003332	1.666	0.000773	0.193
0.01	0.001597	1.597	0.000336	0.168

It can be seen that as $\varepsilon \to 0$ the difference between the numerical and the linearized solutions tends to zero faster than ε. This is clearly most satisfactory since it seems to confirm that the numerical solution and the linearized solution agree up to terms of order ε, as we would hope. It would be even more pleasing to observe the difference between these solutions behaving like ε^2 as $\varepsilon \to 0$; however this does not appear to be the case. The main reason for this is likely to be the lack of accuracy in obtaining a 3-dimensional finite element solution with 9375 degrees of freedom, the number used for these computations. In addition, there are bound to be integration errors present due to the use of 8 point Gaussian quadrature on each element, so it would be unreasonable to expect the finite element solution with fixed values of m and n to behave precisely like the true solution as $\varepsilon \to 0$.

At this point it may also be observed that the order ε terms in (6.3) are independent of the specific values of the constants in (3.12). Hence the pattern of results shown in Table 3 should also be observable for all similar choices of stored-energy function (see (3.8)), not just that given by (3.12) which corresponds to the Lamé moduli

$$\lambda = 1.8 \quad \text{and} \quad \mu = 2.2.$$

For all of the examples of possible stored-energy functions of this form that we tried this did indeed appear to be qualitatively true. However, the values of ε at which this convergence began to take place was not always the same. The worst case that we encountered was for the choice of constants

$$a_1 = a_2 = b = c = 1, \quad d = 12. \tag{6.4}$$

(Hence $\lambda = 8$ and $\mu = 12$.) Table 4 shows the difference between the computed solutions and (6.3) in this case. As with the results shown in Table 3 it can again be seen that the numerical solution does eventually appear to converge to the linearized solution at a faster rate than ε tends to zero, although smaller values of ε need to be considered. It is still true that there will be errors present in the finite element solution due to the coarseness of the discretization and the use of numerical quadrature, but

Table 4
A comparison between another two numerical solutions ($\hat{y}_1$ when $\delta = 0.1$ and $\hat{y}_2$ when $\delta = 0.2$) and the linearized solution as $\varepsilon \to 0$.

ε/δ	($\delta = 0.1$) $\lVert \hat{y}_1 - (y^{(0)} + \varepsilon u) \rVert$	($\delta = 0.1$) $1/\varepsilon \lVert \hat{y}_1 - (y^{(0)} + \varepsilon u) \rVert$	($\delta = 0.2$) $\lVert \hat{y}_2 - (y^{(0)} + \varepsilon u) \rVert$	($\delta = 0.2$) $1/\varepsilon \lVert \hat{y}_2 - (y^{(0)} + \varepsilon u) \rVert$
0.020	3.5550×10^{-3}	1.777	8.8461×10^{-4}	0.221
0.010	1.7688×10^{-3}	1.769	4.2783×10^{-4}	0.214
0.005	8.8281×10^{-4}	1.766	2.1118×10^{-4}	0.212
0.0025	4.4026×10^{-4}	1.761	1.0514×10^{-4}	0.210
0.00125	2.1782×10^{-4}	1.743	4.6761×10^{-5}	0.187

there is no reason to suspect that they will be any more significant in this case than in that considered in Table 3. A more likely explanation for the need to consider smaller values of ε in Table 4 is that the terms of $o(\varepsilon)$ in the solution to the nonlinear problem (6.1) will themselves depend upon the choice of constants a_1, a_2, b, c and d in (3.8). Hence the significance of these terms will vary with this choice of constants.

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Abstract

The equilibrium of an inhomogeneous elastic body is analyzed theoretically and numerically, with special emphasis on the case when the inhomogeneity arises from a given temperature distribution. The case when the inhomogeneity (or variation in temperature) is small is treated via linearization, the corresponding expansion of the solution in terms of an appropriate small parameter ε being justified by means of the implicit function theorem. For certain stored-energy functions suggested by the problem of cooling basalt rock, an exact solution to the linearized problem is found. A direct minimization of the energy using a finite-element algorithm is found to agree with the linearized solution as $\varepsilon \to 0$.

Résumé

L'équilibre d'un corps élastique inhomogène est étudié théoriquement et numériquement, en particulier dans le cas où l'homogenéité résulte d'une distribution de température donnée. Le cas où l'inhomogenéité (ou variation de la température) est petite est traité par linéarisation, le développement correspondant de la solution en termes d'un paramètre ε convenable étant justifié par le théorème des fonctions implicites. Pour diverses fonctions d'énergie interne suggérées par le problème du refroidissement du basalte, on donne une solution exacte du problème linéarisé. Une minimisation directe de l'énergie utilisant une méthode d'élements finis est en accord avec les solutions linéarisées quand $\varepsilon \to 0$.

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