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## MINIMIZING SEQUENCES IN THERMOMECHANICS

ABSTRACT - A common approach to justifying energy minimization in thermomechanics is to seek an appropriate Lyapunov function for the dynamical equations. Mathematically this leads to the possibility that solutions may have finer and finer structure as time  $t \rightarrow \infty$ .

The purpose of this article is to make some remarks concerning the classical problem of justifying energy minimization in thermomechanics. One popular line of thought (see, for example, Duhem [1911], Ericksen [1966], Coleman & Dill [1973]) involves the observation that the governing equations possess a Lyapunov function  $E$ , the *equilibrium free energy*. To establish that  $E$  is nonincreasing along solutions it is commonly assumed that the body force and mechanical boundary conditions are conservative, that motions obey the second law of thermodynamics in the form of the Clausius-Duhem inequality, that there is no volumetric heat supply, and that the thermal boundary conditions take the form that part of the boundary is perfectly insulated while the remainder is held at a constant temperature  $\theta = \theta_0$ . For spatially varying  $\theta_0$  Ball & Knowles [1986] have found a generalization of  $E$  that remains a Lyapunov function in certain interesting but rather special cases (e.g. thermoelasticity with reference heat flux vector  $q_R = -k(\theta)\text{Grad } \theta$ , where  $\log k(\theta)$  is a concave function of  $\log \theta$ ). Perhaps other useful Lyapunov functions remain to be discovered. The idea is now that equilibrium configurations will be minimizers of  $E$  in an appropriate

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(\*) Dept. of Mathematics - Heriot-Watt University - RICCARTON, EDINBURGH  
EH14 4AS (Great Britain).

function space  $X$ .

It would be useful to have a general theorem about dynamical systems that would lend support to the above reasoning, but I know of no such result. Such a theorem might assert that for certain dynamical systems endowed with a Lyapunov function  $E$ , and having no constants of the motion, for most orbits the states of the system at a sequence of times  $t_n \rightarrow \infty$  will form a 'local minimizing sequence' for  $E$ . A possible definition of a local minimizing sequence  $\{\phi_n\} \subset X$ ,  $X$  a metric space with metric  $d$ , is that for some  $\varepsilon > 0$

$$\lim_{n \rightarrow \infty} [E(\phi_n) - \inf_{d(\psi, \phi_n) \leq \varepsilon} E(\psi)] = 0. \quad (1)$$

When there are constants of motion the phase space  $X$  should be chosen to incorporate these as constraints (cf. Man [1985]).

For many boundary conditions the above motivation leads to consideration of minimizing sequences and minimizers for the energy functional

$$I(x) = \int_{\Omega} W(X, Dx(X)) dX + H(x) \quad (2)$$

obtained from  $E$  by setting the velocity to zero and the temperature to its equilibrium value. (For more details see the above references and Ball [1984].) In (2),  $x(X) \in \mathbb{R}^3$ ,  $W = W(X, A)$  is the stored-energy function, and  $H$  is the potential energy of the body and applied surface forces. Although the picture is far from complete, a substantial amount of information is now available concerning the existence and properties of global minimizers and global minimizing sequences for integrals of the form (2). By contrast the available information concerning local minimizers and minimizing sequences is meagre.

The simplest example of a global minimizing sequence is one consisting of a sequence of global minimizers. To illustrate one possibility we take  $H = 0$  and  $W = W(A)$ . We suppose that

$W: M^{3 \times 3} \rightarrow \overline{\mathbb{R}}$  is Borel measurable and bounded below, where  $M^{3 \times 3}$  denotes the set of real  $3 \times 3$  matrices and  $\overline{\mathbb{R}} = \mathbb{R} \cup \{-\infty\} \cup \{+\infty\}$  the extended real line with its usual topology; these hypotheses cover both compressible and incompressible elasticity, for which it is often assumed that  $W(A) < \infty$  if and only if  $\det A > 0$  and  $\det A = 1$  respectively. Let  $\Omega$  be bounded and open,  $1 \leq p \leq \infty$ ,  $M \in M^{3 \times 3}$  and consider the problem of minimizing

$$I_{\Omega}(x) = \int_{\Omega} W(Dx(X)) dX \quad (3)$$

in the set

$$\mathcal{A}_M^p = \{x: x - MX \in W_0^{1,p}(\Omega; \mathbb{R}^3)\}. \quad (4)$$

Suppose that the global minimum of  $I_{\Omega}$  on  $\mathcal{A}_M^p$  is attained at  $\bar{x}$  and that  $\bar{x}$  is not affine. Provided the boundary  $\partial\Omega$  of  $\Omega$  has zero three-dimensional Lebesgue measure we can construct by the following procedure infinitely many distinct global minimizers of  $I_{\Omega}$  on  $\mathcal{A}_M^p$  having arbitrarily fine structure. By the Vitali covering theorem, given any  $\varepsilon \in (0, 1)$  there exists a finite or countable family  $a_i + \varepsilon_i \Omega$  of disjoint subsets of  $\Omega$ , where  $a_i \in \mathbb{R}^3$ ,  $0 < \varepsilon_i \leq \varepsilon$ , such that  $\text{meas}(\Omega \setminus \bigcup_i (a_i + \varepsilon_i \Omega)) = 0$ . Then

$$x_{\varepsilon}(X) = Ma_i + \varepsilon_i \bar{x} \left( \frac{X - a_i}{\varepsilon_i} \right) \quad \text{for a.e. } X \in a_i + \varepsilon_i \Omega \quad (5)$$

defines a mapping in  $\mathcal{A}_M^p$ , and it is easily verified (Ball & Murat [1984]) that  $I_{\Omega}(x_{\varepsilon}) = I_{\Omega}(\bar{x})$ . Hence  $x_{\varepsilon}$  is also a global minimizer of  $I_{\Omega}$ . We claim that  $x_{\varepsilon} \neq \bar{x}$ . Suppose the contrary; then by (5)

$$\bar{x}(a_i + \varepsilon_i X) = Ma_i + \varepsilon_i \bar{x}(X) \quad \text{for a.e. } X \in \Omega, \text{ all } i, \quad (6)$$

and hence

$$D\bar{x}(a_i + \varepsilon_i X) = D\bar{x}(X) \quad \text{for a.e. } X \in \Omega, \text{ all } i. \quad (7)$$

Define  $L_i X = a_i + \varepsilon_i X$ ,  $X \in \Omega$ . Consider for each  $s=1, 2, \dots$  the partition  $P_s$  of  $\Omega$  into the union of sets  $\left(\prod_{j=1}^s L_{i_j}\right)\Omega$  and a set  $N_s$  of measure zero. Note that each set in the partition except  $N_s$  has the form  $E=c+\delta\Omega$  for some  $c \in \mathbb{R}^3$ ,  $\delta \in (0, \varepsilon^s)$ , where by (7)

$$\frac{1}{\text{meas } E} \int_E D\bar{x}(X) dX = \frac{1}{\text{meas } \Omega} \int_{\Omega} D\bar{x}(X) dX = M. \quad (8)$$

Since  $\text{meas } N_s = 0$ , for a.e.  $X \in \Omega$  there exists a sequence  $E_s = c_s + \delta_s \Omega \in P_s$  with  $X \in E_s$  for all  $s$ . For such an  $X$  that is also a Lebesgue point we have using (8), the Lebesgue differentiation theorem (Saks [1937 p.115]) and the fact that  $\lim_{s \rightarrow \infty} \delta_s = 0$ ,

$$D\bar{x}(X) = \lim_{s \rightarrow \infty} \frac{1}{\text{meas } E_s} \int_{E_s} D\bar{x}(Y) dY = M. \quad (9)$$

Hence  $\bar{x}$  is affine, a contradiction. In the terminology of Ball & Murat [1984], the hypothesis that  $x=MX$  does not globally minimize  $I_{\Omega}$  in  $\mathcal{A}_M^p$  says exactly that  $W$  is not  $W^{1,p}$ -quasiconvex at  $M$ . Even if  $I_{\Omega}$  does not attain a global minimum on  $\mathcal{A}_M^p$ , an obvious modification of the above construction leads to the existence of minimizing sequences with arbitrarily fine structure. This was used in Ball & Murat [1984 Theorem 5.1] to show that if  $I$  given by (2) attains a global minimum on  $\mathcal{A}_M^p$  for every smooth body force potential then necessarily  $W$  is  $W^{1,p}$ -quasiconvex at  $M$ . They also showed that  $\inf_{\mathcal{A}_M^p} I_{\Omega} = \hat{W}_p(M) \text{meas } \Omega$  for some function  $\hat{W}_p : M^{3 \times 3} \rightarrow \bar{\mathbb{R}}$ .

Stored-energy functions for elastic crystals are typically not  $W^{1,\infty}$ -quasiconvex everywhere (Ericksen [1977], James [1981]), and piecewise affine equilibrium configurations are frequently observed. For a nontrivial piecewise affine global minimizer with affine boundary values the above procedure yields mini-

mizers in which the phases are more and more finely distributed. Stored-energy functions that are  $W^{1,p}$ -quasiconvex everywhere only for  $p \geq 3$  have been used to model cavitation in rubber (Ball [1982], Ball & Murat [1984], Gent & Lindley [1958], Sivaloganathan [1986 a,b], Stuart [1985]). It is not known whether for these stored-energy functions  $I$  attains a global minimum on  $\mathcal{A}_M^1$ ; if so, the above procedure would yield minimizers with patterns of more and more finely distributed holes.

The behaviour of global minimizing sequences for certain integrals of the form (1), (2) has been studied by Acerbi & Fusco [1984], Dacorogna [1982], (see also Acerbi, Buttazzo & Fusco [1983], Marcellini [1985]), who showed that global minimizing sequences possess subsequences converging weakly in  $W^{1,1}(\Omega; \mathbb{R}^3)$  to global minimizers for the integrals obtained by replacing  $W$  with its 'quasiconvex envelope'. It would be interesting if versions of these theorems could be proved that allow  $W$  to take infinite values and give information on the behaviour of local minimizing sequences with respect to an appropriate metric.

The existence of minimizers and minimizing sequences with arbitrarily fine structure prompts the question as to whether the dynamic equations of thermomechanics can have solutions giving rise to minimizing sequences with similar behaviour. (Of course we here suppose, as above, that surface energy effects are ignored; these may impose a limit on how fine the structure of a solution may become.) This is tantamount to asking whether as  $t \rightarrow \infty$  solutions can converge weakly, but not strongly, in an appropriate energy space. We end by mentioning some examples of simpler dynamical systems endowed with a Lyapunov function for which this question can be posed, and in some cases resolved.

(a) *One-dimensional viscoelasticity of rate type*

The initial boundary-value problem

$$\left. \begin{aligned} u_{tt} &= (\sigma(u_x) + u_{xt})_x, & 0 < x < 1, \\ u(0, t) &= 0, & \sigma(u_x(1, t)) + u_{xt}(1, t) = P, \\ u(x, 0) &= u_0(x), & u_t(x, 0) = u_1(x), \end{aligned} \right\} \quad (10)$$

was studied by Andrews & Ball [1982]. Here  $u(x, t)$  denotes the longitudinal displacement at time  $t$  of the particle at  $x$  in a reference configuration, and  $P$  the applied force. The stress-strain law  $\sigma$  is not assumed to be monotone. Thus there are in general infinitely many equilibria  $\bar{u}(x)$  solving

$$\sigma(\bar{u}_x) = P \quad \text{a.e. } x \in (0, 1), \quad \bar{u}(0) = 0. \quad (11)$$

The system has the Lyapunov function  $E(u_t, u)$ , where

$$E(v, u) := \int_0^1 \left[ \frac{1}{2} v^2 + W(u_x) \right] dx - Pu(1, t), \quad (12)$$

and  $W' = \sigma$ . If  $\{v_j, u_j\}$  is a global minimizing sequence for  $E$  in

$$\mathcal{A} = \left\{ \{v, u\} \in L^2(0, 1) \times W^{1, \infty}(0, 1) : u(0) = 0 \right\}$$

then  $v_j \rightarrow 0$  strongly in  $L^2(0, 1)$ , but in general one can have  $u_j \rightharpoonup^* \bar{u}$  in  $W^{1, \infty}(0, 1)$  for some  $\bar{u}$  not satisfying (11). Andrews & Ball showed that under certain hypotheses the solution  $u$  of (10) satisfies

$$u_t \xrightarrow{*} 0 \quad \text{in } W^{1, \infty}(0, 1), \quad u \xrightarrow{*} \bar{u} \quad \text{in } W^{1, \infty}(0, 1),$$

as  $t \rightarrow \infty$ , for some  $\bar{u}$ , but left open the question as to whether  $u_x$  can oscillate more and more finely as  $t \rightarrow \infty$  and hence  $\bar{u}$  not satisfy (11). Recently R. Pego [1986] has shown that in fact  $u_x(x, t) \rightarrow \bar{u}_x(x)$  for a.e.  $x \in (0, 1)$ , so that  $\bar{u}$  is an equilibrium. It thus appears that the damping in (10) is too strong to allow increasing oscillations. Perhaps with weaker damping or some other modification to the equation or boundary conditions

increasing oscillations may be possible and generalized curves in the sense of Young [1969] obtained as asymptotic limits of  $u$  as  $t \rightarrow \infty$ .

#### (b) A control problem

The initial-boundary value problem

$$\left. \begin{aligned} u_{tt} - u_{xx} + \left( \int_0^1 uu_t dx \right) u &= 0, & 0 < x < 1, \\ u(0, t) = u(1, t) &= 0, \\ u(x, 0) = u_0(x), & u_t(x, 0) = u_1(x), \end{aligned} \right\} \quad (13)$$

is one of several examples studied by Ball & Slemrod [1979 a, b] and arising in control theory,  $p(t) = \int_0^1 uu_t dx$  being a candidate stabilizing feedback control. By exploiting the Lyapunov function

$$E = \int_0^1 (u_t^2 + u_x^2) dx, \quad (14)$$

they showed that for every solution

$$\{u, u_t\} \rightharpoonup \{0, 0\} \quad \text{in } H_0^1(0, 1) \times L^2(0, 1)$$

as  $t \rightarrow \infty$ . It is an open problem to decide whether the convergence is strong, i.e.  $E \rightarrow 0$  as  $t \rightarrow \infty$ .

#### (c) The Becker-Döring cluster equations

These are the infinite set of coupled ordinary differential equations

$$\left. \begin{aligned} \dot{c}_r &= J_{r-1}(c) - J_r(c), & r > 1, \\ \dot{c}_1 &= -J_1(c) - \sum_{r=1}^{\infty} J_r(c), \end{aligned} \right\} \quad (15)$$



where  $c=(c_r)$ ,  $J_r(c)=a_r c_1 c_r - b_{r+1} c_{r+1}$  and  $a_r, b_r$  are given positive coefficients. In one of several applications of such equations  $c_r(t)$  denotes the expected number of  $r$ -clusters per unit volume at time  $t$  of the minority atoms of a quenched binary alloy. Under certain hypotheses on the coefficients and initial data Ball, Carr & Penrose [1986] have shown that there is a critical density  $\rho_s$  such that if the initial density is  $\sum_{r=1}^{\infty} r c_r(0) = \rho_0$  then the solution satisfies

$$c(t) \xrightarrow{*} c^{\min(\rho_0, \rho_s)} \text{ in } X \text{ as } t \rightarrow \infty,$$

where  $X := \{y = (y_r) : \sum_{r=1}^{\infty} r |y_r| = \|y\| < \infty\}$  and where  $c^\rho$ ,  $0 \leq \rho \leq \rho_s$ , is the unique equilibrium of (15) having density  $\rho$ . Since  $\sum_{r=1}^{\infty} r c_r$  is a conserved quantity it follows that if  $\rho_0 > \rho_s$  then  $c(t) \not\rightarrow c^{\rho_s}$  strongly in  $X$  as  $t \rightarrow \infty$ . The system (15) possesses a Lyapunov function

$$E(c) = \sum_{r=1}^{\infty} c_r \left( \log \left( \frac{c_r}{Q_r} \right) - 1 \right), \quad (16)$$

where  $Q_1 = 1$ ,  $\frac{Q_{r+1}}{Q_r} = \frac{a_r}{b_{r+1}}$  for  $r \geq 1$ . For any value of  $\rho_0 \geq 0$  the solution satisfies

$$\lim_{t \rightarrow \infty} E(c(t)) = \inf_{X_{\rho_0}^+} E, \quad (17)$$

where  $X_{\rho_0}^+ = \{y \in X : y_r \geq 0 \text{ for all } r, \|y\| = \rho_0\}$ . If  $\rho_0 > \rho_s$  the density difference  $\rho_0 - \rho_s$  between the solution and its weak\* asymptotic limit contributes to a 'tail' composed of larger and larger clusters that describes the condensation of the minority component. If we think of  $r$  as a wave number we see that in the corresponding variables the solution oscillates

increasingly as  $t \rightarrow \infty$ . I am not aware of another example where this type of behaviour has been rigorously established.

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