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GRADIENT FLOWS AS A SELECTION PROCEDURE FOR EQUILIBRIA OF NONCONVEX ENERGIES*

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Abstract. For atomistic material models, global minimization gives the wrong qualitative behavior; a theory of equilibrium solutions needs to be defined in different terms. In this paper, a concept based on gradient flow evolutions, to describe local minimization for simple atomistic models based on the Lennard–Jones potential, is presented. As an application of this technique, it is shown that an atomistic gradient flow evolution converges to a gradient flow of a continuum energy as the spacing between the atoms tends to zero. In addition, the convergence of the resulting equilibria is investigated in the case of elastic deformation and a simple damaged state.

Key words. gradient flows, λ-convexity, atomistic models, continuum limit

AMS subject classifications. 35A15, 35B38, 35K55, 26B25

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1. Introduction.

This article is concerned with a possible concept for analyzing elastic energy functionals which do not satisfy the classical coercivity and weak lower semicontinuity conditions of the calculus of variations. The subject of study is the one-dimensional atomistic energy

$$E_{\mathrm{atom}}\big((y_j)_{j=1}^n\big) = \sum_{j=1}^n \big[J(y_j - y_{j-1}) + f_j u_j\big], \tag{1.1}$$

where $n \in \mathbb{N}$, and y_j are the positions of the atoms with $y_0 = 0$. The family (f_j) represents a linear applied force. We assume that the Lennard–Jones type potential $J = J(z)$ satisfies

$$\begin{aligned}
&J \in \mathrm{C}^2(0,\infty),\\
&J(z) = +\infty \text{ if } z \le 0 \text{ and } J(z) \to +\infty \text{ as } z \to 0,\\
&J'(1) = 0, J''(z) > 0 \text{ in } (0, z_1), \text{ and}\\
&J \text{ is concave, increasing and bounded above in } (z_1, \infty),
\end{aligned} \tag{1.2}$$

with $1 < z_1 < +\infty$. The typical shape is shown in Figure 1.1. Note, that the nonconvexity of J is of a much more fundamental type than the geometric nonconvexity of classical elasticity.

It has been noted previously (see, for example, [24]) that, due to the sublinear growth of J, the energy in (1.1) should not be analyzed in terms of global minimization, as this would give unrealistic material behavior. The most popular example given is that a material described by (1.1) would break for arbitrarily small loads if it were to attain its global minimum. We shall describe this in more detail in section 1.1.

In general, for applications in mechanics, it is advantageous to consider metastable states. The difficulty here is that the number of critical points of E_{atom} tends to infinity as $n \to \infty$. Thus, we require a selection criterion to pick the "correct" equilibrium

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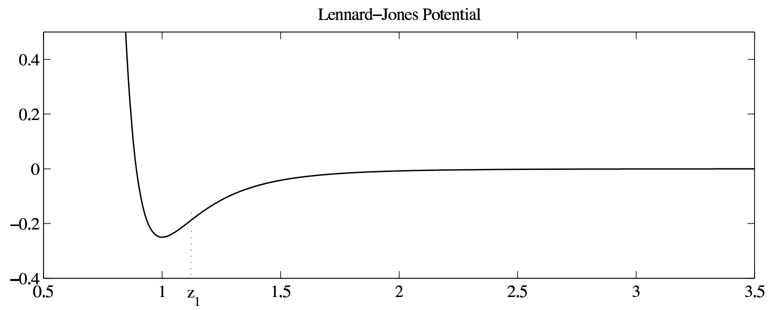

FIG. 1.1. *The shape of natural interaction potentials of Lennard–Jones type.*

points. Theoretically, we should consider the natural dynamics of the material and let time tend to infinity to find its equilibrium state. Here, we take a considerably easier route and use $|\cdot|_{H^1}$-gradient flow dynamics. Our justification for the gradient flow is merely to accept it as a simple model for local minimization. Concerning the choice of the metric, there are also strong mathematical reasons for choosing an $|\cdot|_{H^1}$-gradient flow evolution which are outlined in sections 2 and 3. Note that we do not try to analyze a physical evolution. Our aim is to simply demonstrate a concept which we believe gives better results than the traditional method of global minimization. The ideas in this paper have also important applications for the numerical analysis of coarse-graining techniques such as the QC method [17], as they give an indication how numerical optimization methods can be stabilized [20].

The main goal of the present work is to show that the $|\cdot|_{H^1}$-gradient flow provides a selection criterion for critical points which results in good qualitative properties of the resulting equilibrium model. The simplicity of the one-dimensional model problem makes it possible to give complete results; however, many of the fundamental techniques applied here carry over to much more complicated settings. The additional challenges posed by higher dimensions will be discussed in section 5.

As an application of the idea to use gradient flows to analyze equilibrium points of nonconvex energies, we consider the continuum limit of a rescaled version of the atomistic functional E_{atom} as the number of atoms n tends to infinity. The novelty is that we primarily consider the convergence of the gradient flow evolutions (Theorem 3.1), and obtain the convergence of the equilibria almost as an afterthought (see Theorem 4.1 for elastic deformations and the discussion in section 4.2 for fracture). This procedure gives a different and, one might argue, more realistic continuum limit than previous work; see section 1.2 for a more extensive discussion. In addition, this shows that there is a strong relationship between the atomistic and continuum equilibria.

The local minimizers selected by the gradient flow are weak local minimizers, i.e., local minimizers with respect to the $W^{1,\infty}$-norm. It is clear from the shape of the interaction potential (cf. Figure 1.1) and the comments at the end of section 4.1 that this is in fact the only possibility. In any weaker topology, even the elastic critical points are not local minimizers of the energy. The same is true for fractured states but the interpretation of $W^{1,\infty}$ would be more subtle in this case.

If we replace the Lennard–Jones potential by a potential which is smooth at the origin and therefore J' Lipschitz-continuous, then the convergence analysis of the gradient flow requires only minor modifications of the classical convergence analysis of Galerkin discretizations. For the approach in this paper, however, convergence of the energy is sufficient (cf. Theorem 2.4), which makes a result as general as Theorem 3.1 possible. To achieve this we use some generalizations of ideas in [1, Chapter 4].

For the analysis of equilibria, we use a lim inf condition for the slope of a family of functionals, whose proof is based on the notion of λ-convexity. This condition was also used in [23] to analyze the convergence of gradient flows. Using the techniques of this paper, which has a different aim than the present work, the convergence would have to be obtained by compactness principles (which are not available in our case) rather than λ-convexity.

1.1. The failure of global minimization. The Cauchy–Born hypothesis states that an atomistic body, subjected to a small affine boundary displacement, will follow this displacement in the bulk. Friesecke and Theil demonstrate in [15] a two-dimensional, mathematical version of this important foundation of continuum mechanics by considering global minima of an energy similar to (3.1) but with a quadratic interaction potential. When the potential has sublinear growth, global minimization will typically not reproduce this behavior.

Let us consider the atomistic energy E_{atom} in (1.1) with $f_i \equiv 0$, but apply a "Dirichlet" boundary condition at the right end of the domain as well. For each $\delta > 0$, we consider the minimization problem

$$\min_{y_n = n(1+\delta)} E_{\text{atom}}\big((y_j)_{j=1}^n\big). \tag{1.3}$$

Concerning the formulation of the boundary displacement, note that the minimum of $J(z)$ is attained at $z = 1$. The choice of boundary displacement we have made here scales linearly with the number of atoms. An interesting different choice was made in [6] which we discuss briefly in section 1.2.

PROPOSITION 1.1. *There exist constants $\delta_0, C_0 > 0$, such that, for $\delta_0 > \delta > C_0 n^{-1/2}$, the affine state $y_j = (1+\delta)j$ is not the solution of* (1.3).

Proof. Consider the "fractured" deformation $y_j^f = j$ for $j = 0, 1, \ldots, n-1$ and $y_n^f = n(1+\delta)$. Then,

$$E_f(\delta) = E_{\text{atom}}\big((y_j^f)_{j=1}^n\big) = (n-1)J(1) + J(1+n\delta) \le (n-1)J(1) + \sup_{z\ge 1} J(z).$$

The affine state $y_j^a = (1+\delta)j$ on the other hand has the energy

$$E_a(\delta) = E_{\text{atom}}\big((y_j^a)_{j=1}^n\big) = nJ\big((1+\delta)\big).$$

The assumptions we have made in (1.2) allow us to estimate $J(z)$ from below by a quadratic

$$J(1) + c_0(z-1)^2 \le J(z) \text{ for } 1 \le z < \delta_0,$$

where $c_0 > 0$ and $\delta_0 > 0$ are appropriately chosen. Therefore, for $\delta < \delta_0$, we have $E_a(\delta) \ge n(J(1) + c_0\delta^2)$, and we obtain that $E_a(\delta) > E_f(\delta)$, if

$$\delta^2 > n^{-1}\Big(\frac{\sup_{z\ge 1} J(z) - J(1)}{c_0}\Big) =: C_0^2 n^{-1}. \qquad \square$$

The proof of Proposition 1.1, which is merely a review of well-known facts, actually suggests that not only is the Cauchy–Born hypothesis violated, but in fact any material with a sufficient number of atoms breaks for arbitrarily small boundary displacements or surface forces, if it were to attain its global energy minimum. This behavior is in clear contradiction to observations and, therefore, global minimization should be rejected for models of the type (1.1).

1.2. Continuum limits of atomistic energies. Continuum limits of atomistic models have been studied by many authors in the past. Because it is customary, we consider the case of Dirichlet boundary conditions in this section only. To be able to compute a continuum limit, we need to first rescale the energy (1.1) to a fixed, finite domain. The seemingly naive approach is to use a linear scaling of the energy as well as the boundary condition, which gives

$$E_n^{(1)}\big((y_j)_{j=0}^n\big) = \sum_{j=1}^n \frac{1}{n} J\big(n(y_j - y_{j-1})\big), \quad y_0 = 0, y_n = 1 + \delta. \tag{1.4}$$

If we assume that the body attains its global energy minimum, then for an arbitrarily small boundary displacement δ, the deformation will not be a continuum state (compare Proposition 1.1). This fact is reflected by the Γ-limit of $E_n^{(1)}$ as $n \to \infty$ (see, for example, [4, 5] and references therein) which gives the energy

$$E^{(1)}(y) = \int_0^1 J^{**}(y')\,\mathrm{d}x, y(0) = 0, y(1) = 1 + \delta,$$

where J^{**} is the convex envelope of J.

Motivated by an analysis quite similar to Proposition 1.1, it can be seen that if a different scaling is used, then the Γ-limit becomes more interesting [6]. If we define

$$E_n^{(2)}\big((u_j)_{j=0}^n\big) = \sum_{j=1}^n \Big[J\big(1 + \sqrt{n}(u_j - u_{j-1})\big) - J(1)\Big], \quad u_0 = 0, u_n = \delta,$$

then the Γ-limit turns out to be the Griffiths functional (compare [13])

$$G(u) = \alpha \int_0^1 |u'|^2\,\mathrm{d}x + \beta \sharp S_u, \quad u(0) = 0, u(1) = \delta,$$

where S_u is the set of jump-discontinuities of the displacement u, $\alpha = 1/2J''(1)$ and $\beta = \lim_{z\to\infty} J(z) - J(1)$. The boundary values of the possibly discontinuous functions u can be interpreted in a meaningful way. While it is interesting that the Griffiths functional can be obtained in this way, it should be noted that this model is typically used for crack propagation only, not crack initiation. In one dimension, however, only crack initiation can be analyzed.

The philosophy adopted in the present work is that the scaling of functional $E_n^{(1)}$ is actually the natural one; only the process of passing to the continuum limit is flawed. It will be shown that, if the continuum limit is analyzed in terms of an appropriate evolution, then the resulting model is in fact a very realistic candidate.

One of the problems addressed in this paper (see section 4) is to find the stable equilibrium that the material would "naturally" assume if we started in the reference configuration $y_i^n = x_i^n$, or a perturbation thereof, and then applied forces. In Theorem 4.1 we show that the resulting equilibria represent the correct elastic behavior. For this reason we prefer to work with surface forces rather than a prescribed displacement. This is, however, not a restriction. The entire convergence theory can also be repeated for Dirichlet conditions applied at both ends of the interval.

Closest in spirit to the approach advocated here is the work by Blanc, Le Bris, and Lions [3]. Except for the fact that they consider far more complicated atomistic interactions in three dimensions, their continuum limit is the same. In fact, the present work may be seen as a small step towards a rigorous justification of the approach taken in [3].

From the point of view of numerical analysis, strong connections can be drawn to the local version of the quasicontinuum method [17]. In this respect, the results of E and Ming [11] have some similarities to our own.

For results on the continuum manifestation of some further interesting atomistic effects like finite-range interactions, the reader is referred to [25, 9].

1.3. Outline of the paper. We begin in section 2 by outlining the theoretical tools for the convergence analysis, a theory of gradient flows based on the notion of λ-convexity, and a corresponding approximation theory. We also review the notion of slope which is used to define the concept of critical points.

In section 3, we prove the convergence of an atomistic gradient flow evolution to the $|\cdot|_{\mathrm{H}^1}$-gradient flow of a nonconvex functional defined on H^1, giving a new type of continuum limit for atomistic functionals.

Finally, in section 4, we analyze the resulting equilibrium solutions which are obtained when $t \to \infty$ in the gradient flow. First, we consider the case of small loads and show that the equilibria obtained are the physically reasonable elastic deformations and not the "fractured" global energy minima. Then, we give a brief description of the behavior of the gradient flow evolution in the case when the loads are sufficiently large to create fracture. We demonstrate that the obtained equilibrium is reasonable given that we are always assuming perfect crystals and perfect equilibria. However, these critical points are highly unstable, as is demonstrated also in numerical computations. We may interpret this instability as the uncertainty of where fracture occurs in a material.

1.4. Connections to other models. In section 1.2, some connections to the works of Blanc, Le Bris, and Lions [3] and E and Ming [11] were briefly touched upon. In both of these works, the concept of global minimization of the energy is rejected and alternative means are sought to analyze equilibria of elastic energy functionals. A similar approach is taken by Rieger and Zimmer [22], who use a time-discrete gradient flow evolution of Young-measures to analyze material damage. In the slightly different setting of viscoelasticity [21, 2, 14], it is shown that dynamics can prevent the formation of finer and finer microstructure and therefore the attainment of a global energy minimum.

The model presented here is not to be confused, however, with quasistatic or rate independent evolutions (see, for example, [10, 13] for fracture, [8] for plasticity, or [16] for an abstract analysis). In their time-discrete form, at every timestep an equilibrium (typically a minimum) of a functional of the form

$$D(u_{j-1}, u) + E(u) \tag{1.5}$$

is sought, where D is a so-called dissipation metric. Rather, the gradient flow model we present here should be understood as a simple mechanism to find the equilibrium in the quasistatic evolution (1.5).

2. Approximation of gradient flows of nonconvex energies. Let $\mathscr{H}$ be a Hilbert space with inner product $(\cdot, \cdot)$ and norm $\|\cdot\|$, let $\mathscr{A}$ be a closed convex subset of $\mathscr{H}$, and let $\phi\colon \mathscr{H} \to (-\infty, \infty]$. If ϕ is Fréchet differentiable at a point u, we denote the representation of its derivative, i.e., its gradient, by $\phi'(u)$. Second order derivatives are denoted by $\phi''(u; v_1, v_2)$. We denote the domain of definition of ϕ by $D(\phi) = \{u \in \mathscr{H} : \phi(u) < \infty\}$. By using the convention $+\infty \leq +\infty$, we do in fact not need to make much explicit use of the domain of definition. For example, a functional ϕ would then be convex if and only if $D(\phi)$ is convex and ϕ is convex in $D(\phi)$.

Naively, we may call a curve $u \in \mathrm{C}^1(a, b; \mathscr{H})$ a gradient flow of ϕ, if

$$\dot{u}(t) = -\phi'(u(t)) \quad \forall t \in (a, b). \tag{2.1}$$

Equation (2.1) in infinite-dimensional spaces is usually restated only for convex functionals ϕ. The natural condition on ϕ, under which a considerable part of the theory of gradient flows for convex functionals can be recovered, is the condition of λ-convexity [1]. We say that ϕ is λ-convex in $\mathscr{A}$ if there exists $\lambda \in \mathbb{R}$ such that

$$\begin{aligned} \phi\big((1-t)v_0 + tv_1\big) \le (1-t)\phi(v_0) + t\phi(v_1) - \frac{\lambda}{2} t(1-t)\|v_0 - v_1\|^2 \\ \forall v_0, v_1 \in \mathscr{A} \quad \forall t \in (0,1). \end{aligned} \tag{2.2}$$

To obtain a better feel for the meaning of λ-convexity, consider the following simple proposition (for a proof, see [19]).

PROPOSITION 2.1.

(a) *The functional ϕ is λ-convex in $\mathscr{A}$ if and only if $u \mapsto \phi(u) - \frac{\lambda}{2}\|u\|^2$ is convex in $\mathscr{A}$.*

(b) One-sided Lipschitz continuity of the gradient: *If ϕ is differentiable at every point of $\mathscr{A}$ and satisfies*

$$\big(\phi'(v_1) - \phi'(v_0), v_1 - v_0\big) \ge \lambda\|v_1 - v_0\|^2 \quad \forall\, v_1, v_0 \in \mathscr{A}, \tag{2.3}$$

then ϕ is λ-convex in $\mathscr{A}$.

(c) Boundedness below of the Hessian: *If ϕ is twice differentiable at every nonextremal point of $\mathscr{A}$ and*

$$\phi''(u; v-u, v-u) \ge \lambda\|v - u\|^2 \quad \forall u, v \in \mathscr{A}, \tag{2.4}$$

then ϕ is λ-convex in $\mathscr{A}$.

(d) *If $\phi = \phi_1 + \phi_2$, where $\phi_i \colon \mathscr{A} \to (-\infty, +\infty]$, ϕ_1 is λ_1-convex and ϕ_2 is λ_2-convex, then ϕ is $(\lambda_1 + \lambda_2)$-convex.*

If a functional is λ-convex, then its gradient flows have an alternative characterization. Suppose that a curve $u \in \mathrm{C}^1(a, b; \mathscr{H})$ satisfies (2.1), where ϕ is λ-convex. By a relatively straightforward energy argument, one can show that u also satisfies the evolutionary variational inequality

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t) - v\|^2 + \frac{\lambda}{2}\|u(t) - v\|^2 + \phi(u(t)) \le \phi(v) \quad \forall\, v \in \mathscr{H}, \forall\, t \in (a, b).$$

This inequality is the basis for a powerful theory of gradient flows in metric spaces, then called curves of maximal slope, developed in Chapter 4 of [1]. Note, for example, that it makes sense to consider $u, v \in \mathscr{A}$ only, instead of all of $\mathscr{H}$. Theorem 2.2 is a collection of results in [1] translated to the Hilbert space setting which is sufficient for our purposes.

THEOREM 2.2 (existence and uniqueness). *Let $\mathscr{A}$ be a closed, convex subset of a Hilbert space $\mathscr{H}$ and let $\phi \colon \mathscr{A} \to (-\infty, \infty]$ be (strongly) lower semicontinuous and λ-convex. For each $u_0 \in D(\phi)$, there exists a locally Lipschitz-continuous curve $u \colon [0, \infty) \to \mathscr{A}$ which is the unique solution of*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t) - v\|^2 + \frac{\lambda}{2}\|u(t) - v\|^2 + \phi(u(t)) \le \phi(v) \quad \forall\, v \in \mathscr{A} \text{ for a.e. } t > 0, \tag{2.5}$$

among all curves $v \in \mathrm{AC}_{\mathrm{loc}}(0,\infty;\mathscr{A})$, *satisfying* $v(0+) = u_0$.

For the remainder of the paper, we shall use the following definition for a gradient flow.

Definition 2.3. *Let* $\mathscr{A}$ *be a closed, convex subset of a Hilbert space* $\mathscr{H}$ *and* $\phi\colon \mathscr{A} \to (-\infty,\infty]$ *a lower semicontinuous and* λ*-convex functional. We say that a locally Lipschitz-continuous curve* $u\colon [0,\infty) \to \mathscr{A}$ *is a gradient flow of* ϕ, *if it satisfies* (2.5).

2.1. Approximation of gradient flows. Based on the evolutionary variational inequality stated above, an abstract convergence theory for gradient flows in a general metric setting for λ-convex functionals was developed in [19]. Theorem 2.4 below is one result therein which is relevant for the Hilbert space setting in the present work. For the sake of completeness, we give a sketch of the proof.

Theorem 2.4. *Let* $\mathscr{A}$ *be a closed, convex subset of a Hilbert space* $\mathscr{H}$ *and, for* $n \in \mathbb{N}$, *let* $\phi, \phi_n\colon \mathscr{A} \to (-\infty,\infty]$ *be functionals defined on* $\mathscr{A}$. *Let* $u^0 \in D(\phi)$ *and* $u_n^0 \in D(\phi_n)$ *be given initial values, and assume that the following conditions are satisfied:*

(i) Lower semicontinuity: *The functionals* ϕ *and* ϕ_n $(n \in \mathbb{N})$ *are lower semicontinuous.*

(ii) Uniform λ-convexity: *There exists* $\lambda \in \mathbb{R}$, *such that the* ϕ_n *as well as* ϕ *are* λ*-convex.*

(iii) Equicoercivity: *There exists a point* $u^* \in \mathscr{A}$ *and* $\epsilon > 0$ *such that* $\inf_{n\in\mathbb{N}} \inf_{v\in\mathscr{A}, \|v-u^*\|\le\epsilon} \phi_n(v) > -\infty$.

(iv) Convergence of the initial data: $\sup_{n\in\mathbb{N}} \phi_n(u_n^0) < \infty$ *and* $\|u_n^0 - u^0\| \to 0$ *as* $n \to \infty$.

(v) Consistency: *If* $(w_n)_{n\in\mathbb{N}} \subset \mathscr{A}$ *is bounded in* $\mathscr{H}$, *then there exists a constant* $c_1 > 0$ *such that*

$$\limsup_{n\to\infty} \big(\phi(w_n) - \phi_n(w_n)\big) \le 0, \text{ and } \phi(w_n) \le c_1(1 + [\phi_n(w_n)]^+ + \|w_n\|^2).$$

(vi) Best approximation error: *For every* $n \in \mathbb{N}$, *there exists a Borel-measurable curve* $v_n\colon (0,\infty) \to \mathscr{A}$, *so that* $v_n \to u$ *in* $\mathrm{L}^2_{\mathrm{loc}}([0,\infty);\mathscr{H})$ *and*

$$\phi_n(v_n(t)) \to \phi(u(t)) \text{ and } \phi_n(v_n(t)) \le c_2(1 + [\phi(u(t))]^+ + \|u(t)\|^2),$$

where u *is the gradient flow of* ϕ *with initial data* u^0.

Then the gradient flows (in the sense of Definition 2.3*)* u_n *of* ϕ_n *with initial values* u_n^0 *converge in* $\mathrm{L}^\infty_{\mathrm{loc}}([0,\infty);\mathscr{H})$ *to the gradient flow* u *of* ϕ *with initial value* u^0.

Proof. Let u and u_n, respectively, satisfy

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u(t) - v\|^2 + \frac{\lambda}{2}\|u(t) - v\|^2 + \phi(u(t)) \le \phi(v) \quad \forall\, v \in \mathscr{A}, \text{ and} \tag{2.6}$$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_n(t) - v_n\|^2 + \frac{\lambda}{2}\|u_n(t) - v_n\|^2 + \phi(u_n(t)) \le \phi(v_n) \quad \forall\, v_n \in \mathscr{A}. \tag{2.7}$$

We test (2.6) with $v = u_n$ and choose a recovery sequence v_n satisfying (vi) to test (2.7). Adding (2.6) and (2.7) and some lengthy but relatively straightforward algebra gives the error estimate

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u - u_n\|^2 + \frac{\tilde\lambda}{2}\|u - u_n\|^2 \le \big(\phi_n(v_n) - \phi(u)\big) + \big(\phi(u_n) - \phi_n(u_n)\big) + \frac{|\lambda|}{2}\|v_n - u\|^2 + \frac{1}{2}\|\dot u_n\|\|v_n - u\|,$$

where $\tilde{\lambda} = \lambda - |\lambda|/2$. The λ-convexity can be used to derive an a priori estimate on the $L^2(0,T)$-norm of $\|\dot{u}_n\|$ and $\phi(u_n)$. Using Gronwall's inequality, we obtain

$$e^{2\tilde{\lambda}T}\|u(T) - u_n(T)\|^2 \leq \|u(0) - u_n(0)\|^2 + \int_0^T e^{2\tilde{\lambda}t}(\text{error terms})\,dt.$$

Using Fatou's lemma, the integral term on the right-hand side can be shown to tend to zero as $n \to \infty$, given the hypothesis of the theorem. $\square$

Next, we state a result from [1], concerning the implicit Euler approximation of a gradient flow, which we will use frequently in section 4.

LEMMA 2.5. *Let $t_j = j\tau$, for $j = 0, 1, \ldots,$ define a partition of $[0,\infty)$, with $0 < \tau < 1/\min(0, -\lambda)$. Let $u_0 \in \mathscr{H}$, and let the family $(u_i)_{i=1,2,\ldots}$ be defined by*

$$u_i = \operatorname{argmin}_{\mathscr{A}} \left[v \mapsto \frac{\|v - u_{i-1}\|^2}{2\tau} + \phi(v) \right].$$

Let $u(t)$ be the gradient flow of ϕ with $u(0) = u_0$ and let $\bar{u}_\tau(t)$ be the piecewise constant interpolant of (u_i), i.e.,

$$\bar{u}_\tau(0) = 0 \quad \text{and} \quad \bar{u}_\tau(t) = u_i \quad \text{if } t_{i-1} < t \leq t_i.$$

Then, $\bar{u}_\tau(t) \to u(t)$ in $L^\infty_{\mathrm{loc}}([0,\infty), \mathscr{H})$, as $\tau \to 0$.

2.2. The slope. So far we have only described gradient flow evolutions. However, we are also interested in analyzing the resulting equilibria, which can often be obtained by letting time tend to infinity. A natural concept of equilibrium, or critical point, is given by the concept of local slope,

$$|\partial\phi|(u) = \limsup_{v \to u} \frac{(\phi(u) - \phi(v))^+}{\|u - v\|}. \tag{2.8}$$

We say that $u^* \in \mathscr{H}$ is a critical point of the functional ϕ, if $|\partial\phi|(u^*) = 0$. The following lemma can be used in certain situations to show that an accumulation point of critical points of approximate functionals ϕ_n must again be a critical point.

LEMMA 2.6. *Let $\mathscr{H}$ be a Hilbert space, let $\phi, \phi_n \colon \mathscr{H} \to (-\infty, \infty]$ be λ-convex, with a uniform λ, and suppose that ϕ_n Γ-converges to ϕ in the strong topology of $\mathscr{H}$, i.e.,*

$$v_n \to v \Rightarrow \phi(v) \leq \liminf_{n \to \infty} \phi_n(v_n) \tag{2.9}$$

$$\forall v \in \mathscr{H}\ \exists (v_n)_{n \in \mathbb{N}} \subset \mathscr{H} \text{ s.t. } v_n \to v \text{ and } \phi(v) = \lim_{n \to \infty} \phi(v_n). \tag{2.10}$$

Then, the slopes satisfy the lim inf condition

$$u_n \to u \Rightarrow |\partial\phi|(u) \leq \liminf_{n \to \infty} |\partial\phi_n|(u_n). \tag{2.11}$$

Proof. The crucial observation [1, Theorem 2.4.9] is that for λ-convex functionals, the slope can be rewritten as

$$|\partial\phi|(u) = \sup_{v \neq u} \left[\frac{\phi(u) - \phi(v)}{\|u - v\|} + \frac{\lambda}{2}\|u - v\|^2 \right]^+.$$

Let $u_n \to u$, and for some fixed $v \neq u$ let $(v_n)_{n\in\mathbb{N}}$ be a recovery sequence for v, satisfying (2.10). Then, we have

$$\begin{aligned}
&\left[\frac{\phi(u)-\phi(v)}{\|u-v\|}+\frac{\lambda}{2}\|u-v\|^2\right]^+\\
&\le \left[\frac{\liminf_{n\to\infty}\phi_n(u_n)-\lim_{n\to\infty}\phi_n(v_n)}{\lim_{n\to\infty}\|u_n-v_n\|}+\frac{\lambda}{2}\lim_{n\to\infty}\|u_n-v_n\|^2\right]^+\\
&\le \liminf_{n\to\infty}\left[\frac{\phi_n(u_n)-\phi_n(v_n)}{\|u_n-v_n\|}+\frac{\lambda}{2}\|u_n-v_n\|^2\right]^+\\
&\le \liminf_{n\to\infty}|\partial\phi_n|(u_n).
\end{aligned}$$

Taking the supremum over $v \neq u$, we obtain (2.11). ∎

3. Convergence of an atomistic evolution. In section 1.2, it was outlined that different scalings of the atomistic energy E_{atom} give rise to different continuum limits. We have adopted the point of view that a linear scaling of all terms considered is the most natural choice. For the forces we assume that $f_n = O(1)$ and $f_j = O(1/n)$ for $1 \le j \le n-1$, i.e., f_n represents a boundary force. It is then natural to consider the rescaled energy

$$E_n\big((y_j^n)_{j=1}^n\big) = \sum_{j=1}^n \epsilon_n\left[J\left(\frac{y_j^n - y_{j-1}^n}{\epsilon_n}\right) - f_j^n(y_j^n + y_{j-1}^n)/2\right] - g y_n^n, \tag{3.1}$$

where $\epsilon_n = 1/n$. The family $(f_i^n)_{i=1,\dots,n}$ defines a linear body force, which we assume is obtained by averaging an L^1 function, i.e.,

$$f_i^n = ⨍_{x_{i-1}^n}^{x_i^n} f(x)\,\mathrm{d}x,$$

where $x_i^n = i/n$, for each $i \in \mathbb{Z}$. The scalar g describes a linear surface force. For technical reasons, we may wish to impose an L^∞ bound on the deformations, i.e., we shall assume that $y_i^n \le M$, where $M \in (z_1, \infty]$.

To rewrite E_n as an integral functional it is customary to identify the atomistic deformation with a piecewise affine function. To this end, we define the set of "admissible" atomistic deformations to be

$$\mathscr{A}_n := \big\{v \in \mathrm{H}^1(0,1)\colon v(0) = 0, v \le M, \text{ and } v \text{ is piecewise affine w.r.t. } (x_i^n)\big\}.$$

Letting

$$\begin{aligned}
y_n'(x) &= \frac{y_i^n - y_{i-1}^n}{\epsilon_n} \quad \text{if } x \in (x_{i-1}^n, x_i^n), \text{ and}\\
y_n(x) &= \int_0^x y_n'(x)\,\mathrm{d}x,
\end{aligned}$$

y_n is the piecewise-affine interpolant of (y_i^n) and y_n' is its weak derivative, and we have in particular that $y_n \in \mathscr{A}_n$. Thus, we can rewrite E_n as

$$E_n(y_n) = \int_0^1 \big[J(y_n') - f_n y_n\big]\,\mathrm{d}x - g y_n(1) \qquad \text{for } y_n \in \mathscr{A}_n, \tag{3.2}$$

where f_n is the piecewise constant interpolant of f with

$$f_n(x) = f_n^i \quad \text{for } x \in (x_{i-1}, x_i). \tag{3.3}$$

In the formulation (3.2) it becomes obvious that the nonconvexity is with respect to the deformation gradient. In order to balance it out with the evolution, we need to consider the gradient flow with respect to the $|\cdot|_{\mathrm{H}^1}$-seminorm, which is in fact a norm in the spaces $\mathscr{A}_n$. We shall show below, though it is already quite obvious at this point, that the functionals E_n are uniformly λ-convex in the $|\cdot|_{\mathrm{H}^1}$-seminorm. Therefore, from Theorem 2.4, we expect the correct limit energy with respect to the $|\cdot|_{\mathrm{H}^1}$-gradient flow evolution to be

$$E(y) = \int_0^1 \big[J(y') - fy\big]\,\mathrm{d}x - gy(1), \tag{3.4}$$

defined for $y \in \mathscr{A} := \{v \in \mathrm{H}^1(0,1) \colon v(0) = 0, v \le M\}$.

While it is possible to consider gradient flows with respect to the full H^1-norm as well, the analysis of equilibria becomes significantly more technical. In addition, the $|\cdot|_{\mathrm{H}^1}$-seminorm seems to be the more natural metric for the gradient flow. All results can, however, be translated to the H^1-norm case [18].

Theorem 3.1 states that the (atomistic) $|\cdot|_{\mathrm{H}^1}$-gradient flow of E_n in $\mathscr{A}_n$ converges to the (continuum) $|\cdot|_{\mathrm{H}^1}$-gradient flow of E in $\mathscr{A}$. We embed $\mathscr{A}_n$ in $\mathscr{A}$ by setting $E_n(y) = +\infty$ if $y \in \mathscr{A} \setminus \mathscr{A}_n$.

THEOREM 3.1. *Let $y^0 \in D(E)$, and let $y_n^0 \in \mathscr{A}_n$ be the piecewise affine interpolant of y^0 with respect to the mesh (x_i^n). Then, the $|\cdot|_{\mathrm{H}^1}$-gradient flow y_n of E_n with initial data y_n^0 converges in $\mathrm{L}^\infty_{\mathrm{loc}}([0,\infty);\mathscr{A})$ to the $|\cdot|_{\mathrm{H}^1}$-gradient flow y of E with initial data y^0.*

The convergence proof consists of three steps: first, establishing the λ-convexity of the functionals; second, estimating the perturbations caused by the discrete forcing term; and third, constructing a recovery sequence for the solution which satisfies condition (vi) of Theorem 2.4.

LEMMA 3.2. *With respect to the norm $|\cdot|_{\mathrm{H}^1}$, the functionals E and E_n $(n \in \mathbb{N})$ are λ-convex in $\mathscr{A}$, with $\lambda = \min_{z>0} J''(z)$, and lower semicontinuous.*

Proof. For the λ-convexity as well as the lower semicontinuity, note that the linear, continuous terms need not be considered and we assume without loss of generality that $f, g \equiv 0$. In the spirit of Proposition 2.1, we define $F(z) = J(z) - (\lambda/2)z^2$. By the definition of λ, $F''(y) \ge 0$ whenever $y > 0$, hence F is convex in $(0,\infty)$. Since $F(z) = +\infty$ for $z \le 0$, F is convex on $\mathbb{R}$. Therefore, the functional

$$G(y) = \int_0^1 \Big(J(y') - \frac{\lambda}{2}|y'|^2\Big)\,\mathrm{d}x \;=\; \int_0^1 F(y')\,\mathrm{d}x$$

is convex as well which implies, by Proposition 2.1, that E is λ-convex. Since $E(y) = G(y) - \lambda/2|y|_{\mathrm{H}^1}^2$, a sum of a convex and a continuous functional, E is lower semicontinuous. To see that E_n is lower semicontinuous, simply note that under the assumption that $f, g \equiv 0$, $E_n = E|_{\mathscr{A}_n}$, where $\mathscr{A}_n$ is convex and closed and hence the proof carries over to E_n as well. $\square$

LEMMA 3.3. *If $f \in \mathrm{L}^1(0,1)$, then, for every $v \in \mathscr{A}$, we have*

$$\Big|\int_0^1 (f_n - f)v\,\mathrm{d}x\Big| \le |v|_{\mathrm{H}^1}\|f - f_n\|_{\mathrm{L}^1(0,1)}, \text{ and}$$
$$\|f - f_n\|_{\mathrm{L}^1} \to 0 \quad \text{as } n \to \infty,$$

where f_n *is defined as in* (3.3).

Proof. Hölder's inequality gives

$$\left| \int_0^1 (f_n - f) v \, \mathrm{d}x \right| \le \|v\|_{\mathrm{L}^\infty} \|f - f_n\|_{\mathrm{L}^1(0,1)}.$$

Using $v(0) = 0$, we also have $\|v\|_{\mathrm{L}^\infty} \le \|v'\|_{\mathrm{L}^1} \le |v|_{\mathrm{H}^1}$, which gives the first result. The convergence $\|f_n - f\|_{\mathrm{L}^1} \to 0$ follows from the fact that f_n is the L^2-projection of f onto the piecewise constant functions with respect to the mesh (x_i^n), using also the density of $\mathrm{L}^2(0,1)$ in $\mathrm{L}^1(0,1)$. ▯

LEMMA 3.4. *Let* E *and* E_n *be, respectively, given by* (3.4) *and* (3.2), *where* $f \in \mathrm{L}^1(0,1)$ *and* f_n *satisfies* (3.3). *For every* $y \in \mathscr{A}$ *with* $E(y) < +\infty$, *the piecewise affine, continuous interpolants* v_n *of* y *with respect to the mesh* (x_i^n) *satisfy*

$$\begin{aligned} &|v_n - y|_{\mathrm{H}^1} \to 0, E_n(v_n) \to E(y) \quad \text{as } n \to \infty, \\ &|v_n|_{\mathrm{H}^1} \le |y|_{\mathrm{H}^1}, \text{ and } \; E_n(v_n) \le \left[2\|f\|_{\mathrm{L}^1}^2 + \sup_{z \ge 1} J(z) \right] + E(y) + 2|y|_{\mathrm{H}^1}^2. \end{aligned}$$

Proof. Let $y \in \mathscr{A}$, and let v_n be the piecewise affine interpolant with respect to the mesh (x_i^n). Applying Jensen's inequality to

$$\int_{x_{i-1}^n}^{x_i^n} v_n' \, \mathrm{d}x = \int_{x_{i-1}^n}^{x_i^n} y' \, \mathrm{d}x,$$

and summing over i, we get $\|v_n'\|_{\mathrm{L}^2(0,1)} \le \|y'\|_{\mathrm{L}^2(0,1)}$. It follows from standard interpolation error estimates and a simple density argument that $|y - v_n|_{\mathrm{H}^1} \to 0$ as $n \to \infty$.

To compute the bounds on the energy as well and to show its convergence, we start with the lower-order terms. Jensen's inequality gives $\|f_n\|_{\mathrm{L}^1} \le \|f\|_{\mathrm{L}^1}$ and as in the proof of Lemma 3.3, $\|v_{(n)}\|_{\mathrm{L}^\infty} \le |v_{(n)}|_{\mathrm{H}^1} \le |v|_{\mathrm{H}^1}$. Thus, we have

$$\begin{aligned} -\int_0^1 f_n v_n \, \mathrm{d}x &= -\int_0^1 f y \, \mathrm{d}x + \int_0^1 \left[f(y - v_n) + (f - f_n) v_n \right] \mathrm{d}x \\ &\le -\int_0^1 f y \, \mathrm{d}x + \|f\|_{\mathrm{L}^1} \|y - v_n\|_{\mathrm{L}^\infty} + \|f - f_n\|_{\mathrm{L}^1} \|v_n\|_{\mathrm{L}^\infty} \\ &\le -\int_0^1 f y \, \mathrm{d}x + \|f\|_{\mathrm{L}^1} |y - v_n|_{\mathrm{H}^1} + \|f - f_n\|_{\mathrm{L}^1} |v|_{\mathrm{H}^1} \qquad (3.5) \\ &\le -\int_0^1 f y \, \mathrm{d}x + 2\|f\|_{\mathrm{L}^1}^2 + 2|y|_{\mathrm{H}^1}^2. \qquad (3.6) \end{aligned}$$

Using Lemma 3.3 and the fact that $v_n(1) = y(1)$ for all $n \in \mathbb{N}$, we obtain from (3.5) and (3.6),

$$\begin{aligned} &-\int_0^1 f_n v_n \, \mathrm{d}x - g v_n(1) \to -\int_0^1 f y \, \mathrm{d}x - g y(1) \quad \text{as } n \to \infty, \text{ and} \qquad (3.7) \\ &-\int_0^1 f_n v_n \, \mathrm{d}x - g v_n(1) \le -\int_0^1 f y \, \mathrm{d}x - g y(1) + 2\|f\|_{\mathrm{L}^2(0,1)}^2 + 2|y|_{\mathrm{H}^1}^2. \end{aligned}$$

To deal with the higher-order terms, let $J(z) = J_0(z) + J_1(z)$, where $J_0(z) = J(z)\chi_{(-\infty,1](z)}$. In the interval (x_{i-1}^n, x_i^n), we have $v_n' = n \int_{x_{i-1}^n}^{x_i^n} y' \, \mathrm{d}x$ and, using

Jensen's inequality $J_0(v_n') \le n\int_{x_{i-1}^n}^{x_i^n} J_0(y')\,\mathrm{d}x$ (note that $1/n$ is the length of the interval). If we define

$$a_n(x) = n\int_{x_{i-1}^n}^{x_i^n} J_0(y')\,\mathrm{d}x + \sup_{z\ge 1} J(z) \qquad \text{for } x \in (x_{i-1}^n, x_i^n),$$

then $J(v_n') \le a_n(x)$ a.e. in $(0,1)$ and

$$\int_0^1 a_n(x)\,\mathrm{d}x = \int_0^1 J_0(y')\,\mathrm{d}x + \sup_{z\ge 1} J(z) =: A.$$

In particular, we also have

$$\int_0^1 J(v_n')\,\mathrm{d}x \le \int_0^1 J(y')\,\mathrm{d}x + \sup_{z\ge 1} J(z),$$

which, together with (3.7) gives

$$E_n(v_n) \le \left[2\|f\|_{\mathrm{L}^1}^2 + \sup_{z\ge 1} J(z)\right] + E(y) + 2|y|_{\mathrm{H}^1}^2. \tag{3.8}$$

Since $x \mapsto J_0(y'(x)) \in \mathrm{L}^1(0,1)$, we have, by a slightly stronger version of Lebesgue's differentiation theorem ([12], section 1.7, Corollary 2),

$$\lim_{n\to\infty} a_n(x) = J_0(x) + \sup_{z\ge 1} J(z)$$

for a.e. $x \in (0,1)$, and similarly, $v_n' \to y'$ a.e. in $(0,1)$.

Using Fatou's lemma, and the fact that J is continuous in $(0,\infty)$, we have

$$\begin{aligned} 2A - \limsup_{n\to\infty}\int_0^1 \big|J(v_n') - J(y')\big|\,\mathrm{d}x &= \liminf_{n\to\infty}\int_0^1 \big[2a_n - |J(v_n') - J(y')|\big]\,\mathrm{d}x \\ &\ge \int_0^1 \liminf_{n\to\infty}\big[2a_n - |J(v_n') - J(y')|\big]\,\mathrm{d}x \\ &= 2\int_0^1 \left[J_0(y') + \sup_{z\ge 1} J(z)\right]\mathrm{d}x \\ &= 2A, \end{aligned}$$

and hence, using also (3.7), we have $E(v_n) \to E(y)$ as $n \to \infty$. □

We have now assembled all results required to prove Theorem 3.1.

Proof of Theorem 3.1. The result is a straightforward application of Theorem 2.4, using the preparations of this section.

Conditions (i) and (ii) were shown in Lemma 3.2. Condition (iii), the equi-coercivity, follows from the fact that J is bounded below and the forcing term is Lipschitz continuous. Condition (iv), the convergence of the initial data, is guaranteed by standard interpolation error results as well as Lemma 3.4. Condition (v) is controlled by Lemma 3.3, since E_n and $E|_{\mathscr{A}_n}$ differ only in the forcing term.

Let $v_n(t)$ be the piecewise affine interpolant of $y(t)$. Using Lemma 3.4 to obtain (vi) we only need to show that $t \mapsto v_n(t)$ is Borel measurable. In fact, it is fairly easy to see that it is even continuous. Since in one dimension, $\mathrm{H}^1(0,1)$ is embedded in C[0, 1], the mapping $t \mapsto y(t)$ lies in $C(0,\infty; C[0,1])$ and hence $t \mapsto y(t,x)$ is continuous as well. Since

$$v_n(t,x) = \sum_{j=1}^{n} y(t, x_j^n)\varphi_j^n(x),$$

where the φ_j^n are Lipschitz functions, this shows that $v \in C(0,\infty; H^1)$. □

4. Convergence of equilibria.

4.1. Elastic deformation. In this section we show that the gradient flows are a selection criterion which can be used to recover correct elastic behavior even when the energies are highly nonconvex.

The convergence result of Theorem 3.1 suggests the following procedure: for sufficiently small forces, there should be a critical point y_n^*, in fact a strict local minimum, of the atomistic functional E_n, such that ${y_n^*}' < z_1$, i.e., the deformation gradient lies in the region where J is convex. Hence, the gradient flow for sufficiently close starting points should converge to y_n^* as $t \to \infty$ and the deformation gradient should remain within the region where J is convex. Since the atomistic gradient flow converges to the continuum gradient flow, the continuum deformation gradient should remain in this region as well and therefore converge to a critical point in that set which should be the limit of the y_n^*. By y^* being a critical point of ϕ, we mean that $|\partial\phi|(y^*) = 0$, where $|\partial\phi|(y)$ is the $|\cdot|_{H^1}$-slope of ϕ at y (see section 2.2).

The main difficulty is to show that the critical points y_n^* are "uniform local minimizers" in the sense that we do not require perturbations to tend to zero as $n \to \infty$.

Before we start with the suggested program, let us note that it would be quite easy to show all results for the continuum problem directly. However, we wish to show here that the elastic critical point of the continuum functional (3.4) arises as the limit of the elastic critical points of the atomistic functionals (3.2). Furthermore, it is an interesting feature of the analysis that all information about the continuum functional can be obtained from the knowledge about the atomistic evolution.

THEOREM 4.1. *Let $(E_n)_{n\in\mathbb{N}}, E$ be defined, respectively, by* (3.2) *and* (3.4), *and assume that $|g| + \|f\|_{L^1(0,1)} < J'(z_1)$ (compare* (1.2)*).*

(a) *There exist critical points y_n^* of E_n in $\mathscr{A}_n$, such that ${y_n^*}' < z_1$. These equilibria are stable in the sense that any $|\cdot|_{H^1}$-gradient flow y_n of E_n with $y_n'(0,x) < z_1$ satisfies $\lim_{t\to\infty} y_n(t) = y_n^*$ in $H^1(0,1)$.*

(b) *There exists a critical point $y^* \in \mathscr{A}$ of E such that $\lim_{n\to\infty} y_n^* = y^*$ and $\lim_{t\to\infty} y(t) = y^*$ in H^1, for every $|\cdot|_{H^1}$-gradient flow y of E with $y'(0,x) \le z_1 - \epsilon$ for some $\epsilon > 0$.*

(c) *If, in addition, $f \equiv 0$, then $y_n^* = y^*$ are affine.*

On the one hand, Theorem 4.1 shows that the derived continuum model has the correct qualitative and quantitative behavior for small loads. On the other hand, it shows that in this situation, the atomistic model behaves essentially like a continuum. In particular, note that point (c) is the Cauchy–Born hypothesis for the model presented.

Note also that not all proofs in this section are "optimal." Particularly, the final proof of Theorem 4.1 is more technical than it needs to be. The purpose of this discussion is to show that most of the techniques used here can be applied to far more general problems and are, in particular, dimension independent.

The proof of Theorem 4.1 requires some preparation in the form of several lemmas which assemble information about the atomistic gradient flow. Let $\mathscr{B}$ be the set of all deformations whose gradient remains in the region where J is convex, i.e., we define

$$\mathscr{B}_\epsilon = \{v \in \mathscr{A} : v'(x) \le z_1 - \epsilon \text{ for a.e. } x \in (0,1)\}, \tag{4.1}$$

and $\mathscr{B} = \mathscr{B}_0$.

LEMMA 4.2. *Suppose that* $|g| + \|f\|_{L^1(0,1)} \le J'(z_1 - \epsilon)$ *for some* $\epsilon > 0$*; then there exists a unique critical point* y_n^* *of* E_n *in the set* $\mathscr{B}_\epsilon$*. The point* y_n^* *satisfies*

$$y_n^{*\prime}(x) = (J')^{-1}(F_j^n) \le z_1 - \epsilon \quad \text{ for } x_{j-1}^n < x < x_j^n, \tag{4.2}$$

where F_j^n *is defined by* (4.3).

Proof. We compute the critical point by a change of variables. For $y_n \in \mathscr{A}_n$, let $r_j^n = (y_j^n - y_{j-1}^n)/\epsilon_n$. Then, setting

$$\tilde{f}_i^n = \begin{cases} \frac{1}{2} f_1^n & \text{if } i = 0, \\ \frac{1}{2}(f_i^n + f_{i+1}^n) & \text{if } 1 \le i \le n-1, \\ \frac{1}{2} f_n^n & \text{if } i = n, \end{cases}$$

we have, using $y_0^n = 0$,

$$\begin{aligned} E_n(y_n) &= \sum_{j=1}^n \epsilon_n J(r_j^n) - \sum_{j=0}^n \epsilon_n \tilde{f}_j^n y_j^n - g y_n^n \\ &= \sum_{j=1}^n \epsilon_n J(r_j^n) - \sum_{j=1}^n \epsilon_n \tilde{f}_j^n \sum_{i=1}^j \epsilon_n r_i^n - g \sum_{i=1}^n \epsilon_n r_i^n \\ &= \sum_{j=1}^n \epsilon_n J(r_j^n) - \sum_{i=1}^n \epsilon_n r_i^n \left[g + \sum_{j=i}^n \epsilon_n \tilde{f}_j^n \right] \\ &= \sum_{j=1}^n \epsilon_n \big[J(r_j^n) - F_j^n r_j^n \big], \end{aligned}$$

where

$$F_i^n \ = \ g + \sum_{j=i}^n \epsilon_n \tilde{f}_j^n \ = \ g + \frac{\epsilon_n}{2}(f_i^n + f_n^n) + \sum_{j=i+1}^{n-1} \epsilon_n f_j^n. \tag{4.3}$$

To compute r_j^n, we differentiate E_n with respect to r_j^n, which gives the equation

$$\frac{\partial E_n(y_n)}{\partial r_j^n} = \epsilon_n \big[J'(r_j^n) - F_j^n \big] = 0 \quad \text{for } j = 1, \ldots, n,$$

or, equivalently, $J'(r_j^n) = F_j^n$. We estimate F_j^n, using the assumption that $\|f\|_{L^1} + |g| \le J'(z_1 - \epsilon)$, by

$$\begin{aligned} |F_j^n| &= \left| g + \frac{1}{2} \int_{x_{j-1}^n}^{x_j^n} f(x)\,\mathrm{d}x + \int_{x_j^n}^{x_{n-1}^n} f(x)\,\mathrm{d}x + \frac{1}{2} \int_{x_{n-1}^n}^{1} f(x)\,\mathrm{d}x \right| \\ &\le |g| + \int_{x_{j-1}^n}^{1} |f(x)|\,\mathrm{d}x \\ &\le |g| + \|f\|_{L^1(0,1)} \\ &\le J'(z_1 - \epsilon). \end{aligned} \tag{4.4}$$

In the region $\{z < z_1\}$, $J'(z)$ is strictly increasing and hence invertible. Therefore,

$$r_j^n = (J')^{-1}(F_j^n) \le z_1 - \epsilon$$

describes the unique critical point of E_n in $\mathscr{B}_\epsilon$. ☐

LEMMA 4.3. *Under the conditions of Lemma 4.2, if $y_n\colon [0,\infty) \to \mathscr{A}_n$ is an $|\cdot|_{\mathrm{H}^1}$-gradient flow of E_n with $y_n(0) \in \mathscr{B}_\epsilon$, then $y_n(t) \in \mathscr{B}_\epsilon$ for all $t > 0$.*

Proof. Consider the time-discrete approximation $(U_n(t_j))_{j=0,1,\dots}$, as described in Lemma 2.5, for some fixed, sufficiently small time-step τ. Let $R_n^i(t_j)$ be as in the proof of Lemma 4.2. Then, $R_n(t_j)$ minimizes

$$\frac{1}{2\tau}\|R_n(t_j) - R_n(t_{j-1})\|_{L^2}^2 + E_n(R_n(t_j)). \tag{4.5}$$

As in the proof of Lemma 4.2, we compute the Euler–Lagrange equation in terms of $R_n^i(t_j)$. At the minimum, the equation

$$\frac{1}{\tau}\Big(R_n^i(t_j) - R_n^i(t_{j-1})\Big) = F_j^n - J'(R_n^i(t_j))$$

has to be satisfied. For sufficiently small τ, there is a unique solution. Now assume inductively that $R_n^i(t_{j-1}) \le z_1 - \epsilon$. To show that $R_n^i(t_j) \le z_1 - \epsilon$, assume this is not true. Then $F_j^n - J'(R_n^i(t_j)) < 0$, which gives a contradiction. Hence, we have that for all $i = 1, \dots, n$ and $j \in \mathbb{N}$, $R_n^i(t_j) \le z_1 - \epsilon$. As $\tau \to 0$, the discrete solution converges to the gradient flow y_n and hence $y_n' \le z_1 - \epsilon$ a.e. in $(0,1)$. ☐

COROLLARY 4.4. *Under the conditions of Lemma 4.2, every $|\cdot|_{\mathrm{H}^1}$-gradient flow y_n with $y_n(0) \in \mathscr{B}_\epsilon$ satisfies the evolutionary variational inequality*

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|y_n - v|_{\mathrm{H}^1}^2 + \frac{\alpha}{2}|y_n - v|_{\mathrm{H}^1}^2 + E_n(y_n) \le E_n(v) \quad \forall v \in \mathscr{B}_\epsilon, \tag{4.6}$$

where $\alpha = \min_{z \le z_1 - \epsilon} J''(z) > 0$. In particular, we have

$$|y_n(t) - y_n^*|_{\mathrm{H}^1} \le e^{-\alpha t}|y_n(0) - y_n^*|_{\mathrm{H}^1}.$$

Proof. We set $\tilde{E}_n = E_n|_{\mathscr{B}_\epsilon}$ and show that y_n is also a gradient flow for $\tilde{E}_n$ by considering the minimization problem (4.5) again. (Note that this procedure is equivalent to replacing E_n outside of $\mathscr{B}_\epsilon$ by a uniformly convex functional.) Since the minimizer remains in $\mathscr{B}_\epsilon$, it is also the minimizer of

$$\frac{1}{2\tau}\|R_n(t_j) - R_n(t_{j-1})\|_{\mathrm{L}^2}^2 + \tilde{E}_n(R_n(t_j)),$$

and hence the limit of the time-discretizations must also be the gradient flow of $\tilde{E}_n$. By arguing as in the proof of Lemma 3.2, we find that $\tilde{E}_n$ is α-convex (i.e., λ-convex with $\lambda = \alpha$), and hence y_n satisfies (4.6) if we replace E_n with $\tilde{E}_n$. For $v \in \mathscr{B}_\epsilon$, however, the functionals are the same.

On testing (4.6) with $v = y_n^*$, and multiplying the resulting inequality by $e^{2\alpha t}$, we obtain

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\Big(e^{\alpha t}|y_n(t) - y_n^*|_{\mathrm{H}^1}\Big)^2 \le e^{\alpha t}\big(E_n(y_n^*) - E_n(y_n(t))\big) \le 0.$$

Integrating from 0 to T gives the result. ☐

Proof of Theorem 4.1. Lemmas 4.2 and 4.3 and Corollary 4.4 immediately imply item (a) and we only need to establish the facts about the continuum limit. Note that almost all of the following analysis is independent of the specific structure of the problem. The only crucial condition which we require is that $y_n(t) \to y(t)$ as $n \to \infty$, for every $t \geq 0$, and $y_n(t) \to y_n^*$ as $t \to \infty$, uniformly in n.

For item (b), we first need to show that, given an initial condition $y(0)$ for the "continuum" $|\cdot|_{\mathrm{H}^1}$-gradient flow satisfying the assumptions of the theorem, there exist "atomistic" initial conditions $y_n(0)$ which satisfy the assumptions of Lemma 4.3. Let $y'(0,x) \leq z_1 - \epsilon$ for a.e. $x \in (0,1)$. Letting $y_n(0,x)$ be the piecewise affine interpolant of $y(0,x)$, we have

$$y_n'(0,x) = \frac{1}{\epsilon_n} \int_{x_{i-1}^n}^{x_i^n} y'(0,x)\,\mathrm{d}x \leq z_1 - \epsilon, \quad x \in (x_{i-1}^n, x_i^n).$$

Therefore, the atomistic $|\cdot|_{\mathrm{H}^1}$-gradient flows with starting point $y_n'(0,\cdot)$ converge uniformly in n (compare to Corollary 4.4) to the equilibria y_n^*, computed in item (a) or Lemma 4.2. We use this fact to estimate

$$\begin{aligned} |y_n^* - y_{n'}^*|_{\mathscr{H}} &\leq |y_n^* - y_n(t)|_{\mathscr{H}} + |y_n(t) - y_{n'}(t)|_{\mathscr{H}} + |y_n(t) - y_{n'}^*|_{\mathscr{H}} \\ &\leq 2\mathrm{const.}e^{-\alpha t} + |y_n(t) - y_{n'}(t)|_{\mathscr{H}}, \end{aligned}$$

thus showing that $(y_n^*)_{n\in\mathbb{N}}$ is a Cauchy-sequence. We denote its limit in $\mathscr{A}$ by y^*. To see that $y(t) \to y^*$ as $t \to \infty$, consider

$$|y(t) - y^*|_{\mathscr{H}} \leq \inf_{n\in\mathbb{N}} \left(|y(t) - y_n(t)|_{\mathscr{H}} + |y_n(t) - y_n^*|_{\mathscr{H}} + |y_n^* - y^*|\right) \leq \mathrm{const.}e^{-\alpha t}.$$

We have shown that the "discrete" equilibria y_n^* converge to a "continuum" deformation y^* and that $y(t) \to y^*$.

The fact that y^* is a critical point of E is easily verified by hand, but in fact this follows from the general theory as well, using the concepts introduced in section 2.2. It is straightforward to show that the functionals E_n $\Gamma(\mathrm{H}^1)$-converge to E in the strong H^1 topology. We merely note the limsup condition (2.10) is given by Lemma 3.4 while for the lim inf condition (2.9) E and E_n can be decomposed into a convex, lower semicontinous part and a continuous, uniformly convergent part (compare to the proof of λ-convexity in Lemma 3.2).

Since the functionals E and $(E_n)_{n\in\mathbb{N}}$ are also uniformly λ-convex, Lemma 2.6, shows that

$$|\partial E|(y^*) \leq \liminf_{n\to\infty} |\partial E_n|(y_n^*) = 0,$$

where $|\partial E_{(n)}|$ denotes the $|\cdot|_{\mathrm{H}^1}$-local slope of the functionals $E_{(n)}$. ∎

We conclude the discussion of elastic behavior with a remark on the structure of the elastic critical points. It may not be surprising that the continuum "elastic" critical point computed in section 4.1 are actually not local minimizers with respect to the H^1-topology. Indeed, let us assume that $f \equiv 0$ and $0 < g < J'(z_1)$ and define the curve $s \mapsto v(s)$ by

$$v'(s) = y^{*\prime} + \frac{1}{s}\chi_{(1/2,1/2+s^k)}.$$

It is straightforward to establish that for $k \geq 2p$, $v \in \mathrm{C}^{0,1/p}(0, s_0; \mathrm{W}^{1,p})$ and $E(v(s)) < E(y^*)$, where $s_0 > 0$ and $\mathrm{C}^{0,1/p}$ denotes the usual space of Hölder continuous functions. Thus, the critical point y^* is not an H^1-local minimum of the energy $E(y)$. This is also reflected by the fact that we only allow $\mathrm{W}^{1,\infty}$ perturbations in Theorem 4.1.

Why, we should ask ourselves, is this not in contradiction with Theorem 4.1? If there exists a curve along which the energy decreases, should the gradient flow not find this curve? The explanation is that the curve $v(s)$, which we have constructed, is not absolutely continuous in $\mathrm{H}^1(0,1)$ and hence is not a candidate for the gradient flow evolution. An interesting question is whether there actually can exist an absolutely continuous curve starting in y^* along which the energy decreases strictly. Unfortunately, we are unable to answer this question at this point. A negative answer would lead to an interesting selection criterion for equilibria. It would in particular imply that the choice of evolution is not so crucial after all, as such equilibria would be stable under any "sufficiently smooth" evolution.

4.2. Instability and fracture. If the forces f and g are sufficiently strong, then they will cause the material to break, i.e., the atoms debond. Mathematically, this means that the deformation gradient of the atomistic or continuum deformation enters the region where J is concave. In dimensions higher than one, though, the model is unable to describe fracture. There, effects other than debonding of atoms, most notably dislocations, become highly important and cannot be neglected. The discussion in this section can therefore not be generalized directly to higher dimensions.

If we do not restrict the motion of the material, i.e., if we let $M = \infty$ (compare to section 3), then the gradient flows $y_n(t)$ and $y(t)$ will not converge to a stationary point as $t \to \infty$, but diverge. Hence, we restrict the possible deformations by setting M to be a real number, $z_1 < M < \infty$. We assume throughout this section that $f \equiv 0$ and $g > J'(z_1)$.

PROPOSITION 4.5. *There exists $t_1 > 0$ and $\alpha \in \mathrm{W}^{1,\infty}(0,\infty)$ satisfying $\dot{\alpha}(t) > 0$ if $t < t_1$ and $\alpha(t) = M$ if $t \geq t_1$, such that the solution of the $|\cdot|_{\mathrm{H}^1}$-gradient flow in $\mathscr{A}$ with $y(0,x) = x$ is*

$$y(t,x) = \alpha(t)x.$$

Proof. We change coordinates to $r(t,x) = y'(t,x)$ to obtain, formally for the moment, the equation

$$r_t(t,x) = g - J'(r(t,x)),$$

which is the same ordinary differential equation for every point $x \in (0,1)$. Furthermore, $g - J'(r(t,x)) > 0$ for all x and t, hence $\alpha(t)$ is strictly increasing. Since the solution we have obtained is Lipschitz continuous in time, it is the required gradient flow.

When we reach a time t_1 for which $y(t_1, 1) = M$, the deformation y will be fixed at $y(1,t) = M$ for $t \geq t_1$. To see this, we consider again the time-discretization with initial value $r_0 = M$. The next timestep is the minimizer of

$$\int_0^1 \left[\frac{1}{2\tau} |r - M|^2 + J(r) - gr \right] \mathrm{d}x,$$

subject to $(r) := \int_0^1 r \, \mathrm{d}x \leq M$. If $(r) < M$, then r must satisfy

$$\frac{1}{\tau}(r - M) + J'(r) = g. \tag{4.7}$$

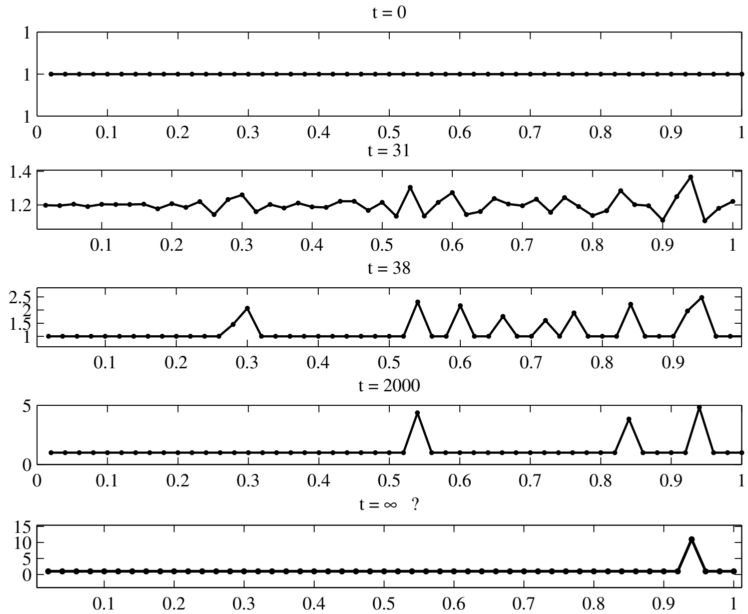

FIG. 4.1. *Snapshots of the deformation gradients of an* $|\cdot|_{H^1}$*-gradient flow evolution, showing the instability of the final state, computed with* 51 *"atoms." The new final state* ($t = \infty$) *after instability sets in is not computed but guessed. This figure shows an* unstable *computation and should not be mistaken for the exact solution of the model! Note also the different scales in the respective plots.*

Since $(r) < m$, there must exist a set of positive measure where $r \le M - \epsilon$ for some $\epsilon > 0$. However, since J' is bounded above, (4.7) cannot be satisfied in this set, if τ is sufficiently small.

By a uniqueness argument, we find that $y(t, x)$ satisfies the partial differential equation

$$-y_t'' = J'(y')' = J''(y')y'', \quad y(t, 0) = 0, \quad y(t, 1) = M, \quad y(t_1, x) = Mx,$$

which can be easily seen to be solved by $y(x, t) = Mx$. Therefore, the evolution remains in the affine state. ◻

Proposition 4.5 suggests that in our model fracture will never occur. However, the analytical solution obtained is highly unstable under perturbation as Figure 4.1, where a numerical computation is shown, demonstrates. In all computations, we chose $J(z)$ to be strictly increasing for $z > z_1$, i.e., there exists no threshold for the deformation gradient beyond which there are no internal forces.

In a second experiment we dominate the numerical round-off errors, and thus the instabilities in the $|\cdot|_{H^1}$-gradient flow computation, by a controlled perturbation which could be interpreted, for example, as an impurity in the material. At time $t = 7.6$, we perturb the position of one node (or atom) by an amount of 10^{-8}. The effect of this is that the "fracture" occurs exactly at this position; see Figure 4.2 for the computational results. The instability of the evolution very much conforms with experimental observation that rupture in many types of materials is a highly unstable

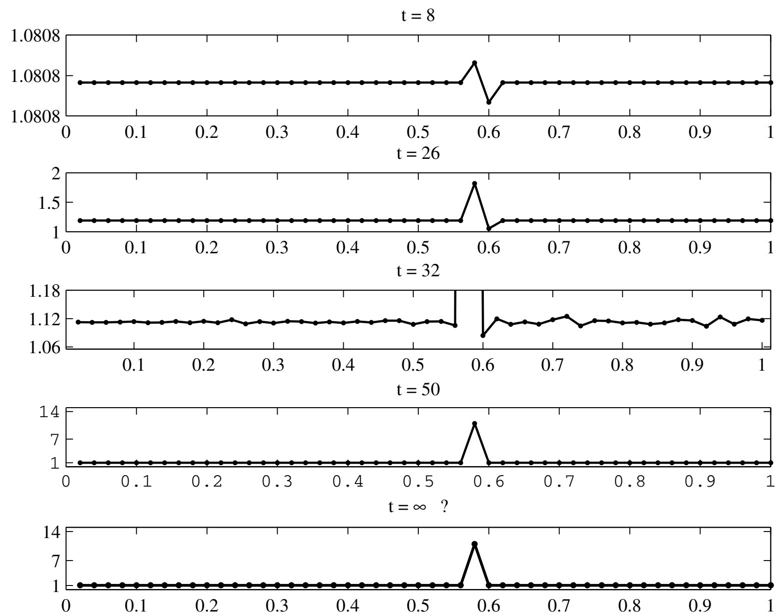

FIG. 4.2. *Snapshots of the deformation gradients of an* $|\cdot|_{H^1}$*-gradient flow evolution, computed with* 51 *"atoms," with a controlled perturbation at time* $t = 7.6$ *by an amount of* 10^{-8}*. The final state* ($t = \infty$) *is not computed but guessed. Note also the different scales in the respective plots.*

process. No fracture experiment can be reproduced exactly. Thus, the instability of the evolution could be thought of as representing the uncertainty of where damage occurs.

5. Remarks on extensions to two and three dimensions. The simple problem we have investigated here has a fair amount of one-dimensional structure. Although most of the techniques developed here can be readily generalized, the extension to two and three dimensions, which is of great importance to the modeling of material behavior, is not entirely trivial.

The first difficulty to notice is that the passage to higher dimensions in a simple nearest-neighbor system based on the Lennard–Jones potential suffers from a loss of λ-convexity, since the atomistic deformations do not necessarily have to remain orientation preserving. By cutting off the Lennard–Jones potential at the origin, a process which is intuitively reasonable but difficult to justify rigorously, the convergence of the gradient flow can be recovered completely. A more interesting, and mathematically much more challenging, alternative would be to consider a gradient flow with respect to a different metric, which may allow the blow-up behavior of the Lennard–Jones potential, but such a metric seems to be presently unavailable.

To analyze elastic equilibria, it is necessary to obtain L^∞ bounds on the deformation gradient. This step poses the biggest challenge in higher dimensions as these bounds cannot be computed explicitly anymore. One possible avenue to obtain them would be to use the implicit function theorem, for which uniform bounds can be constructed with a slightly refined analysis. It would be necessary, however, that the solution of the linearized system lies in $W^{1,\infty}(\Omega)$, which can only be obtained in some very restrictive cases, e.g., with smooth domains and Dirichlet boundary conditions. At re-entrant corners or interfaces between Dirichlet and Neumann boundaries (for example, a crack tip), the nearest neighbor model is too simple to describe the material behavior accurately.

While the convergence theory for gradient flows can still be analyzed if finite-range interactions are added to the energy functional, the analysis of the equilibria seems to be far more difficult if we consider damaged states, but remains essentially unchanged for elastic deformation. The case of infinity-range interactions is completely unclear. For examples of atomistic models with finite-range interactions and their relation to continuum theories, see [25, 9].

Finally, it should be noted that different evolutions can be analyzed as well. For example, it is straightforward to extend the convergence result from the gradient flow evolution to linear viscoelasticity following, for example, the theory developed in [7]. It is more difficult in this setting, however, to analyze the resulting stationary points in similar detail.

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