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Discretization and hysteresis

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Abstract

This paper presents a simple and explicit mathematical example of the effects of discretization on a nonconvex variational problem. We describe a one-dimensional model which we call the Ericksen–Timoshenko bar. The energy includes a term that is nonconvex in the strain, quadratic terms in an internal variable and its derivatives, and the simplest quadratic coupling. In the framework of classical elasticity theory, the model has a strong integral nonlocality. Under special constitutive hypotheses, one can construct a collection of stationary points with an arbitrary number of interfaces between phases. We show that solutions with more than one interface are saddle points of the energy, unstable with respect to motion of the interface. We then discretize the energy and show that the saddle points of the continuum problem all correspond to local minimizers of the discrete problem. Thus, the "energy landscape" of the continuum problem is essentially smooth, while the landscape of the discretization is bumpy. This result, which is due to the constraints imposed by the discretization, is independent of mesh size.

Keywords: Hysteresis; Phase transitions; Discretization; Nonlocality

1. The Ericksen–Timoshenko bar

In this paper we consider a specific model of the longitudinal deformation of an elastic bar. This is a special case of a model we call the Ericksen–Timoshenko bar [1–3] which was also studied in Refs. [4, 5]. It was designed as an alternative to strain-gradient models to simulate finite scale microstructures observed experimentally in wires of shape-memory materials (cf., e.g. [6]). Other examples of works on microstructure in one-dimensional problems include [7–9]. We take the reference configuration to be the interval $[0, l]$. Under longitudinal motion, the reference point $x \in [0, l]$ is mapped to the point $x + u(x)$ where $u : [0, l] \to \mathbb{R}$ is the displacement. We define the longitudinal strain $w : [0, l] \to \mathbb{R}$ by $w(x) := u'(x)$. We assume that $u(0) = 0$ and $u(l) = d$. Thus, the strain must satisfy the constraint

$$\int_0^l w(x)\,\mathrm{d}x = \mathrm{d}. \tag{1}$$

At each reference point x we introduce an internal scalar variable ϕ that measures the deviation from one-dimensional deformation. This variable is analogous to shear in the classical Timoshenko beam. However, other interpretations such as atomic shuffles or shifts may also be considered. Our main concern here is the mathematical effect of the nonlocality induced by this term.

We consider a local stored energy function W: $\mathbb{R} \to [0, \infty]$ of the form

$$W(w) := \begin{cases} \frac{\beta}{2}(w+1)^2 & w < 0, \\ \frac{\beta}{2}(w-1)^2 & w > 0, \end{cases}$$

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where $\beta > 0$. This is similar to the model used in Ref. [9]. We define the Ericksen–Timoshenko energy functional $\mathscr{E}$ to be

$$\mathscr{E}(w,\phi) := \int_0^1 W(w) - \alpha w\phi + \frac{\alpha}{2}(\phi^2 + \xi^2|\phi'|^2)\,\mathrm{d}x, \tag{2}$$

Here $\alpha > 0$ and $\xi > 0$ are given parameters. Up to normalization, α measures the coupling between w and ϕ while ξ introduces an internal length scale. Note that $\mathscr{E}$ has the same mathematical form as the energy of the Timoshenko beam if $W(w) = \alpha w^2/2$.

We wish to consider variational problems for the energy defined above. For a given $d \in \mathbb{R}$ we define the set of admissible strains by

$$\mathscr{A}_d := \left\{ w \in L^2(0,l) \;\middle|\; \int_0^l w(x)\,\mathrm{d}x = d \right\}. \tag{3}$$

We consider any internal variable $\phi \in H^1(0,l)$ to be admissible. If (w,ϕ) is a local minimizer of $\mathscr{E}$ over $\mathscr{A}_d \times H^1(0,l)$, then this pair is a stationary point of $\mathscr{E}$, i.e. there exists $\sigma \in \mathbb{R}$ such that

$$W_w(\bar{w}(x)) - \alpha\phi(x) = \sigma \tag{4}$$

for almost every $x \in [0,l]$. (The constant σ is the Lagrange multiplier of the constraint (1) and can be interpreted as a constant stress in the bar.) Furthermore, ϕ is in $H^2(0,l)$ and is a strong solution of

$$-\xi^2\phi'' + \phi = w \tag{5}$$

and satisfies the natural boundary conditions

$$\phi'(0) = \phi'(1) = 0; \tag{6}$$

an analog of the zero moment boundary condition in the Timoshenko theory.

We also note that by integrating (5) and using (1) and (6) we also get

$$\int_0^1 \phi = \int_0^1 w = \mathrm{d} \tag{7}$$

for any stationary point. Furthermore, the usual jump conditions for weak solutions of a differential equation imply that for a stationary point of $\mathscr{E}$, we have $\phi \in H^2(0,1) \subset C^1(0,1)$ and $W_w(w(\cdot))$ is continuous on $(0,1)$.

2. Calculation of stationary points

If we let $\mathscr{P} \subset [0,1]$ be the set of points where $w < 0$, then we have

$$W(w) = \frac{\beta}{2}(w + 2\chi(\mathscr{P}) - 1)^2, \tag{8}$$

where

$$\chi(\mathscr{P})(x) := \begin{cases} 1 & x \in \mathscr{P}, \\ 0 & x \notin \mathscr{P} \end{cases}$$

is the characteristic function of the set $\mathscr{P}$. Thus, for a given $d \in \mathbb{R}$, stationary points of $\mathscr{E}$ are given by $w \in L^2(0,1)$, $\phi \in H^2(0,1)$, and $\sigma \in \mathbb{R}$ satisfying

$$\beta(w + 2\chi(\mathscr{P}) - 1) - \alpha\phi = \sigma, \tag{9}$$

and Eqs. (1), (5), and (6).

Following Ref. [9], we split the optimization problem in two parts. We first regard the set $\mathscr{P}$ as being given. For a given $\mathscr{P}$ and d, we refer to $w \in L^2(0,1)$, $\phi \in H^2(0,1)$, and $\sigma \in \mathbb{R}$ satisfying Eqs. (1), (5), (6), and (9) (and having $w < 0$ in $\mathscr{P}$) as an elastic equilibrium solution. We call the second step the phase equilibrium problem: finding the set $\mathscr{P}$ for which the elastic equilibrium solution has the lowest energy. We note that the elastic equilibrium problem is linear in w and ϕ. The nonlinearity has been confined to the phase equilibrium problem.

To solve the elastic equilibrium problem for a given $\mathscr{P}$, we integrate both sides of (9) and use (7) and (1) to get

$$\sigma = (\beta - \alpha)d + \beta(2|\mathscr{P}| - 1). \tag{10}$$

Putting this back into (9) yields

$$w = \frac{\alpha}{\beta}\phi + \frac{\beta - \alpha}{\beta}d + 2|\mathscr{P}| - 2\chi(\mathscr{P}) \tag{11}$$

We can now use this to eliminate w in (5) to get

$$-\xi^2\phi'' + \frac{\beta - \alpha}{\beta}\phi = \frac{\beta - \alpha}{\beta}d + 2|\mathscr{P}| - 2\chi(\mathscr{P}). \tag{12}$$

Standard techniques for Strum–Liouville problems can be used to find the general solution of this problem.

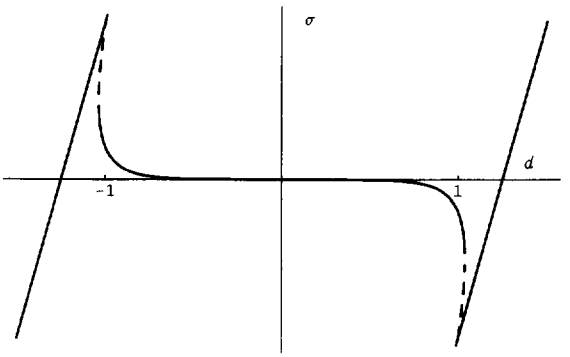

Fig. 1. The stress–strain curves representing the L^2-local minimizers of the Ericksen–Timoshenko nonlocal energy for $\alpha = 2$, $\beta = 10$ and $\xi = 0.1$. The straight lines represent uniform solutions while the interior curve represents a continuum of solutions with a single interface (jump in w). The dashed portions of these curves indicate single interface elastic equilibrium states that are saddles of the energy. All other solutions we have computed are saddle points of the energy, unstable with respect to motion of the interfaces.

$$\phi(x) = d - 4\sum_{k=1}^{\infty} \frac{\cos k\pi x}{\xi^2 k^2 \pi^2 + (\beta - \alpha)/\beta} \times \left(\int_{\mathscr{P}} \cos k\pi s \, ds \right). \tag{13}$$

Now, we can compute the total energy of an elastic equilibrium solution. Using Eqs. (8), (10) and (11), we get

$$\begin{aligned} \hat{\mathscr{E}}(d, \mathscr{P}) &= \int_0^1 \frac{\beta}{2}(w + 2\chi(\mathscr{P}) - 1)^2 - \frac{\alpha}{2} w\phi \\ &= (\beta - \alpha)\frac{d^2}{2} - (\alpha + (2\beta - \alpha)(1 - 2|\mathscr{P}|))\frac{d}{2} \\ &\quad + \frac{\beta}{2}(1 - 2|\mathscr{P}|)^2 + \alpha \int_{\mathscr{P}} \phi. \end{aligned}$$

In a similar spirit to Ref. [9] we compute the energy of elastic equilibrium solutions for sets $\mathscr{P}$ with a finite number of interfaces. Let us assume that we have a sequence of n transition points

$$0 = c_0 < c_1 < c_2 < \cdots < c_n < 1 = c_{n+1}. \tag{14}$$

We define the intervals $I_i = [c_i, c_{i+1}]$, and let $\mathscr{P} = I_0 \cup I_2 \cup \ldots$. One can derive explicit formulas for E as a function of the c_i and its first and second partial derivatives (see Ref. [3] for details).

We have made a number of explicit symbolic calculations for particular choices of the parameters α, β, and ξ, involving up to four interfaces, and then have done numerical calculations of critical points of the energy and the eigenvalues of the Hessian at the critical points. Our observations about these phase equilibria can be summarized as follows:

- Solutions with no interfaces (which are uniform) are L^2-stable for $d < -1$ and $d > 1$.
- The phase equilibrium points with a single interface ($n = 1$) are the most interesting. For $|d| < 1$ there is a unique solution (up to symmetry) and it is a local minimizer. There is a constant $d_0 > 1$, depending on the parameters, such that there is no single interface solution for $|d| > d_0$. There are two such solutions for $1 < |d| < d_0$, one of which is a local minimum and the other a saddle point. In Fig. 1 we have graphed the stress–strain curves of these phase equilibrium points together with the stable equilibria with no interfaces.
- For fixed $n = 2, 3, 4$, there is a unique (again, up to obvious symmetries) critical point of the energy as a function of the interface positions. This critical point is not a local minimizer of E. In fact, the Hessian matrix of E has $n - 1$ negative eigenvalues. For any arrangement of interface points satisfying (14), there is a "path" or "process" of strictly decreasing energy in which "extra" interfaces move to the boundary or anihilate.
- For each of the phase equilibrium solutions, the discontinuities of the function w satisfy the "Maxwell condition", i.e. they jump between $w = \pm 1$.
- For $d \in (-1, 1)$ one can explicitly compute the limiting energy of an infinite number of interfaces (i.e. a "Young-measure" (cf. [8])), and this energy is

higher than the energies of the finite energy solutions we compute.

3. The discretized problem

Now observe that if we eliminate the variable ϕ using a Green's function we can convert our problem to a nonlocal minimization problem for w alone. We derive a nonlocal model similar to those studied in Refs. [4, 10] and the references cited therein. That is, we define

$$\phi(x) = \mathscr{K}[w](x) := \int_0^1 k(x,y)w(y)\,\mathrm{d}y, \tag{15}$$

where

$$k(x,y) := \frac{1}{2\xi}\mathrm{e}^{-|x-y|/\xi} + \frac{1}{\xi(\mathrm{e}^{2/\xi}-1)}\left[\mathrm{e}\cosh\left(\frac{x+y-1}{\xi}\right) + \cosh\left(\frac{x-y}{\xi}\right)\right]. \tag{16}$$

One can easily calculate that for any $w \in \mathscr{A}_d$, $\phi = \mathscr{K}[w]$ satisfies (5) and (6). We define a nonlocal energy $\tilde{\mathscr{E}}$ by

$$\tilde{\mathscr{E}}(w) := \mathscr{E}(w, \mathscr{K}(w)) = \int_0^l W(w(x))\,\mathrm{d}x - \frac{\alpha}{2}\int_0^l\int_0^l k(x,y)w(x)\cdot w(y)\,\mathrm{d}x\,\mathrm{d}y \tag{17}$$

Minimizing $\tilde{\mathscr{E}}$ over $\mathscr{A}_d$ is essentially equivalent to minimizing $\mathscr{E}$ over $\mathscr{A}_d \times H^1(0,l)$ (see Ref. [4] for details).

We now discretize the nonlocal energy. Let

$$\Pi_N := 0 = x_1 < x_2 < \cdots < x_{N-1} < x_N = 1,$$

be a partition of $[0,1]$, and let

$$\int_0^1 f(x)\,\mathrm{d}x \approx \sum_{j=1}^N v_{j,N} f(x_j) \tag{18}$$

be a quadrature formula which converges for all continuous functions. Then the discretized nonlocal energy is given by

$$E(w_j) := \sum_{j=1}^N v_j W(w_j) - \alpha\sum_{j=1}^N\sum_{i=1}^N v_j v_i k(x_i,x_j)w_i w_j, \tag{19}$$

where $w_j \approx w(x_j)$, $j = 1,2,\ldots,N$. The discretization of the constraint (1) is given by

$$\sum_{j=1}^N v_{j,N} w_j = d, \tag{20}$$

Critical points of the energy function (19) subject to the constraint (20) satisfy

$$W_w(w_i) - \alpha\sum_{j=1}^N v_{j,N}k(x_i,x_j)w_j = \sigma, \tag{21}$$

for $i = 1,2,\ldots,N$, where σ is the Lagrange multiplier of (20).

Once again we make use of the "two-parabola" nonlinearity in Eq. (21):

$$W_w(w_i) = \beta w_i - \beta\,\mathrm{sgn}(w_i).$$

Using this, the equations above can be written in matrix form

$$(\beta \boldsymbol{I} - \alpha \boldsymbol{Q})\cdot \boldsymbol{w} = \sigma \boldsymbol{s} + \beta \boldsymbol{p}, \tag{22}$$

$$\boldsymbol{v}\cdot\boldsymbol{w} = d, \tag{23}$$

where

$$\boldsymbol{Q} := \begin{bmatrix} v_{1,N}k(x_1,x_1) & \cdots & v_{N,N}k(x_1,x_N) \\ \vdots & \vdots & \vdots \\ v_{1,N}k(x_N,x_1) & \cdots & v_{N,N}k(x_N,x_N) \end{bmatrix},$$

$$\boldsymbol{v} := \begin{bmatrix} v_{1,N} \\ v_{2,N} \\ \vdots \\ v_{N,N} \end{bmatrix}^T, \quad \boldsymbol{s} := \begin{bmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{bmatrix},$$

$$\boldsymbol{w} := \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix}, \quad \boldsymbol{p} := \begin{bmatrix} \mathrm{sgn}(w_1) \\ \mathrm{sgn}(w_2) \\ \vdots \\ \mathrm{sgn}(w_N) \end{bmatrix}.$$

As in the elastic equilibrium problems above, our equations become linear in the unknowns $\boldsymbol{w}$ and σ if we regard the values $p_i = \pm 1$ as being given.

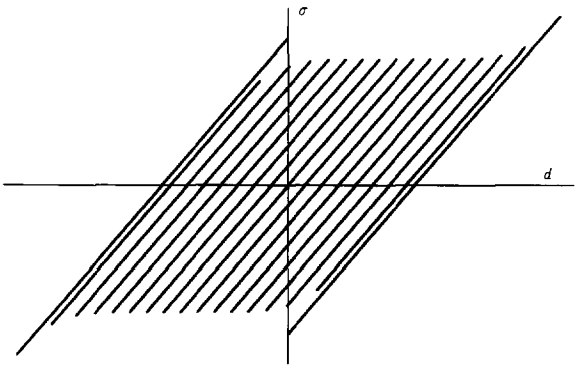

Fig. 2. A typical collection of elastic equilibrium curves for the discretized problem for $\alpha = 2$, $\beta = 10$ and $\xi = 0.1$. Each curve represents a set of solutions with the interface between phases at a particular grid point. Each point on each curve represents a local minimum of the constrained discretized energy. A quasistatic hysteresis loop computed by successive Newton's method calculations as d is varied periodically would traverse the "sawtooth envelope" of the local minimum curves. When a curve ends (so the corresponding solution is no longer admissible) Newton's method produces an "irreversible jump" to the nearest admissible curve.

To find elastic equilibria we observe that if we use trapezoidal-rule weights $v_{i,N} = 1/(N-1)$, $1 = 2, 3, \ldots, N-1$, $v_{1,N} = v_{N,N} = \frac{1}{2}(N-1)$ then the eigenvalues of $\boldsymbol{Q}$ have absolute value less than or equal to one. (This follows from the corresponding estimate for the eigenvalues of $\mathscr{K}$.) Thus, if

$$\beta > \alpha \tag{24}$$

then the matrix $\beta \boldsymbol{I} - \alpha \boldsymbol{Q}$ is positive definite (all eigenvalues are larger than $\beta - \alpha$) and therefore invertible.

We now solve Eq. (22) for $\boldsymbol{w}$, take the dot product of the solution with $\boldsymbol{v}$, and use Eq. (23) to get

$$\sigma = \gamma d + c(\boldsymbol{p}), \tag{25}$$

where

$$\gamma^{-1} := \boldsymbol{v}^{\mathrm{T}} \cdot (\beta \boldsymbol{I} - \alpha \boldsymbol{Q})^{-1} \cdot \boldsymbol{s}, \tag{26}$$

$$c(\boldsymbol{p}) := \gamma \beta \boldsymbol{v}^{\mathrm{T}} \cdot (\beta \boldsymbol{I} - \alpha \boldsymbol{Q})^{-1} \cdot \boldsymbol{p}. \tag{27}$$

Thus, we have the option of thinking of either d or σ as being prescribed and solving for the other parameter. The various choices of $\boldsymbol{p}$ give us parallel line segments relating σ to d. The length of each segment depends on the implicit constraint $p_i = \mathrm{sgn}(w_i)$. The emerging configuration of elastic equilibria reminds us of the picture obtained in the model of noninteracting bistable "snap-springs" [11, 12]. The important difference here is the nonlocal part of the energy, which is responsible for a particular interaction of "snap-spring" elements and allows one to distinguish between configurations with different numbers of interfaces.

It appears that for every choice of $\boldsymbol{p}$ there is a nontrivial segment of the line described in Eq. (25) that represents admissible solutions. We have checked this for small ($n = 1, 2, 3$) and very large ($n = N, N/2$) numbers of interfaces. In Fig. 2, we have graphed the admissible portions of the stress–strain curves for a single interface $\boldsymbol{p}$, i.e. $p_i = -1$ for $i < k$, $p_i = 1$ for $i \geqslant k$, $k = 1, 2, \ldots, N+1$.

The following observations about the elastic equilibria are in order.

- Every elastic equilibrium solution is a local minimizer of the energy since the Hessian is the positive definite matrix $(\beta \boldsymbol{I} - \alpha \boldsymbol{Q})$. This result is completely independent of the mesh size of the discretization.
- The analog of the phase equilibrium problem in this setting would be a search for the discrete location of the interface with the lowest energy: the choice of the set $\mathscr{P}$ in the continuous setting is analogous to the choice of the vector $\boldsymbol{p}$ in the discrete setting. While $\mathscr{P}$ can be varied continuously, there are only a finite number of isolated choices for $\boldsymbol{p}$.

Since we cannot vary the position of the interfaces continuously, the concept of phase equilibrium (and the related hysteresis-free constitutive

behavior) may not be adequate for the description of realistic numerical experiments where the system, unless artificially triggered, will stay on a particular discrete branch of elastic equilibrium until the branch ceases to exist. Only then will the solution jump into the closest discrete branch. Thus, the solutions of the discrete problem describe a hysteresis loop which is given by the sawtooth envelope of the stress–strain curves in Fig. 2.

- The hysteresis loop depends slightly on the mesh size of the discretized problem, but in particular, in the limit of decreasing mesh, the thickness of the loop does not go to zero. We retain essentially the same rhomboidal hysteresis loop as in Fig. 2 for all values of the mesh.

4. Conclusions

This problem is essentially a cautionary tale about the dangers of discretizing a nonconvex variational problem.

Our calculations indicate that for most displacements d, the continuum energy has a unique global and L^2-local minimizer. There is a large collection of stationary points, but they are all saddles, unstable with respect to displacement of the interfaces. During a quasistatic, displacement controlled experiment, a physical bar reflecting this model would be expected to adopt a configuration that was a local minimizer of the energy. Outside the narrow interval of d where there are two local minima, the system should exhibit a hysteresis-free stress–strain curve like the one indicated in Fig. 1. On the other hand, the discretized problem exhibits a very different behavior. Here again, the energy has a large collection of critical points (which are each approximations of a stationary points of the continuous problem). These critical points are not saddles, but local minimizers. The result is that the solutions of the discretized problem trace a full hysteresis loop which persists in the limit as the mesh size goes to zero.

Although the discreteness in our problem is caused by numerical approximation, we suggest that the observed effect may have a physical nature. Thus, there are several levels of microstructure in generic solids, ranging from the crystal lattice to the almost macroscopic regular defect patterns. The fact that the interface may only occupy discrete set of positions is compatible with physical ideas of lattice trapping and defect pinning.

Acknowledgments

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