THE FORMATION OF FILAMENTARY VOIDS IN SOLIDS

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and

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RICHARD D. JAMES[†] & SCOTT J. SPECTOR[‡]

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1. Introduction. In 1958 GENT & LINDLEY observed a striking rupture phenomena in short rubber cylinders that were bonded at their ends to parallel steel plates and pulled in tension. At a load that was in many cases less than a fourth of the ultimate breaking load, they observed the appearance of small, approximately spherical holes in the interior of the test-piece.¹

To analyze this phenomenon, they first calculated the maximum hydrostatic tension P_{max} (the maximum trace of the Cauchy stress) in a bonded cylinder pulled in tension, using an approximate stress analysis. The value P_{max} that they obtained from their calculation depended on the material parameters and the dimensions of the cylinder. They gave these parameters definite numerical values based upon the known dimensions of the test-piece and upon the independently measured energy functions of the rubbers used in the tests.

They then considered a different theoretical problem. They supposed that an infinite, incompressible elastic body contained a finite hole at the origin and was loaded at infinity by a pure hydrostatic tension P . They found an equilibrated radial deformation that solved this problem and which of course depended on P . At a critical value $P = P_{crit}^{radial}$ they found that the deformed hole radius became infinite. Even though the cylinders in their experiments were not in a state of pure hydrostatic tension, GENT & LINDLEY theorized that the hydrostatic part of the stress is most important and they, in effect, proposed the criterion that macroscopic holes will form in an inhomogeneous deformation at any place where the hydrostatic part of the stress reaches a critical value obtained in the *radial* problem with pure hydrostatic stress at infinity; in short, their criterion for void formation is

$$(1.1) \quad P_{max} = P_{crit}^{radial}.$$

Here “max” refers to a maximization over all points in the body. This criterion involves no free parameters once the energy function for the rubber and the test-piece dimensions are assigned. GENT & LINDLEY compared the criterion (1.1) with experiment and the agreement between theory and experiment was truly remarkable considering the range of dimensions and rubbers tested.²

A different point of view of this phenomena was made in 1982 in a fundamental paper by BALL. He considered a *finite* ball of compressible elastic material, with no hole present initially, subject to a pure radial displacement of amount $\hat{\lambda} - 1$ at its boundary. He found

¹GENT & LINDLEY measured the load at which these internal flaws appeared as a function of the dimensions of the cylinder and of the type of rubber. They found that this load varied linearly with the Young’s modulus of the rubber, for eight rubber formulations with Young’s modulus varying from 10 to 60 kg/cm², and nonlinearly with the length.

²Subsequent experiments by LINDSEY [1967] and GENT & TOMPKINS [1969a] have confirmed the above criterion, with some interesting qualifications in the work of GENT & THOMPSON [1969b], GENT & PARK [1984] and CHO & GENT [1988].

that for appropriate materials and for $\hat{\lambda}$ sufficiently large the minimizer of the total stored energy among radial deformations contains a spherical cavity. For incompressible elastic materials, he considered the problem of given radial traction P on the boundary of a finite ball. He found that the equilibrium equations admit a weak solution with a traction-free cavity when $P > P_{crit}^{radial}$, the same critical value as given by GENT & LINDLEY.³

A major conceptual notion in BALL'S work is that holes do not have to be present initially. Hence, the idea is applicable in principle to inhomogeneous deformations since it removes the necessity of having to judge the effect of introducing (in the reference configuration) a sufficiently small hole at an arbitrary point in the body, surely a computational nightmare. Instead one can minimize the total stored energy in a sufficiently large space (*e.g.*, an appropriate subset of the Sobolev space $W^{1,p}$, $1 \leq p < 3$ for a three dimensional body) so that deformations with voids can compete for a minimum. Then one views the formation of voids as a (nonsmooth) bifurcation phenomenon. Of course, it must be determined that in such large spaces the expression for the total energy reasonably measures this energy.⁴

To our knowledge all analyses of the phenomenon of void formation in elastic materials⁵ have been concerned with the radial problem in which all deformations $\mathbf{f} : \Omega \rightarrow \mathbf{R}^n$ that compete for a minimum are required to have the special form

$$(1.2) \quad \mathbf{f}(\mathbf{x}) = \frac{r(R)}{R} \mathbf{x}, \quad R = |\mathbf{x}|.$$

To realize the program of actually predicting the formation of voids at a stress concentration in an elastomer two questions naturally arise:

- 1) Are the radial solutions with holes minimizers of the energy when nonradial deformations are allowed to compete for a minimum?
- 2) What information from the analyses of homogeneous boundary value problems in which $\mathbf{f}(\mathbf{x}) = \mathbf{F}_0 \mathbf{x}$ on $\partial\Omega$ can be carried over to inhomogeneous deformations that happen to take on the deformation gradient $\mathbf{F}_0$ at some point $\mathbf{x}_0 \in \Omega$? More specifically, under what conditions does GENT & LINDLEY'S criterion (1.1) follow from a minimum energy criterion?

³The reason for this agreement, which is based upon the scaling laws for finite elasticity, is explained by BALL [1982]. BALL also analyzed the dynamic (radial) stability of the solutions with cavities and briefly considered the effect of surface energies.

⁴Questions of this nature are highly nontrivial and have been considered by BALL & MURAT [1984]. We discuss this point in Section 2 and the Appendix.

⁵Analyses by HORGAN & ABEYARATNE [1986], HORGAN & PENCE [1989], PODIO-GUIDUGLI, VERGARA CAFFARELLI, & VIRGA [1986], SIVALOGANATHAN [1986a,b], and STUART [1985] have provided a rather complete picture of the radial problem for isotropic materials, while ANTMAN & NEGRON-MARRERO [1987] have obtained results for radially or azimuthally reinforced materials. PERICAK-SPECTOR & SPECTOR [1988] have shown that the equations of nonlinear elastodynamics can be used to predict the spontaneous formation of spherically symmetric holes.

In this paper we give partial answers to both of these questions. Regarding question 2 we show that if a void of any kind, not necessarily radially symmetric, reduces the energy in the boundary value problem with linear boundary conditions $\mathbf{f}(\mathbf{x}) = \mathbf{F}_0\mathbf{x}$, $\mathbf{x} \in \partial\Omega$, then one can find a closely related deformation that reduces the energy of an inhomogeneous deformation that assumes the deformation gradient $\mathbf{F}_0$ at some interior point.

The answer to question 1 clearly depends on the stored energy function. We show that, for a large and realistic class of stored energy functions, the answer is no. Our method is based on the following ideas. Consider first the radial problem with boundary conditions $\mathbf{f}(\mathbf{x}) = \hat{\lambda}\mathbf{x}$ at $|\mathbf{x}| = 1$. The homogeneous deformation satisfying these boundary conditions, $\mathbf{f}(\mathbf{x}) = \hat{\lambda}\mathbf{x}$, $|\mathbf{x}| \leq 1$, induces a large volume change when $\hat{\lambda}$ is large. A material may find it energetically unfavorable to undergo such a large change in volume and will instead open a spherical hole at its center. That is, the typical radial deformation that creates a traction-free hole has principal stretches of the form

$$(1.3) \quad \alpha(R), \lambda(R), \lambda(R), \quad R = |\mathbf{x}|,$$

with $\alpha\lambda^2$ bounded and $\lambda(R) \rightarrow +\infty$ as $R \rightarrow 0^+$. Our analysis involves the same idea carried one step further. A deformation with principal stretches of the form (1.3) might also be judged energetically unfavorable because of the large change in *area* $\lambda(R)^2$ as $R \rightarrow 0^+$. We show that for a large class of stored energy functions the material would “prefer” to have principal stretches of the form

$$(1.4) \quad \alpha, \lambda_1, \lambda_2$$

with $\lambda_1\lambda_2 < \lambda^2(R)$. In order to realize a competitor with principal stretches (1.4), we construct, just outside of the hole, a short but very thin *filamentary void*, which points in the radial direction. Roughly, the filamentary void turns stretches of the form (1.3) into those of the form (1.4) and reduces the energy.

The analysis of BALL [1982], as well as the analyses of SIVALOGANATHAN [1986a] and STUART [1985], contains certain growth assumptions that may be interpreted as saying that the materials are “soft” with respect to changes of single stretches (shear), but “stiff” with respect to changes in the product of the principal stretches (dilatation). In our assumptions the growth of the energy with respect to pairwise products of the principal stretches is important. These assumptions rule out the class of compressible materials originally studied by BALL, but do not rule out the materials studied by SIVALOGANATHAN & STUART. To emphasize the distinction between spherical and filamentary voids, we note that our assumptions that promote the formation of filamentary voids allow any behavior whatsoever of the stored energy for pure dilatation.

As noted above, BALL’s analysis (in the incompressible case) and GENT & LINDLEY’s analysis deliver the same critical hydrostatic tension for spherical cavitation. Further support for this connection is provided by an analysis of SIVALOGANATHAN [1986a], who

considers a finite ball subject to a radial displacement of amount $\hat{\lambda} - 1$ at its boundary with and without a pre-existing cavity of radius R_0 at the origin. He shows that the graph of hole radius *vs.* $\hat{\lambda}$ for radial minimizers tends to the analogous graph with no initial cavity as $R_0 \rightarrow 0$. This may be interpreted as saying that critical conditions for void formation and sudden growth of a pre-existing void are identical. This conclusion must be tempered by results of GENT & PARK [1984] and CHO & GENT [1988]. They find that the critical conditions for cavitation near a *very small* inclusion are not given by (1.1), and they interpret this to mean that the probability of finding a relatively large (large enough to omit surface energy) precursor void within the small region of stress concentration is small.

The filamentary void provides another mechanism for energy reduction, different from cavitation. A striking example of a rupture process that produces something resembling a filamentary void is the phenomenon of crazing in polymers. In fact, after writing the present paper, we found a striking photograph of DONALD, CHEN & KRAMER [1981 Fig.1] that shows tiny filamentary voids in thin sheets of polystyrene pulled in tension. This prompted us to write Section 7 which relates our results to crazing. A weakness of our results, which prevents a quantitative comparison, is that we do not give critical conditions for the formation of a filamentary void, but we only say that if certain combinations of principal stretches are sufficiently large, then a filamentary void will reduce the energy. Furthermore, all polymers are to some extent viscoelastic, as is true of the elastomers studied by GENT & LINDLEY, and our thinking relies on the notion that most viscoelasticity theories have a Lyapunov functional which has the form of a nonlinear elastic energy. In a subsequent paper we shall examine in more detail the connection between the formation of a filamentary void and crazing.

2. Notation. We let

$\text{Lin} :=$ space of all linear transformations (tensors) from $\mathbb{R}^n$ into $\mathbb{R}^n$

with norm

$$|\mathbf{H}| = [\text{trace}(\mathbf{H}\mathbf{H}^T)]^{1/2},$$

where $\mathbf{H}^T$ denotes the transpose of $\mathbf{H}$. We write

$$\begin{aligned}\text{Lin}^> &= \{\mathbf{H} \in \text{Lin} : \det \mathbf{H} > 0\}, \\ \text{Lin}^{\leq} &= \{\mathbf{H} \in \text{Lin} : \det \mathbf{H} \leq 0\},\end{aligned}$$

where $\det$ denotes the determinant. Given two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^n$ we write $\mathbf{a} \otimes \mathbf{b}$ for the tensor product of $\mathbf{a}$ and $\mathbf{b}$; in components

$$(\mathbf{a} \otimes \mathbf{b})_{ij} = a_i b_j.$$

We write ∇ for the gradient operator in $\mathbf{R}^n$: for a vector field $\mathbf{u}$, $\nabla \mathbf{u}$ is the tensor field with components $(\nabla \mathbf{u})_{ij} = \partial u_i / \partial x_j$. Given any function $\Phi(\mathbf{a}, \mathbf{b}, \dots, \mathbf{c})$ with vector or tensor arguments, we write, *e.g.*, $\partial \Phi / \partial \mathbf{a}$ for the partial Frechet derivative with respect to $\mathbf{a}$ holding the remaining arguments fixed.

We call a bounded open region $\Omega \subset \mathbf{R}^n$ **regular** provided that $\partial \Omega$ has measure zero. For $1 \leq p \leq \infty$ we let $\|\cdot\|_{\Omega, m, p}$ denote the $W^{m, p}$ -norm on Ω and $\|\cdot\|_{\Omega, p}$ denote the L^p -norm on Ω . Thus, in particular,

$$\|\mathbf{f}\|_{\Omega, p} := \|\mathbf{f}\|_{\Omega, 0, p} = \begin{cases} [\int_{\Omega} |\mathbf{f}(\mathbf{x})|^p d\mathbf{x}]^{1/p}, & 1 \leq p < \infty \\ \text{ess sup}_{\mathbf{x} \in \Omega} |\mathbf{f}(\mathbf{x})|, & p = \infty \end{cases}$$

$$\|\mathbf{f}\|_{\Omega, 1, p} = \{ \int_{\Omega} [|\mathbf{f}(\mathbf{x})|^p + |\nabla \mathbf{f}(\mathbf{x})|^p] d\mathbf{x} \}^{1/p}, \quad 1 \leq p < \infty.$$

For $1 \leq p < \infty$ we define

$$W^{1, p}(\Omega) = \text{completion of } \{\mathbf{f} \in C^\infty(\Omega, \mathbf{R}^n) : \|\mathbf{f}\|_{\Omega, 1, p} < +\infty\}$$

with respect to the $W^{m, p}$ -norm and let

$$W_0^{1, p}(\Omega) = \text{closure of } C_0^\infty(\Omega, \mathbf{R}^n) \text{ in } W^{1, p}(\Omega).$$

3. Deformation, Stress and Stored Energy. We consider a *homogeneous* body that, for convenience, we identify with the region $\bar{\Omega}$ that it occupies in a fixed homogeneous reference configuration. Let $1 \leq p < n$. We call a function $\mathbf{f} : \bar{\Omega} \rightarrow \mathbf{R}^n$ a **deformation** of the body provided that

- (i) $\mathbf{f}$ is one-to-one on $\bar{\Omega}$;
- (ii)⁷ $\mathbf{f} \in W^{1, p}(\Omega) \cap L^\infty(\Omega)$.

We denote by $\text{Def}(\Omega)$ the set of all such deformations.

Remark 3.1. The set of deformations has been chosen so that the energy will be well-defined, voids can form in the material, and the interpenetration of matter is prohibited. For $p < n$ the spaces $W^{1, p}$, even with the added requirement that the deformation gradient have positive determinant almost everywhere, is too large a space for nonlinear elasticity. One major difficulty is that such functions are not necessarily invertible. Furthermore, such functions can arise as the absolute minimizer of the energy in certain compression problems since the body is able to relax severe compressive strains by overlapping material (see the

⁷More precisely, the *function* $\mathbf{f}$ belongs to an equivalence class that is contained in the indicated spaces.

Appendix). The spaces $W^{1,p}$ for $p > n$ do not suffer this pathology, but unfortunately do not permit the formation of voids.

Remark 3.2. Additional restrictions are needed in order to insure that a function $\mathbf{f} \in \text{Def}(\Omega)$ corresponds to a reasonable physical notion of a deformation. One such restriction is that for every $\mathcal{D} \subset \Omega$, $\mathbf{f}(\mathcal{D})$ has measure zero whenever $\mathcal{D}$ has measure zero. Without such a restriction one can construct (cf. BESICOVITCH [1950]) a function that is equal to the identity everywhere except on a flat surface, contained in Ω , which is mapped onto the unit cube. The fact that such a deformation is equal to the identity almost everywhere is one of the reasons we require our deformations to be functions rather than equivalence classes.

We assume that the body is hyperelastic with continuous **stored energy** function $W : \text{Lin}^> \longrightarrow \mathbb{R}^{\geq} \cup \{+\infty\}$. W gives the energy stored per unit volume in Ω ,

$$W(\nabla \mathbf{f}(\mathbf{x}))$$

at any point $\mathbf{x} \in \Omega$ when the body is deformed by a smooth deformation $\mathbf{f}$.

We further assume that W restricted to $\text{Lin}^>$ is C^2 and that $W = +\infty$ on $\text{Lin}^{\leq}$. The derivative

$$\mathbf{S}(\mathbf{F}) := \frac{d}{d\mathbf{F}} W(\mathbf{F})$$

is the **Piola-Kirchhoff stress** while the **Cauchy stress** is defined by

$$(3.1) \quad \mathbf{T}(\mathbf{F}) := \mathbf{S}(\mathbf{F})\mathbf{F}^T / \det \mathbf{F}.$$

We assume that the response of the material is invariant under a change in observer and hence that

$$(3.2) \quad W(\mathbf{QF}) = W(\mathbf{F})$$

for every $\mathbf{F} \in \text{Lin}^>$ and $\mathbf{Q} \in \text{Lin}^>$ with $\mathbf{Q}\mathbf{Q}^T = \mathbf{I}$. One consequence of this assumption is that $\mathbf{T}$ is symmetric. The eigenvalues of $\mathbf{T}$ are called the *principal stresses*.

In Sections 5-8 we will consider *isotropic materials* that is, materials for which there is a symmetric function $\Phi : (\mathbb{R}^>)^n \longrightarrow \mathbb{R}^{\geq}$ with the property that for every $\mathbf{F} \in \text{Lin}^>$

$$(3.3) \quad W(\mathbf{F}) = \Phi(\lambda_1(\mathbf{F}), \lambda_2(\mathbf{F}), \dots, \lambda_n(\mathbf{F})),$$

where $\lambda_1(\mathbf{F})$ are the *principal stretches*, i.e. the eigenvalues of $(\mathbf{F}\mathbf{F}^T)^{1/2}$.

4. Results on the Local Reduction of Energy. We assume that there is a potential $\beta \in C^1(\overline{\Omega} \times \mathbb{R}^n, \mathbb{R})$ such that

$$\mathbf{b}_f(\mathbf{x}) := \frac{\partial}{\partial \mathbf{f}} \beta(\mathbf{x}, \mathbf{f}(\mathbf{x}))$$

gives the **body force** exerted by the environment on the material at the point $\mathbf{x}$ when the body is deformed by a smooth deformation $\mathbf{f}$. We let

$$(4.1) \quad E(\mathbf{f}, \Omega) = \int_{\Omega} [W(\nabla \mathbf{f}(\mathbf{x})) - \beta(\mathbf{x}, \mathbf{f}(\mathbf{x}))] d\mathbf{x}$$

denote the **total energy** when the body is deformed by $\mathbf{f}$. Later, we shall introduce restrictions on W and β so that the total energy is defined for all $\mathbf{f}$ in $\text{Def}(\Omega)$. We use the term **total stored energy** for the right hand side of (4.1) with β omitted.

Let $\mathbf{d} \in C^1(\overline{\Omega})$ be one-to-one. We are interested in deformations that are local minimizers of the total energy and that have the *same boundary-values and orientation* as $\mathbf{d}$. We therefore let

$$\text{Kin}_d(\Omega) = \{\mathbf{f} \in \text{Def}(\Omega) : (\mathbf{f} - \mathbf{d}) \in W_0^{1,p}(\Omega), \mathbf{f}(\Omega) \subset \mathbf{d}(\Omega)\};$$

the set of *kinematically admissible* deformations.

Remark 4.1. The constraint $\mathbf{f}(\Omega) \subset \mathbf{d}(\Omega)$ is used in the proof of Theorem 4.3, where a certain deformation is altered on a sphere in Ω . It seems to us a reasonable restriction on deformations that are allowed to compete for a minimum. This constraint may be a consequence (in the sense that it is satisfied almost everywhere) of other conditions one might impose in order to insure that a function $\mathbf{f} \in \text{Def}(\Omega)$ corresponds to a reasonable physical notion of a deformation that has finite energy and satisfies the boundary condition $\mathbf{f} = \mathbf{d}$ on $\partial\Omega$.

Let $\mathbf{f} \in \text{Kin}_d(\Omega)$ satisfy $E(\mathbf{f}, \Omega) < +\infty$. We say that $\mathbf{f}$ is a **strong local minimizer** (in $W^{1,p}(\Omega) \cap L^\infty(\Omega)$) of the energy E provided that there is an $\varepsilon > 0$ such that

$$E(\mathbf{f}, \Omega) \leq E(\mathbf{g}, \Omega)$$

for every $\mathbf{g} \in \text{Kin}_d(\Omega)$ that satisfies

$$(4.2) \quad \|\mathbf{f} - \mathbf{g}\|_{\Omega, \infty} + \|\mathbf{f} - \mathbf{g}\|_{\Omega, 1, p} < \varepsilon.$$

THEOREM 4.2. *Let $\mathbf{f} \in \text{Kin}_d(\Omega)$ be a strong local minimizer of $E(\cdot, \Omega)$. Suppose that $\mathbf{f}$ is C^1 in a neighborhood of $\mathbf{x}_0 \in \Omega$ and let*

$$\mathbf{F}_0 := \nabla \mathbf{f}(\mathbf{x}_0); \quad \mathbf{f}_0(\mathbf{x}) := \mathbf{F}_0(\mathbf{x} - \mathbf{x}_0) + \mathbf{f}(\mathbf{x}_0), \quad \mathbf{x} \in \mathbb{R}^n.$$

Assume that $W(\mathbf{F}_0) < \infty$. Then for every regular region $\mathcal{D} \subset \mathbb{R}^n$

$$(4.3) \quad \int_{\mathcal{D}} W(\mathbf{F}_0) d\mathbf{x} \leq \int_{\mathcal{D}} W(\mathbf{F}_0 + \nabla \mathbf{u}(\mathbf{x})) d\mathbf{x}$$

whenever $\mathbf{f}_0 + \mathbf{u} \in \text{Kin}_{\mathbf{f}_0}(\mathcal{D})$.

In other words a necessary condition for $\mathbf{f}$ to be a strong local minimizer is that, at each point $\mathbf{x}_0$ of smoothness of $\mathbf{f}$, the affine deformation $\mathbf{f}_0(\mathbf{x}) = \nabla \mathbf{f}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0) + \mathbf{f}(\mathbf{x}_0)$ is a global minimizer of the total energy of any body that is composed of the same material but is not subjected to body forces.

Remark 4.3. Theorem 4.2 remains valid if the constraint $\mathbf{f}(\Omega) \subset \mathbf{d}(\Omega)$ and the hypothesis of invertibility are dropped. In the terminology of BALL & MURAT [1984] our proof of Theorem 4.2 shows that if $\mathbf{f}$ is a strong local minimizer then the stored energy function W must be $W^{1,p}$ -quasiconvex at $\mathbf{F}_0 = \nabla \mathbf{f}(\mathbf{x}_0)$ for every point $\mathbf{x}_0$ at which $\mathbf{f}$ is smooth. If the variations $\mathbf{u}$ are required to be C^∞ then eq. (4.3) is MORREY'S [1952] quasiconvexity condition and Theorem 4.2 is therefore related to a result of MEYERS [1952, pp.128-131] who shows that quasiconvexity is a necessary condition for a local minimum.

Remark 4.4. We do not know if Theorem 4.2 is true for general integrands $W(\mathbf{x}, \mathbf{f}, \nabla \mathbf{f})$. The technique used in our proof requires that W be independent of its first two arguments, although we have included body forces.

Remark 4.5. Theorem 4.2 remains valid if the definition of a strong local minimizer omits the term $\|\mathbf{f} - \mathbf{g}\|_{\Omega, \infty}$ provided a growth condition is put on the body force potential β .

Remark 4.6. Theorem 4.2 shows that the introduction of a new hole as a method of energy reduction is a local phenomena; that is, it is possible to introduce such a hole at any point in the body without changing the deformation outside of a small neighborhood of that point.⁸ We think that the introduction of new holes in *incompressible* bodies is global in nature since we expect that the total volume of the body should not change in an isochoric deformation (even if the deformation is only contained in $W^{1,1}$) and hence the introduction of a new hole can only be achieved by allowing the boundary of the body to move. This fact makes a rigorous justification of a failure criterion such as GENT & LINDLEY'S [1958] difficult for incompressible materials.

Remark 4.7. In section 5 we introduce constitutive hypotheses on the stored energy W that promote the formation of voids by forcing (4.3) to be violated at certain $\mathbf{F}_0$. Thus these constitutive hypotheses, as well the hypotheses of all the other authors who consider deformations that create holes, imply that W is not $W^{1,p}$ -quasiconvex. A result of BALL

⁸Of course when equilibrium solutions are considered the introduction of a new hole will cause changes in the solution at all points in the body.

& MURAT [1984, Corollary 3.2] then implies that, for such energy functions, $E(\cdot, \Omega)$ is not sequentially weakly lower semicontinuous. Therefore it is not clear that a minimizer of $E(\cdot, \Omega)$ need exist (*cf.* BALL & MURAT [1984, Theorem 5.1]). Even if a minimizer does indeed exist it may be difficult to construct since it may be approached weakly by only very special minimizing sequences, a situation that arises in the study of phase transitions (*cf.* BALL & JAMES [1987]).

Proof of Theorem 4.2. Let $\mathbf{f} \in \text{Kin}_d(\Omega)$ be C^1 in a neighborhood of $\mathbf{x}_0$ with $W(\mathbf{F}_0)$ finite. Then our basic assumptions on W imply that there is an $\varepsilon > 0$ such $\mathbf{f}$ is C^1 with $\det \nabla \mathbf{f} > 0$ and $W(\nabla \mathbf{f}(\cdot))$ finite on $\mathcal{B}_{3\varepsilon}$. (Here, and in what follows, $\mathcal{B}_\rho = \mathcal{B}_\rho(\mathbf{x}_0)$ the open ball of radius $\rho > 0$ centered at $\mathbf{x}_0$.)

We will prove this theorem by showing that if (4.3) is not satisfied then $\mathbf{f}$ is not a strong local minimizer of the total energy. To do this we construct a family of deformations $\mathbf{f}_\alpha \in \text{Kin}_d(\Omega)$, each of which has less energy than $\mathbf{f}$, that converge to $\mathbf{f}$ in $W^{1,p}(\Omega) \cap L^\infty(\Omega)$ as $\alpha \rightarrow 0^+$.

Let $\theta \in C^\infty(\mathbb{R}, \mathbb{R})$ be a monotone decreasing bridging function satisfying

$$(4.4) \quad \theta(t) = \begin{cases} 1, & t \leq 1 \\ 0, & t \geq 4 \end{cases}.$$

Let $\mathcal{B} := \mathcal{B}_{2\varepsilon}$ and define $\mathbf{h}_\alpha \in C^1(\overline{\mathcal{B}}, \mathbb{R}^n)$, for $0 < \alpha < \varepsilon$, by

$$(4.5) \quad \mathbf{h}_\alpha(\mathbf{x}) := \theta(\alpha^{-2}|\mathbf{x} - \mathbf{x}_0|^2)\mathbf{f}_0(\mathbf{x}) + [1 - \theta(\alpha^{-2}|\mathbf{x} - \mathbf{x}_0|^2)]\mathbf{f}(\mathbf{x})$$

and note that

$$(4.6) \quad \nabla \mathbf{h}_\alpha = \nabla \mathbf{f} + \theta[\mathbf{F}_0 - \nabla \mathbf{f}] + 2\alpha^{-2}\dot{\theta}[\mathbf{f} - \mathbf{f}_0] \otimes [\mathbf{x} - \mathbf{x}_0].$$

We claim that for α sufficiently small $\mathbf{h}_\alpha \in \text{Kin}_f(\mathcal{B})$. To show this we first combine (4.4) and (4.6) to conclude that

$$(4.7) \quad \max_{\overline{\mathcal{B}}} |\nabla \mathbf{h}_\alpha - \nabla \mathbf{f}| \leq \max_{\overline{\mathcal{B}_{2\alpha}}} |\mathbf{F}_0 - \nabla \mathbf{f}| + 4\alpha^{-1}(\max |\dot{\theta}|) \max_{\overline{\mathcal{B}_{2\alpha}}} |\mathbf{f} - \mathbf{f}_0|.$$

Since $\mathbf{f} \in C^1(\overline{\mathcal{B}}, \mathbb{R}^n)$, $\mathbf{f}(\mathbf{x}_0) = \mathbf{f}_0(\mathbf{x}_0)$, and $\nabla \mathbf{f}_0(\mathbf{x}) = \nabla \mathbf{f}(\mathbf{x}_0)$, we find that

$$\alpha^{-1} \max_{\overline{\mathcal{B}_{2\alpha}}} |\mathbf{f} - \mathbf{f}_0| \rightarrow 0 \quad \text{as} \quad \alpha \rightarrow 0^+$$

and thus, with the aid of (4.7), we find that $\nabla \mathbf{h}_\alpha \rightarrow \nabla \mathbf{f}$ uniformly on $\overline{\mathcal{B}}$. We note that $\mathbf{f}$ is one-to-one with $\det \nabla \mathbf{f} > 0$ on $\overline{\mathcal{B}}$ and $\mathbf{h}_\alpha = \mathbf{f}$ on $\partial \mathcal{B}$. Thus a standard theorem (*cf.*, *e.g.*, CIARLET [1988, Theorem 5.5-1]) yields an $\alpha_0 \in (0, \varepsilon)$ such that $\mathbf{h}_\alpha$ is one-to-one on $\overline{\mathcal{B}}$ with $\mathbf{h}_\alpha(\mathcal{B}) = \mathbf{f}(\mathcal{B})$ for $0 < \alpha < \alpha_0$. Thus, $\mathbf{h}_\alpha \in \text{Kin}_\alpha(\mathcal{B})$.

We now suppose that $\mathcal{D} \subset \mathbb{R}^n$ is a regular region and $\mathbf{g} \in \text{Kin}_{\mathbf{f}_0}(\mathcal{D})$ is a deformation satisfying

$$(4.8) \quad \int_{\mathcal{D}} [W(\nabla \mathbf{g}(\mathbf{x})) - W(\mathbf{F}_0)] d\mathbf{x} =: -\gamma < 0.$$

Choose $\delta > 0$ so that (see figure 1)

$$\mathbf{x}_0 + \mathcal{D}_\delta \subset \mathcal{B}, \quad \mathcal{D}_\delta := \delta \mathcal{D}.$$

Figure 1. Construction used in the proof of Theorem 4.2

For $0 < \alpha < \alpha_0$ and $\mathbf{x} \in \mathbf{x}_0 + \alpha \mathcal{D}_\delta$, let

$$(4.9) \quad \mathbf{e}_\alpha(\mathbf{x}) := \alpha \delta [\mathbf{g}((\mathbf{x} - \mathbf{x}_0)/\alpha \delta) - \mathbf{f}_0((\mathbf{x} - \mathbf{x}_0)/\alpha \delta)] + \mathbf{f}_0(\mathbf{x})$$

and define $\mathbf{f}_\alpha : \overline{\Omega} \longrightarrow \mathbb{R}^n$ by

$$(4.10) \quad \mathbf{f}_\alpha(\mathbf{x}) := \begin{cases} \mathbf{e}_\alpha(\mathbf{x}), & \mathbf{x} \in \mathbf{x}_0 + \alpha\mathcal{D}_\delta \\ \mathbf{h}_\alpha(\mathbf{x}), & \mathbf{x} \in \overline{\mathcal{B}} - (\mathbf{x}_0 + \alpha\mathcal{D}_\delta) \\ \mathbf{f}(\mathbf{x}), & \mathbf{x} \in \overline{\Omega} - \overline{\mathcal{B}} \end{cases}.$$

Since $\mathbf{f} \in \text{Kin}_{\mathbf{d}}(\Omega)$, $\mathbf{h}_\alpha \in \text{Kin}_{\mathbf{f}}(\mathcal{B})$ for $0 < \alpha < \alpha_0$, and $\mathbf{g} \in \text{Kin}_{\mathbf{f}_0}(\mathcal{D})$, we conclude that $\mathbf{f}_\alpha \in \text{Kin}_{\mathbf{d}}(\Omega)$ for $0 < \alpha < \alpha_0$.

We next show that $\mathbf{f}_\alpha \longrightarrow \mathbf{f}$ in $W^{1,p}(\Omega) \cap L^\infty(\Omega)$ as $\alpha \longrightarrow 0^+$. First, by (4.9) we note that for $\mathbf{x} \in \mathbf{x}_0 + \alpha\mathcal{D}_\delta$,

$$|\mathbf{e}_\alpha(\mathbf{x}) - \mathbf{f}(\mathbf{x})| \leq \alpha\delta[|\mathbf{g}((\mathbf{x} - \mathbf{x}_0)/\alpha\delta)| + |\mathbf{f}_0((\mathbf{x} - \mathbf{x}_0)/\alpha\delta)|] + |\mathbf{f}_0(\mathbf{x}) - \mathbf{f}(\mathbf{x})|,$$

and so we find, with the aid of (4.4), (4.5), and (4.10), that

$$\|\mathbf{f}_\alpha - \mathbf{f}\|_{\Omega,\infty} \leq \alpha\delta \{ \|\mathbf{g}\|_{\mathcal{D},\infty} + \|\mathbf{f}_0\|_{\mathcal{D},\infty} \} + \|\mathbf{f}_0 - \mathbf{f}\|_{\mathcal{B}_{2\alpha},\infty}.$$

Since $\mathbf{f}$ is continuous on $\mathcal{B}$ we conclude that $\mathbf{f}_\alpha \longrightarrow \mathbf{f}$ in $L^\infty(\Omega)$ as $\alpha \longrightarrow 0^+$. By (4.9), the triangle inequality, Hölders inequality and the change of variables $\mathbf{y} = (\mathbf{x} - \mathbf{x}_0)/\alpha$ we find that

$$(4.11) \quad \|\nabla \mathbf{e}_\alpha - \nabla \mathbf{f}\|_{\mathbf{x}_0 + \alpha\mathcal{D}_\delta, p} \leq \alpha^{n/p} \left\{ \left(\int_{\mathcal{D}_\delta} |\nabla \mathbf{g} - \mathbf{F}_0|^p d\mathbf{y} \right)^{1/p} + \text{vol}(\mathcal{D}_\delta)^{1/p} \|\mathbf{F}_0 - \nabla \mathbf{f}\|_{\mathcal{B},\infty} \right\}.$$

Therefore, since $\mathbf{h}_\alpha \longrightarrow \mathbf{f}$ and $\nabla \mathbf{h}_\alpha \longrightarrow \nabla \mathbf{f}$ uniformly on $\overline{\mathcal{B}}$ (4.11) shows that $\mathbf{f}_\alpha \longrightarrow \mathbf{f}$ in $W^{1,p}(\Omega)$.

Finally, we compute the total energy of the deformations $\mathbf{f}_\alpha$, $0 < \alpha < \alpha_0$. The definition (4.10) of $\mathbf{f}_\alpha$ gives

$$(4.12) \quad \int_{\Omega} [W(\nabla \mathbf{f}_\alpha) - W(\nabla \mathbf{f})] d\mathbf{x} = \left\{ \begin{aligned} & \int_{\mathbf{x}_0 + \alpha\mathcal{D}_\delta} [W(\nabla \mathbf{e}_\alpha) - W(\mathbf{F}_0)] d\mathbf{x} \\ & + \int_{\mathcal{B}_\alpha} [W(\mathbf{F}_0) - W(\nabla \mathbf{f})] d\mathbf{x} \\ & + \int_{\mathcal{B}_{2\alpha} - \mathcal{B}_\alpha} [W(\nabla \mathbf{h}_\alpha) - W(\nabla \mathbf{f})] d\mathbf{x} \end{aligned} \right\}.$$

If we define

$$\sigma_\alpha := \|W(\mathbf{F}_0) - W(\nabla \mathbf{f})\|_{\mathcal{B}_\alpha,\infty} + \|W(\nabla \mathbf{h}_\alpha) - W(\nabla \mathbf{f})\|_{\mathcal{B},\infty},$$

and make the change of variables $\mathbf{y} = (\mathbf{x} - \mathbf{x}_0)/\alpha\delta$ in the first integral on the right hand side of (4.12) we find, with the aid of (4.8) and (4.9), that

$$(4.13) \quad \int_{\Omega} [W(\nabla \mathbf{f}_{\alpha}) - W(\nabla \mathbf{f})] d\mathbf{x} \leq \alpha^n [-\gamma\delta^n + 2^n \text{vol}(\mathcal{B}_1)\sigma_{\alpha}].$$

Similarly, (4.10) implies that

$$(4.14) \quad \int_{\Omega} [\beta(\mathbf{x}, \mathbf{f}_{\alpha}(\mathbf{x})) - \beta(\mathbf{x}, \mathbf{f}(\mathbf{x}))] d\mathbf{x} = \left\{ \begin{array}{l} \int_{\mathbf{x}_0 + \alpha\mathcal{D}_{\delta}} [\beta(\mathbf{x}, \mathbf{e}_{\alpha}(\mathbf{x})) - \beta(\mathbf{x}, \mathbf{f}_0(\mathbf{x}))] d\mathbf{x} \\ + \int_{\mathcal{B}_{\alpha}} [\beta(\mathbf{x}, \mathbf{f}_0(\mathbf{x})) - \beta(\mathbf{x}, \mathbf{f}(\mathbf{x}))] d\mathbf{x} \\ + \int_{\mathcal{B}_{2\alpha} - \mathcal{B}_{\alpha}} [\beta(\mathbf{x}, \mathbf{h}_{\alpha}(\mathbf{x})) - \beta(\mathbf{x}, \mathbf{f}(\mathbf{x}))] d\mathbf{x} \end{array} \right\}.$$

Let

$$\tau_{\alpha} := \|\beta(\cdot, \mathbf{f}_0(\cdot)) - \beta(\cdot, \mathbf{f}(\cdot))\|_{\mathcal{B}_{\alpha}, \infty} + \|\beta(\cdot, \mathbf{h}_{\alpha}(\cdot)) - \beta(\cdot, \mathbf{f}(\cdot))\|_{\mathcal{B}, \infty},$$

and

$$\omega_{\alpha} := \int_{\mathcal{D}} [\beta(\mathbf{x}_0 + \alpha\delta\mathbf{y}, \alpha\delta[\mathbf{g}(\mathbf{y}) - \mathbf{f}_0(\mathbf{y})] + \mathbf{f}_0(\mathbf{x}_0 + \alpha\delta\mathbf{y})) - \beta(\mathbf{x}_0 + \alpha\delta\mathbf{y}, \mathbf{f}_0(\mathbf{x}_0 + \alpha\delta\mathbf{y}))] d\mathbf{y}$$

We make the change of variables $\mathbf{y} = (\mathbf{x} - \mathbf{x}_0)/\alpha\delta$ in the first integral on the right hand side of (4.14). Then we combine (4.13) with (4.14) to get

$$(4.15) \quad E(\mathbf{f}_{\alpha}, \Omega) - E(\mathbf{f}, \Omega) \leq \alpha^n [(-\gamma + |\omega_{\alpha}|)\delta^n + 2^n \text{vol}(\mathcal{B}_1)(\sigma_{\alpha} + \tau_{\alpha})].$$

Now, $\nabla \mathbf{h}_{\alpha} \rightarrow \nabla \mathbf{f}$ uniformly on $\overline{\mathcal{B}}$ and $\nabla \mathbf{f}$ is continuous on $\mathcal{B}$ with $\nabla \mathbf{f}(\mathbf{x}_0) = \mathbf{F}_0$. Thus since W is continuous we find that

$$\sigma_{\alpha} \rightarrow 0 \quad \text{as} \quad \alpha \rightarrow 0^+.$$

Also $\mathbf{h}_{\alpha} \rightarrow \mathbf{f}$ uniformly on $\overline{\mathcal{B}}$ and $\mathbf{f}_0$ and $\mathbf{f}$ are continuous on $\mathcal{B}$ with $\mathbf{f}(\mathbf{x}_0) = \mathbf{f}_0(\mathbf{x}_0)$. Thus since β is continuous we conclude that

$$\tau_{\alpha} \rightarrow 0 \quad \text{as} \quad \alpha \rightarrow 0^+.$$

Finally, $\mathbf{g} \in L^{\infty}(\mathcal{D})$ and β and $\mathbf{f}_0$ are continuous. Therefore, by the bounded convergence theorem we find that

$$\omega_{\alpha} \rightarrow 0 \quad \text{as} \quad \alpha \rightarrow 0^+.$$

Thus (4.15) implies that $\mathbf{f}_{\alpha}$ has strictly less energy than $\mathbf{f}$ when α is sufficiently small, completing the proof. $\square$

5. The Energetics of Filamentary Voids.

a. Constitutive assumptions

The formation of filamentary voids is promoted by assumptions that limit the growth of the stored energy for large, nearly isochoric shears while at the same time require fairly strong growth for large equibiaxial stretches. Also, we wish to differentiate the phenomenon of the formation of filamentary voids from the formation of spherical voids by being completely noncommittal about the behavior of the energy for dilatation. We will *henceforth assume that the body is three dimensional and isotropic* and write the stored energy

$$(5.1) \quad \Phi(\alpha, \beta, \gamma) = \phi(\alpha) + \phi(\beta) + \phi(\gamma) + \psi(\alpha\beta) + \psi(\alpha\gamma) + \psi(\beta\gamma) + \chi(\alpha\beta\gamma) + \Delta(\alpha, \beta, \gamma),$$

where $\psi \in C^1(\mathbb{R}^+, \mathbb{R})$, $\phi : \mathbb{R}^+ \rightarrow \mathbb{R}$, $\chi : \mathbb{R}^+ \rightarrow \mathbb{R}$, and $\Delta : (\mathbb{R}^+)^3 \rightarrow \mathbb{R}$. The assumption (5.1) entails no restrictions on Φ so far because Δ is arbitrary.

Our main constitutive assumptions are:

S1. Stiffness for Equibiaxial Stretch.

- (a) ψ is convex,
- (b) $\psi(t) \rightarrow +\infty$ as $t \rightarrow +\infty$,
- (c) χ is nondecreasing,
- (d) ϕ, ψ , and Δ are nonnegative.

S2. Softness for Isochoric Families of Shear. There are constants $q \in (0, 2)$ and $c > 0$ and a function $h \in C^0(\mathbb{R}^+, \mathbb{R})$ such that

- (a) $\phi(t) \leq c[t^q + t^{-q}]$ for all $t > 0$,
- (b) $\psi(t) \leq c[t^q + 1]$ for all $t > 0$,
- (c) $\Delta(\alpha, \beta, \gamma) \leq h(\alpha\beta\gamma)[1 + \alpha^q + \beta^q + \gamma^q + (\alpha\beta)^{q/2} + (\alpha\gamma)^{q/2} + (\beta\gamma)^{q/2}]$ for all $\alpha > 0, \beta > 0$, and $\gamma > 0$.

The convexity of ψ together with the nonnegativity of ϕ, ψ and Δ insure that the material is *stiff for equibiaxial stretch*; i.e., that $\Phi(\alpha, \lambda, \lambda)$ grows at least quadratically in λ , uniformly in α , for large λ . The upper bounds on ϕ, ψ , and Δ insure that the material is *soft for isochoric families of shear*, i.e., that $\Phi(\alpha, \beta, k/\alpha\beta)$ grows subquadratically in α and β for each $k > 0$. These upper bounds also insure that certain deformations, which open cylindrical holes in the material, have finite energy.

Remark 5.1. The subquadratic growth of $\Phi(\alpha, \beta, k/\alpha\beta)$ is necessary for the formation of essentially cylindrical holes as is evident from the work of BALL [1982] specialized to the case $n = 2$. At the expense of complicating our proofs greatly, our results remain valid when the constant c in S2 is different on different lines and when the value of $q \in (0, 2)$ changes from term to term.

The constitutive hypotheses S1 and S2 yield a comparison between the energy of a certain triaxial stretch and the energy of a related biaxial stretch.

LEMMA 5.2. Let $S1$ and $S2$ be satisfied. Suppose that $\alpha, \lambda, r', \omega$, and a are real numbers that satisfy

$$(5.2) \quad \left. \begin{aligned} 1 < a, & \quad 0 < r' \leq \omega < 1 \\ 1 < \lambda, & \quad 0 < \alpha < a \end{aligned} \right\}.$$

Then

$$\Phi(\lambda r', \lambda \omega / r', \alpha) - \Phi(\lambda, \lambda, \alpha) \leq 8a^q \lambda^q (r')^{-q} [c + h(\omega \alpha \lambda^2)] - \lambda^2 (1 - \omega) \psi'(\omega \lambda^2).$$

Proof. If we evaluate Φ at the indicated arguments we find, with the aid of (5.1), (5.2)₂, $S1(c) - (d)$, and $S2$ that

$$\Phi(\lambda r', \lambda \omega / r', \alpha) - \Phi(\lambda, \lambda, \alpha) \leq k \lambda^q (r')^{-q} + \psi(\omega \lambda^2) - \psi(\lambda^2),$$

$$k := \left\{ \begin{aligned} & c \left[(r')^{2q} + \lambda^{-2q} + \omega^q + \lambda^{-2q} (r'/\omega)^q (r')^q \right] \\ & + h(\omega \alpha \lambda^2) \left[\lambda^{-q} (r')^q + (r')^{2q} + \omega^q + \alpha^q \lambda^{-q} (r')^q + \omega^{q/2} (r')^q \right] \\ & + \alpha^{q/2} \lambda^{-q/2} (r')^{3q/2} + \alpha^{q/2} \lambda^{-q/2} \omega^{q/2} (r')^{q/2} \end{aligned} \right\}.$$

The desired result then follows from (5.2) and the convexity of ψ , *i.e.*,

$$\psi(\lambda^2) \geq \psi(\omega \lambda^2) + \lambda^2 (1 - \omega) \psi'(\omega \lambda^2).$$

□

b. Formation of a cylindrical hole through a plate

Let $\Gamma \subset \mathbb{R}^2$ be a regular region with $(0, 0) \in \Gamma$. Given $L > 0$ define

$$(5.3) \quad \mathcal{P}_{-L}^L := \Gamma \times (-L, L)$$

A *plane radial deformation* of the plate $\mathcal{P}_{-L}^L$ is a deformation $\mathbf{f} \in \text{Def}(\mathcal{P}_{-L}^L)$ that satisfies

$$(5.4) \quad \mathbf{f}(\mathbf{x}) = r(R) \mathbf{e}_R(\mathbf{x}) + \alpha x_3 \mathbf{e}_3, \quad \mathbf{x} \in \mathcal{P}_{-L}^L, R > 0,$$

for some $\alpha > 0$ and $r \in C^0(\mathbb{R}^{\geq}, \mathbb{R}^{\geq})$. Here $R = (x_1^2 + x_2^2)^{1/2}$ and

$$(5.5)^9 \quad \mathbf{e}_R(\mathbf{x}) := \begin{cases} (x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2) / R, & R > 0 \\ \mathbf{e}_1, & R = 0 \end{cases},$$

the radial unit vector. The special plane radial deformation given by (5.4) with the choice

$$r(R) = \lambda R, \quad \lambda = \text{constant} > 0,$$

⁹We have put $\mathbf{e}_R(0) = \mathbf{e}_1$ in (5.5) so that $\mathbf{f}$ is well defined at $R = 0$

is called an *equibiaxial stretch*.

Let $R_0 > 0$ be sufficiently small so that

$$\{(x_1, x_2) : x_1^2 + x_2^2 \leq R_0^2\} \subset \Gamma.$$

Fix $\omega \in (0, 1)$ and define $r \in C^0(\mathbf{R}^{\geq}, \mathbf{R}^>)$ by

$$(5.6) \quad r(R) := \begin{cases} [\omega R^2 + (1 - \omega)R_0^2]^{1/2}, & 0 \leq R < R_0 \\ R, & R_0 \leq R \end{cases}.$$

Then, for each $\alpha > 0$ and $\lambda > 0$,

$$(5.7) \quad \mathbf{p}_\lambda^\alpha(\mathbf{x}) = \lambda r(R) \mathbf{e}_R(\mathbf{x}) + \alpha x_3 \mathbf{e}_3, \quad \mathbf{x} \in \mathcal{P}_{-L}^L,$$

is a plane radial deformation of $\mathcal{P}_{-L}^L$ (cf. Proposition 5.4) that satisfies the boundary condition

$$\mathbf{p}_\lambda^\alpha = \mathbf{b}_\lambda^\alpha \quad \text{on} \quad \partial\Gamma \times [-L, L],$$

where

$$(5.8) \quad \mathbf{b}_\lambda^\alpha(\mathbf{x}) := \lambda R \mathbf{e}_R(\mathbf{x}) + \alpha x_3 \mathbf{e}_3$$

is the *equibiaxial stretch associated with $\mathbf{p}_\lambda^\alpha$* . The deformation $\mathbf{p}_\lambda^\alpha$ opens a circular cylindrical hole of radius $\lambda(1 - \omega)^{1/2}R_0$ in the plate. The principal stretches of $\nabla \mathbf{p}_\lambda^\alpha$ are (in no special order)

$$(5.9) \quad \lambda_1 = \lambda r'(R), \quad \lambda_2 = \lambda r(R)/R, \quad \lambda_3 = \alpha,$$

where prime denotes differentiation with respect to R .

We now show that, for λ sufficiently large, the deformation (of a material governed by $S1$ and $S2$) that introduces a hole in the plate has less energy than the associated equibiaxial stretch.

PROPOSITION 5.3. *Let the stored energy satisfy constitutive hypotheses $S1$ and $S2$. Let $a > 1$ and suppose that $\hat{\alpha} : (1, \infty) \rightarrow (0, a)$ is such that both*

$$(5.10) \quad 0 < \inf_{\lambda > 1} [\hat{\alpha}(\lambda) \lambda^2] \quad \text{and} \quad \sup_{\lambda > 1} [\hat{\alpha}(\lambda) \lambda^2] < +\infty,$$

or

$$(5.11) \quad \sup_{\lambda > 1} h(\hat{\alpha}(\lambda) \lambda^2) < +\infty$$

(cf. S2(c)). Then there is a $\lambda_0 > 1$ and a $\kappa > 0$, which are independent of λ and L , such that

$$\int_{\mathcal{P}_{-L}^L} [W(\nabla \mathbf{p}_\lambda^{\hat{\alpha}}(\mathbf{x})) - W(\nabla \mathbf{b}_\lambda^{\hat{\alpha}}(\mathbf{x}))] d\mathbf{x} \leq -2\kappa L \lambda^q$$

for all $\lambda \geq \lambda_0$. Here $\mathbf{p}_\lambda^{\hat{\alpha}}$ is the plane radial deformation given by (5.7), with $\alpha = \hat{\alpha}(\lambda)$, and $\mathbf{b}_\lambda^{\hat{\alpha}}$ is the associated equibiaxial stretch given by (5.8)

Proof. We first note that (5.10) and the continuity of h imply (5.11). Next, by (5.6), $0 < r'(R) < \omega$ and $r'(R) = \omega R/r(R)$ provided $0 < R < R_0$. Thus (5.9) and Lemma 5.2 imply that for $0 < R < R_0$

$$(5.12) \quad W(\nabla \mathbf{p}_\lambda^{\hat{\alpha}}) - W(\nabla \mathbf{b}_\lambda^{\hat{\alpha}}) \leq 8a^q \lambda^q \omega^q (r/R)^q [c + h(\omega \alpha \lambda^2)] - \lambda^2 (1 - \omega) \psi'(\omega \lambda^2).$$

The definition (5.6) of $r(\cdot)$ shows that

$$(5.13) \quad \int_0^{R_0} \left| \frac{r(R)}{R} \right|^q R dR \leq \int_0^{R_0} \left| \frac{R_0}{R} \right|^q R dR < +\infty,$$

for $q < 2$, and hence that the function $|r(R)/R|^q$ is integrable on $\mathcal{P}_{-L}^L$. Also, S1(a) and S2(b) imply that $\psi'(t)$ is positive and nondecreasing for large t . Thus, if we integrate (5.12) over $\mathcal{P}_{-L}^L$ we conclude, with the aid of (5.11), that there are $c_1 > 0$ and $c_2 > 0$, which are independent of L and λ , such that

$$\int_{\mathcal{P}_{-L}^L} [W(\nabla \mathbf{p}_\lambda^{\hat{\alpha}}) - W(\nabla \mathbf{b}_\lambda^{\hat{\alpha}})] d\mathbf{x} \leq 2L(c_1 \lambda^q - c_2 \lambda^2).$$

The desired result is now immediate since $q < 2$. $\square$

c. Kinematic description of the caps

The deformation $\mathbf{p}_\lambda^\alpha$ of the preceeding section opens a hole through a plate and reduces the total energy relative to the associated equibiaxial stretch. We intend to use a deformation like $\mathbf{p}_\lambda^\alpha$ to show that the conclusion of Theorem 4.2 is violated and therefore that any deformation that at some point has principal stretches λ, λ , and α (with suitable assumptions on $\alpha = \hat{\alpha}(\lambda)$ and with λ sufficiently large) is unstable. In particular this will sometimes occur outside a spherical cavity. At this point we cannot use $\mathbf{p}_\lambda^\alpha$ for this purpose because it does not satisfy linear boundary conditions at $x_3 = \pm L$. The linear boundary conditions are essential for applying Theorem 4.2. The problem is that the hole pierces the top and bottom of the plate. To circumvent this difficulty we shall, in this section, place *caps* on the ends of the holes. Eventually, we will find it necessary to make the void very long and thin ($R_0 \ll L$) in order to take advantage of the energy reducing nature of the cylindrical void relative to the caps.

Fix $\omega \in (0, 1)$ and let $\theta \in C^\infty(\mathbf{R}, \mathbf{R})$ be a bridging function with

$$(5.14) \quad \begin{aligned} \theta(t) &= \begin{cases} \omega, & t \leq 1 \\ 1, & t \geq 2 \end{cases} \\ \dot{\theta}(t) &> 0, 1 < t < 2. \end{aligned}$$

PROPOSITION 5.4. Fix $\alpha > 0, \lambda > 0$ and $L > 0$. Define

$$(5.15) \quad \mathbf{c}_\lambda^\alpha(\mathbf{x}) := \lambda r(R, x_3) \mathbf{e}_R(\mathbf{x}) + \alpha x_3 \mathbf{e}_3, \mathbf{x} \in \mathcal{P}_L^{L+3},$$

where

$$(5.16) \quad r(R, z) := \begin{cases} [\theta(z - L)R^2 + (1 - \theta(z - L))R_0^2]^{1/2}, & 0 \leq R < R_0, \\ R, & R_0 \geq R \end{cases}.$$

Then, $\mathbf{c}_\lambda^\alpha \in \text{Def}(\mathcal{P}_L^{L+3})$, i.e. $\mathbf{c}_\lambda^\alpha \in W^{1,p}(\mathcal{P}_L^{L+3}) \cap L^\infty(\mathcal{P}_L^{L+3})$ and $\mathbf{c}_\lambda^\alpha$ is one-to-one. Moreover, if the stored energy function satisfies S2 then there is a $K_1 > 0$, which does not depend on L , such that

$$(5.17) \quad \int_{\mathcal{P}_L^{L+3}} W(\nabla \mathbf{c}_\lambda^\alpha) d\mathbf{x} \leq K_1.$$

Proof. It is clear from (5.15) and (5.16) that $\mathbf{c}_\lambda^\alpha$ is bounded and one-to-one. We claim that $\mathbf{c}_\lambda^\alpha \in W^{1,p}(\mathcal{P}_L^{L+3})$ with weak derivative

$$(5.18) \quad \mathbf{C}_\lambda^\alpha := \lambda r_R \mathbf{e}_R \otimes \mathbf{e}_R + \lambda(r/R) \mathbf{e}_T \otimes \mathbf{e}_T + \alpha \mathbf{e}_3 \otimes \mathbf{e}_3 + \lambda r_z \mathbf{e}_R \otimes \mathbf{e}_3 \quad a.e.,$$

where r_R and r_z are the classical partial derivatives of r , and $\mathbf{e}_T(\mathbf{x}) := \mathbf{e}_3 \times \mathbf{e}_R(\mathbf{x})$ is the tangential unit vector. To prove the above claim we first show that $\mathbf{C}_\lambda^\alpha \in L^p(\mathcal{P}_L^{L+3})$.

If we square both sides of (5.16), take the partial derivatives, and square the results we find that for $0 < R < R_0$ and $L + 1 < z < L + 2$,

$$(5.19) \quad \begin{aligned} r_R^2 &= \frac{\theta^2 R^2}{\theta R^2 + (1 - \theta)R_0^2} \leq \frac{\theta^2 R^2}{\theta R^2} = \theta, \\ r_z^2 &= \frac{\dot{\theta}^2 (R^2 - R_0^2)^2}{4[\theta R^2 + (1 - \theta)R_0^2]} \leq \frac{\dot{\theta}^2 R_0^4}{4(1 - \theta)R_0^2} = \frac{\dot{\theta}^2 R_0^2}{4(1 - \theta)}. \end{aligned}$$

L'Hospital's rule shows that

$$\lim_{t \rightarrow 2^-} \frac{[\dot{\theta}(t)]^2}{1 - \theta(t)} = \lim_{t \rightarrow 2^-} \frac{2\dot{\theta}(t)\ddot{\theta}(t)}{-\dot{\theta}(t)} = 0.$$

Using the definition (5.14) of θ , we conclude that r_R and r_z are bounded on $\mathcal{P}_L^{L+3}$. The argument leading to (5.13) can be repeated with ω replaced by θ and q replaced by p to show that $|r(R)/R|^p$ is integrable on $\mathcal{P}_L^{L+3}$. It follows that $\mathbf{C}_\lambda^\alpha \in L^p(\mathcal{P}_L^{L+3})$.

To show that $\mathbf{C}_\lambda^\alpha$ is the weak derivative of $\mathbf{c}_\lambda^\alpha$, we let $\psi \in C_0^\infty(\mathcal{P}_L^{L+3})$ and let $\mathcal{C}_\varepsilon = \{\mathbf{x} \in \mathcal{P}_L^{L+3} : x_1^2 + x_2^2 \leq \varepsilon\}$. Then, by (5.14) - (5.16) and the divergence theorem

$$\begin{aligned}
(5.20) \quad \int_{\mathcal{P}_L^{L+3}-\mathcal{C}_\varepsilon} [\psi \mathbf{C}_\lambda^\alpha + \mathbf{c}_\lambda^\alpha \otimes \nabla \psi] d\mathbf{x} &= \int_{\mathcal{P}_L^{L+3}-\mathcal{C}_\varepsilon} \operatorname{div} [\psi \mathbf{c}_\lambda^\alpha] d\mathbf{x} \\
&= \int_{\partial(\mathcal{P}_L^{L+3}-\mathcal{C}_\varepsilon)} \psi \mathbf{c}_\lambda^\alpha \cdot \mathbf{n} da \\
&= \varepsilon \int_L^{L+3} \int_0^{2\pi} \psi \mathbf{c}_\lambda^\alpha \cdot \mathbf{e}_R d\Theta dx_3,
\end{aligned}$$

where (R, Θ, x_3) are the cylindrical coordinates of the point $\mathbf{x}$. The functions ψ , $\mathbf{c}_\lambda^\alpha$, and $\mathbf{e}_R$ are bounded on $\mathcal{P}_L^{L+3}$. Thus, if we let $\varepsilon \rightarrow 0^+$ in (5.20) and use the dominated convergence theorem, we get

$$\int_{\mathcal{P}_L^{L+3}} [\psi \mathbf{C}_\lambda^\alpha + \mathbf{c}_\lambda^\alpha \otimes \nabla \psi] d\mathbf{x} = \lim_{\varepsilon \rightarrow 0} \int_{\mathcal{P}_L^{L+3}-\mathcal{C}_\varepsilon} [\psi \mathbf{C}_\lambda^\alpha + \mathbf{c}_\lambda^\alpha \otimes \nabla \psi] d\mathbf{x} = 0,$$

which proves that $\nabla \mathbf{c}_\lambda^\alpha = \mathbf{C}_\lambda^\alpha$.

We now assume that the stored energy satisfies *S2* and we show that $\mathbf{c}_\lambda^\alpha$ has finite total stored energy. The definition (5.18) of $\mathbf{C}_\lambda^\alpha$ yields

$$\begin{aligned}
\mathbf{C}_\lambda^\alpha (\mathbf{C}_\lambda^\alpha)^T &= \lambda^2 (r_R^2 + r_z^2) \mathbf{e}_R \otimes \mathbf{e}_R + \lambda^2 \left(\frac{r}{R}\right)^2 \mathbf{e}_T \otimes \mathbf{e}_T \\
&\quad + \alpha^2 \mathbf{e}_3 \otimes \mathbf{e}_3 + \alpha \lambda r_z (\mathbf{e}_3 \otimes \mathbf{e}_R + \mathbf{e}_R \otimes \mathbf{e}_3),
\end{aligned}$$

so the eigenvalues $\{\lambda_1^2, \lambda_2^2, \lambda_3^2\}$ of $\mathbf{C}_\lambda^\alpha (\mathbf{C}_\lambda^\alpha)^T$ satisfy

$$\lambda_1^2 = \lambda^2 \left(\frac{r}{R}\right)^2, \quad \lambda_{2,3}^4 - \lambda_{2,3}^2 (\alpha^2 + \lambda^2 r_R^2 + \lambda^2 r_z^2) + \alpha^2 \lambda^2 r_R^2 = 0.$$

Hence,

$$(5.21) \quad \lambda_1 = \lambda \frac{r}{R}, \quad \lambda_2^2 + \lambda_3^2 = \alpha^2 + \lambda^2 r_R^2 + \lambda^2 r_z^2, \quad \lambda_2 \lambda_3 = \alpha \lambda r_R,$$

and therefore

$$\begin{aligned}
(5.22) \quad \lambda_1 &= \lambda(r/R), \\
\lambda_2 &= \alpha \lambda r_R / \lambda_3, \\
\lambda_3 &= \frac{1}{2} \{[(\alpha + \lambda r_R)^2 + \lambda^2 r_z^2]^{1/2} + [(\alpha + \lambda r_R)^2 + \lambda^2 r_z^2]^{1/2}\}.
\end{aligned}$$

We also note that

$$\lambda_1 \lambda_2 \lambda_3 = \alpha \lambda^2 r_R \left(\frac{r}{R} \right) = \alpha \lambda^2 \theta \in (\alpha \lambda^2 w, \alpha \lambda^2).$$

By (5.1) and S2, there is a constant $\bar{c} > 0$ such that

$$\Phi(\lambda_1, \lambda_2, \lambda_3) \leq \bar{c} \{ 1 + \sum_i (\lambda_i^q + \lambda_i^{-q}) + \sum_{j \neq k} (\lambda_j^q \lambda_k^q + (\lambda_j \lambda_k)^{q/2}) \}.$$

Therefore, in order to prove that the deformation $\mathbf{c}_\lambda^\alpha$ has finite total stored energy, we shall show that $R\lambda_i(R, z)^q$, $R\lambda_i(R, z)^{-q}$ and $R(\lambda_j(R, z)\lambda_k(R, z))^q$, are integrable on $(0, R_0) \times (L, L+3)$.

By (5.22)₃ $\lambda_3 \geq \alpha$. Since also r_R and r_z are bounded on $\mathcal{P}_L^{L+3}$ we find from (5.21) that λ_2 and λ_3 are bounded on $\mathcal{P}_L^{L+3}$. The argument above, which shows that $\mathbf{C}_\lambda^\alpha \in L^p(\mathcal{P}_L^{L+3})$, also shows that λ_1^q is integrable on $\mathcal{P}_L^{L+3}$. Putting these facts together, we have established the integrability of

$$\begin{aligned} & \lambda_i^q, \quad i = 1, 2, 3, \\ & \lambda_3^{-q}, \\ & (\lambda_j \lambda_k)^q, j, k \in \{1, 2, 3\}, j \neq k. \end{aligned}$$

It remains to examine the integrability of λ_1^{-q} and λ_2^{-q} . We note that (5.14) and (5.16) imply that $r(R, z) \geq \omega R$ which yields the integrability of λ_1^{-q} . The integrability of λ_2^{-q} follows from the identity

$$\lambda_2^{-q} = \frac{\lambda_3^q}{\alpha^q \lambda^q \theta^q} \left(\frac{r}{R} \right)^q,$$

and (5.13). Finally, it is clear from (5.15) and (5.16) that the total stored energy $E(\mathbf{c}_\lambda^\alpha, \mathcal{P}_L^{L+3})$ is independent of L . $\square$

d. Main result

We now use Theorem 4.2, Proposition 5.3 and Proposition 5.4 to show that by introducing a filamentary void at a point $\mathbf{x}_0 \in \Omega$ of large equibiaxial stretch, we can reduce the energy.

THEOREM 5.5. *Let the stored energy function Φ satisfy constitutive hypotheses S1 and S2. Let $a > 1$ and suppose that $\hat{\alpha} : (1, \infty) \rightarrow (0, a)$ is such that both*

$$0 < \inf_{\lambda > 1} [\hat{\alpha}(\lambda) \lambda^2] \quad \text{and} \quad \sup_{\lambda > 1} [\hat{\alpha}(\lambda) \lambda^2] < \infty$$

or

$$\sup_{\lambda > 1} h(\hat{\alpha}(\lambda) \lambda^2) < \infty$$

(cf. S2(c)). Let λ_0 be as in Proposition 5.3 and let $\mathbf{f} \in \text{Kin}_{\mathbf{d}}(\Omega)$ be C^1 in a neighborhood of $\mathbf{x}_0 \in \Omega$. Suppose that $\mathbf{f}$ is a sufficiently large equibiaxial stretch at $\mathbf{x}_0$ up to a rigid rotation: for some unit vector $\mathbf{e}$, some proper orthogonal tensor $\mathbf{Q}$, and some $\lambda \geq \lambda_0$,

$$\mathbf{Q} \nabla \mathbf{f}(\mathbf{x}_0) = \lambda \mathbf{I} + (\hat{\alpha}(\lambda) - \lambda) \mathbf{e} \otimes \mathbf{e}.$$

Then $\mathbf{f}$ is not a strong local minimizer of the total energy $E(\cdot, \Omega)$.

Proof. Suppose on the contrary that $\mathbf{f}$ is a strong local of $E(\cdot, \Omega)$. Then by Theorem 4.2, we have that for every regular region $\mathcal{D} \subset \mathbb{R}^3$,

$$(5.23) \quad \int_{\mathcal{D}} W(\nabla \mathbf{f}(\mathbf{x}_0)) d\mathbf{x} \leq \int_{\mathcal{D}} W(\nabla \mathbf{f}(\mathbf{x}_0) + \nabla \mathbf{u}(\mathbf{x})) d\mathbf{x}$$

whenever $\mathbf{f}_0 + \mathbf{u} \in \text{Kin}_{\mathbf{f}_0}(\mathcal{D})$. Here,

$$\mathbf{f}_0(\mathbf{x}) := \mathbf{f}(\mathbf{x}_0) + \nabla \mathbf{f}(\mathbf{x}_0)(\mathbf{x} - \mathbf{x}_0), \mathbf{x} \in \mathcal{D}.$$

However, we can apply Proposition 5.3 to show that for any $L > 0$ and any $\lambda \geq \lambda_0$,

$$(5.24) \quad \int_{\mathcal{P}_{-L}^L} [W(\nabla \mathbf{p}_{\lambda}^{\hat{\alpha}}) - W(\mathbf{Q} \nabla \mathbf{f}(\mathbf{x}_0))] d\mathbf{x} \leq -2\kappa L \lambda^q$$

where $\mathbf{p}_{\lambda}^{\hat{\alpha}}$ is defined by (5.7) with R_0 fixed and κ is independent of λ and L . Note that $\mathbf{Q}^T \mathbf{p}_{\lambda}^{\hat{\alpha}}$ cannot be used as a competitor in (5.23) because it does not satisfy the linear boundary conditions. We put “caps” on $\mathbf{Q}^T \mathbf{p}_{\lambda}^{\hat{\alpha}}$ by defining for each $L > 0$ the function $\mathbf{f}^L : \mathcal{P}_{-L-3}^{L+3} \rightarrow \mathbb{R}^3$ by

$$\mathbf{f}^L(\mathbf{x}) = \begin{cases} \mathbf{Q}^T \mathbf{c}_{\lambda}^{\hat{\alpha}}(x_1, x_2, x_3), & L \leq x_3 < L+3, \\ \mathbf{Q}^T \mathbf{p}_{\lambda}^{\hat{\alpha}}(x_1, x_2, x_3), & -L < x_3 < L, \\ \mathbf{Q}^T \mathbf{c}_{\lambda}^{\hat{\alpha}}(x_1, x_2, -x_3), & -L-3 < x_3 \leq -L, \end{cases}$$

(cf. (5.3), (5.5), (5.7), (5.14) - (5.16)). Here, x_1, x_2, x_3 are components relative to the basis $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 = \mathbf{e}$. It is clear from Proposition 5.3 and 5.4 that $\mathbf{f}^L \in \text{Def}(\mathcal{P}_{-L-3}^{L+3})$ and $\mathbf{f}^L(\mathbf{x}) = \nabla \mathbf{f}(\mathbf{x}_0) \mathbf{x}, \mathbf{x} \in \partial \mathcal{P}_{-L-3}^{L+3}$. Therefore, if we define $\mathbf{u}^L(\mathbf{x}) := \mathbf{f}^L(\mathbf{x}) - \nabla \mathbf{f}(\mathbf{x}_0) \mathbf{x}, \mathbf{x} \in \mathcal{P}_{-L-3}^{L+3}$, then $\mathbf{f}_0 + \mathbf{u}^L \in \text{Kin}_{\mathbf{f}_0}(\mathcal{P}_{-L-3}^{L+3})$.

We now combine (3.1), (5.24), and Proposition 5.4 to conclude that

$$(5.25) \quad \int_{\mathcal{P}_{-L-3}^{L+3}} [W(\nabla \mathbf{f}(\mathbf{x}_0) + \nabla \mathbf{u}^L(\mathbf{x})) - W(\nabla \mathbf{f}(\mathbf{x}_0))] d\mathbf{x} \leq 2K_1 - 2\kappa \lambda^q L,$$

with K_1 and κ independent of L . For L sufficiently large (5.25) contradicts (5.23). $\square$

Remark 5.6. In the proof of Theorem 5.5 we have fixed R_0 and we have let $L \rightarrow \infty$ in order to take advantage of the energy reducing nature of the cylindrical deformation relative to the caps. At the expense of a slightly more complicated argument, we could have fixed L and let $R_0 \rightarrow 0$. The important point is that the void must be very long and thin to force it to be energy reducing, which motivates the term “filamentary void”.

Remark 5.7. Our construction of the filamentary void shows that the conclusions of Theorem 5.5 are valid for certain anisotropic materials. The crucial assumptions are: that the material at the point $\mathbf{x}_0$ is transversely isotropic in the plane perpendicular to $\mathbf{e}$, and that the stored energy function W satisfies both

$$(i) \quad W(\mathbf{F}) \leq c(\det \mathbf{F}) \left[\sum_i (\lambda_i^q + \lambda_i^{-q}) + \sum_{i \neq k} (\lambda_i \lambda_k)^q \right]$$

for every $\mathbf{F} \in \text{Lin}^>$ and some $q \in (0, 2)$ and $c : \mathbb{R}^> \rightarrow \mathbb{R}$, and

$$(ii) \quad W(\mathbf{F}) = \phi(\alpha) + \phi(\beta) + \phi^*(\gamma) + \psi(\alpha\beta) + \psi^*(\alpha\gamma) + \psi^*(\alpha\gamma) + \chi(\alpha\beta\gamma) + \Delta(\alpha, \beta, \gamma)$$

whenever α, β, γ are the eigenvalues of $\mathbf{F}\mathbf{F}^T$, $\mathbf{F}\mathbf{F}^T \mathbf{e} = \gamma^2 \mathbf{e}$, and ϕ, ψ, χ , and Δ satisfy $S1$ and $S2$.

Our description of the filamentary void as well as our proof of its energy reducing property appears to require that the underlying smooth deformation be an equibiaxial stretch at the point where the void is to be inserted. This requirement is not essential, but was made to simplify both the analysis and the conceptual description of our results. In a more general deformation it is possible to achieve a reduction of energy by introducing a filamentary void with elliptical cross section. More precisely, given $0 < \alpha < \lambda_1 \leq \lambda_2$, let

$$(5.26) \quad \begin{aligned} \mathbf{g}(\mathbf{x}) &:= \lambda_1 x_1 \mathbf{e}_1 + \lambda_2 x_2 \mathbf{e}_2 + \alpha x_3 \mathbf{e}_3, \\ \mathbf{f}(\mathbf{x}) &= r(R) \mathbf{e}_R(\mathbf{x}) + x_3 \mathbf{e}_3, \quad R = (x_1^2 + x_2^2)^{1/2}, \end{aligned}$$

be deformations of the plate $\mathcal{P}_{-L}^L$ (cf. (5.3)), where r is given by (5.6) and $\mathbf{e}_R$ is the radial unit vector (cf. (5.5)). Then $\mathbf{g} \in \text{Def}(\mathcal{P}_{-L}^L)$, $\mathbf{g} \circ \mathbf{f} \in \text{Def}(\mathcal{P}_{-L}^L)$, and $(\mathbf{g} \circ \mathbf{f})(\mathbf{x}) = \mathbf{g}(\mathbf{x})$ for $x_1^2 + x_2^2 \geq R_0^2$.

Let $\mathbf{x}_0 \in \mathcal{P}_{-L}^L$, $\mathbf{x}_0 \times \mathbf{e}_3 \neq \mathbf{o}$, and denote the principal stretches of $\nabla(\mathbf{g} \circ \mathbf{f})(\mathbf{x}_0)$ by ν_1, ν_2 , and ν_3 . Then it is not difficult to show that

$$(5.27) \quad \begin{aligned} \lambda_1 r' &\leq \nu_1 \leq \lambda_2 r / R, & \nu_3 &= \alpha, \\ \lambda_1 r' &\leq \nu_2 \leq \lambda_2 r / R, & \nu_1 \nu_2 &= \omega \lambda_1 \lambda_2, \end{aligned}$$

and hence that (cf. Lemma 5.2)

$$(5.28) \quad W(\nabla(\mathbf{g} \circ \mathbf{f})(\mathbf{x}_0)) - W(\nabla \mathbf{g}(\mathbf{x}_0)) \leq \left[\begin{aligned} &8a^q \lambda_2^q (r')^{-q} (c + h(\omega \alpha \lambda_1 \lambda_2)) \\ &- \lambda_1 \lambda_2 (1 - \omega) \psi'(\omega \lambda_1 \lambda_2) \end{aligned} \right],$$

provided $1 < a, \alpha \in (0, a)$, and $\lambda_1 \in [a^{-1}, \lambda_2]$.

The energy reduction achieved by the introduction of the filamentary void $\mathbf{g} \circ \mathbf{f}$ is now clear from (5.28). For example if we let $\lambda_2 = \lambda, \lambda_1 = \varepsilon \lambda$, for some $\varepsilon \in (0, 1]$ and suppose that $h(w\alpha\varepsilon\lambda^2)$ is bounded uniformly in λ for $\lambda \geq 1$ then the right hand side of (5.28) will be negative for sufficiently large λ .

Finally, a computation similar to that done in the proof of Proposition 5.4 shows that the “cap” $\mathbf{g} \circ \mathbf{c}_1^1$ is contained in $\text{Def}(\mathcal{P}_L^{L+3})$ and has finite total stored energy that is independent of L . Thus we arrive at the following result.

THEOREM 5.8. *Let the stored energy function Φ satisfy constitutive hypotheses S1 and S2. Let $a > 1$, and suppose that $\hat{\alpha} : (1, \infty) \rightarrow (0, a)$ is such that both*

$$0 < \inf_{\lambda > 1} [\hat{\alpha}(\lambda)\lambda^2] \quad \text{and} \quad \sup_{\lambda > 1} [\hat{\alpha}(\lambda)\lambda^2] < +\infty,$$

or

$$(5.29) \quad \sup_{\substack{\lambda > 1 \\ \varepsilon \in [\varepsilon_0, 1]}} h(\varepsilon \hat{\alpha}(\lambda)\lambda^2) < +\infty.$$

Then there is a $\lambda^* > 1$ such that any $\mathbf{f} \in \text{Kin}_{\mathbf{d}}(\Omega)$ that satisfies property LS given below is not a strong local minimizer of the total energy $E(\cdot, \Omega)$.

(LS) f is C^1 in a neighborhood of a point $\mathbf{x}_0 \in \Omega$ where the principal stretches λ_1, λ_2 and λ_3 of $\nabla \mathbf{f}(\mathbf{x}_0)$ satisfy

$$\lambda_1 \geq \lambda^*, \quad \lambda_2 \in [\varepsilon \lambda_1, \lambda_1], \quad \lambda_3 = \hat{\alpha}(\lambda).$$

Remark 5.9. If h is convex then hypothesis (5.29) is equivalent to (5.11).

6. An application. Instability of radial minimizers. In 1982, BALL considered the problem of minimizing the total energy of a ball composed of a homogeneous, isotropic, compressible hyperelastic material among those deformations that are radial, orientation preserving, and satisfy given displacement or traction conditions on the boundary. In particular BALL showed that when the load on the boundary is sufficiently large, the global radial minimizer of the energy will exhibit a spherical hole at its center for a large class of stored energy functions.

Motivated by BALL’s work others have shown that both radial minimizers and radial solutions of the equilibrium equations can exhibit spherical cavities under a wide range of constitutive hypotheses. However, it is still not known whether the minimizer of the energy among radial deformations is a global minimizer of the energy.

Although it may be true that the radial minimizer is indeed a global minimizer for many stored energy functions, we show in this section that *a radial deformation that exhibits cavitation cannot be a global minimizer of the energy* for materials that satisfy constitutive

hypotheses $S1$ and $S2$ of Section 5. We also show that the constitutive hypotheses of SIVALOGANATHAN [1986a] and STUART [1985] include some polyconvex materials satisfying $S1$ and $S2$. Hence, for these materials the radial solutions that exhibit cavitation are not global minimizers of the total energy.

We now assume that the body in its reference configuration occupies the ball of radius P_0 ,

$$\mathcal{B} := \{\mathbf{x} \in \mathbb{R}^3; |\mathbf{x}| < P_0\}.$$

A *radial deformation* of $\mathcal{B}$ is a deformation $\mathbf{f} \in \text{Def}(\mathcal{B})$ that satisfies

$$(6.1) \quad \mathbf{f}(\mathbf{x}) = \frac{\rho(P)}{P} \mathbf{x}, \quad P = |\mathbf{x}| \neq 0,$$

for some $\rho : [0, P_0] \rightarrow \mathbb{R}$. We say that a radial deformation is *smooth* provided that $\rho \in C^0([0, P_0], \mathbb{R}) \cap C^1((0, P_0), \mathbb{R})$. A radial deformation will *exhibit cavitation* provided that

$$(6.2) \quad 0 < \rho(0) := \lim_{P \rightarrow 0^+} \rho(P).$$

LEMMA 6.1. (BALL [1982, p.566]). *Let $\mathbf{f} : \mathcal{B} \rightarrow \mathbb{R}^3$ satisfy (6.1). Then $\mathbf{f} \in W^{1,q}(\mathcal{B})$ if and only if ρ is absolutely continuous on every closed subinterval of $(0, P_0)$ and*

$$(6.3) \quad \int_0^{P_0} [|\dot{\rho}(P)|^q + |\frac{\rho(P)}{P}|^q] P^2 dP < +\infty.$$

In this case the weak derivatives of $\mathbf{f}$ are given by

$$\nabla \mathbf{f}(\mathbf{x}) = \frac{\rho(P)}{P} \mathbf{I} + (\dot{\rho}(P) - \frac{\rho(P)}{P}) \frac{\mathbf{x}}{P} \otimes \frac{\mathbf{x}}{P} \quad \text{a.e. } \mathbf{x} \in \mathcal{B}$$

and hence the principal stretches are given by

$$(6.4) \quad |\dot{\rho}(P)|, \left| \frac{\rho(P)}{P} \right|, \left| \frac{\rho(P)}{P} \right|, \quad \text{a.e. } \mathbf{x} \in \mathcal{B}.$$

It follows from (6.4) that $\det \nabla f(\mathbf{x}) = \dot{\rho}(P) \rho^2(P) / P^2$ a.e. $\mathbf{x} \in \mathcal{B}$. Thus we will call a smooth radial deformation *orientation preserving* provided that

$$(6.5) \quad \dot{\rho}(P) > 0 \quad \text{for every } P > 0.$$

We next note that by (6.4) almost every $\mathbf{x} \in \mathcal{B}$ in a radial deformation experiences an equibiaxial stretch. In addition, in radial deformations that exhibit cavitation this stretch becomes infinite at the center of the ball. The following result is therefore a consequence of Theorem 5.5

THEOREM 6.2. *Let the stored energy satisfy constitutive hypotheses S1 and S2. Suppose that $\mathbf{f} \in \text{Def}(\mathcal{B})$ is a smooth, orientation preserving,¹⁰ radial deformation that exhibits cavitation. If there is a sequence of radii $P_i \rightarrow 0^+$ such that*

$$(6.6) \quad 0 < \lim_{i \rightarrow \infty} \dot{\rho}(P_i) \frac{\rho(P_i)^2}{P_i^2} < +\infty,$$

or

$$(6.7) \quad \lim_{i \rightarrow \infty} \dot{\rho}(P_i) < +\infty \quad \text{and} \quad \lim_{i \rightarrow \infty} h(\dot{\rho}(P_i) \frac{\rho(P_i)^2}{P_i^2}) < +\infty,$$

then $\mathbf{f}$ is not a strong local minimizer of the total energy $E(\cdot, \mathcal{B})$.

Proof. Equations (6.2) and (6.5) show that (6.6) implies $\dot{\rho}(P_i) \rightarrow 0$ as $i \rightarrow \infty$. Therefore (6.6) implies (6.7) and so we consider assumption (6.7) only. By (6.2) $\rho(P)/P \rightarrow +\infty$ as $P \rightarrow 0^+$ and hence there is a subsequence $P'_i \rightarrow 0^+$ of $\{P_i\}$ such that

$$(6.8) \quad \left. \begin{aligned} P'_{i+1} &< P'_i, \\ \rho(P'_{i+1})/P'_{i+1} &> \rho(P'_i)/P'_i. \end{aligned} \right\}$$

Let

$$a := 1 + \sup_i \dot{\rho}(P'_i), \quad v_1 := \dot{\rho}(P'_1) \rho(P'_1)^2 / (P'_1)^2$$

and define $\hat{\alpha} : (1, \infty) \rightarrow (0, a)$ by

$$(6.9) \quad \hat{\alpha}(\lambda) := \begin{cases} \dot{\rho}(P'_i) & \text{if } \lambda = \rho(P'_i)/P'_i \\ v_1/\lambda^2 & \text{otherwise} \end{cases}.$$

Then by (6.8) $\hat{\alpha}$ is well defined and using (6.9) we find that

$$\sup_{\lambda > 1} h(\hat{\alpha}(\lambda) \lambda^2) \leq h(v_1) + \sup_i h(\dot{\rho}(P_i) \frac{\rho(P_i)^2}{P_i^2}) < +\infty.$$

Therefore, by Theorem 5.5 $\mathbf{f}$ is not a strong local minimizer. $\square$

We will next replace (6.6) or (6.7) by an alternative physical assumption, which can be more easily adapted to the analyses found in the literature. In particular, in order for a radial deformation that creates a hole to be at equilibrium we would expect, in the case of a vacuum hole, that there are no radial forces on the surface of the hole. More precisely, let $\mathbf{f} \in \text{Def}(\mathcal{B})$ be a smooth radial deformation that exhibits cavitation. If $\mathbf{f}$ is the global minimizer of the energy then BALL [1982] and SIVALOGANATHAN [1986a] have

¹⁰ A smooth radial deformation that is not orientation preserving has infinite total energy.

shown, under various constitutive hypotheses, that the radial component of the Cauchy stress is zero on the surface of the cavity. In order to allow for cavities with contents¹¹ we will make the slightly more general assumption that the radial component of the Cauchy stress is bounded as one approaches the surface of the cavity.

We now consider a class of stored energy functions for which we are able to deduce the conditions (6.7) from the aforementioned bound on the radial component of the Cauchy stress at the surface of the cavity. This class of stored energy functions satisfies our $S1$ and $S2$ and at the same time can be further restricted to satisfy the constitutive hypotheses of other authors. We assume

$$\Phi(\alpha, \beta, \gamma) = \phi(\alpha) + \phi(\beta) + \phi(\gamma) + \psi(\alpha\beta) + \psi(\alpha\gamma) + \psi(\beta\gamma) + \delta(\alpha\beta\gamma)$$

where ϕ, ψ , and δ are C^1 , nonnegative and satisfy

- (G1) ϕ is convex and $\phi(t) \leq c[t^q + t^{-r}]$;
- (G2) ψ is convex, $\lim_{t \rightarrow \infty} \psi(t) = +\infty$, and $\psi(t) \leq c[t^s + 1]$;
- (G3) $\delta'(t) \rightarrow +\infty$ as $t \rightarrow +\infty$;

for some $c > 0, q \in [1, 2), r \in (0, 2)$, and $s \in [1, 2)$. For such a material the radial component of the Cauchy stress in a radial deformation is given by

$$(6.11) \quad T(P) := P^{-2} \mathbf{x} \cdot \mathbf{T} \mathbf{x} = \frac{P^2}{\rho^2} \phi'(\dot{\rho}) + \frac{2P}{\rho} \psi'(\dot{\rho} \frac{\rho}{P}) + \delta'(\dot{\rho} \frac{\rho^2}{P^2}),$$

for $P \in (0, P_0)$.

THEOREM 6.3. *Let the stored energy satisfy constitutive hypotheses G1 – G3. Suppose that $\mathbf{f} \in \text{Def}(\mathcal{B})$ is a smooth, orientation preserving radial deformation that exhibits cavitation and for which*

$$(6.12) \quad \lim_{P \rightarrow 0^+} \sup |T(P)| < +\infty.$$

Then $\mathbf{f}$ is not a strong local minimizer of the total energy $E(\cdot, \mathcal{B})$.

Proof. By G3 there is a $\tau > 0$ such that $\delta'(t) \geq 0$ for all $t > \tau$. Define

$$\chi(t) := \begin{cases} 0, & 0 < t < \tau \\ \delta(t) - \delta(\tau), & \tau \leq t < \infty \end{cases}, \quad h(t) := \begin{cases} \delta(t), & 0 < t < \tau \\ \delta(\tau), & \tau \leq t < \infty \end{cases}.$$

¹¹We note that GENT & TOMPKINS [1969a,b] have studied the creation of holes in an unloaded material that has been subject to high pressure over a long period of time. They modified criterion (1.1) to account for a pressure in the hole equal to the pressure that was imposed.

Then it is clear that $G1 - G3$ imply that $S1$ and $S2$ are satisfied. We show that (6.12) together with $G1 - G3$ imply that (6.7) is also satisfied so that the desired result follows from Theorem 6.2.

Let $\mathbf{f} \in \text{Def}(\mathcal{B})$ be a smooth orientation preserving radial deformation that exhibits cavitation and for which (6.12) is satisfied. Then it is clear from (6.2), (6.11), (6.12), and $G1 - G3$ that

$$(6.13) \quad \dot{\rho}(P) \longrightarrow 0^+ \quad \text{as} \quad P \longrightarrow 0^+$$

If there is a sequence of radii $P_i \longrightarrow 0^+$ such that

$$v(P_i) = \dot{\rho}(P_i) \frac{\rho(P_i)^2}{P_i^2} \geq \varepsilon > 0$$

then we are done since $h(v(P_i))$ is uniformly bounded. Thus we only need to consider the case

$$(6.14) \quad v(P) \longrightarrow 0 \quad \text{as} \quad P \longrightarrow 0^+.$$

We claim that, given (6.14), equations (6.12), (6.13), $G1$, and $G2$ imply that the constitutive function δ must satisfy

$$(6.15) \quad \liminf_{t \longrightarrow 0^+} \delta'(t) > -\infty.$$

If not, (6.14) and the continuity of v yield a sequence $P'_i \longrightarrow 0^+$ such that

$$(6.16) \quad \delta'(v(P'_i)) \longrightarrow -\infty.$$

However, (6.14) and the continuity of ρ and $\dot{\rho}$ imply that

$$a(P) := \dot{\rho}(P) \frac{\rho(P)}{P} \longrightarrow 0^+ \quad \text{as} \quad P \longrightarrow 0^+$$

and hence we conclude, with the aid of (6.13), $G1$, and $G2$, that $\phi'(\dot{\rho}(P'_i))$ and $\psi'(a(P'_i))$ are uniformly bounded. These uniform bounds and (6.16) contradict (6.12), *i.e.* for this sequence $T(P'_i) \longrightarrow -\infty$. Therefore (6.15) must hold.

Finally, we note that (6.15) yields for $0 < s < \sigma$ and σ sufficiently small

$$0 < \delta(s) = \delta(\sigma) + \int_s^\sigma -\delta'(t) dt \leq \delta(\sigma) + k(\sigma - s),$$

which shows that (6.7)₂ is satisfied. $\square$

Before stating our final theorem, we quote a result of SIVALOGANATHAN [1986a] which establishes the existence of radial minimizers that open a hole.

PROPOSITION 6.4. (SIVALOGANATHAN [1986a]). Suppose the stored energy function $\Phi \in C^3((\mathbb{R}^+)^3)$ satisfies $\Phi_{,i}(1, 1, 1) = 0$ as well as the following constitutive hypotheses (in the notation of [1986a]):

- (H1) $\Phi_{,11}(\lambda_1, \lambda_2, \lambda_3) > 0$;
- (H2) $\frac{\lambda_i \Phi_{,i}(\lambda_1, \lambda_2, \lambda_3) - \lambda_j \Phi_{,j}(\lambda_1, \lambda_2, \lambda_3)}{\lambda_i - \lambda_j} \geq 0, \lambda_i \neq \lambda_j$;
- (H5) $\Phi_{,1}(\lambda, a, a) \longrightarrow \begin{cases} +\infty \\ -\infty \end{cases}$ as $\lambda \longrightarrow \begin{cases} +\infty \\ 0 \end{cases}$ for fixed $a \in (0, \infty)$;
- (H7) $\frac{\Phi_{,i}(\lambda_1, \lambda_2, \lambda_3) - \Phi_{,j}(\lambda_1, \lambda_2, \lambda_3)}{\lambda_i - \lambda_j} + \Phi_{,ij}(\lambda_1, \lambda_2, \lambda_3) \geq 0$ for $\lambda_i \neq \lambda_j$;
- (H9) $\frac{\lambda^2}{(\lambda^3 - 1)^2} \Phi(\lambda^{-2}, \lambda, \lambda) \in L^1(2, \infty)$;
- (H10) There are constants $k, M > 0$ such that $\frac{\Phi(\lambda, \lambda, \lambda)}{\lambda^3} \geq M$ for $\lambda \geq k$;
- (E1) $\Phi(\lambda_1, \lambda_2, \lambda_3) \geq \sum_{i=1}^3 \Psi(\lambda_i)$ where
 - (i) $\Psi \in C^0((0, \infty), (0, \infty))$,
 - (ii) $\Psi(\lambda)/\lambda \longrightarrow +\infty$ as $\lambda \longrightarrow +\infty$,
 - (iii) $\Psi(\lambda) \longrightarrow +\infty$ as $\lambda \longrightarrow 0^+$;
- (E2) There exist constants $M, \varepsilon_0 \in (0, \infty)$ such that
 $|\Phi_{,i}(\lambda_1, \alpha_2 \lambda_2, \alpha_3 \lambda_3) \lambda_i| < M(\Phi(\lambda_1, \lambda_2, \lambda_3) + 1)$ if $|\alpha_i - 1| < \varepsilon_0, i = 2, 3$.

Then,

$$I(\rho) := \int_0^1 \Phi(\dot{\rho}(P), \frac{\rho(P)}{P}, \frac{\rho(P)}{P}) P^2 dP$$

attains its infimum on the set

$$A_\lambda := \{\rho \in W^{1,1}(0, 1) : \rho(1) = \lambda, \dot{\rho} > 0 \text{ a.e.}, \rho(0) \geq 0\}.$$

If $\rho_\lambda \in A_\lambda$ is an absolute minimizer of I on A_λ then $\rho \in C^0([0, 1]) \cap C^2((0, 1])$, and ρ_λ satisfies the corresponding Euler-Lagrange equation. Moreover, there is a $\lambda_0 > 0$ such that, for all $\lambda > \lambda_0$, ρ_λ exhibits cavitation and

$$\lim_{P \rightarrow 0^+} T(P) = 0,$$

where T is the radial component of the Cauchy stress in the radial deformation ρ_λ .

Remark 6.5. For $P_0 = 1$ Lemma 6.1 implies that for any radial deformation $\mathbf{f}(\mathbf{x}) = [\rho(P)/P]\mathbf{x}$, $P = |\mathbf{x}|$, with finite stored energy,

$$\int_{\mathbb{B}} W(\nabla \mathbf{f}(\mathbf{x})) d\mathbf{x} = 4\pi I(\rho).$$

Therefore Proposition 6.4 establishes the existence of a radial minimizer.

Remark 6.6. A difficulty with the application of Proposition 6.4 to our constitutive hypotheses is that the natural choice of Ψ in E1 is our ϕ . However, if we put $\Psi = \phi$, the condition (E1)_(iii) would violate simple known sufficient conditions for polyconvexity (*cf.* BALL [1977]), these conditions being that ϕ and ψ are convex and *increasing* and δ is convex. We would clearly like to include many polyconvex and therefore elliptic stored energy functions in our hypotheses. For this purpose we note that Proposition 6.4 remains valid when (E1) is replaced by the following hypotheses:

$$(E1)' \left\{ \begin{array}{l} \Phi(\alpha, \beta\gamma) \geq \phi(\alpha) + \phi(\beta) + \phi(\gamma) + \psi(\alpha\beta) + \psi(\beta\gamma) \\ \quad + \psi(\alpha\gamma) + \delta(\alpha\beta\gamma), \\ \text{where } \phi, \psi \text{ and } \delta \text{ belong to } C^0(\mathbf{R}^>, \mathbf{R}^{\geq}) \text{ and satisfy} \\ (i) \quad \lim_{v \rightarrow 0^+} \delta(v) = \lim_{v \rightarrow +\infty} [\delta(v)/v] = +\infty; \\ (ii) \quad \lim_{\lambda \rightarrow +\infty} \phi(\lambda) = +\infty \text{ or } \lim_{\xi \rightarrow +\infty} \psi(\xi) = +\infty. \end{array} \right.$$

To see that this is true, we note that (E1) is only used in the proof of Proposition 6.4 at one place, *i.e.* in SIVOLOGANATHAN'S proof of his Proposition 4.1 [1986a], which establishes the existence of minimizers of $I(\rho)$ in A_λ . An alternate proof of existence is given by BALL [1982, Theorem 7.1] which can be easily adapted to the hypotheses (E1)' and (H1).

Finally, we use Proposition 6.4 and Theorem 6.3 to obtain a class of stored energy functions for which the radial minimizer is not a local minimizer among general deformations.

THEOREM 6.7. *Suppose that the stored energy function is given by*

$$(6.19) \quad \Phi(\alpha, \beta, \gamma) = \phi(\alpha) + \alpha(\beta) + \phi(\gamma) + \psi(\alpha\beta) + \psi(\beta\gamma) + \psi(\alpha\gamma) + \delta(\alpha\beta\gamma),$$

where ϕ, ψ , and δ are C^3 , nonnegative and satisfy (G1), (G2), and (G3) with $c > 0, q \in [1, 2), r \in (0, 3/2), s \in [1, 3/2)$. In addition, assume that $\Phi_{,i}(1, 1, 1) = 0$ and

$$(G4) \quad \left\{ \begin{array}{l} [t\phi'(t)]' \geq 0, \\ |t\phi'(\alpha t)| \leq c[\phi(t) + 1] \text{ whenever } |\alpha - 1| < c^{-1} \end{array} \right\};$$

$$(G5) \quad \left\{ \begin{array}{l} [t\psi'(t)]' \geq 0, \\ |t\psi'(\alpha t)| \leq c[\psi(t) + 1] \text{ whenever } |\alpha - 1| < c^{-1} \end{array} \right\};$$

$$(G6) \quad \left\{ \begin{array}{l} \delta''(t) > 0, \quad \lim_{t \rightarrow 0^+} \delta(t) = +\infty, \\ |t\delta'(\alpha t)| \leq c[\delta(t) + 1] \text{ whenever } |\alpha - 1| < c^{-1} \end{array} \right\}.$$

Then there is a $\lambda_0 > 0$ such that for $\lambda > \lambda_0$ the infimum of

$$I(\rho) := \int_0^1 \Phi(\dot{\rho}(P), \frac{\rho(P)}{P}, \frac{\rho(P)}{P}) P^2 dP$$

on the set $A_\lambda := \{\rho \in W^{1,1}(0,1) : \rho(1) = \lambda, \dot{\rho} > 0 \text{ a.e.}, \rho(0) \geq 0\}$ is attained by a function $\rho_\lambda \in A_\lambda$ and ρ_λ exhibits cavitation. However, the radial deformation $\mathbf{f}_\lambda \in \text{Def}(\mathcal{B})$, $\mathcal{B} := \{\mathbf{x} : |\mathbf{x}| < 1\}$, defined by

$$(6.20) \quad \mathbf{f}_\lambda(\mathbf{x}) := \frac{\rho_\lambda(P)}{P} \mathbf{x}, P = |\mathbf{x}| < 1,$$

is not a strong local minimizer of the total energy $E(\cdot, \mathcal{B})$ on the set $\text{Kind}(\mathcal{B})$ where $\mathbf{d}(\mathbf{x}) = \lambda \mathbf{x}$, $\mathbf{x} \in \overline{\mathcal{B}}$.

Remark 6.8. A simple class of stored energy functions that satisfies the hypotheses of Theorem 6.7 is given by

$$(6.21) \quad \begin{aligned} \Phi(\alpha, \beta, \gamma) = & c_1(\alpha^q + \beta^q + \gamma^q) + c_2((\alpha\beta)^s + (\beta\gamma)^s + (\gamma\delta)^s) \\ & + c_3(\alpha\beta\gamma)^l + c_4(\alpha\beta\gamma)^{-m} + c_5(\alpha\beta\gamma), \end{aligned}$$

where $c_1 \geq 0, c_i > 0, i = 2, 3, 4, q \in [1, 2), s \in [1, 3/2), l \in (1, \infty), m \in (0, \infty)$ and $c_5 = mc_4 - lc_3 - sc_2 - qc_1$. (The term $c_5\alpha\beta\gamma$ is a null Lagrangian and is included so that Φ satisfies the condition $\Phi_{,i}(1, 1, 1) = 0$.) The function (6.21) with the restrictions listed above is also polyconvex, quasiconvex (but not $W^{1,p}$ -quasiconvex (cf. Remark 4.7)) and rank-one convex (cf. Remark 6.6).

Proof of Theorem 6.7. To prove this theorem it is sufficient to show that a function $\Phi \in C^3((\mathbf{R}^>)^3)$ of the form (6.19) satisfying (G1)-(G6) with $q \in [1, 2), r \in (0, 3/2)$ and $s \in [1, 3/2)$ necessarily satisfies SIVALOGANATHAN'S hypotheses (H1), (H2), (H5), (H7), (H9), (H10), (E2), and either (E1) or (E1)'. If so, then by Theorem 6.3 $\mathbf{f}_\lambda$ is not a strong local minimizer, whereas by Proposition 6.4 there is a $\rho_\lambda \in A_\lambda$ which minimizes $I(\cdot)$ on A_λ , and for $\lambda > \lambda_0$ ρ_λ exhibits cavitation.

Assume (G1)-(G6) is satisfied by Φ having the form (6.19) with ϕ, ψ and δ in $C^3(\mathbf{R}^>, \mathbf{R}^\geq)$. By (G1), (G2) and (G6) we have $\phi'' \geq 0, \psi'' \geq 0, \delta'' > 0$. Hence, (H1) is satisfied. The condition (H2) applied to a function of the form (6.19) becomes

$$(6.22) \quad \frac{\lambda_i \phi'(\lambda_i) - \lambda_j \phi'(\lambda_j)}{\lambda_i - \lambda_j} + \frac{\lambda_k^2 [\lambda_i \psi'(\lambda_i \lambda_k) - \lambda_j \psi'(\lambda_j \lambda_k)]}{\lambda_k \lambda_i - \lambda_k \lambda_j} \geq 0,$$

for $\lambda_i \neq \lambda_j$ and $k \neq i, k \neq j$. Clearly, (G4), and (G5), imply (6.22) and therefore (H2). By (6.19)

$$\Phi_{,1}(\lambda, a, a) = \phi'(\lambda) + 2a\psi'(\lambda a) + a^2\delta'(\lambda a^2).$$

Thus since ϕ and ψ are convex and nonnegative (G3) implies that the first part of (H5) holds. The second part of (H5) follows from the convexity of ϕ, ψ , and δ together with (G6)₂. The condition (H7) applied to (6.19) becomes

$$(6.23) \quad \begin{aligned} \frac{\phi'(\lambda_i) - \phi'(\lambda_j)}{\lambda_i - \lambda_j} + \frac{\lambda_k^2 [\psi'(\lambda_i \lambda_k) - \psi'(\lambda_j \lambda_k)]}{\lambda_i \lambda_k - \lambda_j \lambda_k} \\ + \lambda_i \lambda_j \psi''(\lambda_i \lambda_j) + \lambda_i \lambda_j \lambda_k^2 \delta''(\lambda_i \lambda_j \lambda_k) \geq 0 \end{aligned}$$

for $\lambda_i \neq \lambda_j$ and $k \neq i, k \neq j$. Thus the conditions $\psi'' \geq 0, \psi'' \geq 0$, and $\delta'' \geq 0$ imply (6.23) and therefore (H7). Sufficient conditions for (H9) are

$$(6.24) \quad \begin{aligned} \frac{\lambda^2}{(\lambda^3 - 1)^2} \phi(\lambda) &\in L^1(2, \infty), \\ \frac{\lambda^2}{(\lambda^3 - 1)^2} \phi(\lambda^{-2}) &\in L^1(2, \infty), \\ \frac{\lambda^2}{(\lambda^3 - 1)^2} \psi(\lambda) &\in L^1(2, \infty), \\ \frac{\lambda^2}{(\lambda^3 - 1)^2} \psi(\lambda^{-1}) &\in L^1(2, \infty), \end{aligned}$$

However (G1) with $q \in [1, 2)$ and $r \in (0, 3/2)$ implies (6.24)_{1,2}, while (G2) with $s \in [1, 3/2)$ implies (6.24)_{3,4}. The conditions $\delta'' > 0$ (from (G7)) and $\delta'(t) \rightarrow +\infty$ as $t \rightarrow +\infty$ (from (G3)) and the nonnegativity of ϕ and ψ imply (H10). Recalling Remark 6.6, we verify (E1)' rather than (E1). Clearly, (G2) implies (E1)_{ii}, while the convexity of δ yields

$$(6.25) \quad \delta(t) \geq \delta\left(\frac{t}{2}\right) + \frac{t}{2} \delta'\left(\frac{t}{2}\right).$$

We divide (6.25) by t and let $t \rightarrow +\infty$; it then follows from (G3) that (E1)_i' is satisfied, completing the verification of (E1)'. Finally, (E2) follows from (G4)₂, (G5)₂, (G6)₃, the triangle inequality, and the fact that ϕ and ψ are nonnegative. $\square$

Remark 6.9. STUART [1985] gives existence theorems for radial equilibrium solutions with cavities under constitutive hypotheses that differ from those of SIVALOGANATHAN. STUART does not examine the stability of his solutions but he does compare the energy of the homogeneous deformation $\mathbf{h}(\mathbf{x}) = \lambda \mathbf{x}, \mathbf{x} \in \mathcal{B}$, with the energy of solutions $\mathbf{f}_\lambda$ that exhibit cavitation and satisfy $\mathbf{f}_\lambda(\mathbf{x}) = \lambda \mathbf{x}, \mathbf{x} \in \partial \mathcal{B}$. He also gives similar results for boundary conditions of pressure and dead loading, which we do not discuss here. In our terminology his existence theorem states that under his constitutive hypotheses A1 - A7 (discussed below) there is a radial deformation $\mathbf{f}_\lambda(\mathbf{x}) = [\rho_\lambda(P)/P] \mathbf{x}$ that satisfies

$$(6.26) \quad \begin{aligned} \rho_\lambda &\in C^0([0, 1]) \cap C^2((0, 1)), \\ \rho_\lambda(1) &= \lambda > 0, \quad \rho'_\lambda > 0 \text{ on } (0, 1), \end{aligned}$$

$$[\rho^2 \Phi_1, (\rho'_\lambda(P), \rho_\lambda(P)/P, \rho_\lambda(P)/P)]' = 2P \Phi_{,2}(\rho'_\lambda(P), \rho_\lambda(P)/P, \rho_\lambda(P)/P).$$

Furthermore, he shows that there is $\lambda_0 > 0$ such that for $0 < \lambda \leq \lambda_0$

$$(6.27) \quad \rho_\lambda(P) = \lambda P,$$

while for $\lambda > \lambda_0$ there are exactly two solutions of (6.26), one given by (6.27) and the other of which exhibits cavitation and satisfies $T(P) \rightarrow 0$ as $P \rightarrow 0$. Here, $T(P)$ is the radial component of the Cauchy stress defined by (6.11).

Thus, according to Theorem 6.3 STUART's equilibrium solutions will be unstable relative to the formation of filamentary voids in the case where the stored energy function satisfies both his (A1)-(A7) and our (S1) and (S2). A relatively easy special case to work-out is the case of a function $\Phi(\alpha, \beta, \gamma)$ of the form (6.19) with ϕ, ψ, δ in $C^3((0, \infty))$ and satisfying (G1), (G2), and (G3) with $c > 0, r = 0, q \in [1, 2)$, and $s \in (1, 3/2)$. A lengthy computation shows that this stored energy function also satisfies STUART's (A1)-(A7) if

$$\begin{aligned} \text{(J1)} \quad & \phi' \geq 0, \phi'' \geq 0, \\ & \phi'(t) \leq A + Bt^v, \\ & t\phi''(t) \leq A + Bt^v, \\ \text{(J2)} \quad & \psi' \geq 0, \psi'' > 0 \\ & t\psi''(t) \leq A + Bt^w, \\ \text{(J3)} \quad & \delta''(t) > \delta_0 > 0, \\ & \delta'(t) < -A/t, 0 < t < t_0, \end{aligned}$$

for some constants $A > 0, B > 0, v \in (0, 2), w \in (0, 1/2)$, and $t_0 > 0$. A simple function satisfying all the hypotheses is given by (6.21) with $s > 1, l \geq 2$, and the qualifications listed there. Note that for the function (6.21) SIVALOGANATHAN's constitutive hypotheses are also satisfied so that in this case the cavitating equilibrium solutions found by STUART are also radial minimizers.

7. The Filamentary Void and Crazing in Glassy Polymers. We have shown that under appropriate constitutive hypotheses, a material that at some point has principal stretches $\lambda, \lambda, \alpha(\lambda)$ with $0 < c_1 < \lambda^2 \alpha(\lambda) < c_2$ and λ sufficiently large is unstable relative to the formation of a filamentary void. These constitutive hypotheses embody the idea that the material is stiff for large equibiaxial stretches and is soft for a certain isochoric family of shear deformations. The generalization of our results given at the end of Section 5 shows that a similar instability involving the formation of a filamentary void with elliptical cross-section is possible with principal stretches

$$\left. \begin{aligned} \lambda_1 &= k_1 \lambda \\ \lambda_2 &= k_2 \lambda \\ \lambda_3 &= \alpha(\lambda) \end{aligned} \right\}, \quad k_1 > 0, k_2 > 0, 0 < c_1 < \lambda^2 \alpha(\lambda) < c_2$$

and with λ sufficiently large. The void is termed a *filamentary void* because our methods require that it be made long and thin in order that the energy reducing nature of the essentially cylindrical deformation compensates for the energy excess in the tip region. Our hypotheses that promote the formation of filamentary voids as $\lambda \rightarrow +\infty$ place no restriction on the dilatational behavior of the stored energy; h in S2 is an assignable function.

The geometry of the filamentary void suggests a possible connection with the phenomena of crazing in polymers such as polystyrene (low molecular weight), polycarbonate, and

polymethyl methacrylate. In this section we present some qualitative evidence both for and against this connection.

Many authors who have studied crazing have interpreted it in terms of a material instability. That is, it is found to be an instability that occurs when certain conditions on stress, strain, and temperature are met locally and is independent of the nature of the loading device or the boundary conditions, unlike a buckling instability or the Treloar (*cf.*, *e.g.* CHEN [1987]) instability. This is especially clear from work of DEKKERS & HEIKENS [1983] who compare a variety of crazing criteria to tensile experiments on polystyrene containing either well-adhering or poorly adhering glass beads. The adherence of the beads does not directly affect their criteria although it drastically changes the local stress distribution. Our treatment of filamentary voids similarly treats them as material instabilities, this idea being directly embodied in Theorem 4.2.

An early and influential treatment of crazing was given by STERNSTEIN, ONGCHIN, & SILVERMAN [1968] and later modified by STERNSTEIN & ONGCHIN [1969]. They drilled 1/16" holes in 1/2" $\times$ 2" $\times$ 1/31" strips of polymethyl methacrylate and pulled them in tension. Crazes (long thin voids) appeared in the specimen in regions adjacent to the hole; the crazes assumed curvilinear trajectories beginning at the surface of the hole. Most of the crazes occurred in two symmetric regions that were near poles of the hole that were connected by a diameter that was *perpendicular* to the tensile axis. STERNSTEIN, ONGCHIN, & SILVERMAN [1968] observed both the directions of the crazes and the shape of the region of predominantly crazed material. To arrive at a criterion for crazing, they calculated a linear elastic solution for the stress field near a hole in an infinite plate pulled in tension. They found that the individual crazes pointed in the direction of the principal axis of stress corresponding to the *minimum* principal stress, while the first formation of a craze was governed by the *value* of the maximum principal stress σ_1 . They also inferred from the absence of crazing in compression that conditions of dilatation ($\text{tr}\mathbf{T} > 0$, *cf.* (3.1)) were necessary for craze formation. It is clear from their principal stress contours that various other criteria besides $\sigma_1 = \sigma_{crit}$ would also fit the shape of the crazed zone and in [1969] STERNSTEIN & ONGCHIN formulated a craze criterion based on $\text{tr}\mathbf{T} := \sigma_1 + \sigma_2 + \sigma_3$ and the *stress bias* $\sigma_1 - \sigma_2$. Here $\sigma_3 \leq \sigma_2 \leq \sigma_1$ represent the principal Cauchy stresses. STERNSTEIN, ONGCHIN, & SILVERMAN also state [1968] : "... [T]he craze always propagates transverse to the major principal stress vector, thereby maximizing the spreading stress on the tip of the craze. ... The requirement that the formation of a craze necessitates an anisotropic driving force is stated by eq. (15) [$\sigma_1 \neq \sigma_2, \sigma_1 \neq \sigma_3$]"'. These remarks and our calculation seem to reflect a similar point of view.

DEKKERS & HEIKENS [1983] also compare various crazing criteria to results of their experiments on $10^{-5}m$ glass beads embedded in polystyrene. They find that either a criterion for the maximum principal stress or the dilatation ($\lambda_1 + \lambda_2 + \lambda_3$) can match their experimental results; they do not examine the stress-bias criterion of STERNSTEIN & ONGCHIN, nor do they compare principal stress axes with the trajectories of the crazes.

The idea that dilatation alone is a criterion for crazing seems to us to be inconsistent with the ideas of STERNSTEIN, ONGCHIN, & SILVERMAN quoted above, and also does not relate very well to our calculation, as discussed below.

In recent years a great deal of information on the microstructure of crazes has emerged, as presented for example in the review article by KRAMER [1983]. It is found that the crazes observed for example by STERNSTEIN, ONGCHIN, & SILVERMAN and DEKKERS & HEIKENS consist of thin bands of fibrous material with the fibers lying in a direction perpendicular to the band. As pictured by KRAMER [1983, Fig. 2c], a craze in its early stages of formation consists of many small filamentary voids. A striking photograph of these voids is shown by DONALD, CHEN & KRAMER [1981, Fig 1c]. Once a craze band is established, a meniscus instability similar to the Saffman-Taylor instability is regarded as a mechanism for the advance of the craze tip. This mechanism is based on surface energy considerations at the craze tip and contains no bulk energy contribution of the polymer; in the analysis the polymer is modelled as a non-Newtonian fluid. This theory does not fit very well with our suggestion, which would be more in line with the idea that during advance of the craze tip, the local stress field nearby would satisfy conditions so as to form a filamentary void.

GENT [1970] proposes a rather different criterion for crazing. Noting that crazing only occurs in glassy polymers that are capable of transformation to the rubbery state, he proposes a mechanism whereby the material at a stress concentration first experiences a stress-induced phase transformation and then undergoes cavitation. Using his criterion for (spherical) cavitation (eq. (1.1)) in the rubbery region, he then is able to account for the effect of pressure, preorientation and the presence of craze inducing liquids and vapors on crazing. The agreement between his theory and experiment, covering several very different physical phenomena, cannot be ignored. However, his cavitation criterion for the rubbery region could be replaced by a criterion for the formation of a filamentary void, rather than a spherical one.

The idea that the material undergoes a stress-induced phase transformation at a flaw could easily be built into a stored energy function. For example, stored energy functions that exhibit martensitic and other structural phase transformations have been studied by ERICKSEN [1988] JAMES [1986] and many others. In these studies, calculations of the effect of stress on transformation temperature are in excellent agreement with experiment. The hypotheses on the stored energy function $\Phi(F, T)$ needed to cause a stress-induced phase transformation do not contradict our hypotheses S1 and S2, which promote the formation of a filamentary void. Thus, a single stored energy function could be defined that necessarily gives a stress-induced phase transformation at an appropriate flaw and that also promotes void formation in the transformed zone, although at this time we would be more inclined to search for the possibility of a filamentary void in this zone.

Indirect support for both GENT's hypothesis and the use of thermoelastic energy functions comes from recent work of PLUMMER & DONALD [1989]. They show that in some polymers that exhibit high entanglement density and low molecular weight (such as polycarbonate) crazes will heal. That is, upon heating the crazed material to above the glass transition, the crazes disappear in the optical microscope and the material recovers its original material properties.

Several studies¹² have focussed on the competition between crazing and shear yielding in polycarbonate, polystyrene, and polyphenylene oxide. Presumably a stored energy function could be defined that exhibited both the formation of filamentary voids and shear bands, the latter being a material instability associated with a loss of ellipticity of the stored energy function¹³. Such a competition does not seem to be inconsistent with GENT's hypotheses, since many of the energy functions appropriate for materials that undergo stress-induced phase transformations in fact lose ellipticity at some deformation gradient.

Although the filamentary void forming deformation is not in general an energy minimizer, it is interesting to determine the energy reduction per unit volume achieved by different distributions of filamentary voids. In order to obtain more energy reduction it is clear that one should use as little cap (see Section 5c) as possible, since there is an energy penalty proportional to the volume of the cap for each one used. More precisely, suppose that the unit cube is subject to a pure stretch with principal stretches $(\lambda, \lambda, \hat{\alpha}(\lambda))$ with $\lambda \geq \lambda_0$ (see Proposition 5.3). The deformation $\mathbf{f}^L$ used in Theorem 5.5 creates a filamentary void with domain

$$0 < R < R_0, -(L+3) < x_3 < L+3,$$

and achieves an energy reduction

$$\Delta E_1 \leq 2(K_1 - \kappa \lambda^q L),$$

where K_1 and κ are independent of L . If we scale $\mathbf{f}^L$ using the usual scaling laws of nonlinear elasticity, we find that the deformation $\mathbf{f}_\mu^L(\mathbf{x}) := \mu \mathbf{f}^L(\mu^{-1}\mathbf{x})$ occupies the domain

$$0 < R < R_0, -\mu(L+3) < x_3 < \mu(L+3)$$

and achieves an energy reduction

$$\Delta E_\mu \leq 2\mu^3(K_1 - \kappa \lambda^q L).$$

¹²*cf.*, *e.g.* DONALD & KRAMMER [1982], DEKKERS & HEIKENS [1985], DONALD [1985], and PLUMMER & DONALD [1989].

¹³Analyses of the formation of shear bands in nonlinear elasticity due to a loss of ellipticity are given by many authors, see *e.g.* KNOWLES & STERNBERG [1978], ABEYARATNE [1980].

Thus, in order to insert a periodic array of $n \times n$ filamentary voids in the unit cube we set $\mu := (2nR_0)^{-1}$ and $L := nR_0 - 3$ to achieve the energy reduction

$$(7.1) \quad \begin{aligned} n^2 \Delta E_{(2nR_0)^{-1}} &\leq 2n^2 (2nR_0)^{-3} (K_1 - \kappa \lambda^q (nR_0 - 3)) \\ &= \frac{1}{4R_0^3} \left(\frac{K_1 + 3\kappa \lambda^q}{n} - \kappa \lambda^q R_0 \right), \end{aligned}$$

which shows that many filamentary voids lowers the energy more than a few voids occupying the same volume. This should be contrasted with a similar calculation due to BALL (private communication ; *cf.* also BALL & MURAT [1984, Prop. 2.3]) which shows that a single spherical void at the center of a ball gives the *same* energy reduction as a ball filled with small spherical voids. The reason for this is due to the caps which scale differently than the cylindrical holes and which are regions of excess energy. The inclusion of surface energy proportional to the area of the new surface formed would contribute a positive term proportional to n to the right hand side of (7.1) and therefore would mediate against the formation of infinitely many voids. It is interesting (but perhaps misleading) to note that crazes often consist of bands containing many fine parallel voids.

An unsatisfactory aspect of the present analysis is that the behavior of the material appears to be crucially dependent on the growth of the stored energy function for arbitrarily large stretches and this growth can never be directly examined experimentally (This point is also discussed BALL [1982].) This feature is really a defect of the analysis. That is, it is extremely likely that all materials satisfy “slow” growth hypotheses for large stretches and therefore permit the formation of various kind of spherical, elliptical, and filamentary voids. For example, Cauchy’s molecular theory of elasticity gives the stored energy function

$$(7.2) \quad \Phi(\mathbf{F}) = \frac{m}{(\mathbf{e}_1 \times \mathbf{e}_2) \cdot \mathbf{e}_3} \sum_{n^1, n^2, n^3} \phi(|n^i \mathbf{F} \mathbf{e}_i|),$$

where $\mathbf{F}$ is the deformation gradient ($\mathbf{e}_i$) are reference lattice vectors, m is the mass of an atom, and the sum is taken over all triples of integers. A popular choice of the central force potential ϕ gives $\phi(r) \sim r^{-6}$, for large r , which implies that for every fixed $\mathbf{F} \in \text{Lin}^>$

$$(7.3) \quad \Phi(t\mathbf{F}) \longrightarrow 0 \quad \text{as} \quad t \longrightarrow \infty.$$

It is then realized that at sufficiently large stretches voids may occur (as well as the possibility of shear instability¹⁴) and the other features of the stored energy become important in deciding which instability comes first. For example, GENT & LINDLEY’S [1958] criterion for spherical cavitation $P_{crit} = -5E/6$ only depends on the single easily accessible constant E , the Young’s modulus, but behind this criterion is the assumption that the stored

¹⁴Cauchy’s energy (7.2) fails the condition of strong ellipticity, as discussed, for example, by ERICKSEN [1977].

energy has a simple form (verified experimentally for moderate stretches) that satisfies the crucial growth hypothesis

$$\int_1^\infty \left[\frac{d\hat{\Phi}/dv}{v^3 - 1} \right] dv < \infty,$$

where $\hat{\Phi}(v) = \Phi(v^{-2}, v, v)$ and the material is assumed to be incompressible.

A final objection against the present approach could be the failure to account for viscoelastic properties of the polymer, particularly for T near T_g , the glass transition temperature, although many of the above mentioned criteria for crazing have relied on interpreting the experiments in terms of pure elasticity. This objection does not appear particularly difficult in that most viscoelasticity theories have a Lyapunov function consisting of a nonlinear elastic energy. If it is possible to reduce this energy by inserting a void, then it is likely that the associated viscoelasticity theory will have a dynamic solution¹⁵ involving the creation and evolution of a similar void. Of course, verifying this property for general theories of viscoelasticity involves great mathematical difficulties. In special cases, however, this hope is often borne out, for example, in the analysis by CALDERER [1986] of the radial motion of a viscoelastic sphere containing a void. Her principal hypothesis is a slow growth assumption on the underlying elastic energy, and under sufficiently large imposed hydrostatic tension a pre-existing hole grows suddenly to infinite size. The physical interpretation of the nonlinear elastic/viscoelastic relation described here is that under appropriate time independent boundary conditions, a void or filamentary void eventually appears.

In summary, the formation of a filamentary void warrants further study as a possible explanation for crazing in glassy polymers. To test the idea, critical conditions for the formation of a filamentary void must be determined and meaningful stored energy functions for polymers must be found. Ideally, these functions would also model the glass transition (including the observed effect of stress on transition temperature) so a direct connection with GENT'S [1970] proposal could be established. Measurements of mechanical properties under carefully controlled conditions of multiaxial stress are particularly important. The difficulty with obtaining critical conditions for void formation from the theory is that the filamentary void has a complex geometry, particularly near the tip of the void. With a leap of faith, we would guess that in the equibiaxial case such critical conditions might turn out to be

$$\lambda_{crit}^\alpha, \lambda_{crit}^\alpha, \alpha,$$

where λ_{crit}^α is the critical condition for *circular* void formation in the radial deformation of a two-dimensional elastic material defined by

$$\Phi^\alpha(\lambda_1, \lambda_2) = \Phi(\lambda_1, \lambda_2, \alpha).$$

¹⁵PERICAK-SPECTOR & SPECTOR [1988] show that the equations of dynamic nonlinear elasticity have a time-dependent solution involving the creation and evolution of a spherical void.

This guess is mainly based upon the observation in Theorem 5.5 that the energy contribution of the caps scales away for long thin voids. The formation of a filamentary void also seems to be possible (under different constitutive hypotheses) when λ_1 and λ_2 are fixed and $\alpha > \alpha_{crit}$. A further speculation is that essentially the same critical conditions would be obtained for a sufficiently small preexisting filamentary void. This speculation is based on the fact that a similar connection between the creation of spherical voids and the growth of a preexisting spherical void has been established by SIVALOGANATHAN [1986a]. A criterion such as the one given above would seem to indicate that commonly quoted criteria such as a “dilatational stress field” or “adequate free volume” are not sufficient conditions for crazing. Finally, a potential advantage of the present approach is the same advantage enjoyed by GENT & LINDLEY’S criterion for spherical voids - that conditions for instability are only dependent on measureable nonlinear elastic properties of the solid.¹⁶

8. Appendix. Interpenetration of Matter and Function Spaces for Elasticity. In our definition of a deformation we explicitly included the hypothesis that deformations are 1-1, a reasonable requirement for elasticity. In this Appendix we show that if this requirement is dropped and one just minimizes the total energy in the space

$$\{\mathbf{f} \in W^{1,p}(\Omega) \cap L^\infty(\Omega) : \det \nabla \mathbf{f} > 0 \text{ a.e.}\},$$

$1 \leq p < 3$, then one will obtain physically unreasonable results for very simple boundary value problems under very mild constitutive hypotheses.

The idea behind these results is that the local invertibility constraint $\det \nabla \mathbf{f} > 0$ a.e. is not sufficiently strong to prevent interpenetration of matter in the space $W^{1,p}(\Omega) \cap L^\infty(\Omega)$, $1 \leq p < 3$, and under severe compressive boundary conditions, the material can relax severe compressive strains and therefore reduce the energy by interpenetrating.

We do not know what is the appropriate function space for elasticity. However, we think that such a space should allow for the formation of spherical and filamentary voids, should satisfy the constraint $\mathbf{f}(\Omega) \subset \mathbf{d}(\Omega)$, should restrict minimizers to be 1-1, and should permit $h_\lambda(\mathbf{x}) := \lambda \mathbf{x}$, $\lambda \ll 1$, to be a minimizer for the displacement problem for a large class of reasonable stored energy functions.

Remark 8.1. BALL [1981] & SVERAK [1988] have obtained results in which the global invertibility of a function is a consequence of the local constraint $\det \nabla \mathbf{f} > 0$. However the underlying function spaces that they use do not allow deformations that create holes.

For simplicity we now assume that the body in its reference configuration occupies the unit ball

$$\mathcal{B} := \{\mathbf{x} \in \mathbb{R}^3 : |\mathbf{x}| < 1\}$$

¹⁶Another advantage is the accessibility of the present approach to comprehensive parameter studies which can be directly compared with experiment. For example, the effect of superimposed hydrostatic or nonhydrostatic pressure, and of changes in the linearized moduli (Young’s modulus and Poisson’s ratio) on the critical conditions for the formation of a filamentary void can be studied.

and, for $1 \leq p \leq \infty$, we let

$$A_\lambda^p := \{\mathbf{f} \in W^{1,p}(\mathcal{B}) \cap L^\infty(\mathcal{B}) : \det \nabla \mathbf{f} > 0 \text{ a.e. and } \mathbf{f}(\mathbf{x}) = \lambda \mathbf{x} \text{ on } \partial \mathcal{B}\}.$$

PROPOSITION 8.2. *Suppose that the stored energy satisfies the following constitutive hypotheses:¹⁷*

- (I1) $\lim_{\lambda \rightarrow 0^+} \Phi(\lambda, \lambda, \lambda) = +\infty$,
- (I2) $t \mapsto \Phi(t^{1-q}, t, t) t^{1-q} \in L^1((0, 1))$,
- (I3) $t \mapsto \Phi(t^{1-r}, t, t) t^{-4} \in L^1((1, \infty))$,

for some $q \in (1, \infty)$ and $r \in (0, \infty)$. Then there is a $\lambda_0 > 0$ such that for every $\lambda \in (0, \lambda_0)$

$$(8.1) \quad \inf_{\mathbf{f} \in A_\lambda^p} E(\mathbf{f}, \mathcal{B}) < E(\lambda \mathbf{x}, \mathcal{B})$$

whenever $p < \min\{3, q/(q-1)\}$.

Remark 8.3. The competitor $\mathbf{f}_\lambda$ used to prove Proposition 8.2 belongs to A_λ^p and therefore satisfies $\det \nabla \mathbf{f}_\lambda > 0$ a.e. but is not 1-1. However, $\mathbf{f}_\lambda$ does satisfy the constraint $\mathbf{f}_\lambda(\mathcal{B}) \subset \mathbf{d}_\lambda(\mathcal{B})$ where $\mathbf{d}_\lambda(\mathbf{x}) = \lambda \mathbf{x}$, $\mathbf{x} \in \overline{\mathcal{B}}$ (see Remark 4.1). Note that the constitutive hypotheses (I1)-(I3) are extremely mild.

For an elastic fluid we obtain a more precise result.

PROPOSITION 8.4. *Let the stored energy be given by*

$$(8.2) \quad W(\mathbf{F}) = \delta(\det \mathbf{F}),$$

where δ has a strict global minimum at $\Delta > 0$. Then, for $p \in [1, 3/2)$ and $\lambda^3 \neq \Delta$,

$$(8.3) \quad \inf_{\mathbf{f} \in A_\lambda^p} E(\mathbf{f}, \mathcal{B}) < E(\lambda \mathbf{x}, \mathcal{B}).$$

Moreover, a global minimizer of the total energy $E(\cdot, \mathcal{B})$ in A_λ^p is given by

$$(8.4) \quad \mathbf{f}_\lambda(\mathbf{x}) := \frac{\rho(P)}{P} \mathbf{x}, \quad \rho(P) := (P^3 + \lambda^3 - \Delta)^{1/3},$$

which exhibits interpenetration of matter for $\lambda^3 < \Delta$ and cavitation for $\lambda^3 > \Delta$. If $\lambda^3 > \Delta$, $\mathbf{f}_\lambda$ as defined by (8.4) is a global minimizer of the total energy $E(\cdot, \mathcal{B})$ in A_λ^p for $1 \leq p < 3$.

Remark 8.5. In the terminology of BALL & MURAT [1984] Proposition 8.4 implies that, for $1 \leq p < 3/2$, the stored energy given by (8.2) is not $W^{1,p}$ -quasiconvex at $\lambda \mathbf{I}$

¹⁷Actually we need not make I1 as a separate hypotheses since it is a consequence of the continuity of W and the fact that $W(\mathbf{F}) = +\infty$ for $\det \mathbf{F} \leq 0$.

unless λ^3 is the global minimizer of δ . A related result of BALL & MURAT [1984, Theorem 4.1 (iii)] is that, for $1 \leq p < 3$, W as given by (8.2) is $W^{1,p}$ -quasiconvex at *every* $\mathbf{A} \in \text{Lin}$ if and only if h is constant.

Proof of Proposition 8.2. Let $\lambda \in (0, 1/3)$, consider the function

$$(8.5) \quad \mathbf{f}_\lambda(\mathbf{x}) := \frac{\rho(P)}{P} \mathbf{x}, \quad \rho(P) := \begin{cases} -(\lambda^r - P^r)^{r^*}, & 0 \leq P < \lambda 2^{-r^*} \\ -(A^q - P^q)^{q^*}, & \lambda 2^{-r^*} \leq P < A \\ (P^q - A^q)^{q^*}, & A \leq P < \hat{\lambda} A \\ \lambda P, & \hat{\lambda} A \leq P < 1 \end{cases},$$

where $A := \lambda/2^{(r^*-q^*)}$, $\hat{\lambda} := (1 - \lambda^q)^{-q^*}$, $q^* := 1/q$, and $r^* := 1/r$.

We will show that $\mathbf{f}_\lambda \in W^{1,p}(\mathcal{B})$ and that, for λ sufficiently small $\mathbf{f}_\lambda$ has less total energy than the homogeneous deformation $\mathbf{f}(\mathbf{x}) = \lambda \mathbf{x}$.

We first compute the total energy of $\mathbf{f}_\lambda$. By Lemma 6.1 we find, with the aid of (3.2) and (8.5), that

$$E(\mathbf{f}_\lambda, \mathcal{B}) = 4\pi\lambda^3[E_1 + E_2 + E_3 + E_4],$$

$$(8.6) \quad \begin{aligned} E_1 &:= \lambda^{-3} \int_0^{\lambda/2^{r^*}} \Phi(\dot{\rho}, -\frac{\rho}{P}, -\frac{\rho}{P}) P^2 dP, \quad E_2 := \int_{\lambda/2^{r^*}}^A \Phi(\dot{\rho}, -\frac{\rho}{P}, -\frac{\rho}{P}) P^2 dP, \\ E_3 &:= \lambda^{-3} \int_A^{\hat{\lambda}A} \Phi(\dot{\rho}, \frac{\rho}{P}, \frac{\rho}{P}) P^2 dP, \quad E_4 := \lambda^{-3} \int_{\hat{\lambda}A}^1 \Phi(\dot{\rho}, \frac{\rho}{P}, \frac{\rho}{P}) P^2 dP. \end{aligned}$$

In order to compute E_1 we make the change of variables $w = -\rho/P$ and note that, by (8.5)

$$\dot{\rho} = w^{1-r}, \quad P = \lambda/(1 + w^r)^{r^*}$$

and hence

$$E_1 = \int_1^\infty \Phi(w^{1-r}, w, w) g_r(w) dw, \quad g_r(w) := \frac{w^{r-1}}{(1 + w^r)^{\frac{r+3}{r}}}.$$

Similarly, the change of variables $w = -\rho/P$ in E_2 and the change of variables $v = \rho/P$ in E_3 yield

$$E_2 = K \int_0^1 \Phi(w^{1-q}, w, w) g_q(w) dw, \quad E_3 = K \int_0^{\hat{\lambda}} \Phi(v^{1-q}, v, v) g_q(v) dv,$$

where $K = K(q, r) = 8^{q^*-r^*}$. It is now clear that I2 and I3 are necessary and sufficient for E_1 , E_2 , and E_3 to be finite.

We next compute

$$\begin{aligned} E(\lambda \mathbf{x}, \mathcal{B}) &= 4\pi\lambda^3[\lambda^{-3} \int_0^{\lambda A} \Phi(\lambda, \lambda, \lambda) P^2 dP + E_4] \\ &= 4\pi\lambda^3[K\Phi(\lambda, \lambda, \lambda)/3(1 - \lambda^q)^{3/q} + E_4]. \end{aligned}$$

Thus

$$E(\mathbf{f}_\lambda, \mathcal{B}) - E(\lambda \mathbf{x}, \mathcal{B}) \leq 4\pi\lambda^3[E_1 + E_2 + E_3 - k\Phi(\lambda, \lambda, \lambda)]$$

for $\lambda \in (0, 2^{-r^*})$, where $k > 0$ is independent of λ .

We note that I2 and I3 imply that E_1 , E_2 , and E_3 are bounded independently of λ and hence that I1 implies that

$$E(\mathbf{f}_\lambda, \mathcal{B}) < E(\lambda \mathbf{x}, \mathcal{B})$$

for sufficiently small λ .

In order to prove that $\mathbf{f}_\lambda \in A_\lambda^p$ we first note that it is clear from (8.5) that $\mathbf{f}_\lambda \in L^\infty(\mathcal{B})$ and that $\mathbf{f}_\lambda(\mathbf{x}) = \lambda \mathbf{x}$ for $\mathbf{x} \in \partial \mathcal{B}$. In addition the definition (8.4) shows that ρ is continuous and piecewise differentiable. Thus, by Lemma 6.1, all we need to show is that ρ , as given by (8.5), satisfies

$$(8.7) \quad \hat{E} := \int_0^1 [|\dot{\rho}(P)|^p + 2|\frac{\rho(P)}{P}|^p] P^2 dP < +\infty.$$

Consider the function

$$\hat{W}(\mathbf{F}) = \hat{\Phi}(\lambda_1(\mathbf{F}), \lambda_2(\mathbf{F}), \lambda_3(\mathbf{F})) = \lambda_1^p + \lambda_2^p + \lambda_3^p.$$

Then, by (8.5), (8.7), and the changes of variables used in the first part of this proof we find that

$$\int_{\mathcal{B}} \hat{W}(\nabla \mathbf{f}_\lambda) d\mathbf{x} = 4\pi \hat{E} = 4\pi\lambda^3[\hat{E}_1 + \hat{E}_2 + \hat{E}_3 + \hat{E}_4],$$

$$\begin{aligned} \hat{E}_1 &:= \int_1^\infty (w^{p(1-p)} + 2w^p) g_r(w) dw, \quad \hat{E}_2 := K \int_0^1 (w^{p(1-q)} + 2w^p) g_q(w) dw, \\ \hat{E}_3 &:= K \int_0^\lambda (v^{p(1-q)} + 2v^p) g_q(v) dv, \quad \hat{E}_4 := \lambda^{-3} \int_{\lambda A}^1 3\lambda^p P^2 dP. \end{aligned}$$

Thus $\hat{E}_1 < +\infty$ provided $p < 3$ while $\hat{E}_2 < +\infty$ and $\hat{E}_3 < +\infty$ follow from $p < q/(q-1)$. $\square$

Proof of Proposition 8.4. If we cube (8.5) and then differentiate with respect to P we find that

$$\dot{\rho}(P) \frac{\rho(P)^2}{P^2} = \Delta, \quad 0 < P < 1.$$

Thus by Lemma 6.1, (8.2), and the fact that δ has a strict global minimum at Δ we conclude that $\mathbf{f}_\lambda$, as given by (8.4), is a global minimizer of the total energy. It is clear that $\mathbf{f}_\lambda$ exhibits interpenetration of matter for $\lambda^3 < \Delta$ and cavitation for $\lambda^3 > \Delta$.

In order to complete the proof we must determine the values of p for which $\mathbf{f}_\lambda \in A_\lambda^p$. If $\lambda^3 > \Delta$ then $\dot{\rho}$ is bounded on $(0,1)$ and hence it is clear from (6.3) and (8.4) that $1 \leq p < 3$. If $\lambda^3 < \Delta$ then $\dot{\rho}$ is singular at $P^3 = (\Delta - \lambda^3)/\Delta$. In this case the changes of variables used in Proposition 8.2 can be used to show that $\mathbf{f}_\lambda \in A_\lambda^p$ for $1 \leq p < 3/2$. $\square$

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**FEEDBACK, DELAYS AND THE ORIGIN
OF BLOOD CELL DYNAMICS**

By

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Feedback, Delays and the Origin of Blood Cell Dynamics

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ABSTRACT

This paper reviews a variety of models for the regulation of hematopoiesis that are most naturally framed as nonlinear differential delay equations, and which are often obtained from partial differential equations. We review the development of these models, and point out a number of interesting mathematical questions raised by the biology, including the effects of multiple delays, distributions of delays, state dependent delays, and nonconstant initial functions. The range of insight given by the modelling to experimentally and clinically observed dynamics is discussed.

INTRODUCTION

The dynamics of many biological variables, $x(t)$, can be modeled by the differential equation¹⁻²

$$\begin{aligned}\frac{dx}{dt} &= \text{Production rate} - \text{Destruction rate} \\ &= P-D\end{aligned}\tag{1}$$

Typically P and/or D are highly nonlinear functions of the state variable at some time, τ in the past, $x(t - \tau)$, as well as depending on the current value of $x(t)$, i.e.

$$\frac{dx}{dt} = P(x(t), x(t - \tau), \mu_1, \mu_2, \dots) - D(x(t), x(t - \tau), \mu'_1, \mu'_2, \dots)\tag{2}$$

where the $\mu_i, \mu'_i, i = 1, 2, \dots$ are control parameters which, in comparison to the state variable, either do not change with time, or change so slowly that they can be regarded as constant by the investigator. In order to solve the differential delay equation (2) it is necessary to specify an initial function on the interval $[-\tau, 0]$. In this sense differential delay equations like eq. (2) are infinite dimensional systems. Differential delay equations have a rich literature³⁻⁴.

Equation (2) is to be contrasted with models typically encountered in the physical sciences where the dynamics are often described by differential equations in which the right hand side is an instantaneous function of $x(t)$. In biology, the time delays are often inherent properties of the control mechanisms and arise, for example, because of non-zero conduction times in the nervous system, the cell cycle time or maturation time in replicating cellular populations, delays due to transcription or translation in the genome and circulatory times in the cardiovascular system⁵⁻⁸.

Differential delay equations have been used to model the control of respiration⁵⁻⁶, the pupil light reflex⁹⁻¹², blood cell dynamics¹³⁻²⁵, simple neural networks²⁶⁻²⁸, population

growth²⁹, protein synthesis^{30–31}, optical^{32–33} and acousto-optical³⁴ bistability and the dynamics of economic commodity markets^{35–36}. Here we focus on applications of Eq. (2) for modelling the control of blood cell numbers with references to other physiological contexts. Mathematical investigations of the control of blood cell dynamics continue to provide important insights into the properties of the hematological regulatory systems. In addition, we draw attention to experimental and clinical observations which suggest the importance of extending these studies to situations which, to our knowledge, have not been explored mathematically.

CONTROL OF HEMATOPOIESIS

The formation of red blood cells (erythrocytes), white blood cells (granulocytes) and platelets (thrombocytes) primarily occurs in the bone marrow (see references 37-39 for a general discussion). A simplified schematic representation of normal hematopoiesis is shown in Figure 1. As depicted there, a self-maintaining pluripotential stem cell population (PPSC) is thought to exist which is capable of producing committed stem cells (CSC) specialized for the erythroid, granuloid and thromboid cell lines. The influx of cells from the PPSC to the CSC lines is regulated in two ways: 1) long range humoral mechanisms (labeled LR in Figure 1); and 2) local environmental mechanisms which are as yet poorly understood

The long range humoral substances regulating the erythroid (erythropoietin) and thromboid (thrombopoietin) cell lines are primarily produced by the kidney, but extra-renal sites such as liver may also be of importance. A variety of substances possessing granulopoietic activity have been isolated from T lymphocytes, monocytes, endothelial cells and fibroblasts. An intrinsic property of these feedback mechanisms is the presence of time delays which range from seconds (e.g. circulatory time) to days (e.g. maturational times).

Under normal circumstances marked fluctuations in blood cell number do not seem to be present. In humans abnormal oscillations in blood cell number occur in a group of disorders collectively referred to as periodic hematological diseases (for a recent review see reference 40). The periodic hematological diseases include periodic hematopoiesis (also referred to as cyclic neutropenia)^{41–42}, cyclic thrombocytopenia⁴³, cyclic eosinophilic myositis and hyper-immunoglobulin E syndrome⁴⁴ and the periodic variants of chronic myelogenous leukemia^{45–46} and autoimmune hemolytic anemia^{47,48}. In addition, oscillations in granulocyte number have been observed following the administration of chemotherapeutic agents to patients with chronic myelogenous leukemia⁴⁹.

Experimental study of the periodic hematological diseases has sometimes been facilitated by the availability of suitable animal models. For example, all gray collies have periodic hematopoiesis^{50–51}, and periodic erythropoiesis can be induced in mice^{52–53} by the administration of a single dose of the marrow-seeking radioisotope ⁸⁹Sr and in rabbits⁵⁴ by the administration of red blood cell auto-antibodies.

In principle, there are three types of mechanisms which can account for oscillations in peripheral blood cell number.

1. Oscillations can occur because of instabilities in the long range feedback mechanisms.
2. Oscillations in peripheral blood cell number may simply be a reflection of oscillations in PPSC number due to abnormalities in PPSC regulatory mechanisms.
3. Oscillations in blood cell number may arise because of interactions between two or more cell lines.

In the following, we survey the work that has been done in each of these areas, as well as offering some possible unexplored, or incompletely explored, extensions.

LONG RANGE HUMORAL MECHANISMS

a). Delayed negative feedback: Single delay

The control of erythrocyte production can be characterized as a delayed negative feedback mechanism³⁷ (Figure 2a). Hypoxia (due, for example, to a fall in erythrocyte number) induces the release the hormone erythropoietin from the kidney. Erythropoietin, in turn, increases the production rate within the early committed erythroid series cells, ultimately augmenting circulating erythrocyte numbers (i.e. negative feedback). There is a significant delay between the receipt of this erythropoietin signal and a consequent change in the influx of circulating erythrocytes. This is because once a cell from the PPSC is committed to the erythroid series it takes an average of $\tau_m \sim 5.7$ days for it to complete a series of nuclear divisions and undergo maturation before being released into the circulation.

Oscillations in erythrocyte number, E , are rarely observed in humans^{47–48}, but can be induced in rabbits by using a red blood cell auto-antibody to increase the peripheral erythrocyte destruction rate⁵⁴. In terms of eq. (2), a possible model for induced rabbit auto-immune hemolytic anemia (AIHA) is

$$\frac{dE}{dt} = f(E_{\tau_m}) - \gamma E, \quad (3)$$

where

$$f(E_{\tau_m}) = \frac{\beta_o \theta^n}{\theta^n + E_{\tau_m}^n}, \quad (4)$$

$\gamma > 0$ is the random rate of erythrocyte destruction, and n, β_o , and θ are constants (i.e. control parameters) characterizing the erythrocyte production function¹⁴. The notation E_{τ_m} denotes E at a time τ_m in the past, i.e. $E_{\tau_m} = E(t - \tau_m)$. A monotone decreasing $f(E_{\tau_m})$ is consistent with *in vivo* measurements of erythrocyte production rates in rats⁵⁵. Increasing the parameter n increases the maximal slope of the feedback function f , the

parameter θ controls the location of the point of maximum slope, while β_0 controls the maximal erythroid production rate. Increases in n are equivalent to increasing the gain in the feedback loop^{10–11}.

The properties of eq. (3) have been extensively studied using analytical and numerical methods^{5–6,56}. Two types of stable solutions are known to exist: 1) a locally stable equilibrium point, $E^* > 0$, defined by $dE/dt = 0$, and given implicitly by

$$\gamma E^* = \frac{\beta_0 \theta^n}{\theta^n + (E^*)^n}; \quad (5)$$

and 2) a stable limit cycle oscillation of simple type, i.e. one maximum per period⁵⁶. A supercritical Hopf bifurcation between these two types of solutions occurs¹¹ when the control parameters n , γ , and τ_m satisfy

$$\omega \tau_m = \cos^{-1} \left(\frac{\gamma}{f'(E^*)} \right), \quad (6a)$$

where

$$\omega^2 = [f'(E^*)]^2 - \gamma^2 \quad (6b)$$

and $f'(E^*) = (\partial f / \partial E_{\tau_m})_{E_{\tau_m} = E^*}$. The period, $T_H = 2\pi/\omega$, of the oscillatory solution at the Hopf bifurcation⁵⁷ is easily shown to be bounded by $2\tau_m \leq T_H \leq 4\tau_m$. For $\tau_m \sim 6$ days, these bounds predict oscillations with periods between 12–24 days, but use of the strict relation $T_H = 2\pi/\omega$ with estimates of the other parameters¹⁴ sharpens the estimated period to about 21 days which is in good agreement with the observed period of 16–17 days in induced AIHA.

Because of the nonlinear nature of the problem, numerical calculations must be used to explore the global behavior of the solutions of eq. (3) as the control parameters are increased beyond the Hopf bifurcation. To obtain insight into the nature of the dynamics

of AIHA, changes in γ are important since red cell auto-antibody causes random erythrocyte lysis. As γ is increased, there is a progressive fall in the steady state number of circulating erythrocytes as would be expected. However, the other feature that appears as γ is increased is related to a loss of the stability of this steady state for some biologically important ranges of the parameters β_0, n , and τ_m . In these ranges, for small values of γ , the steady state is locally stable. At a critical value of $\gamma = \gamma_{crit,1}$ which may be calculated exactly from eqs. (6a,b), there is a supercritical Hopf bifurcation and the steady state E^* is locally unstable. This instability persists for all $\gamma_{crit,1} < \gamma < \gamma_{crit,2}$. Finally, at $\gamma = \gamma_{crit,2}$ there is a reverse Hopf bifurcation, and the (depressed) steady state E^* is once again stable for $\gamma > \gamma_{crit,2}$ (Figure 2b). This sequence explains the observation in rabbit AIHA that reticulocyte levels may be either depressed at constant levels or oscillate around depressed levels depending on the severity of the hemolytic anemia⁵⁴.

Once the supercritical Hopf bifurcation has occurred and the positive steady state E^* is unstable ($\gamma_{crit,1} < \gamma < \gamma_{crit,2}$), it is found numerically that increasing the control parameters n and β_0 controlling the gain changes the shape of the oscillation with little change in frequency^{10–11}. The more complex waveforms typically associated with the occurrence of higher-order bifurcations⁵⁸, such as period-doubling bifurcations or bifurcations from a limit cycle to a two torus, are not seen and the results of Kaplan and Yorke⁵⁶ make it likely that no other bifurcations exist.

In the special case of piecewise constant negative feedback, when $f(E_{\tau_m})$ is replaced by $F(E_{\tau_m})$ given by

$$F(E_{\tau_m}) = \begin{cases} \alpha & \text{if } E_{\tau_m} < \theta \\ 0 & \text{if } E_{\tau_m} > \theta, \end{cases} \quad (7)$$

and α, θ are positive constants, it has been possible to prove that only one type of stable oscillatory solution exists¹.

These results indicate that this model accurately replicates the essential elements of the dynamic behaviour of induced AIHA. However, the oscillations in erythrocyte number observed in AIHA show variations in both waveform morphology and inter-peak interval. Recently the possibility that noise-like fluctuations of these types may be of deterministic origin, i.e. ‘chaotic’, has attracted a great deal of attention^{5-7,59-61}. Thus, these modeling observations further indicate that chaotic dynamics can not be produced by nonlinear negative feedback mechanisms of the type described by eq. (3) in the absence of stochastic inputs.

b). Mixed feedback: Single delay

The type of feedback which arises in the regulation of neutrophil numbers differs from that involved in the regulation of erythrocyte numbers. At sufficiently high neutrophil numbers, the neutrophil production rate decreases as the number of neutrophils increases (i.e. negative feedback). However, at low neutrophil numbers the production rate falls to zero. Thus in the range of low neutrophil numbers, the production rate increases as the neutrophil number increases (i.e. positive feedback). The resulting feedback function has the ‘humped’ shape shown in Figure 2a. This type of feedback has been referred to as ‘mixed’ feedback¹⁻². Though the feedback function for neutrophil regulation has a different functional characteristic (mixed) than does the one for erythrocytes (negative), they are similar in that the feedback in both is delayed. For the neutrophils, there is once again a significant delay of $\tau_m \simeq 5-7$ days between when the feedback signal is sensed by the primitive neutrophil precursors and when the effect of this signal is seen in the periphery. Finally, from studies utilizing labeled neutrophils, it is known that these cells have an exponential disappearance from the circulation, consistent with random destruction at a constant rate.

Oscillations in neutrophil number occur in a type of human leukemia referred to as periodic chronic myelogenous leukemia (CML). A simple model for the regulation of neutrophil number, N , which incorporates the delayed mixed feedback is⁵⁻⁶

$$\frac{dN}{dt} = g(N_{\tau_m}) - \gamma N \quad (8)$$

where γ is again the random destruction rate and the delayed production function is

$$g(N_{\tau_m}) = \frac{\beta_0 N_{\tau_m} \theta^n}{\theta^n + N_{\tau_m}^n}. \quad (9)$$

In contrast to the erythroid control system, this model predicts that there are potentially two steady state levels of neutrophil numbers: $N_1^* = 0$, and a second positive steady state N_2^* given explicitly by

$$N_2^* = \theta \left[\frac{\beta_0 - \gamma}{\gamma} \right]^{1/n}$$

which exists whenever $\beta_0 > \gamma$. As for the model of erythroid production, it is possible to analyze the local stability of both of these steady states, and the results of this analysis indicate that whenever $N_2^* > 0$ exists, the steady state corresponding to no neutrophils, $N_1^* = 0$, is unstable. For fixed values of the random peripheral neutrophil destruction rate γ , increases in either β_0 and/or n , which both increase the gain of the system at the steady state, and in τ_m will eventually lead to a loss of stability of N_2^* through a supercritical Hopf bifurcation and the onset of limit cycle behaviour. The criteria for this bifurcation are given by eqs. (6a,b) with g replacing f .

The behaviour of eq. (8) has been studied numerically⁵⁻⁶, and these studies indicate that the dynamics of eqs. (8) and (9) is much richer than for the simple negative feedback model of erythrocyte production. Increases in τ_m are of particular interest since a prolongation of the neutrophil maturation time is inferred in patients with CML⁶². As τ_m is increased an initially stable equilibrium becomes unstable and stable periodic solutions

appear. Further increases in τ_m lead to a sequence of period-doubling bifurcations which ultimately culminates in an apparently chaotic or aperiodic regime (an example of which is shown in Figure 2c). In the aperiodic regime, the choice of the initial function determines the evolution of the dynamics. In addition, for some choices of initial functions stable, but complex periodic oscillations may also be observed. Precisely the same mathematical observations have been made⁶³ using a different analytic mixed feedback form for the function g .

Figure 2c compares a computer simulation of eq. (8), when the maturation time is increased from a normal value of ~ 5 -7 days to 20 days, to the changes in neutrophil number measured for a CML patient. Not only does the simulation correctly predict the overall period of the observed oscillations in neutrophil number, but it also duplicates the irregular fluctuations. Thus in the case of mixed feedback it is not easy to distinguish fluctuations which arise from stochastic inputs (“noise”) from the inherent dynamics of the control mechanism. To our knowledge, this simple model for the production of neutrophils was the first association of “intrinsic” chaos in a continuous time deterministic equation with a pathological process.

As in the case of negative feedback, it has been possible to obtain greater analytical insight into the properties of mixed feedback by considering the special case of piecewise constant mixed feedback¹. In particular, $g(N_{\tau_m})$ in eq. (8) is replaced by $G(N_{\tau_m})$ where

$$G(N_{\tau_m}) = \begin{cases} 0 & \text{if } N_{\tau_m} \leq \theta_1 \\ \alpha & \text{if } \theta_1 < N_{\tau_m} < \theta_2 \\ \delta & \text{if } \theta_2 \leq N_{\tau_m}, \end{cases} \quad (10)$$

and $\alpha > \delta > 0$. In this case it has been proved¹ that for constant initial functions there exist stable equilibria, stable and unstable limit cycles, Li and Yorke⁶⁴ type chaos, and mixing and exact motions for various parameter values.

c). Multiple delays

In the models for erythrocyte and neutrophil regulation, the destruction rates only accounted for cell loss due to random processes in the circulation such as immune-mediated cytolysis and loss of cells in hemostatic-thrombotic events. For neutrophils this is an accurate representation of the underlying physiology, but erythrocytes also age and are removed from circulation as a consequence of senescence. Laboratory studies indicate that in humans, the lifespan of erythrocytes is on the order of 120 days³⁷. Figure 3a illustrates a possible model for erythrocyte production which incorporates loss due to senescence. If we denote the erythrocyte senescence time by τ_s , then the dynamics will be more accurately described by

$$\frac{dE}{dt} = f(E_{\tau_m}) - \gamma E - f(E_{\tau_m+\tau_s})e^{-\gamma\tau_s} \quad (11)$$

In contrast to eq. (3), eq. (11) contains two different time delays, τ_m and τ_s . Numerical simulations of eq. (11) indicate that for $\tau_s = 120$ days, the dynamics do not differ significantly from those produced by eq. (3) (M.C. Mackey, unpublished data). This is not surprising since for large τ_s , $\gamma\tau_s \gg 1$ and $e^{-\gamma\tau_s} \sim 0$, so eq. (11) is approximated by eq. (3).

However, in other situations multiple delays may have profound effects on the predicted dynamics. One example comes from a model for the production of platelets, whose dynamics are of interest because of the as yet unexplained condition of cyclical thrombocytopenia⁴³. In this disease, platelet levels oscillate from high to low levels with a period of approximately 28 days. If the platelet count at the nadir of the oscillation is sufficiently low, the patient is at risk for a stroke, and indeed this is the cause of death for many of these patients. Initial reports of this condition were in women, and it was thought that the oscillation might be driven by the menstrual cycle. However, there are

other clinical studies of the same disease in men thus ruling out this explanation for all cases.

Platelets are produced from megakaryocytes by a fragmentation processes⁶⁵. Normally, the total time between the appearance of a recognizable megakaryocyte and when it starts to produce platelets is $\tau_m \sim 9$ days⁶⁵. Once released into the circulation, the platelet lifetime is $\tau_s \sim 10$ days³⁷. Thus two delays arise: one associated with the platelet lifetime (τ_s) and another with the megakaryocyte maturation time (τ_m). In contrast to the situation for erythrocyte production, these two delays are of comparable magnitude.

A simple yet realistic model for platelet production is shown schematically in Figure 3b and can be expressed mathematically¹⁶ as

$$\frac{dP}{dt} = -\gamma P + e^{-\delta\tau_m} [\beta(P_{\tau_m}) - \beta(P_{\tau_s+\tau_m})e^{-\gamma\tau_s}] \quad (12)$$

where the feedback function β is of the mixed form like that described by eq.(9), γ is the random rate of destruction of platelets in the circulation, and δ is the random rate of megakaryocyte destruction.

As in the model for neutrophil dynamics of the previous section, this model has two steady state values of platelet levels, one zero ($P_1^* = 0$) which always exists, and a second positive one ($P_2^* > 0$) that exists for all values of γ satisfying $0 < \gamma < \gamma_{crit}$. However, the existence of the two time delays controlling the dynamics makes the stability analysis at these steady states much more complicated than the analysis when only one delay is present⁶⁶. One of the surprising predictions of the model for platelet regulation is that the nonzero platelet steady state is *unstable* for low platelet destruction rates γ , and that increases in γ , in addition to decreasing the unstable steady state platelet levels, will ultimately result in a reverse supercritical Hopf bifurcation so that the platelet numbers are eventually stabilized by increasing platelet destruction rates. Precisely the

same behaviour is found following increases in δ . These results suggest that a possible, but certainly non-intuitive, treatment for the potentially life-threatening condition of cyclical thrombocytopenia might be to increase platelet and/or megakaryocyte destruction rates in a carefully controlled fashion.

d). Distributed delays

In writing eqs. (3), (8), (11) and (12) we have assumed that the maturation time is the same for all cells. In general, however, this is not the case and there will be a distribution of maturation times. Similar problems arise in the modeling of recurrent inhibitory pathways in the nervous system, where there is not a single delay but rather a distribution of delays due to a distribution of fibre diameters and conduction path lengths, and a consequent distribution of conduction times in the feedback pathways.

Considerations like these lead to models framed in terms of integro-differential equations. For example, eq. (3) becomes

$$\frac{dE}{dt} = f(y(t)) - \gamma E \quad (13a)$$

where

$$y(t) = \int_{-\infty}^{t-\tau_{min}} \phi(t-u)E(u) du, \quad (13b)$$

the kernel ϕ gives the distribution of maturation times and $\tau_{min} \geq 0$ is the minimum maturation time. Clearly if ϕ is a dirac delta function, $\phi(t-u) = \delta(t-u-\tau_m)$ with $\tau_m \geq \tau_{min}$, then we just have $y(t) = E(t-\tau_m)$ and the original model of eq. (3) is recovered.

It has been known for some time^{8,67-68} that if a smooth kernel corresponding to a gamma distribution of maturation times is chosen,

$$\phi(q) = \frac{a^{m+1}}{m!} q^m e^{-aq}, \quad a, m \geq 0,$$

with m an integer, then the system (13) can be rewritten as a system of m linear differential equations coupled to one nonlinear differential delay equation. In the case that $\tau_{min} = 0$, then the system just reduces to a system of ordinary differential equations. Furthermore, in this latter case it is easy to calculate that the average delay corresponding to the gamma distribution kernel is simply $\tau_{av} = (m + 1)/a$ and thus taking the double limit $m, a \rightarrow \infty$ with τ_{av} held constant we have

$$\lim_{\substack{m, a \rightarrow \infty \\ \tau_{av} \text{const}}} \phi(q) \simeq \delta(t - \tau_{av}),$$

so $y(t) \simeq E(t - \tau_{av})$. The dynamics of systems with no minimum delay ($\tau_{min} = 0$) and a continuous gamma distribution of delays as the parameter m is increased have been studied⁶⁹. Mackey (unpublished) has compared the numerical behaviour of differential delay equations with delta function delays (both negative and mixed feedback) with that of the same equations but with a gamma distribution of delays and $\tau_{av} = \tau_{min}$, and found that there seemed to be no new qualitative behaviors introduced by the distribution of delays. The system (13) with very general kernels ϕ may be approximated by systems of ordinary differential equations⁷⁰.

e). State-dependent delays

To now we have assumed that the time delays are constant. However, in the case of platelet production there is clear evidence that the megakaryocyte age at which platelets are produced is, in fact, not constant but is a function of platelet number⁷¹. Megakaryocytes mature by undergoing repeated nuclear divisions without cytokinesis to the point of disintegration in three principal ploidy classes⁶⁵: $8n$, $16n$, and $32n$. Since more nuclear divisions are required to produce a $32n$ versus a $8n$ megakaryocyte, ploidy is a convenient marker of megakaryocyte age. In the normal situation the majority of circulating platelets are produced by $16n$ megakaryocytes. In response to a fall in platelet number⁷¹, there

is a poorly characterized increase in the velocity of megakaryocyte maturation leading to an eventual decrease in τ_m . In addition τ_m may be altered under pathological conditions because the different ploidy classes respond differently to stimulation and suppression of thrombopoiesis⁷², i.e. differing proportions of circulating platelets may be derived from the various ploidy classes in these situations.

In view of these observations, eq. (12) should be modified to read

$$\frac{dP}{dt} = -\gamma P + e^{-\delta\tau_m(P)}[\beta(P_{\tau_m(P)}) - \beta(P_{\tau_s+\tau_m(P)})e^{-\gamma\tau_s}] \quad (14)$$

where the dependence of τ_m on platelet number is explicitly recognized⁷³. Now, the platelet dynamics are described by a nonlinear differential delay equation with two delays, one of which is constant (τ_s) and the second of which is a monotone increasing function of the state variable, $\tau_m(P) \geq 0$.

Though little is presently known about the dynamics of the solutions of problems with state dependent delays^{74–75}, a local stability analysis of the positive steady state of eq. (14) indicates that when the megakaryocyte destruction rate is positive, $\delta > 0$, the inclusion of the state dependent delay $\tau_m(P)$ is equivalent to an augmentation of the random platelet destruction rate γ . Thus, if the positive steady state P_2^* of the original platelet model given by eq. (12) was unstable, the effect of the state dependent delay would be to move the steady state closer to the stability boundary. This stabilizing effect of the state dependent delay is a consequence of the fact that the delay is an increasing function of the circulating platelet numbers.

State-dependent delays also arise in models of economic commodity dynamics and of recurrent inhibition in the nervous system. In the economic context, the state dependent delays arise because producers are able to store commodities for a period of time that is dependent on market price³⁵. In this situation, it would be expected that the delay would

be a decreasing function of the state variable, market price. In the recurrent inhibitory models, the average value of the distribution of delays mentioned in the previous section is expected to be a decreasing function of the state variable which is the difference between the excitatory and inhibitory potentials in a population of post synaptic cells. In both of these models, based on a local stability analysis the existence of the state dependent delay is a destabilizing factor.

REGULATION OF PLURIPOTENTIAL STEM CELL PRODUCTION

The most common periodic hematological disease in humans is periodic hematopoiesis (PH)^{41–42}. PH is characterized by 17-28 day periodic oscillations in all the formed elements of the blood and is currently thought to be due to a defect in the regulation of the pluripotential stem cells (PPSC)^{76–77}. Although control mechanisms within the PPSC populations are not well understood, there is evidence that short range interactions are more important than long range circulating regulators for limiting stem cell numbers.

A schematic representation of a possible model for the production of PPSC is shown in Figure 4. Stem cells are classified as being in either a proliferative (cycling) phase (C) or resting phase (R). Cells travel through proliferation to undergo mitosis after a fixed time (τ). Proliferating cells entering R may exit randomly to either re-enter proliferation at a rate β (known to be a monotone decreasing function of the number of resting phase cells) or to be irreversibly lost via differentiation into the hematopoietic cell lines at an approximately constant rate δ . In addition proliferating cells may be lost from any phase of the cell cycle at a rate γ .

The dynamics of this PPSC population is governed by the pair of coupled differential delay equations^{13,15}

$$\frac{dC}{dt} = -\gamma C + \beta(R)R - e^{-\gamma\tau}\beta(R_\tau)R_\tau \quad (15a)$$

$$\frac{dR}{dt} = -(\beta(R) + \delta)R + 2e^{-\gamma\tau}\beta(R_\tau)R_\tau \quad (15b)$$

where τ is the time required for a cell to traverse the proliferative phase, and the resting to proliferative phase feedback rate is taken to be

$$\beta(R) = \frac{\beta_0 \theta^n}{\theta^n + R^n}.$$

An examination of eq. (15b) shows that this equation could be interpreted as describing the control of a population with a delayed mixed feedback type production term $[2e^{-\gamma\tau}\beta(R_\tau)R_\tau]$ and a destruction rate $[\beta(R) + \delta]$ that is a decreasing function of R .

Once again, this model has two possible steady states. There is a steady state corresponding to no cells, $(C_1^*, R_1^*) = (0, 0)$ which is stable if it is the only steady state, and which becomes unstable whenever the second positive steady state (C_2^*, R_2^*) exists. The stability of the non-zero steady state depends on the value of γ . When $\gamma = 0$ (assumed to characterize the normal situation), this steady state cannot be destabilized to produce dynamics characteristic of PH. On the other hand for $\gamma > 0$, increases in γ lead to a decrease in the PPSC numbers and a consequent decrease in the cellular efflux (given by δR) into the differentiated cell lines. This diminished efflux becomes unstable when a critical value of γ is reached, $\gamma = \gamma_{crit,1}$, at which a supercritical Hopf bifurcation occurs. For all values of γ satisfying $\gamma_{crit,1} < \gamma < \gamma_{crit,2}$, there is a periodic solution of eq. (15) whose period is in good agreement with that seen in PH. At $\gamma = \gamma_{crit,2}$, a reverse bifurcation occurs and the greatly diminished PPSC numbers as well as cellular efflux again becomes stable. These results suggest that PH is likely related to defects, possibly genetic, within the PPSC population that lead to an abnormal ($\gamma > 0$) losses of cells from the proliferative phase of the cell cycle. Indeed oscillations can be induced in the peripheral reticulocyte number of mice^{52–53} using ⁸⁹Sr to increase γ .

Numerical simulations of eqs. (15) bear out the results of the above local stability analyses. When all the parameters in the model are set to the values estimated from laboratory and clinical data, no other types of bifurcations are found. Although these simulations also indicate the existence of multiple bifurcations and chaotic behaviors, these more complex dynamics are only observed for non-physiological choices of the parameters (M. C. Mackey, unpublished). Thus the observed irregularities in the fluctuations in blood cell numbers in PH cannot be related to chaotic solutions of eq. (15).

CHAOS IN MATURING CELL LINES

The model for the regulation of the PPSC population given by eqs. (15) was derived by balancing cellular fluxes in each of the cell compartments. The fact that cells are both maturing (or aging) and proliferating simultaneously suggests that a model for PPSC production might be better expressed in terms of partial differential equations rather than differential delay equations. However for biologically appropriate boundary conditions it has been previously shown¹⁵ that the description of PPSC production in terms of partial differential equations reduces to the differential delay equations given by eqs. (15). Since complex and chaotic dynamics are observed for eqs. (15), this observation suggests that similar dynamics might also be observed in partial differential equations. This is indeed the case. Here we illustrate this point by considering a model for a population of cells that are proliferating and maturing in a continuous manner. A similar model for a single cellular population has appeared previously⁷⁸.

Characterize each cell in the population by two internal variables: a , the age of the cell in the cell cycle, and m , the maturation level of the cell. For concreteness and convenience, one could think of erythroid cells and take the intracellular hemoglobin content as an index of maturation. At birth, cells have age $a = 0$ and their age increases with a velocity V_a

until cell division occurs at age $a = a_D$. In terms of maturation, cells are assumed to first become identifiable members of the population under consideration at a maturation level $m = m_0$. These cells mature at a velocity V_m until they reach the maturation level $m = m_1$ of a totally mature cell. During this entire process of maturation, the cells proliferate and they may, in addition, also die at a constant random rate γ . It is important to emphasize that this process explicitly allows cellular movement through the cell cycle to proceed hand in hand with cellular maturation. This hypothesis is sufficient to explain existing hematopoietic cell kinetic data⁷⁹.

Denote the number of cells of age a and maturation level m at time t by $n(t, m, a)$. By our description of the assumed progression of cells through the age- maturation space, $n(t, m, a)$ must satisfy a continuity equation of the form

$$\frac{\partial n}{\partial t} + \frac{\partial(V_m n)}{\partial m} + \frac{\partial(V_a n)}{\partial a} = -\gamma n(t, m, a) \quad (18)$$

along with the mitotic flux condition

$$V_a(t, m, 0)n(t, m, 0) = 2V_a(t, m, a_D)n(t, m, a_D). \quad (19)$$

At any given time t and maturation level m the total number of cells of all ages is simply

$$N(t, m) = \int_0^{a_D} n(t, m, a) da. \quad (20)$$

If the velocity of maturation, V_m , is independent of cellular position within the cell cycle, then eq. (18) may be integrated over cellular age a and the result combined with (19) and (20) to yield a corresponding continuity equation for N :

$$\frac{\partial N}{\partial t} + V_m \frac{\partial N}{\partial m} = \left[\beta(t, m, N) - \frac{\partial V_m}{\partial m} - \gamma \right] N. \quad (21)$$

In (21), the *relative proliferation rate* β is defined by

$$\beta(t, m, N) = \frac{V_a(t, m, a_D)n(t, m, a_D)}{N(t, m)}, \quad (22)$$

and plays a role analogous to the function β in the PPSC model of the previous section.

We assume that the maturation velocity V_m , as a function of maturation level m , is given by

$$V_m(t, m) = r(m - m_0), \quad (23)$$

where $m_0 \leq m \leq m_1$ and $r > 0$ is constant. Equations (21) through (23), in addition to the initial condition

$$N(0, m) = \tilde{v}(m), \quad (24)$$

complete the specification of the model.

One of the parameters is superfluous and may be eliminated by a judicious choice of variables. To this end we first define a dimensionless maturation variable x by

$$x = \frac{m - m_0}{m_1 - m_0},$$

so $0 \leq x \leq 1$. With this change, equations (21) through (23) may be transformed and combined to yield

$$\frac{\partial N}{\partial t} + rx \frac{\partial N}{\partial x} = [\beta(t, x, N) - r - \gamma] N. \quad (25)$$

with the associated initial condition

$$N(0, x) = v(x). \quad (26)$$

Partial differential equations of the form⁸⁰

$$\frac{\partial u}{\partial t} + c(x) \frac{\partial u}{\partial x} = f(x, u) \quad (27)$$

with the initial condition $u(0, x) = v(x)$ have a unique solution only if $c(0) = 0$. However, this requirement for the uniqueness of the solution has some other surprising consequences.

Namely, under certain mild regularity conditions on the function $f(x, u)$ one of two behaviours may occur. If the initial function $v(x)$ satisfies $v(0) > 0$, then there is always a *stable* unique solution $u(t, x)$. However, this stability is lost if the initial function is such that $v(0) = 0$, and the solutions are chaotic in a function space.

Our cell proliferation and maturation model is described by an equation (25) exactly of the type of eq. (27), and it is rather easy to illustrate the nature of the unstable solutions that Lasota's results⁸⁰ guarantee. To this end, we pick a relative proliferation rate given by $\beta = \beta_0 - N$, where $\beta_0 > 0$ is constant. Then, eq. (25) takes the form

$$\frac{\partial N}{\partial t} + rx \frac{\partial N}{\partial x} = [\beta_0 - r - \gamma - N] N. \quad (28)$$

With the initial condition (26), it is straightforward to show that the solution of eq. (28) is given by

$$N(t, x) = \alpha \frac{v(xe^{-rt})e^{\alpha t}}{1 - v(xe^{-rt})[1 - e^{\alpha t}]}, \quad (29)$$

where we have set $\alpha = \beta_0 - r - \gamma$. Clearly, if the solutions $N(t, x)$ are to be biologically meaningful, then we must have $\alpha > 0$ and under this condition it is an immediate consequence that $\lim_{t \rightarrow \infty} N(t, x) = \alpha$ whenever $v(0) > 0$, thus illustrating the stability result of Lasota⁸⁰.

If, however, $v(0) = 0$ then a much different situation occurs. Let ν denote the exponential rate at which $v(xe^{-rt})$ approaches 0. Then it is clear that

$$\lim_{t \rightarrow \infty} N(t, x) = \begin{cases} 0 & 0 < \alpha < \nu \\ \alpha \frac{v(x)}{1 + v(x)} & \nu = \alpha \\ \alpha & \nu < \alpha, \end{cases} \quad (30)$$

which shows the nature of the instability and the sensitive dependence of the eventual behaviour of $N(t, x)$ on the initial function $v(x)$.

The situation of $v(0) = 0$ is quite likely in hematopoietic systems since, for example, it is known from *in vitro* observations that if cell numbers within the PPSC fall to low values

then differentiation into the neutrophilic and erythroid cell lines ceases. When this occurs, the result would be precisely $v(0) = 0$ and the instability predicted by the mathematical results of Lasota⁸⁰ and demonstrated by equation (30) could easily be observed if there were fluctuations in α sufficiently large to cause switching between various dynamic behaviours. These fluctuations could arise, for example, because of fluctuations in the rate r of cell maturation or in the rate γ of cell death within the simultaneously proliferating and maturing cells. The consequent switching in dynamic behaviour would be mirrored in the output flux of cells from this compartment, proportional to $N(t, 1)$, and eventually in the numbers of circulating mature cells.

INTERACTIONS BETWEEN DEVELOPING CELL LINES

Interactions between different committed stem cell compartments occur⁸¹. For example, *in vivo* experimental maneuvers expected to increase (decrease) the erythropoietin drive to the CSC-E, there is an accompanying decrease (increase) in the number of circulating neutrophils as well as their primitive precursors. Thus changes in the proliferative activity in one population gives rise to changes in the proliferative activity in another. Here we examine whether certain periodic hematological diseases arise from abnormalities in the interactions between different stem cell compartments.

This question has recently been examined⁸² in the context of n coupled first- order partial differential equations of the form of eq. (21). The coupling of proliferative activity between different committed stem cell compartments is mediated by cell number⁸¹. This coupling will be reflected through the dependence of the relative proliferative rate, β , on the numbers, N_i of the various stem cells. For N_i stem cell populations coupled in this way

$$\frac{\partial N_i}{\partial t} + V_m \frac{\partial N_i}{\partial m} = \left[\beta(t, m, N_1, \dots, N_i) - \frac{\partial V_m}{\partial m} \right] N_i \quad (31)$$

In the special case that

$$\beta(t, m, N_1, \dots, N_i) = \frac{\theta_i^{n_i}(m)}{\theta_i^{n_i} + (\sum_j B_{ij}(m)N_j)^{n_i}} \quad (32)$$

it has been possible to show using local stability results (K. Loskot, unpublished) and numerical simulations, that oscillatory dynamics do not occur. This observation suggests that periodic hematological diseases likely have their origin in other destabilizing mechanisms.

CONCLUDING REMARKS

Here we have discussed the origins of periodic hematological diseases from the context of the properties of nonlinear delay and partial differential equations. These disorders likely arise as a result of destabilization of feedback control mechanisms. In the case of diseases such as AIHA and CML this destabilization may occur in the long range humoral feedback control mechanisms, whereas for diseases such as PH it probably occurs within the short range feedback mechanisms in the PPSC compartment. In contrast, it is unlikely that oscillations in blood cell number arise because of abnormalities in the interactions between different stem cell compartments.

Under certain conditions, nonlinear delay and partial differential equations can produce (in addition to regular oscillations) complex, aperiodic, irregular fluctuations in blood cell numbers. These “chaotic” dynamics are so complex that in some cases they could be misinterpreted as, or mistaken for, noise and/or experimental error. This observation has caused many investigators to search for a deterministic origin for all of the complex, noisy fluctuations seen in the real world^{83–84}. However attractive these claims may be, obtaining solid evidence to support them has been problematic. The strongest case can be made in those experimental situations in which it is possible to observe theoretically predicted dynamics (periodic as well as chaotic) for corresponding parameter values^{7,85–86}. The study of hematological control mechanisms is well suited for this approach. In this

case the nature of the control mechanisms are well understood experimentally, a variety of qualitatively different dynamics are observed in both clinical and laboratory settings, and the values of the relevant control parameters can either be measured directly, or readily estimated.

In all the models discussed in this review, oscillations in blood cell number which resemble those observed in human disease and laboratory animals are produced. The fact that these dynamics are observed in the model for the measured ranges of the control parameters indicates that these models provide, at the very least, plausible explanations for the observed dynamics. However, these models do not, in general, readily account for the observed irregular fluctuations in blood cell number. Delayed negative feedback mechanisms (eq. 3) are incapable of generating chaotic dynamics and in the case of the PPSC model (eqs. 15) complex dynamics are not observed for physiologically relevant values of the control parameters. Only in the case of the mixed feedback model for CML (eq. 8) is a deterministic origin of irregular blood cell fluctuations plausible. These observations provide little evidence to support the possibility of a deterministic origin to noise-like fluctuations in blood cell number.

An alternate point of view is that complex, noisy dynamics observed in the real world reflect an interplay between deterministic and stochastic processes. Indeed in order to compare the predictions of any model to experimental and/or clinical data it would seem to be prudent to explore the predictions of the model in the face of noisy perturbations (additive and/or multiplicative). The study of the stochastic nonlinear delay and partial differential equations that arise in the description of physiological phenomena has received little attention.

From a clinical point of view, the potentially most important observation gained from

modelling studies is the realization that qualitative changes can occur in blood cell dynamics as quantitative changes are made in control parameters. This suggests the possibility of treating certain periodic hematological diseases by careful manipulation of control parameters^{5-7,87-88}. Given the rapid advances in understanding the molecular biology of hematological control mechanisms and the development of molecular probes, such an approach may soon be feasible. It can be anticipated that modelling studies, such as those reviewed here, will play an important role in implementing these treatment strategies.

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FIGURE LEGENDS

Figure 1.

Hematopoietic Regulation Architecture. A schematic representation of the control of platelet (P), erythrocyte (RBC), and white blood cell (WBC) production⁴⁰. The peripheral control loops are mediated by the various poietins, and there are in addition local regulatory (LR) loops within the various stem cell compartments. CFU stands for the various colony forming units (M = megakaryocytic, E = erythroid, C = granulocyte/macrophage) which are thought to be the *in vitro* analogs of the *in vivo* committed stem cell (CSC) populations, all of which arise from the pluripotent stem cells (PPSC).

Figure 2.

Peripheral Hematopoietic Regulation. a). The generic peripheral regulatory system of Figure 1, with the qualitative dependence of the feedback mechanisms (right) on circulating cell numbers for erythrocyte (top) and neutrophil (bottom) production. γ is the rate of random loss of cells from the circulation. b). Computer simulations of the model for erythrocyte production, defined by eqs. (3,4), for four different peripheral destruction rates, γ . The predicted reticulocyte numbers have been plotted relative to their normal steady state values. See the text for further discussion. c). A comparison between the temporal evolution of WBC numbers in a patient with periodic CML (from ref. 45) and the predictions of the model defined by eqs. (8,9) when the neutrophil production delay is abnormally long^{5,6}. See text for further discussion.

Figure 2.

Peripheral Hematopoietic Regulation. a). The generic peripheral regulatory system of Figure 1, with the qualitative dependence of the feedback mechanisms (right) on circulating cell numbers for erythrocyte (top) and neutrophil (bottom) production. γ is the rate of random loss of cells from the circulation. b). Computer simulations of the model for erythrocyte production, defined by eqs. (3,4), for four different peripheral destruction rates, γ . The predicted reticulocyte numbers have been plotted relative to their normal steady state values. See the text for further discussion. c). A comparison between the temporal evolution of WBC numbers in a patient with periodic CML (from ref. 45) and the predictions of the model defined by eqs. (8,9) when the neutrophil production delay is abnormally long^{5,6}. See text for further discussion.

Figure 3.

Peripheral Regulation—Variation on a Theme. a). An elaboration of the erythroid peripheral control, taking into account the senescence time τ_s of circulating erythrocytes which leads to a two delay problem as in eqn. (11). b). The peripheral control of platelet production, including the variable maturation time $\tau_m(P)$ within the megakaryocyte compartment and the senescence time τ_s of circulating platelets, as described by eq. (12).

Figure 4.

Central Hematopoietic Regulation. A schematic representation of the control of PPSC regeneration. Proliferating phase (C) cells include those cells in G_1 , S (DNA synthesis), G_2 , and M (mitosis) while the resting phase (R) cells are in the G_0 phase. Local regulatory influences are exerted via a cell number dependent variation $[R\beta(R)]$ in the flux of cells reentering proliferation. δ is the **normal** rate of differentiation into all of the CSC populations, while γ represents an **abnormal loss** of proliferating phase cells. See the text for further details.

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